



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:56 PM UTC

PDB ID : 1K8Z / pdb_00001k8z
Title : CRYSTAL STRUCTURE OF THE TRYPTOPHAN SYNTHASE BETA-SER178PRO MUTANT COMPLEXED WITH N-[1H-INDOL-3-YL-ACETYL]GLYCINE ACID
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Deposited on : 2001-10-26
Resolution : 1.70 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

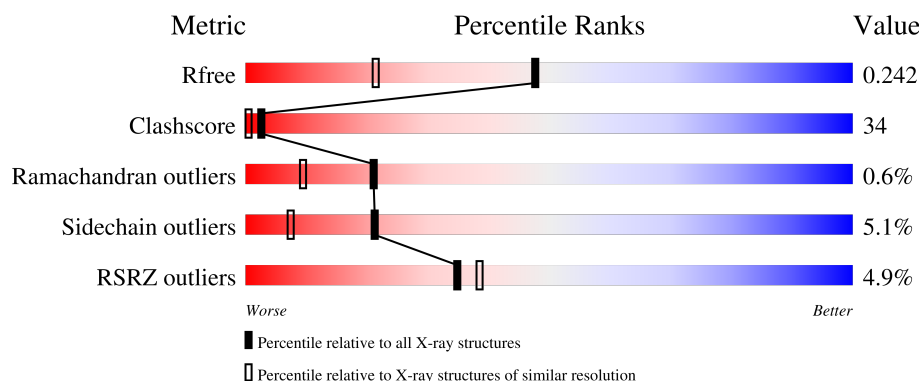
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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

Mol	Chain	Length	Quality of chain
1	A	268	
2	B	396	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	IAG	A	501	-	X	-	-
5	PLP	B	502	-	X	-	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5352 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 TRYPTOPHAN SYNTHASE ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	2	0
			1955	1248	334	365	8			

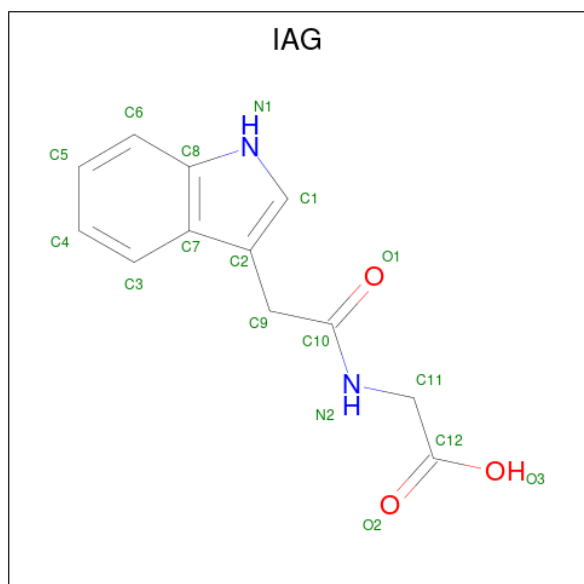
- Molecule 2 is a protein called TRYPTOPHAN SYNTHASE BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	394	Total	C	N	O	S	0	1	0
			2987	1877	527	564	19			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	34	SER	ARG	cloning artifact	UNP P0A2K1
B	178	PRO	SER	engineered mutation	UNP P0A2K1

- Molecule 3 is N-[1H-INDOL-3-YL-ACETYL]GLYCINE ACID (CCD ID: IAG) (formula: $C_{12}H_{12}N_2O_3$).

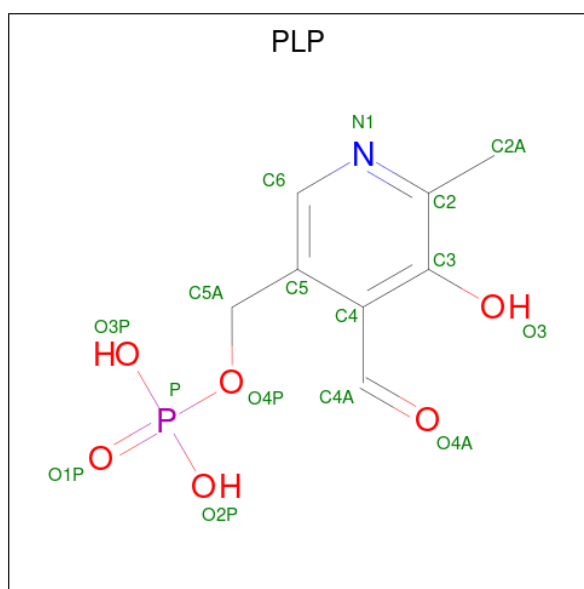


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	12	2	3		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Na	0	0
			1	1		

- Molecule 5 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C₈H₁₀NO₆P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

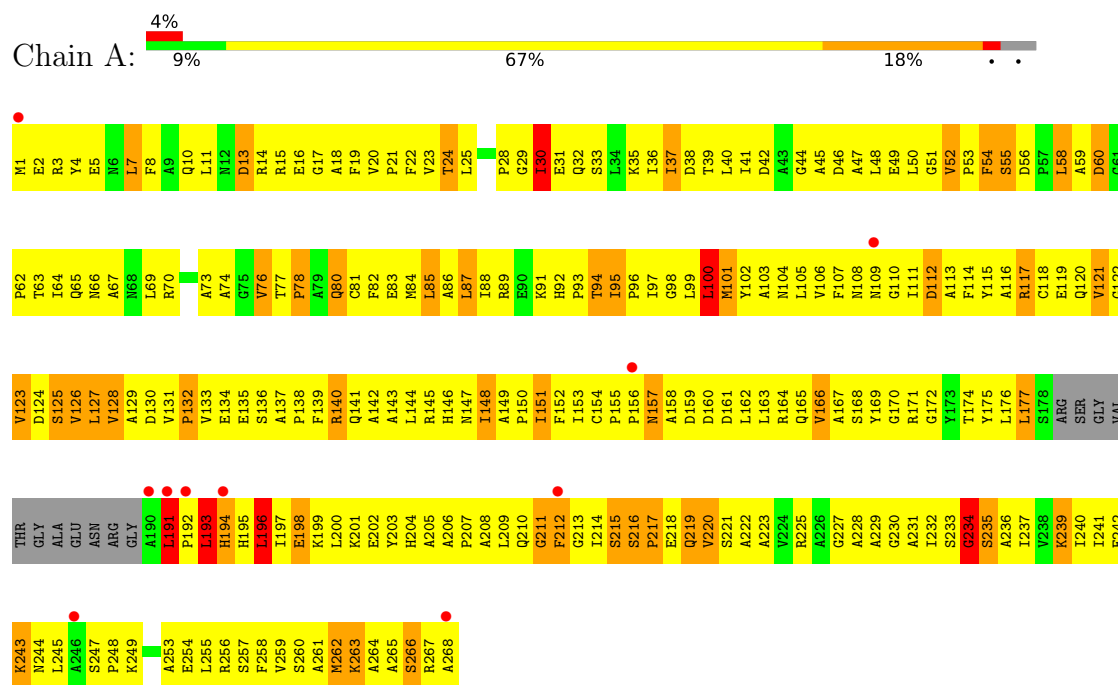
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	129	Total	O	0	0
			129	129		
6	B	248	Total	O	0	0
			248	248		

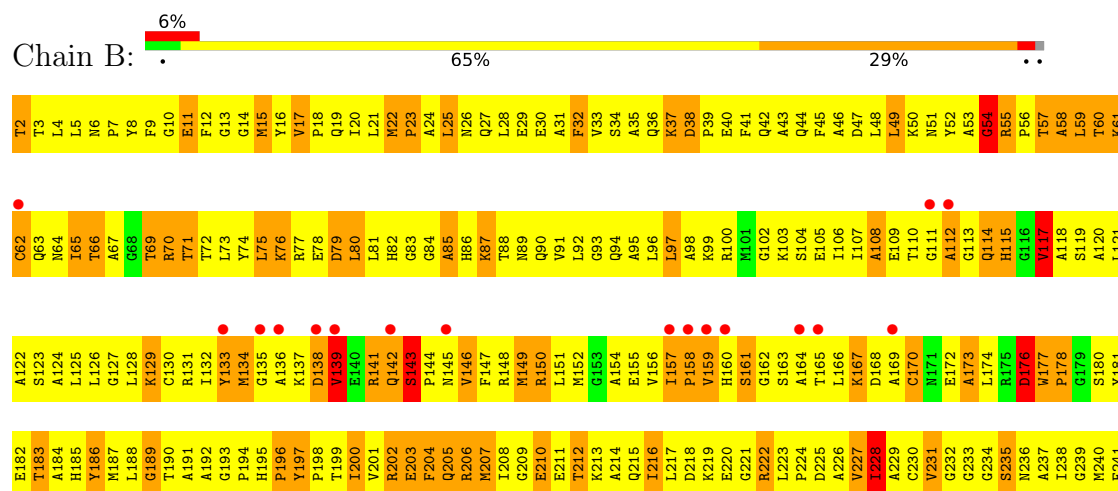
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: TRYPTOPHAN SYNTHASE ALPHA CHAIN



• Molecule 2: TRYPTOPHAN SYNTHASE BETA CHAIN



A242	A302	K362
D243	G303	R363
F244	I304	E364
I245	D305	Q365
N246	F306	P366
D247	P307	E367
T248	S308	K368
S249	V309	E369
V250	G310	Q370
G251	F311	L371
L252	Q312	L372
I253	H313	V373
G254	A314	V374
V255	Y315	N375
E256	L316	L376
P257	N317	S377
G258	S318	G378
G259	I319	R379
H260	G320	G380
G261	R321	D381
I262	A322	K382
E263	D323	D383
T264	Y324	I384
G265	V325	F385
E266	S326	T386
H267	I327	V387
G268	T328	H388
A269	D329	D389
P270	D330	I390
L271	E331	L391
K272	A332	K392
H273	L333	A393
G274	E334	R394
R275	A335	G395
V276	F336	GLU
G277	K337	ILE
I278	T338	
Y279	L339	
F280	C340	
G281	R341	
M282	H342	
K283	E343	
A284	G344	
P285	I345	
M286	L346	
M287	P347	
Q288	A348	
T289	L349	
A290	E350	
D291	S351	
G292	S352	
Q293	H353	
I294	A354	
E295	L355	
E296	A356	
S297	H357	
Y298	A358	
S299	L359	
I300	K360	
S301	M361	

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	184.42Å 61.03Å 67.53Å 90.00° 94.69° 90.00°	Depositor
Resolution (Å)	20.00 – 1.70 20.00 – 1.70	Depositor EDS
% Data completeness (in resolution range)	96.4 (20.00-1.70) 96.3 (20.00-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 1.70Å)	Xtriage
Refinement program	CNS, REFMAC	Depositor
R, R_{free}	0.209 , 0.265 0.200 , 0.242	Depositor DCC
R_{free} test set	4065 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	20.8	Xtriage
Anisotropy	0.592	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 53.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5352	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, IAG, PLP

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	4.41	408/2004 (20.4%)	3.42	359/2722 (13.2%)
2	B	5.82	1056/3052 (34.6%)	4.73	1017/4123 (24.7%)
All	All	5.31	1464/5056 (29.0%)	4.26	1376/6845 (20.1%)

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	1
2	B	0	1
All	All	0	2

All (1464) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	72	THR	CA-CB	-24.91	1.19	1.53
1	A	52	VAL	CA-C	23.08	1.73	1.52
2	B	70	ARG	CA-C	22.13	1.81	1.53
2	B	361	MET	SD-CE	-21.34	1.26	1.79
2	B	61	LYS	N-CA	21.27	1.72	1.46
2	B	255	VAL	CA-CB	21.25	1.80	1.53
2	B	22	MET	SD-CE	-21.12	1.26	1.79
2	B	59	LEU	CA-C	20.71	1.77	1.52
2	B	59	LEU	N-CA	20.49	1.71	1.46
2	B	362	MET	SD-CE	-20.44	1.28	1.79
2	B	51	ASN	CA-C	-20.16	1.25	1.52
2	B	208	ILE	CA-CB	-19.84	1.33	1.54
1	A	123	VAL	CA-CB	19.68	1.76	1.54
2	B	252	LEU	C-O	19.34	1.46	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	17	VAL	CA-C	19.16	1.68	1.52
2	B	282	MET	SD-CE	-19.04	1.31	1.79
1	A	151	ILE	CA-CB	-18.98	1.30	1.54
2	B	135	GLY	C-O	18.87	1.43	1.23
2	B	319	ILE	C-O	18.84	1.45	1.24
1	A	98	GLY	CA-C	18.78	1.69	1.52
1	A	54	PHE	CA-C	18.53	1.75	1.52
2	B	233	GLY	C-N	18.51	1.55	1.33
2	B	6	ASN	CA-C	-18.31	1.29	1.52
2	B	152	MET	SD-CE	-18.16	1.34	1.79
2	B	308	SER	C-O	18.09	1.43	1.24
2	B	252	LEU	CA-C	-18.03	1.29	1.52
2	B	203	GLU	CA-C	17.85	1.77	1.52
1	A	127	LEU	CA-C	17.79	1.73	1.52
2	B	106	ILE	CA-C	-17.75	1.30	1.52
2	B	254	GLY	CA-C	-17.75	1.39	1.52
2	B	351	SER	CA-C	17.59	1.76	1.52
2	B	373	VAL	C-O	17.53	1.42	1.24
2	B	6	ASN	C-O	17.50	1.47	1.24
2	B	117	VAL	CA-C	-17.41	1.30	1.52
2	B	328	THR	CA-C	17.33	1.77	1.53
2	B	314	ALA	C-O	17.23	1.44	1.24
2	B	286	MET	CB-CG	17.18	2.04	1.52
2	B	202	ARG	NE-CZ	17.00	1.51	1.33
2	B	368	LYS	CA-C	16.92	1.75	1.52
2	B	27	GLN	CA-C	16.72	1.74	1.52
2	B	254	GLY	C-O	16.53	1.43	1.23
2	B	287	MET	SD-CE	-16.50	1.38	1.79
2	B	31	ALA	N-CA	16.46	1.66	1.46
1	A	229	ALA	CA-C	-16.43	1.30	1.52
2	B	262	ILE	CA-CB	-16.42	1.36	1.54
2	B	29	GLU	C-N	16.21	1.55	1.33
2	B	128	LEU	CA-C	-16.14	1.32	1.52
2	B	243	ASP	N-CA	-16.14	1.24	1.46
2	B	105	GLU	CA-C	16.06	1.72	1.52
1	A	77	THR	CA-C	16.00	1.68	1.52
1	A	97	ILE	C-N	15.96	1.52	1.33
2	B	77	ARG	NE-CZ	15.92	1.50	1.33
2	B	85	ALA	N-CA	15.90	1.65	1.46
2	B	205	GLN	C-O	15.88	1.45	1.24
2	B	95	ALA	C-O	15.81	1.43	1.24
2	B	138	ASP	C-O	15.55	1.42	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	9	PHE	CA-C	15.47	1.71	1.53
2	B	117	VAL	CA-CB	15.31	1.75	1.54
2	B	195	HIS	N-CA	-15.27	1.28	1.45
2	B	353	HIS	CA-CB	15.27	1.77	1.53
2	B	335	ALA	CA-C	15.23	1.73	1.52
1	A	149	ALA	C-N	-15.22	1.20	1.33
2	B	25	LEU	CA-C	-15.19	1.33	1.52
1	A	24	THR	CA-CB	15.16	1.75	1.53
1	A	125	SER	CA-C	15.05	1.71	1.52
2	B	55	ARG	CA-C	-15.03	1.35	1.53
2	B	21	LEU	CA-C	-15.00	1.32	1.52
1	A	262	MET	SD-CE	-14.98	1.42	1.79
2	B	231	VAL	C-N	14.93	1.55	1.33
1	A	21	PRO	CA-CB	-14.92	1.37	1.54
1	A	94	THR	CA-CB	14.87	1.75	1.54
2	B	291	ASP	CB-CG	-14.81	1.15	1.52
2	B	228	ILE	CA-CB	14.79	1.72	1.54
2	B	367	GLU	C-O	14.69	1.42	1.24
2	B	199	THR	N-CA	-14.69	1.28	1.46
1	A	210	GLN	C-N	14.68	1.54	1.33
2	B	86	HIS	CA-C	14.67	1.73	1.52
2	B	353	HIS	CA-C	-14.67	1.33	1.52
2	B	3	THR	CA-C	-14.65	1.34	1.52
2	B	212	THR	N-CA	14.49	1.63	1.46
2	B	360	LYS	C-O	14.49	1.42	1.24
2	B	58	ALA	CA-CB	14.48	1.75	1.53
2	B	229	ALA	CA-C	-14.47	1.34	1.52
2	B	336	PHE	CA-C	14.42	1.71	1.52
2	B	19	GLN	CA-C	14.41	1.72	1.52
2	B	120	ALA	CA-CB	-14.36	1.30	1.53
2	B	207	MET	C-O	14.35	1.42	1.24
2	B	321	ARG	C-O	14.34	1.43	1.24
2	B	141	ARG	C-O	14.26	1.43	1.24
2	B	280	PHE	CA-C	-14.20	1.33	1.52
1	A	171	ARG	CA-C	-14.10	1.35	1.52
2	B	284	ALA	C-N	14.05	1.50	1.33
2	B	197	TYR	CA-CB	-14.05	1.34	1.53
2	B	253	ILE	CA-CB	14.04	1.71	1.54
2	B	356	ALA	CA-CB	-14.04	1.31	1.53
2	B	52	TYR	N-CA	-14.02	1.28	1.46
2	B	227	VAL	C-O	13.99	1.40	1.24
2	B	269	ALA	CA-CB	13.96	1.69	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	194	PRO	CA-C	-13.94	1.34	1.52
2	B	283	LYS	CA-C	13.94	1.70	1.52
2	B	257	PRO	N-CD	13.90	1.67	1.47
2	B	390	ILE	CA-C	-13.89	1.35	1.52
1	A	165	GLN	CA-C	-13.80	1.35	1.52
2	B	215	GLN	N-CA	13.76	1.63	1.46
2	B	268	GLY	CA-C	-13.74	1.32	1.51
1	A	230	GLY	CA-C	13.64	1.65	1.52
2	B	78	GLU	C-O	13.61	1.41	1.24
1	A	101	MET	CG-SD	-13.60	1.46	1.80
1	A	97	ILE	N-CA	13.58	1.65	1.46
2	B	255	VAL	N-CA	-13.57	1.29	1.46
2	B	285	PRO	CA-C	-13.57	1.36	1.52
2	B	362	MET	C-O	13.53	1.39	1.24
2	B	211	GLU	CA-C	13.49	1.71	1.52
2	B	130	CYS	CA-C	-13.47	1.36	1.52
2	B	325	VAL	CA-CB	13.45	1.72	1.54
2	B	276	VAL	CA-CB	-13.42	1.36	1.54
1	A	139	PHE	CA-C	13.38	1.70	1.52
1	A	143	ALA	CA-CB	13.37	1.74	1.53
2	B	227	VAL	N-CA	13.37	1.62	1.46
2	B	245	ILE	C-O	13.36	1.39	1.24
2	B	53	ALA	CA-C	13.32	1.71	1.52
2	B	245	ILE	N-CA	13.32	1.62	1.46
2	B	241	PHE	C-N	13.30	1.50	1.33
2	B	315	TYR	CE2-CZ	13.30	1.70	1.38
1	A	120	GLN	CA-C	-13.30	1.35	1.52
2	B	100	ARG	CA-C	13.30	1.70	1.52
2	B	118	ALA	N-CA	-13.29	1.30	1.46
2	B	30	GLU	CA-CB	13.22	1.74	1.53
2	B	29	GLU	CA-C	-13.21	1.35	1.52
2	B	309	VAL	CA-CB	13.21	1.69	1.55
2	B	157	ILE	N-CA	13.20	1.58	1.46
1	A	116	ALA	CA-C	-13.16	1.35	1.52
2	B	24	ALA	N-CA	13.15	1.62	1.46
2	B	237	ALA	C-N	13.12	1.48	1.34
2	B	194	PRO	C-O	13.11	1.38	1.23
1	A	50	LEU	CA-C	13.08	1.68	1.52
2	B	323	ASP	CA-C	-13.08	1.37	1.52
2	B	374	VAL	N-CA	-13.06	1.30	1.46
1	A	121	VAL	N-CA	-13.02	1.28	1.46
2	B	82	HIS	CG-CD2	13.01	1.50	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	5	GLU	N-CA	13.01	1.62	1.46
2	B	235	SER	CA-CB	12.97	1.74	1.53
2	B	48	LEU	CA-C	12.95	1.69	1.52
2	B	108	ALA	CA-CB	12.92	1.78	1.54
2	B	93	GLY	C-O	12.91	1.39	1.23
2	B	314	ALA	N-CA	12.83	1.61	1.46
2	B	316	LEU	C-O	12.78	1.40	1.24
2	B	6	ASN	C-N	-12.77	1.20	1.34
2	B	375	ASN	C-N	12.75	1.51	1.33
2	B	238	ILE	CA-CB	12.74	1.73	1.54
1	A	166	VAL	CA-C	12.71	1.69	1.52
1	A	158	ALA	CA-CB	12.70	1.73	1.53
2	B	76	LYS	C-N	12.68	1.50	1.33
2	B	71	THR	CA-CB	-12.65	1.34	1.53
2	B	376	LEU	CA-CB	12.64	1.68	1.52
2	B	324	TYR	C-O	12.64	1.39	1.24
2	B	76	LYS	CA-CB	12.63	1.71	1.53
2	B	151	LEU	C-O	12.61	1.39	1.24
2	B	32	PHE	N-CA	12.56	1.61	1.46
1	A	126	VAL	N-CA	12.55	1.61	1.46
2	B	95	ALA	CA-CB	12.54	1.73	1.53
1	A	121	VAL	CA-CB	12.53	1.71	1.54
2	B	49	LEU	C-O	12.51	1.39	1.24
2	B	337	LYS	C-O	12.51	1.39	1.24
2	B	341	ARG	N-CA	12.48	1.62	1.46
2	B	203	GLU	N-CA	-12.47	1.29	1.46
2	B	7	PRO	CA-C	12.43	1.71	1.52
2	B	157	ILE	CA-CB	12.42	1.69	1.54
1	A	131	VAL	CA-CB	12.41	1.66	1.53
2	B	165	THR	C-O	12.40	1.39	1.24
2	B	379	ARG	CA-C	-12.40	1.35	1.53
2	B	196	PRO	CA-C	12.38	1.77	1.52
2	B	340	CYS	CA-CB	-12.35	1.34	1.53
2	B	278	ILE	CA-CB	12.33	1.70	1.54
1	A	18	ALA	CA-C	12.32	1.69	1.52
2	B	281	GLY	C-N	12.29	1.49	1.33
2	B	282	MET	CA-CB	12.24	1.77	1.54
2	B	192	ALA	CA-C	12.21	1.69	1.53
1	A	96	PRO	CA-CB	-12.21	1.37	1.53
1	A	102	TYR	CA-CB	12.20	1.72	1.53
1	A	208	ALA	CA-C	-12.16	1.36	1.52
1	A	130	ASP	CA-C	-12.13	1.36	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	61	LYS	CA-C	-12.13	1.37	1.52
1	A	136	SER	CA-C	12.12	1.69	1.52
2	B	73	LEU	CA-C	12.12	1.67	1.52
2	B	279	TYR	CA-C	12.11	1.67	1.52
2	B	71	THR	CA-C	12.09	1.68	1.52
1	A	84	MET	C-O	12.05	1.38	1.24
2	B	323	ASP	C-O	12.05	1.38	1.24
2	B	30	GLU	CD-OE2	12.05	1.48	1.25
2	B	26	ASN	CA-CB	11.96	1.73	1.53
2	B	44	GLN	N-CA	-11.96	1.32	1.46
1	A	128	VAL	N-CA	11.92	1.60	1.46
2	B	82	HIS	C-O	11.90	1.38	1.23
2	B	225	ASP	N-CA	11.90	1.61	1.46
1	A	145	ARG	C-O	11.89	1.39	1.24
2	B	256	GLU	C-O	11.88	1.38	1.23
2	B	242	ALA	CA-C	-11.85	1.37	1.52
2	B	384	ILE	CA-CB	11.83	1.70	1.54
2	B	134	MET	C-O	11.82	1.37	1.23
2	B	243	ASP	CA-C	11.81	1.69	1.52
1	A	126	VAL	C-N	11.80	1.49	1.33
2	B	289	THR	CB-OG1	11.79	1.62	1.43
2	B	354	ALA	CA-C	11.77	1.67	1.52
1	A	37	ILE	CA-C	11.76	1.69	1.52
2	B	223	LEU	C-O	11.68	1.39	1.23
2	B	201	VAL	CA-CB	-11.68	1.39	1.54
2	B	206[A]	ARG	CA-C	11.68	1.68	1.52
2	B	206[B]	ARG	CA-C	11.68	1.68	1.52
2	B	313	HIS	N-CA	11.68	1.60	1.46
2	B	345	ILE	C-O	11.68	1.37	1.24
2	B	182	GLU	CA-C	11.67	1.69	1.52
2	B	353	HIS	C-O	11.67	1.38	1.24
2	B	58	ALA	CA-C	11.67	1.69	1.53
2	B	256	GLU	C-N	-11.64	1.22	1.33
2	B	255	VAL	C-O	11.64	1.36	1.24
2	B	19	GLN	CA-CB	11.63	1.72	1.53
2	B	106	ILE	C-N	11.63	1.50	1.33
2	B	119	SER	CA-C	11.62	1.68	1.52
2	B	79	ASP	CG-OD2	11.62	1.47	1.25
2	B	12	PHE	CA-C	11.62	1.66	1.52
2	B	13	GLY	C-O	-11.61	1.16	1.24
2	B	369	GLU	CA-CB	-11.61	1.36	1.53
2	B	231	VAL	CA-C	-11.60	1.38	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	317	ASN	CA-CB	-11.56	1.35	1.53
2	B	69	THR	CA-C	-11.56	1.37	1.53
2	B	139	VAL	CA-C	-11.55	1.38	1.52
2	B	207	MET	CA-C	11.54	1.68	1.52
2	B	80	LEU	N-CA	11.50	1.61	1.46
2	B	59	LEU	CA-CB	-11.48	1.35	1.53
1	A	220	VAL	CA-C	11.44	1.66	1.52
2	B	260	HIS	CA-CB	-11.43	1.33	1.53
2	B	286	MET	CA-CB	11.35	1.77	1.54
2	B	343	GLU	C-N	-11.34	1.19	1.33
1	A	210	GLN	CA-C	-11.32	1.38	1.52
1	A	130	ASP	C-N	11.30	1.44	1.33
2	B	215	GLN	CA-C	11.30	1.67	1.52
2	B	60	THR	CA-CB	-11.30	1.37	1.53
2	B	46	ALA	CA-C	11.29	1.67	1.52
2	B	120	ALA	N-CA	11.28	1.60	1.46
2	B	120	ALA	C-O	11.27	1.37	1.24
2	B	29	GLU	N-CA	-11.26	1.32	1.46
1	A	137	ALA	CA-CB	-11.24	1.35	1.53
2	B	369	GLU	C-O	11.24	1.37	1.24
2	B	63	GLN	C-O	11.22	1.37	1.24
2	B	338	THR	CA-CB	11.22	1.71	1.53
1	A	74	ALA	CA-CB	11.22	1.71	1.53
1	A	104	ASN	N-CA	11.22	1.60	1.46
2	B	305	ASP	CG-OD1	11.21	1.46	1.25
1	A	138	PRO	CA-CB	11.20	1.69	1.53
2	B	205	GLN	CG-CD	11.17	1.79	1.52
1	A	140	ARG	C-O	11.11	1.36	1.24
1	A	169	TYR	CA-CB	11.11	1.71	1.53
1	A	232	ILE	C-N	-11.10	1.18	1.33
2	B	361	MET	CA-C	11.07	1.67	1.52
2	B	234	GLY	C-N	11.02	1.50	1.33
2	B	327	ILE	N-CA	11.01	1.59	1.46
2	B	192	ALA	CA-CB	-11.01	1.39	1.53
2	B	362	MET	C-N	-10.99	1.19	1.33
2	B	335	ALA	N-CA	-10.98	1.31	1.46
1	A	259	VAL	CA-CB	10.97	1.68	1.54
1	A	141	GLN	CA-C	-10.97	1.38	1.52
1	A	38	ASP	N-CA	10.97	1.60	1.46
2	B	285	PRO	C-O	10.97	1.37	1.23
2	B	367	GLU	N-CA	-10.96	1.33	1.46
2	B	60	THR	CA-C	10.96	1.66	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	312	GLN	CA-C	10.91	1.66	1.52
2	B	349	LEU	CA-CB	-10.89	1.36	1.53
2	B	311	PRO	C-O	10.88	1.38	1.24
2	B	49	LEU	CA-C	10.88	1.66	1.52
2	B	266	GLU	C-O	10.86	1.38	1.23
2	B	149	MET	CG-SD	10.83	2.07	1.80
2	B	122	ALA	CA-C	10.82	1.67	1.52
2	B	257	PRO	N-CA	-10.82	1.34	1.47
2	B	55	ARG	CZ-NH2	10.74	1.47	1.33
2	B	332	ALA	C-N	-10.73	1.19	1.33
2	B	70	ARG	N-CA	-10.72	1.33	1.46
2	B	8	TYR	CE1-CZ	10.71	1.64	1.38
1	A	51	GLY	N-CA	10.69	1.57	1.45
2	B	33	VAL	CA-CB	10.68	1.67	1.54
2	B	152	MET	CA-C	10.68	1.68	1.52
2	B	343	GLU	CA-C	10.63	1.67	1.52
2	B	260	HIS	CA-C	-10.62	1.38	1.52
2	B	57	THR	CA-C	10.62	1.66	1.52
2	B	51	ASN	C-O	10.61	1.38	1.24
1	A	211	GLY	CA-C	10.60	1.63	1.51
2	B	228	ILE	N-CA	-10.58	1.33	1.46
2	B	57	THR	C-N	10.58	1.47	1.33
2	B	297	SER	CA-CB	-10.56	1.38	1.53
2	B	61	LYS	CB-CG	10.56	1.84	1.52
1	A	139	PHE	N-CA	-10.53	1.33	1.46
2	B	270	PRO	CA-CB	10.52	1.68	1.53
1	A	55	SER	N-CA	10.48	1.59	1.46
2	B	232	GLY	CA-C	10.46	1.66	1.51
1	A	103	ALA	CA-CB	-10.45	1.36	1.53
2	B	125	LEU	CA-C	10.45	1.66	1.52
1	A	116	ALA	CA-CB	10.44	1.69	1.53
2	B	39	PRO	C-O	10.44	1.37	1.24
2	B	196	PRO	N-CD	10.44	1.62	1.47
2	B	20	ILE	N-CA	10.44	1.60	1.46
2	B	373	VAL	N-CA	10.43	1.58	1.46
2	B	214	ALA	CA-CB	10.43	1.70	1.53
2	B	287	MET	CA-C	10.42	1.66	1.52
1	A	10	GLN	N-CA	-10.42	1.33	1.46
2	B	198	PRO	C-O	10.42	1.37	1.24
2	B	310	GLY	C-O	10.41	1.38	1.24
2	B	149	MET	CA-CB	10.39	1.70	1.53
2	B	330	ASP	CA-C	-10.39	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	138	ASP	CA-C	10.33	1.66	1.52
2	B	103	LYS	N-CA	-10.32	1.32	1.45
1	A	39	THR	C-O	10.31	1.36	1.24
2	B	262	ILE	N-CA	10.31	1.58	1.46
1	A	140	ARG	NE-CZ	-10.29	1.21	1.33
1	A	206	ALA	CA-CB	10.29	1.68	1.53
2	B	104	SER	C-O	10.28	1.37	1.24
2	B	240	MET	CA-C	10.28	1.65	1.52
2	B	188	LEU	CA-C	10.27	1.66	1.52
2	B	65	ILE	C-N	-10.27	1.19	1.33
2	B	340	CYS	N-CA	10.26	1.58	1.46
2	B	204	PHE	CD1-CE1	10.24	1.69	1.38
2	B	394	ARG	CZ-NH1	10.24	1.47	1.32
2	B	302	ALA	CA-CB	10.24	1.69	1.53
2	B	339	LEU	CA-C	10.24	1.66	1.52
1	A	162	LEU	N-CA	-10.24	1.33	1.46
2	B	388	HIS	C-O	-10.24	1.12	1.24
2	B	225	ASP	CG-OD2	10.23	1.44	1.25
2	B	297	SER	CA-C	10.23	1.67	1.53
2	B	20	ILE	CA-CB	-10.23	1.39	1.54
1	A	112	ASP	CA-C	-10.22	1.39	1.52
1	A	261	ALA	CA-C	-10.18	1.39	1.52
2	B	221	GLY	CA-C	10.17	1.65	1.51
2	B	65	ILE	N-CA	10.15	1.59	1.46
2	B	317	ASN	N-CA	10.14	1.58	1.46
2	B	360	LYS	CA-C	-10.12	1.39	1.52
1	A	125	SER	CA-CB	10.12	1.71	1.53
2	B	216	ILE	CA-C	-10.11	1.38	1.52
2	B	222	ARG	N-CA	10.10	1.57	1.46
2	B	123	SER	CA-C	10.10	1.65	1.52
2	B	375	ASN	N-CA	10.10	1.58	1.46
2	B	35	ALA	N-CA	10.10	1.58	1.46
2	B	176	ASP	CA-CB	10.09	1.69	1.53
2	B	268	GLY	C-N	10.08	1.47	1.33
2	B	352	SER	N-CA	10.07	1.58	1.46
1	A	170	GLY	C-O	10.06	1.38	1.23
2	B	357	HIS	CD2-NE2	10.06	1.49	1.37
2	B	189	GLY	N-CA	10.05	1.58	1.45
1	A	117	ARG	CG-CD	10.04	1.82	1.52
2	B	247	ASP	N-CA	10.04	1.60	1.46
2	B	359	LEU	N-CA	10.02	1.58	1.46
2	B	229	ALA	C-O	10.01	1.36	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	60	THR	N-CA	9.99	1.58	1.46
2	B	365	GLN	CA-C	9.98	1.65	1.52
2	B	368	LYS	C-N	-9.97	1.19	1.33
2	B	339	LEU	CA-CB	9.96	1.69	1.53
2	B	309	VAL	N-CA	-9.96	1.34	1.46
2	B	371	LEU	N-CA	9.95	1.58	1.46
2	B	303	GLY	N-CA	-9.94	1.31	1.45
2	B	327	ILE	CA-C	-9.93	1.40	1.52
1	A	92	HIS	C-O	9.93	1.35	1.24
1	A	150	PRO	CA-C	9.92	1.61	1.52
2	B	19	GLN	C-N	-9.91	1.23	1.34
1	A	109	ASN	CA-C	-9.90	1.40	1.53
1	A	143	ALA	CA-C	9.90	1.65	1.52
2	B	95	ALA	CA-C	-9.90	1.40	1.52
2	B	24	ALA	CA-CB	-9.90	1.37	1.53
2	B	63	GLN	N-CA	9.89	1.58	1.46
1	A	141	GLN	C-O	9.87	1.35	1.24
2	B	79	ASP	CA-C	9.86	1.66	1.52
2	B	200	ILE	CA-C	9.86	1.65	1.52
1	A	145	ARG	CZ-NH2	9.85	1.46	1.33
1	A	219	GLN	CB-CG	9.85	1.82	1.52
1	A	95	ILE	C-O	9.84	1.37	1.25
2	B	100	ARG	N-CA	-9.84	1.33	1.46
2	B	50	LYS	CA-CB	-9.84	1.36	1.53
2	B	231	VAL	N-CA	9.83	1.59	1.46
1	A	13	ASP	CB-CG	9.82	1.76	1.52
2	B	260	HIS	C-O	9.82	1.36	1.24
2	B	256	GLU	CG-CD	9.81	1.76	1.52
2	B	208	ILE	N-CA	9.80	1.57	1.46
1	A	100	LEU	CA-C	9.78	1.64	1.52
1	A	81	CYS	CA-C	9.77	1.65	1.52
2	B	106	ILE	N-CA	9.76	1.57	1.46
2	B	230	CYS	CA-C	9.76	1.66	1.53
2	B	67	ALA	CA-CB	9.75	1.69	1.53
2	B	331	GLU	N-CA	-9.75	1.34	1.46
2	B	356	ALA	N-CA	9.74	1.58	1.46
2	B	376	LEU	CG-CD2	9.72	1.84	1.52
2	B	18	PRO	C-N	9.71	1.47	1.34
2	B	45	PHE	CE1-CZ	9.69	1.67	1.38
1	A	145	ARG	CD-NE	9.69	1.59	1.46
2	B	220	GLU	N-CA	9.67	1.59	1.45
2	B	321	ARG	C-N	-9.66	1.20	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	349	LEU	CA-C	9.65	1.65	1.52
1	A	153	ILE	CA-C	-9.63	1.41	1.52
2	B	80	LEU	CB-CG	9.63	1.72	1.53
2	B	323	ASP	CA-CB	9.63	1.70	1.53
2	B	280	PHE	CD2-CE2	9.63	1.67	1.38
2	B	207	MET	CA-CB	9.60	1.70	1.53
1	A	99	LEU	N-CA	9.59	1.57	1.45
1	A	117	ARG	CA-C	9.59	1.65	1.52
2	B	201	VAL	N-CA	9.59	1.58	1.46
2	B	37	LYS	CA-C	9.58	1.66	1.52
2	B	85	ALA	CA-C	-9.57	1.41	1.52
2	B	347	PRO	C-N	9.57	1.46	1.33
1	A	221	SER	CA-C	-9.56	1.40	1.52
1	A	120	GLN	CA-CB	9.55	1.68	1.53
2	B	260	HIS	CB-CG	9.54	1.63	1.50
2	B	318	SER	N-CA	9.52	1.58	1.46
2	B	329	ASP	CA-C	9.50	1.65	1.52
2	B	4	LEU	CA-C	9.47	1.65	1.52
2	B	123	SER	N-CA	9.47	1.58	1.46
2	B	236	ASN	C-O	-9.46	1.12	1.24
1	A	104	ASN	CA-CB	9.45	1.69	1.53
2	B	287	MET	CA-CB	9.44	1.65	1.53
2	B	333	LEU	CA-CB	-9.44	1.38	1.53
2	B	130	CYS	C-N	9.44	1.48	1.33
2	B	311	PRO	N-CD	9.43	1.60	1.47
2	B	371	LEU	C-O	9.41	1.35	1.24
2	B	235	SER	C-O	-9.40	1.11	1.24
2	B	71	THR	N-CA	9.33	1.58	1.46
2	B	208	ILE	C-O	9.33	1.34	1.24
2	B	16	TYR	CE2-CZ	9.32	1.60	1.38
1	A	143	ALA	C-O	9.32	1.34	1.24
2	B	110	THR	CA-CB	9.30	1.70	1.53
2	B	329	ASP	CA-CB	-9.29	1.39	1.53
2	B	65	ILE	CA-CB	9.27	1.67	1.54
2	B	193	GLY	C-N	9.26	1.45	1.33
2	B	256	GLU	CA-CB	9.26	1.68	1.52
2	B	53	ALA	CA-CB	9.25	1.70	1.53
2	B	280	PHE	C-N	9.24	1.48	1.33
2	B	304	LEU	CG-CD1	9.24	1.83	1.52
2	B	10	GLY	C-O	9.23	1.36	1.24
2	B	376	LEU	N-CA	-9.22	1.35	1.46
1	A	261	ALA	C-O	9.22	1.34	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	121	LEU	C-N	9.22	1.47	1.33
2	B	242	ALA	CA-CB	9.22	1.67	1.53
2	B	205	GLN	CA-C	-9.20	1.40	1.52
2	B	15	MET	SD-CE	9.18	2.02	1.79
2	B	85	ALA	C-O	9.18	1.34	1.23
2	B	157	ILE	C-N	-9.18	1.21	1.33
2	B	312	GLN	N-CA	-9.18	1.35	1.46
1	A	99	LEU	C-N	9.17	1.46	1.33
2	B	317	ASN	CG-OD1	9.17	1.41	1.23
1	A	96	PRO	CA-C	9.16	1.64	1.52
1	A	222	ALA	CA-CB	9.16	1.67	1.53
2	B	82	HIS	CA-CB	9.15	1.67	1.53
1	A	142	ALA	N-CA	-9.14	1.35	1.46
2	B	227	VAL	CA-C	-9.13	1.42	1.52
2	B	136	ALA	N-CA	9.12	1.57	1.46
2	B	12	PHE	CD1-CE1	9.11	1.66	1.38
2	B	237	ALA	CA-CB	9.11	1.67	1.53
1	A	17	GLY	N-CA	9.10	1.57	1.44
2	B	282	MET	CA-C	9.10	1.63	1.52
2	B	210	GLU	N-CA	-9.10	1.34	1.46
1	A	245	LEU	CA-C	-9.09	1.40	1.52
2	B	316	LEU	CA-CB	9.09	1.68	1.53
1	A	47	ALA	N-CA	9.08	1.57	1.46
1	A	212	PHE	CD1-CE1	9.07	1.65	1.38
2	B	91	VAL	N-CA	9.07	1.57	1.46
2	B	53	ALA	C-N	-9.07	1.21	1.33
2	B	80	LEU	CA-C	9.07	1.65	1.52
2	B	197	TYR	CA-C	9.06	1.64	1.52
2	B	87	LYS	CA-CB	-9.06	1.38	1.53
1	A	117	ARG	N-CA	-9.05	1.34	1.46
2	B	47	ASP	C-O	9.05	1.34	1.24
1	A	92	HIS	CA-C	-9.04	1.41	1.52
2	B	73	LEU	CA-CB	-9.04	1.37	1.53
2	B	334	GLU	CA-C	-9.04	1.41	1.52
1	A	4	TYR	CA-C	9.01	1.64	1.52
1	A	11	LEU	CA-CB	9.00	1.68	1.53
2	B	218	ASP	C-O	8.99	1.35	1.24
2	B	371	LEU	CA-CB	-8.97	1.41	1.53
2	B	97	LEU	CA-C	8.96	1.64	1.52
2	B	13	GLY	CA-C	8.96	1.64	1.52
2	B	373	VAL	CB-CG1	8.95	1.82	1.52
1	A	29	GLY	CA-C	8.94	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	253	ALA	CA-CB	-8.94	1.39	1.53
1	A	20	VAL	CA-C	8.93	1.62	1.52
1	A	65	GLN	CG-CD	8.93	1.74	1.52
1	A	49[A]	GLU	CA-C	8.93	1.63	1.52
1	A	49[B]	GLU	CA-C	8.93	1.63	1.52
2	B	6	ASN	CA-CB	8.93	1.69	1.53
2	B	151	LEU	CA-C	-8.92	1.40	1.52
1	A	30	ILE	CA-C	8.90	1.63	1.52
2	B	45	PHE	C-O	8.90	1.34	1.24
2	B	123	SER	CB-OG	8.89	1.59	1.42
1	A	89	ARG	C-O	8.88	1.34	1.24
1	A	138	PRO	CA-C	-8.88	1.37	1.52
2	B	96	LEU	CA-C	8.87	1.64	1.52
2	B	146	VAL	C-O	8.87	1.34	1.24
2	B	192	ALA	N-CA	8.87	1.59	1.46
2	B	230	CYS	N-CA	-8.87	1.34	1.45
2	B	32	PHE	CG-CD1	8.86	1.57	1.38
2	B	125	LEU	N-CA	-8.85	1.35	1.46
2	B	291	ASP	CA-CB	8.85	1.69	1.53
2	B	348	ALA	C-N	-8.83	1.22	1.33
2	B	301	SER	CA-C	8.81	1.64	1.52
2	B	271	LEU	C-O	8.81	1.34	1.24
1	A	86	ALA	CA-CB	8.80	1.67	1.53
2	B	282	MET	CG-SD	8.80	2.02	1.80
1	A	33	SER	CA-C	8.80	1.64	1.52
2	B	210	GLU	CA-C	8.80	1.64	1.52
2	B	294	ILE	CA-CB	-8.79	1.43	1.54
2	B	180	SER	CA-C	-8.78	1.43	1.52
2	B	348	ALA	CA-C	8.78	1.64	1.52
2	B	36	GLN	CG-CD	8.77	1.74	1.52
2	B	276	VAL	N-CA	8.77	1.57	1.46
2	B	86	HIS	C-N	-8.77	1.22	1.34
1	A	7	LEU	CA-CB	8.76	1.67	1.53
1	A	212	PHE	CD2-CE2	8.76	1.65	1.38
2	B	45	PHE	CA-C	8.75	1.64	1.52
2	B	347	PRO	CA-C	-8.75	1.40	1.52
2	B	89	ASN	N-CA	-8.74	1.36	1.46
2	B	215	GLN	CA-CB	-8.74	1.39	1.53
2	B	293	GLN	CA-CB	-8.74	1.39	1.53
2	B	294	ILE	CB-CG1	8.74	1.71	1.53
2	B	372	LEU	CA-CB	-8.73	1.37	1.53
2	B	59	LEU	CB-CG	8.73	1.71	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	85	LEU	CA-CB	-8.72	1.39	1.53
1	A	83	GLU	CA-CB	8.71	1.66	1.53
2	B	190	THR	CB-OG1	8.71	1.57	1.43
2	B	199	THR	CA-C	8.69	1.63	1.52
2	B	346	ILE	N-CA	-8.68	1.39	1.46
2	B	372	LEU	CB-CG	8.68	1.70	1.53
1	A	161	ASP	CG-OD1	8.66	1.41	1.25
2	B	252	LEU	CB-CG	-8.65	1.36	1.53
2	B	350	GLU	CA-CB	8.64	1.67	1.53
2	B	57	THR	CA-CB	-8.63	1.40	1.53
2	B	165	THR	CA-CB	8.62	1.68	1.53
1	A	227	GLY	CA-C	8.62	1.64	1.51
2	B	126	LEU	CA-C	8.60	1.64	1.52
2	B	30	GLU	CA-C	8.60	1.63	1.52
2	B	231	VAL	CA-CB	8.60	1.65	1.54
2	B	49	LEU	CG-CD2	8.60	1.80	1.52
2	B	276	VAL	C-N	8.60	1.44	1.33
1	A	121	VAL	CA-C	8.58	1.65	1.52
1	A	107	PHE	CA-C	8.57	1.64	1.52
1	A	105	LEU	CA-CB	-8.57	1.39	1.53
2	B	339	LEU	CG-CD2	8.57	1.80	1.52
2	B	209	GLY	CA-C	-8.56	1.41	1.52
1	A	84	MET	CA-C	8.55	1.63	1.52
2	B	324	TYR	CE1-CZ	8.55	1.58	1.38
2	B	23	PRO	CA-C	8.55	1.65	1.52
2	B	78	GLU	CD-OE1	8.54	1.41	1.25
1	A	205	ALA	CA-CB	8.53	1.67	1.53
1	A	144	LEU	C-O	8.53	1.34	1.24
1	A	154	CYS	CA-C	8.52	1.62	1.52
2	B	184	ALA	CA-CB	-8.52	1.38	1.53
1	A	229	ALA	C-N	8.51	1.41	1.33
1	A	7	LEU	CA-C	8.49	1.63	1.52
1	A	223	ALA	CA-C	8.49	1.64	1.52
2	B	333	LEU	N-CA	8.49	1.56	1.46
1	A	114	PHE	N-CA	-8.48	1.35	1.46
2	B	246	ASN	CA-C	8.48	1.64	1.52
2	B	212	THR	CA-C	-8.48	1.41	1.52
2	B	352	SER	CB-OG	8.48	1.59	1.42
2	B	383	ASP	C-N	8.47	1.44	1.33
2	B	298	TYR	N-CA	8.44	1.56	1.46
2	B	366	PRO	CA-C	-8.43	1.37	1.52
1	A	82	PHE	CD1-CE1	-8.43	1.13	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	111	ILE	C-O	8.43	1.33	1.24
2	B	319	ILE	CB-CG1	8.43	1.70	1.53
2	B	121	LEU	CA-C	-8.43	1.41	1.52
2	B	55	ARG	C-O	8.42	1.34	1.23
1	A	106	VAL	CA-CB	8.42	1.66	1.54
2	B	362	MET	CA-CB	8.42	1.66	1.53
2	B	94	GLN	CA-CB	-8.41	1.39	1.53
1	A	199	LYS	CA-C	8.40	1.63	1.52
2	B	213	LYS	C-N	8.40	1.45	1.34
2	B	355	LEU	CB-CG	8.40	1.70	1.53
2	B	36	GLN	CA-CB	8.39	1.68	1.53
2	B	143	SER	CA-CB	-8.38	1.41	1.54
2	B	17	VAL	CA-CB	8.38	1.64	1.55
2	B	272	LYS	N-CA	8.37	1.57	1.46
2	B	177	TRP	N-CA	-8.37	1.36	1.46
1	A	140	ARG	N-CA	8.36	1.56	1.46
2	B	90	GLN	CD-OE1	8.34	1.39	1.23
2	B	362	MET	CG-SD	8.34	2.01	1.80
1	A	141	GLN	N-CA	8.33	1.56	1.46
2	B	76	LYS	CD-CE	8.32	1.77	1.52
2	B	7	PRO	N-CA	-8.32	1.36	1.47
2	B	238	ILE	N-CA	-8.32	1.34	1.46
2	B	240	MET	C-O	-8.30	1.14	1.24
1	A	150	PRO	CA-CB	-8.28	1.43	1.53
2	B	214	ALA	C-N	-8.28	1.22	1.33
1	A	45	ALA	C-O	8.25	1.33	1.23
2	B	93	GLY	CA-C	8.25	1.62	1.51
2	B	190	THR	N-CA	8.25	1.57	1.46
1	A	200	LEU	CA-C	8.25	1.63	1.52
1	A	171	ARG	N-CA	8.24	1.56	1.45
1	A	119	GLU	N-CA	8.24	1.56	1.46
2	B	253	ILE	N-CA	-8.24	1.36	1.46
2	B	86	HIS	CG-CD2	8.23	1.45	1.35
2	B	358	ALA	CA-C	8.23	1.63	1.52
2	B	372	LEU	C-O	-8.23	1.14	1.24
2	B	43	ALA	CA-CB	-8.21	1.40	1.53
2	B	13	GLY	N-CA	8.21	1.54	1.45
2	B	98	ALA	CA-C	8.20	1.63	1.52
1	A	20	VAL	CA-CB	-8.20	1.43	1.54
2	B	258	GLY	C-N	8.19	1.45	1.33
2	B	295	GLU	CG-CD	8.19	1.72	1.52
2	B	28	LEU	N-CA	8.19	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	152	PHE	CA-CB	-8.18	1.35	1.53
2	B	334	GLU	CA-CB	8.18	1.66	1.53
2	B	139	VAL	CB-CG2	8.17	1.79	1.52
2	B	327	ILE	C-O	8.16	1.32	1.24
2	B	363	ARG	CA-C	8.15	1.63	1.52
2	B	219	LYS	CG-CD	-8.14	1.28	1.52
2	B	211	GLU	C-N	-8.14	1.23	1.33
1	A	123	VAL	C-N	8.14	1.45	1.33
1	A	217	PRO	CA-C	-8.14	1.40	1.52
2	B	287	MET	CB-CG	8.13	1.76	1.52
1	A	124	ASP	C-N	8.12	1.43	1.33
1	A	142	ALA	CA-CB	8.11	1.66	1.53
1	A	53	PRO	N-CA	8.11	1.56	1.47
1	A	257	SER	N-CA	8.11	1.56	1.46
2	B	9	PHE	CD2-CE2	8.10	1.62	1.38
2	B	55	ARG	CD-NE	8.10	1.57	1.46
1	A	134	GLU	C-N	-8.09	1.23	1.33
2	B	59	LEU	C-N	-8.09	1.22	1.33
2	B	87	LYS	N-CA	8.08	1.56	1.46
1	A	108	ASN	CG-OD1	-8.07	1.08	1.23
1	A	70	ARG	NE-CZ	-8.07	1.24	1.33
2	B	360	LYS	CB-CG	-8.06	1.28	1.52
2	B	342	HIS	N-CA	-8.05	1.35	1.46
2	B	323	ASP	C-N	-8.04	1.22	1.33
1	A	140	ARG	CG-CD	8.04	1.76	1.52
2	B	328	THR	CB-OG1	8.04	1.56	1.43
2	B	360	LYS	N-CA	8.04	1.56	1.46
2	B	363	ARG	N-CA	8.04	1.56	1.46
2	B	81	LEU	CA-CB	8.04	1.66	1.53
2	B	177	TRP	CD2-CE3	8.04	1.53	1.40
2	B	231	VAL	CB-CG1	8.03	1.79	1.52
1	A	214	ILE	CA-CB	8.03	1.61	1.53
2	B	121	LEU	C-O	8.02	1.34	1.24
2	B	322	ALA	C-O	8.02	1.33	1.23
2	B	216	ILE	N-CA	8.02	1.56	1.46
2	B	271	LEU	N-CA	-8.00	1.36	1.46
2	B	281	GLY	CA-C	-7.99	1.40	1.51
1	A	199	LYS	C-O	7.99	1.33	1.24
2	B	133	TYR	CA-CB	7.99	1.68	1.53
2	B	60	THR	CB-OG1	7.98	1.56	1.43
2	B	132	ILE	CA-CB	-7.98	1.43	1.55
1	A	174	THR	C-O	7.98	1.33	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	341	ARG	CZ-NH1	7.97	1.44	1.32
2	B	380	GLY	C-O	-7.97	1.13	1.23
2	B	177	TRP	C-O	-7.97	1.17	1.24
2	B	138	ASP	CA-CB	-7.97	1.40	1.53
2	B	342	HIS	CA-C	-7.97	1.41	1.52
1	A	253	ALA	CA-C	-7.95	1.42	1.52
2	B	236	ASN	CA-CB	7.95	1.66	1.53
1	A	220	VAL	N-CA	7.94	1.55	1.46
2	B	195	HIS	CA-C	7.94	1.62	1.53
2	B	216	ILE	CB-CG1	7.94	1.69	1.53
2	B	98	ALA	CA-CB	-7.93	1.41	1.53
1	A	221	SER	CA-CB	7.89	1.65	1.53
2	B	314	ALA	CA-C	-7.88	1.42	1.52
1	A	207	PRO	C-O	7.88	1.32	1.23
1	A	7	LEU	CG-CD2	7.87	1.78	1.52
1	A	101	MET	CB-CG	7.87	1.76	1.52
2	B	115	HIS	CA-C	7.87	1.63	1.52
1	A	48	LEU	C-N	7.86	1.44	1.33
2	B	74	TYR	N-CA	7.85	1.55	1.45
1	A	59	ALA	CA-CB	-7.85	1.41	1.53
2	B	131	ARG	CZ-NH2	7.84	1.43	1.33
2	B	311	PRO	CA-C	-7.84	1.38	1.52
2	B	321	ARG	NE-CZ	7.84	1.41	1.33
2	B	330	ASP	C-O	7.84	1.33	1.24
1	A	25	LEU	N-CA	7.84	1.55	1.46
2	B	320	GLY	C-N	7.84	1.45	1.33
2	B	59	LEU	C-O	7.84	1.32	1.24
2	B	78	GLU	N-CA	7.83	1.56	1.46
1	A	263	LYS	CA-C	7.83	1.63	1.52
2	B	195	HIS	ND1-CE1	-7.83	1.24	1.32
2	B	21	LEU	C-N	7.83	1.44	1.33
2	B	22	MET	N-CA	-7.83	1.39	1.46
2	B	28	LEU	CB-CG	7.83	1.69	1.53
2	B	275	ARG	CA-C	7.82	1.62	1.52
2	B	123	SER	CA-CB	-7.80	1.40	1.53
2	B	37	LYS	CG-CD	7.80	1.75	1.52
2	B	10	GLY	CA-C	-7.80	1.38	1.51
2	B	339	LEU	C-N	-7.80	1.23	1.33
1	A	135	GLU	N-CA	7.80	1.55	1.46
2	B	172	GLU	N-CA	7.79	1.56	1.46
1	A	129	ALA	N-CA	7.78	1.56	1.46
2	B	46	ALA	CA-CB	-7.78	1.41	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	230	GLY	N-CA	-7.78	1.37	1.45
2	B	366	PRO	C-O	7.77	1.34	1.24
1	A	140	ARG	CB-CG	-7.77	1.29	1.52
2	B	72	THR	C-O	7.77	1.33	1.24
2	B	129	LYS	CA-CB	7.76	1.63	1.53
2	B	62	CYS	C-N	-7.76	1.23	1.33
2	B	85	ALA	CA-CB	-7.74	1.41	1.53
2	B	375	ASN	CA-CB	7.74	1.62	1.53
1	A	194	HIS	N-CA	-7.74	1.36	1.46
2	B	195	HIS	CB-CG	-7.73	1.39	1.50
2	B	237	ALA	C-O	-7.73	1.15	1.24
1	A	47	ALA	CA-C	7.73	1.61	1.52
1	A	255	LEU	CA-C	7.73	1.62	1.52
2	B	302	ALA	N-CA	7.72	1.55	1.46
2	B	145	ASN	C-O	7.72	1.32	1.24
2	B	225	ASP	C-O	7.72	1.33	1.24
2	B	353	HIS	CD2-NE2	-7.70	1.29	1.37
2	B	353	HIS	N-CA	7.70	1.55	1.46
2	B	67	ALA	CA-C	7.69	1.63	1.52
1	A	91	LYS	C-N	-7.69	1.22	1.33
2	B	365	GLN	N-CA	-7.69	1.38	1.46
1	A	132	PRO	C-O	7.67	1.33	1.23
1	A	133	VAL	CA-CB	7.66	1.66	1.54
2	B	48	LEU	C-O	-7.66	1.15	1.24
2	B	380	GLY	N-CA	-7.66	1.34	1.45
2	B	308	SER	C-N	-7.64	1.26	1.33
2	B	369	GLU	CA-C	7.64	1.63	1.52
1	A	14	ARG	C-O	-7.64	1.13	1.24
1	A	130	ASP	CA-CB	7.63	1.63	1.53
1	A	39	THR	CA-CB	7.62	1.65	1.53
2	B	97	LEU	N-CA	7.62	1.55	1.46
2	B	264	THR	CA-C	7.62	1.63	1.52
2	B	264	THR	C-N	-7.61	1.22	1.33
2	B	261	GLY	CA-C	7.61	1.62	1.51
2	B	283	LYS	N-CA	7.61	1.55	1.46
2	B	207	MET	N-CA	-7.61	1.36	1.46
2	B	370	GLN	CA-C	7.60	1.61	1.52
2	B	109	GLU	CA-CB	7.60	1.71	1.53
2	B	371	LEU	C-N	-7.59	1.23	1.33
2	B	373	VAL	CA-C	-7.58	1.43	1.52
1	A	239	LYS	CA-C	-7.58	1.42	1.52
1	A	223	ALA	CA-CB	7.58	1.65	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	78	GLU	CD-OE2	-7.58	1.10	1.25
2	B	345	ILE	CA-CB	-7.57	1.44	1.54
2	B	114	GLN	N-CA	-7.56	1.37	1.46
2	B	216	ILE	CA-CB	7.56	1.65	1.54
2	B	359	LEU	CB-CG	7.56	1.68	1.53
1	A	113	ALA	CA-CB	7.55	1.65	1.53
1	A	153	ILE	C-N	7.55	1.45	1.33
2	B	129	LYS	CG-CD	7.55	1.75	1.52
2	B	183	THR	CA-C	7.54	1.62	1.52
2	B	204	PHE	N-CA	7.54	1.55	1.46
1	A	95	ILE	N-CA	7.53	1.56	1.47
1	A	231	ALA	C-N	7.52	1.43	1.33
2	B	69	THR	CB-OG1	7.52	1.55	1.43
2	B	195	HIS	CE1-NE2	7.52	1.40	1.32
2	B	355	LEU	C-N	-7.51	1.24	1.33
2	B	387	VAL	CA-CB	-7.51	1.44	1.54
1	A	114	PHE	CA-C	7.51	1.62	1.52
2	B	199	THR	CB-OG1	7.51	1.55	1.43
1	A	213	GLY	CA-C	7.51	1.62	1.51
2	B	55	ARG	CG-CD	7.50	1.75	1.52
1	A	204	HIS	C-N	-7.49	1.23	1.33
2	B	302	ALA	C-O	7.49	1.32	1.24
2	B	11	GLU	CD-OE2	7.48	1.39	1.25
2	B	4	LEU	N-CA	-7.48	1.36	1.46
1	A	118	CYS	C-N	-7.48	1.24	1.33
2	B	325	VAL	CA-C	-7.47	1.43	1.52
1	A	20	VAL	C-N	-7.47	1.24	1.33
1	A	209	LEU	C-O	7.47	1.33	1.24
1	A	261	ALA	N-CA	7.47	1.55	1.46
2	B	52	TYR	CZ-OH	-7.47	1.22	1.38
2	B	248	THR	C-O	-7.47	1.14	1.24
1	A	113	ALA	N-CA	-7.47	1.36	1.46
1	A	119	GLU	CA-CB	-7.46	1.41	1.53
2	B	84	GLY	N-CA	7.46	1.56	1.45
2	B	381	ASP	CA-CB	7.46	1.65	1.53
2	B	38	ASP	C-N	-7.46	1.24	1.33
1	A	87	LEU	N-CA	-7.45	1.37	1.46
2	B	234	GLY	C-O	-7.45	1.16	1.24
1	A	149	ALA	CA-CB	7.44	1.65	1.52
2	B	212	THR	CB-CG2	7.44	1.77	1.52
1	A	166	VAL	CB-CG2	7.43	1.77	1.52
2	B	71	THR	CB-CG2	7.43	1.77	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	146	HIS	N-CA	-7.42	1.37	1.46
2	B	12	PHE	CD2-CE2	7.41	1.60	1.38
2	B	243	ASP	CG-OD1	7.41	1.39	1.25
2	B	46	ALA	C-O	7.41	1.32	1.24
2	B	345	ILE	N-CA	7.40	1.55	1.46
1	A	257	SER	CA-C	-7.39	1.43	1.52
2	B	319	ILE	C-N	-7.39	1.23	1.33
2	B	244	PHE	CA-C	7.39	1.63	1.52
2	B	348	ALA	C-O	7.38	1.33	1.23
2	B	107	ILE	C-O	-7.38	1.15	1.24
2	B	121	LEU	CG-CD1	-7.38	1.28	1.52
2	B	150	ARG	CB-CG	7.37	1.74	1.52
2	B	209	GLY	C-N	7.37	1.44	1.33
1	A	97	ILE	CA-CB	-7.37	1.44	1.53
2	B	284	ALA	N-CA	7.36	1.56	1.46
1	A	102	TYR	C-O	7.36	1.32	1.23
1	A	116	ALA	C-O	7.36	1.32	1.24
1	A	76	VAL	C-O	7.36	1.32	1.24
1	A	120	GLN	CG-CD	7.36	1.70	1.52
2	B	112	ALA	CA-C	7.35	1.62	1.52
2	B	89	ASN	CA-C	7.34	1.61	1.52
1	A	137	ALA	N-CA	7.33	1.56	1.46
2	B	29	GLU	CD-OE2	7.33	1.39	1.25
1	A	40	LEU	CA-C	7.33	1.62	1.52
2	B	86	HIS	CA-CB	7.32	1.67	1.53
2	B	197	TYR	C-O	7.32	1.31	1.24
1	A	118	CYS	C-O	-7.31	1.15	1.24
2	B	20	ILE	C-N	7.30	1.44	1.33
2	B	349	LEU	C-O	7.30	1.32	1.24
2	B	77	ARG	CB-CG	7.30	1.74	1.52
1	A	258	PHE	C-O	7.29	1.32	1.24
2	B	66	THR	N-CA	7.29	1.55	1.46
2	B	277	GLY	CA-C	7.29	1.60	1.51
2	B	349	LEU	N-CA	7.29	1.55	1.46
2	B	78	GLU	CA-CB	7.29	1.66	1.53
1	A	67	ALA	CA-C	7.28	1.62	1.52
2	B	119	SER	CA-CB	7.28	1.65	1.53
2	B	57	THR	C-O	-7.27	1.15	1.23
2	B	204	PHE	CB-CG	7.26	1.67	1.50
2	B	328	THR	C-N	-7.26	1.24	1.33
2	B	312	GLN	CD-NE2	-7.26	1.18	1.33
2	B	360	LYS	CG-CD	7.25	1.74	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	78	GLU	C-N	7.25	1.43	1.33
2	B	15	MET	C-O	7.24	1.33	1.23
2	B	115	HIS	CG-ND1	-7.24	1.30	1.38
1	A	264	ALA	C-O	7.23	1.32	1.24
2	B	167	LYS	CE-NZ	7.23	1.71	1.49
1	A	216	SER	N-CA	7.23	1.52	1.45
2	B	241	PHE	CA-C	-7.22	1.42	1.52
1	A	109	ASN	CG-OD1	7.22	1.37	1.23
2	B	277	GLY	C-N	7.22	1.43	1.33
2	B	250	VAL	CA-CB	7.22	1.62	1.54
1	A	216	SER	CA-C	7.21	1.60	1.52
2	B	128	LEU	CA-CB	7.21	1.64	1.53
2	B	196	PRO	C-N	-7.20	1.24	1.33
1	A	103	ALA	C-O	-7.20	1.15	1.24
1	A	112	ASP	CB-CG	-7.20	1.34	1.52
1	A	157	ASN	CA-CB	7.20	1.63	1.53
2	B	88	THR	C-N	7.19	1.42	1.33
1	A	4	TYR	C-O	7.18	1.32	1.24
2	B	372	LEU	CA-C	7.18	1.61	1.52
1	A	15	ARG	CA-CB	7.18	1.64	1.53
2	B	17	VAL	C-N	-7.16	1.24	1.33
1	A	114	PHE	C-N	-7.16	1.23	1.33
1	A	124	ASP	CA-C	-7.15	1.43	1.52
1	A	218	GLU	CA-C	-7.15	1.42	1.52
1	A	53	PRO	CA-CB	-7.15	1.44	1.53
1	A	11	LEU	N-CA	-7.14	1.37	1.46
2	B	147	PHE	C-O	7.14	1.32	1.24
2	B	188	LEU	CA-CB	7.14	1.64	1.53
2	B	363	ARG	CA-CB	-7.14	1.42	1.53
1	A	110	GLY	CA-C	7.13	1.61	1.51
2	B	129	LYS	N-CA	-7.13	1.37	1.46
2	B	355	LEU	C-O	7.13	1.32	1.24
1	A	219	GLN	CA-CB	7.13	1.65	1.53
2	B	223	LEU	CA-CB	7.12	1.63	1.53
1	A	33	SER	N-CA	-7.12	1.37	1.46
1	A	21	PRO	CA-C	7.12	1.59	1.52
2	B	88	THR	CA-CB	7.12	1.65	1.53
2	B	363	ARG	CB-CG	7.11	1.73	1.52
2	B	321	ARG	CA-C	7.10	1.62	1.52
2	B	265	GLY	C-O	7.10	1.34	1.24
1	A	67	ALA	N-CA	7.09	1.55	1.46
1	A	148	ILE	C-O	-7.09	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	305	ASP	CA-C	7.08	1.61	1.53
2	B	20	ILE	CG1-CD1	-7.08	1.24	1.51
2	B	357	HIS	CE1-NE2	-7.08	1.25	1.32
2	B	8	TYR	C-N	7.06	1.42	1.33
2	B	293	GLN	CA-C	7.05	1.62	1.52
2	B	351	SER	CA-CB	7.05	1.65	1.53
2	B	231	VAL	C-O	-7.04	1.16	1.24
2	B	33	VAL	N-CA	-7.03	1.38	1.46
1	A	25	LEU	CB-CG	7.03	1.67	1.53
2	B	308	SER	CA-CB	7.03	1.64	1.53
2	B	102	GLY	C-N	7.02	1.43	1.33
2	B	66	THR	CA-CB	-7.02	1.42	1.53
2	B	99	LYS	C-O	7.02	1.32	1.24
2	B	202	ARG	CD-NE	-7.01	1.36	1.46
2	B	260	HIS	CG-ND1	7.01	1.46	1.38
2	B	258	GLY	CA-C	-7.00	1.39	1.51
2	B	319	ILE	CB-CG2	7.00	1.75	1.52
2	B	385	PHE	C-O	-7.00	1.16	1.24
2	B	351	SER	C-N	-6.99	1.24	1.34
2	B	354	ALA	N-CA	-6.99	1.38	1.46
2	B	124	ALA	C-O	6.97	1.32	1.24
2	B	156	VAL	C-N	6.97	1.39	1.33
2	B	61	LYS	C-O	6.97	1.32	1.23
1	A	126	VAL	CB-CG1	6.95	1.75	1.52
2	B	66	THR	CB-CG2	6.95	1.75	1.52
2	B	342	HIS	C-N	6.94	1.44	1.33
2	B	8	TYR	CA-C	6.94	1.61	1.52
2	B	148	ARG	CB-CG	6.94	1.73	1.52
2	B	26	ASN	CA-C	6.93	1.62	1.52
2	B	115	HIS	C-N	-6.92	1.23	1.33
2	B	313	HIS	C-O	6.92	1.32	1.24
1	A	65	GLN	C-O	6.90	1.32	1.24
2	B	240	MET	SD-CE	6.90	1.96	1.79
2	B	79	ASP	CA-CB	6.89	1.65	1.53
2	B	210	GLU	CA-CB	6.89	1.64	1.53
2	B	333	LEU	CG-CD2	6.89	1.75	1.52
2	B	105	GLU	C-O	-6.88	1.15	1.23
2	B	394	ARG	CZ-NH2	6.88	1.42	1.33
2	B	125	LEU	CB-CG	-6.87	1.39	1.53
2	B	3	THR	C-N	6.86	1.44	1.33
2	B	25	LEU	CG-CD2	6.86	1.75	1.52
2	B	366	PRO	C-N	6.86	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	227	VAL	CA-CB	6.86	1.63	1.54
1	A	103	ALA	N-CA	-6.85	1.38	1.46
2	B	269	ALA	N-CA	-6.85	1.39	1.46
2	B	28	LEU	C-N	6.85	1.43	1.33
2	B	363	ARG	CD-NE	6.85	1.55	1.46
2	B	365	GLN	CD-NE2	6.84	1.47	1.33
2	B	88	THR	N-CA	6.84	1.54	1.46
2	B	270	PRO	CA-C	-6.84	1.41	1.52
2	B	332	ALA	CA-C	6.84	1.61	1.52
2	B	264	THR	CB-CG2	6.84	1.75	1.52
2	B	365	GLN	C-O	-6.83	1.16	1.24
1	A	136	SER	CA-CB	6.81	1.65	1.53
2	B	88	THR	C-O	6.81	1.32	1.24
2	B	114	GLN	CB-CG	6.81	1.72	1.52
2	B	281	GLY	N-CA	-6.81	1.34	1.45
2	B	97	LEU	CA-CB	6.80	1.64	1.53
1	A	52	VAL	CB-CG1	6.80	1.75	1.52
2	B	318	SER	C-N	6.79	1.41	1.34
2	B	40	GLU	CA-CB	6.78	1.63	1.53
2	B	63	GLN	CG-CD	6.78	1.69	1.52
2	B	352	SER	C-O	-6.78	1.15	1.24
1	A	263	LYS	CA-CB	6.78	1.64	1.53
1	A	145	ARG	NE-CZ	-6.77	1.25	1.33
2	B	355	LEU	CA-C	6.76	1.61	1.52
2	B	388	HIS	CA-C	-6.76	1.44	1.52
2	B	202	ARG	N-CA	-6.76	1.38	1.46
2	B	143	SER	C-O	-6.75	1.18	1.24
1	A	87	LEU	CG-CD1	6.75	1.74	1.52
2	B	151	LEU	CA-CB	6.75	1.64	1.53
1	A	45	ALA	CA-CB	6.74	1.64	1.53
2	B	79	ASP	C-N	-6.74	1.23	1.33
2	B	56	PRO	C-O	6.73	1.36	1.23
2	B	351	SER	N-CA	-6.73	1.37	1.46
2	B	183	THR	CB-CG2	6.72	1.74	1.52
2	B	296	GLU	CB-CG	6.71	1.72	1.52
2	B	117	VAL	N-CA	6.71	1.54	1.46
2	B	15	MET	CA-C	-6.71	1.42	1.53
2	B	158	PRO	N-CA	6.71	1.55	1.47
1	A	146	HIS	C-O	-6.70	1.15	1.24
2	B	16	TYR	CG-CD1	6.69	1.53	1.39
2	B	190	THR	CA-CB	-6.69	1.43	1.53
2	B	331	GLU	CA-C	6.69	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	162	LEU	C-O	-6.69	1.16	1.24
2	B	168	ASP	CA-CB	-6.69	1.42	1.53
2	B	244	PHE	CB-CG	6.68	1.66	1.50
1	A	140	ARG	CA-CB	6.67	1.63	1.53
2	B	73	LEU	CB-CG	6.67	1.66	1.53
2	B	72	THR	N-CA	6.66	1.54	1.46
1	A	76	VAL	CA-CB	6.66	1.61	1.54
1	A	139	PHE	CB-CG	6.65	1.66	1.50
2	B	159	VAL	N-CA	6.65	1.54	1.46
2	B	30	GLU	CG-CD	6.65	1.68	1.52
1	A	64	ILE	CB-CG1	6.65	1.66	1.53
2	B	211	GLU	CD-OE2	6.64	1.38	1.25
1	A	171	ARG	NE-CZ	-6.63	1.25	1.33
2	B	353	HIS	CB-CG	-6.62	1.40	1.50
2	B	337	LYS	CA-C	-6.62	1.44	1.52
2	B	322	ALA	CA-C	-6.61	1.44	1.52
1	A	10	GLN	C-O	6.59	1.31	1.24
2	B	115	HIS	CA-CB	6.59	1.64	1.53
2	B	255	VAL	CA-C	-6.59	1.44	1.52
1	A	198	GLU	CA-C	-6.59	1.44	1.52
2	B	76	LYS	N-CA	6.58	1.54	1.46
2	B	273	HIS	N-CA	-6.58	1.36	1.45
1	A	118	CYS	CA-C	6.58	1.61	1.52
1	A	134	GLU	N-CA	-6.58	1.37	1.46
1	A	133	VAL	CA-C	-6.58	1.43	1.52
2	B	77	ARG	CA-CB	6.58	1.64	1.53
2	B	52	TYR	C-N	6.57	1.43	1.33
2	B	97	LEU	CG-CD1	6.57	1.74	1.52
1	A	100	LEU	CB-CG	6.55	1.66	1.53
2	B	333	LEU	C-O	6.55	1.31	1.24
2	B	378	GLY	N-CA	6.54	1.52	1.45
1	A	235	SER	CA-C	-6.52	1.44	1.52
2	B	304	LEU	C-N	-6.52	1.24	1.33
1	A	169	TYR	CA-C	-6.52	1.43	1.52
2	B	203	GLU	C-O	6.52	1.32	1.24
2	B	17	VAL	CB-CG1	6.51	1.74	1.52
1	A	148	ILE	CA-C	6.50	1.60	1.52
2	B	322	ALA	CA-CB	6.49	1.67	1.54
2	B	152	MET	N-CA	-6.49	1.37	1.46
2	B	285	PRO	CG-CD	6.48	1.72	1.50
2	B	188	LEU	N-CA	6.48	1.54	1.45
2	B	200	ILE	C-O	6.47	1.31	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	166	VAL	N-CA	-6.47	1.38	1.46
1	A	54	PHE	CA-CB	-6.46	1.38	1.53
1	A	131	VAL	N-CA	-6.46	1.41	1.46
2	B	356	ALA	C-O	6.46	1.31	1.24
2	B	306	PHE	N-CA	6.46	1.55	1.46
2	B	106	ILE	CA-CB	6.45	1.62	1.54
2	B	15	MET	C-N	-6.44	1.25	1.33
2	B	186	TYR	CA-C	6.43	1.60	1.52
2	B	378	GLY	CA-C	6.42	1.58	1.51
2	B	5	LEU	C-N	6.42	1.43	1.33
2	B	357	HIS	CB-CG	6.42	1.59	1.50
1	A	51	GLY	CA-C	6.41	1.58	1.52
1	A	169	TYR	CG-CD2	6.41	1.52	1.39
1	A	195	HIS	CA-C	6.39	1.61	1.52
2	B	94	GLN	N-CA	6.39	1.54	1.46
2	B	360	LYS	CA-CB	6.38	1.63	1.53
2	B	112	ALA	C-O	6.38	1.32	1.24
2	B	368	LYS	N-CA	6.38	1.54	1.46
2	B	188	LEU	CG-CD1	6.38	1.73	1.52
2	B	274	GLY	N-CA	6.38	1.54	1.45
2	B	10	GLY	N-CA	6.38	1.54	1.45
2	B	238	ILE	C-O	-6.37	1.15	1.24
2	B	267	HIS	CB-CG	6.37	1.59	1.50
2	B	100	ARG	CZ-NH2	-6.36	1.25	1.33
2	B	52	TYR	CB-CG	-6.36	1.37	1.51
2	B	8	TYR	N-CA	6.36	1.53	1.45
2	B	340	CYS	CA-C	6.36	1.61	1.52
2	B	315	TYR	CB-CG	-6.35	1.37	1.51
2	B	342	HIS	C-O	-6.35	1.15	1.24
2	B	267	HIS	C-N	-6.35	1.24	1.33
2	B	98	ALA	C-O	6.34	1.31	1.24
1	A	213	GLY	N-CA	6.33	1.54	1.45
2	B	201	VAL	C-N	6.33	1.42	1.33
2	B	204	PHE	CD2-CE2	6.33	1.57	1.38
1	A	130	ASP	CG-OD1	6.33	1.37	1.25
1	A	165	GLN	C-O	6.32	1.31	1.24
2	B	361	MET	N-CA	-6.31	1.38	1.46
1	A	115	TYR	N-CA	6.30	1.54	1.46
2	B	54	GLY	C-N	6.30	1.42	1.33
2	B	207	MET	SD-CE	-6.30	1.63	1.79
2	B	288	GLN	C-O	6.29	1.31	1.23
2	B	34	SER	C-N	-6.29	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	165	THR	N-CA	6.29	1.54	1.46
2	B	256	GLU	N-CA	-6.29	1.36	1.45
1	A	124	ASP	CG-OD2	-6.28	1.13	1.25
2	B	176	ASP	C-O	6.27	1.32	1.24
2	B	220	GLU	C-O	6.27	1.32	1.24
1	A	171	ARG	CZ-NH2	-6.26	1.25	1.33
1	A	62	PRO	N-CD	6.26	1.56	1.47
1	A	151	ILE	N-CA	6.26	1.54	1.46
1	A	218	GLU	C-O	6.26	1.32	1.24
1	A	229	ALA	N-CA	-6.26	1.38	1.46
1	A	163	LEU	CA-CB	6.25	1.63	1.53
1	A	60	ASP	CG-OD1	6.25	1.37	1.25
2	B	234	GLY	CA-C	-6.25	1.41	1.51
2	B	345	ILE	CB-CG1	-6.25	1.41	1.53
2	B	198	PRO	CG-CD	6.25	1.72	1.50
2	B	63	GLN	CD-OE1	6.24	1.35	1.23
2	B	376	LEU	CA-C	6.24	1.60	1.52
2	B	264	THR	N-CA	-6.24	1.38	1.46
2	B	202	ARG	CG-CD	6.24	1.71	1.52
2	B	355	LEU	CA-CB	6.23	1.63	1.53
2	B	346	ILE	CA-C	6.23	1.58	1.53
1	A	77	THR	C-N	-6.22	1.24	1.33
1	A	128	VAL	CA-CB	-6.22	1.46	1.53
2	B	59	LEU	CG-CD2	-6.22	1.32	1.52
1	A	11	LEU	C-O	6.22	1.31	1.24
2	B	198	PRO	CA-C	-6.22	1.43	1.52
2	B	75	LEU	C-O	-6.21	1.17	1.24
2	B	215	GLN	CB-CG	6.21	1.71	1.52
1	A	59	ALA	N-CA	-6.20	1.38	1.46
2	B	40	GLU	CG-CD	6.20	1.67	1.52
2	B	238	ILE	CB-CG2	6.20	1.73	1.52
2	B	12	PHE	CA-CB	6.20	1.64	1.53
2	B	345	ILE	CA-C	-6.20	1.44	1.52
1	A	171	ARG	CA-CB	6.20	1.65	1.53
2	B	103	LYS	C-N	-6.20	1.23	1.33
2	B	294	ILE	N-CA	6.19	1.53	1.46
1	A	45	ALA	C-N	-6.19	1.24	1.33
2	B	388	HIS	CA-CB	6.19	1.62	1.53
2	B	37	LYS	CD-CE	6.17	1.71	1.52
2	B	324	TYR	CG-CD2	6.17	1.52	1.39
2	B	23	PRO	CB-CG	6.17	1.80	1.49
2	B	44	GLN	CG-CD	6.17	1.67	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	212	THR	C-N	6.17	1.41	1.33
2	B	178	PRO	CA-C	6.17	1.61	1.52
1	A	145	ARG	N-CA	6.16	1.54	1.46
2	B	343	GLU	CD-OE2	6.16	1.37	1.25
2	B	289	THR	N-CA	6.16	1.54	1.45
2	B	188	LEU	CG-CD2	6.15	1.72	1.52
1	A	20	VAL	CB-CG1	6.15	1.72	1.52
2	B	32	PHE	C-N	6.15	1.41	1.34
2	B	106	ILE	CB-CG2	6.14	1.72	1.52
2	B	363	ARG	CZ-NH2	6.14	1.41	1.33
1	A	97	ILE	CA-C	-6.13	1.44	1.52
2	B	236	ASN	CA-C	6.13	1.61	1.52
1	A	107	PHE	CG-CD1	-6.13	1.25	1.38
2	B	47	ASP	C-N	6.13	1.41	1.33
2	B	260	HIS	CD2-NE2	6.12	1.44	1.37
2	B	287	MET	CG-SD	6.12	1.96	1.80
1	A	31	GLU	CD-OE2	6.12	1.36	1.25
1	A	66	ASN	N-CA	-6.12	1.38	1.46
2	B	213	LYS	N-CA	-6.12	1.39	1.46
2	B	251	GLY	C-O	6.11	1.32	1.23
1	A	104	ASN	CA-C	6.10	1.60	1.52
2	B	14	GLY	C-O	6.10	1.32	1.24
2	B	86	HIS	CB-CG	-6.09	1.41	1.50
1	A	244	ASN	N-CA	-6.09	1.39	1.46
2	B	80	LEU	C-N	6.08	1.41	1.33
2	B	214	ALA	CA-C	6.08	1.60	1.52
2	B	385	PHE	C-N	-6.08	1.25	1.33
1	A	89	ARG	CA-CB	-6.08	1.43	1.53
2	B	34	SER	CA-CB	6.08	1.62	1.53
1	A	53	PRO	CG-CD	6.07	1.71	1.50
2	B	11	GLU	C-N	6.06	1.41	1.33
1	A	240	ILE	CA-CB	6.06	1.62	1.54
2	B	151	LEU	C-N	6.06	1.41	1.33
1	A	239	LYS	CG-CD	6.05	1.70	1.52
2	B	56	PRO	CA-C	-6.05	1.40	1.52
2	B	324	TYR	CA-CB	6.05	1.64	1.53
1	A	15	ARG	C-N	6.05	1.42	1.33
2	B	130	CYS	C-O	6.04	1.31	1.24
2	B	47	ASP	CA-CB	6.04	1.62	1.53
2	B	149	MET	CA-C	6.04	1.60	1.52
1	A	127	LEU	C-N	-6.04	1.25	1.33
2	B	288	GLN	CA-CB	6.04	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	143	ALA	N-CA	-6.03	1.39	1.46
2	B	258	GLY	N-CA	6.02	1.53	1.45
1	A	3	ARG	N-CA	-6.02	1.38	1.46
1	A	234	GLY	N-CA	6.02	1.54	1.45
2	B	200	ILE	CA-CB	6.02	1.61	1.54
1	A	200	LEU	CA-CB	-6.02	1.43	1.53
1	A	210	GLN	CA-CB	6.01	1.62	1.53
2	B	241	PHE	CA-CB	6.01	1.63	1.53
1	A	18	ALA	C-N	-6.01	1.25	1.33
2	B	275	ARG	N-CA	6.01	1.53	1.46
2	B	186	TYR	CA-CB	6.00	1.61	1.53
2	B	307	PRO	C-N	-6.00	1.28	1.33
1	A	161	ASP	C-O	-6.00	1.17	1.24
2	B	266	GLU	CA-CB	-6.00	1.44	1.52
1	A	69	LEU	CA-C	-5.99	1.45	1.52
2	B	5	LEU	CA-C	5.99	1.60	1.52
2	B	81	LEU	C-O	-5.99	1.16	1.23
2	B	223	LEU	CA-C	-5.99	1.45	1.52
2	B	127	GLY	CA-C	5.99	1.59	1.51
2	B	90	GLN	C-O	5.98	1.31	1.24
2	B	250	VAL	CA-C	-5.98	1.45	1.52
1	A	60	ASP	N-CA	-5.98	1.38	1.46
1	A	107	PHE	C-O	5.98	1.31	1.24
2	B	121	LEU	CG-CD2	5.97	1.72	1.52
2	B	117	VAL	CB-CG1	5.95	1.72	1.52
2	B	81	LEU	N-CA	5.95	1.53	1.45
2	B	310	GLY	CA-C	5.94	1.60	1.51
2	B	203	GLU	C-N	-5.93	1.25	1.33
1	A	262	MET	N-CA	-5.93	1.38	1.46
2	B	252	LEU	CG-CD1	5.93	1.72	1.52
1	A	133	VAL	C-N	5.92	1.42	1.33
2	B	69	THR	C-O	5.92	1.32	1.23
1	A	56	ASP	CA-CB	-5.91	1.46	1.53
2	B	219	LYS	CA-CB	-5.91	1.44	1.53
1	A	107	PHE	CE1-CZ	5.91	1.56	1.38
2	B	22	MET	CA-CB	5.91	1.60	1.53
1	A	10	GLN	CA-CB	-5.90	1.43	1.53
2	B	106	ILE	CB-CG1	-5.90	1.41	1.53
1	A	48	LEU	CG-CD2	5.89	1.72	1.52
1	A	154	CYS	CA-CB	5.89	1.61	1.53
1	A	263	LYS	N-CA	5.89	1.53	1.46
1	A	14	ARG	CA-C	5.89	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	124	ASP	CG-OD1	5.89	1.36	1.25
2	B	327	ILE	CA-CB	5.88	1.63	1.54
2	B	168	ASP	CG-OD1	5.88	1.36	1.25
2	B	278	ILE	CG1-CD1	5.88	1.74	1.51
2	B	31	ALA	CA-C	5.88	1.60	1.52
1	A	46	ASP	CA-CB	-5.87	1.44	1.53
2	B	226	ALA	CA-CB	-5.87	1.43	1.53
2	B	50	LYS	N-CA	5.87	1.53	1.46
2	B	337	LYS	N-CA	5.87	1.53	1.46
2	B	343	GLU	CA-CB	5.86	1.63	1.54
1	A	249	LYS	C-O	5.86	1.30	1.24
1	A	36	ILE	CA-C	5.86	1.60	1.52
1	A	262	MET	C-O	-5.86	1.16	1.24
2	B	37	LYS	CE-NZ	5.85	1.67	1.49
2	B	283	LYS	CA-CB	5.84	1.61	1.53
1	A	136	SER	C-N	-5.83	1.21	1.33
2	B	315	TYR	N-CA	-5.83	1.39	1.46
2	B	347	PRO	N-CA	5.83	1.54	1.47
2	B	365	GLN	CA-CB	5.82	1.61	1.53
1	A	105	LEU	C-N	-5.82	1.26	1.33
2	B	245	ILE	CB-CG2	5.82	1.71	1.52
1	A	168	SER	C-O	5.82	1.30	1.24
2	B	12	PHE	CB-CG	5.81	1.64	1.50
1	A	128	VAL	CA-C	5.81	1.60	1.52
2	B	94	GLN	CB-CG	5.80	1.69	1.52
2	B	110	THR	CB-CG2	-5.80	1.33	1.52
2	B	253	ILE	C-O	5.80	1.30	1.24
2	B	293	GLN	C-O	-5.80	1.16	1.23
1	A	233	SER	CA-C	-5.80	1.45	1.52
1	A	131	VAL	C-O	5.80	1.31	1.24
2	B	377	SER	C-O	5.80	1.31	1.24
2	B	315	TYR	CZ-OH	-5.79	1.25	1.38
1	A	212	PHE	N-CA	5.79	1.53	1.46
2	B	69	THR	CB-CG2	-5.79	1.33	1.52
2	B	163	SER	CA-C	5.79	1.60	1.52
2	B	9	PHE	CA-CB	5.78	1.62	1.53
2	B	89	ASN	CG-ND2	5.78	1.45	1.33
1	A	133	VAL	C-O	5.78	1.31	1.24
2	B	241	PHE	CG-CD1	5.78	1.50	1.38
2	B	341	ARG	C-O	5.78	1.31	1.24
1	A	249	LYS	CG-CD	5.77	1.69	1.52
2	B	122	ALA	CA-CB	5.77	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	292	GLY	C-N	5.76	1.41	1.33
1	A	264	ALA	N-CA	5.76	1.53	1.46
2	B	55	ARG	NE-CZ	-5.76	1.26	1.33
2	B	347	PRO	C-O	-5.75	1.16	1.24
1	A	113	ALA	C-N	5.75	1.41	1.33
2	B	283	LYS	CE-NZ	5.75	1.66	1.49
2	B	166	LEU	CG-CD1	5.74	1.71	1.52
2	B	200	ILE	CB-CG2	5.74	1.71	1.52
2	B	28	LEU	CA-CB	-5.73	1.44	1.53
2	B	58	ALA	N-CA	5.73	1.53	1.45
2	B	371	LEU	CB-CG	5.73	1.65	1.53
1	A	176	LEU	CG-CD2	5.72	1.71	1.52
2	B	250	VAL	N-CA	-5.72	1.39	1.46
2	B	69	THR	N-CA	5.72	1.54	1.46
2	B	233	GLY	CA-C	-5.72	1.43	1.51
2	B	323	ASP	CG-OD1	5.72	1.36	1.25
1	A	92	HIS	CB-CG	-5.72	1.42	1.50
2	B	245	ILE	CA-C	-5.71	1.45	1.52
2	B	219	LYS	CA-C	5.71	1.60	1.52
1	A	145	ARG	CA-C	-5.71	1.45	1.52
2	B	113	GLY	CA-C	-5.70	1.43	1.51
1	A	24	THR	N-CA	5.70	1.53	1.46
1	A	237	ILE	CA-C	5.70	1.60	1.52
2	B	137	LYS	C-O	5.70	1.30	1.24
2	B	357	HIS	CG-CD2	-5.70	1.29	1.35
2	B	286	MET	C-N	-5.68	1.25	1.33
2	B	374	VAL	CA-CB	-5.68	1.47	1.54
1	A	148	ILE	CA-CB	5.68	1.62	1.54
2	B	219	LYS	CD-CE	5.68	1.69	1.52
1	A	19	PHE	CA-CB	-5.67	1.45	1.53
1	A	168	SER	CA-CB	-5.67	1.44	1.53
2	B	62	CYS	CA-C	5.67	1.58	1.53
2	B	283	LYS	C-O	-5.67	1.17	1.24
2	B	159	VAL	CB-CG1	5.67	1.71	1.52
2	B	376	LEU	CG-CD1	5.67	1.71	1.52
2	B	96	LEU	N-CA	-5.66	1.39	1.46
2	B	31	ALA	C-N	5.65	1.41	1.33
2	B	117	VAL	C-N	5.64	1.41	1.33
2	B	295	GLU	N-CA	5.64	1.53	1.45
1	A	69	LEU	N-CA	5.64	1.53	1.46
2	B	339	LEU	C-O	5.64	1.31	1.24
1	A	268	ALA	C-O	5.64	1.34	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	170	CYS	C-O	-5.64	1.17	1.24
2	B	274	GLY	C-N	5.64	1.41	1.33
2	B	362	MET	N-CA	5.64	1.53	1.46
2	B	198	PRO	CA-CB	5.63	1.62	1.53
2	B	94	GLN	CA-C	5.63	1.60	1.52
1	A	105	LEU	CB-CG	5.63	1.64	1.53
1	A	256	ARG	N-CA	5.63	1.53	1.46
2	B	286	MET	N-CA	-5.62	1.38	1.45
2	B	102	GLY	CA-C	-5.62	1.43	1.51
2	B	226	ALA	C-N	-5.62	1.25	1.33
2	B	56	PRO	CB-CG	5.61	1.73	1.51
1	A	165	GLN	CA-CB	5.60	1.62	1.53
2	B	218	ASP	CB-CG	5.59	1.66	1.52
2	B	55	ARG	C-N	5.59	1.44	1.34
2	B	182	GLU	CG-CD	5.59	1.66	1.52
1	A	219	GLN	CD-OE1	5.59	1.34	1.23
1	A	177	LEU	CA-C	5.58	1.60	1.52
1	A	203	TYR	C-O	5.58	1.31	1.24
2	B	26	ASN	N-CA	-5.58	1.39	1.46
2	B	368	LYS	CB-CG	5.58	1.69	1.52
1	A	56	ASP	N-CA	-5.57	1.40	1.46
2	B	207	MET	C-N	-5.57	1.27	1.33
1	A	104	ASN	CB-CG	5.57	1.66	1.52
2	B	154	ALA	N-CA	5.57	1.53	1.45
2	B	329	ASP	CG-OD2	-5.57	1.14	1.25
2	B	165	THR	CA-C	5.56	1.60	1.52
2	B	48	LEU	CA-CB	5.55	1.61	1.53
2	B	148	ARG	CD-NE	5.55	1.54	1.46
2	B	5	LEU	CA-CB	5.55	1.65	1.54
2	B	191	ALA	C-O	5.55	1.32	1.23
2	B	253	ILE	CA-C	-5.54	1.45	1.52
1	A	25	LEU	C-N	-5.54	1.25	1.33
1	A	11	LEU	CA-C	5.54	1.60	1.52
2	B	131	ARG	C-O	5.53	1.30	1.23
2	B	158	PRO	CA-CB	5.53	1.60	1.53
2	B	326	SER	CA-C	5.53	1.59	1.52
2	B	182	GLU	CA-CB	5.53	1.62	1.53
2	B	350	GLU	C-O	5.52	1.30	1.24
2	B	372	LEU	C-N	5.52	1.40	1.33
2	B	114	GLN	C-O	5.52	1.30	1.24
2	B	281	GLY	C-O	-5.52	1.16	1.24
2	B	296	GLU	CA-CB	5.51	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	107	ILE	CA-CB	5.51	1.60	1.54
2	B	96	LEU	CA-CB	-5.50	1.44	1.53
1	A	99	LEU	CG-CD2	-5.50	1.34	1.52
1	A	260	SER	N-CA	5.50	1.53	1.46
2	B	304	LEU	N-CA	5.50	1.52	1.46
2	B	326	SER	CA-CB	-5.50	1.42	1.54
2	B	186	TYR	C-N	5.50	1.41	1.33
2	B	106	ILE	C-O	-5.49	1.18	1.24
1	A	113	ALA	CA-C	-5.49	1.45	1.52
2	B	275	ARG	C-O	5.49	1.30	1.23
2	B	292	GLY	C-O	5.49	1.31	1.23
2	B	273	HIS	CA-C	5.49	1.59	1.52
2	B	379	ARG	CZ-NH2	-5.49	1.26	1.33
2	B	152	MET	CA-CB	5.48	1.62	1.53
2	B	197	TYR	N-CA	5.48	1.52	1.46
2	B	41	PHE	CA-CB	5.48	1.61	1.53
2	B	195	HIS	C-O	-5.48	1.17	1.24
2	B	9	PHE	CD1-CE1	5.48	1.55	1.38
2	B	187	MET	C-N	5.47	1.40	1.33
2	B	374	VAL	CB-CG2	5.46	1.70	1.52
1	A	17	GLY	C-N	5.45	1.41	1.33
2	B	34	SER	CA-C	5.44	1.59	1.52
2	B	92	LEU	CA-CB	5.44	1.61	1.53
2	B	131	ARG	N-CA	-5.44	1.39	1.46
2	B	336	PHE	CD1-CE1	5.44	1.54	1.38
1	A	169	TYR	CG-CD1	-5.43	1.27	1.39
2	B	181	TYR	CA-C	-5.43	1.45	1.52
2	B	355	LEU	N-CA	5.42	1.53	1.46
2	B	300	ILE	CA-CB	5.42	1.62	1.54
2	B	204	PHE	CA-C	5.42	1.61	1.52
2	B	202	ARG	C-N	5.41	1.42	1.33
2	B	182	GLU	C-N	-5.41	1.25	1.33
2	B	25	LEU	CB-CG	-5.40	1.42	1.53
2	B	271	LEU	CG-CD2	5.40	1.70	1.52
1	A	202	GLU	N-CA	-5.40	1.39	1.46
2	B	279	TYR	CE2-CZ	5.40	1.51	1.38
2	B	311	PRO	C-N	5.40	1.41	1.33
2	B	28	LEU	CA-C	-5.40	1.46	1.52
1	A	63	THR	CA-C	5.39	1.59	1.52
2	B	213	LYS	C-O	-5.39	1.17	1.24
2	B	355	LEU	CG-CD2	5.39	1.70	1.52
1	A	198	GLU	CA-CB	5.39	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	385	PHE	CB-CG	-5.39	1.38	1.50
2	B	189	GLY	C-O	-5.39	1.20	1.24
2	B	115	HIS	CD2-NE2	-5.39	1.31	1.37
2	B	313	HIS	CG-CD2	5.38	1.41	1.35
2	B	112	ALA	CA-CB	5.38	1.62	1.53
2	B	131	ARG	CG-CD	5.38	1.68	1.52
2	B	257	PRO	CA-C	-5.38	1.47	1.52
2	B	100	ARG	CB-CG	-5.37	1.36	1.52
2	B	303	GLY	C-O	-5.37	1.16	1.24
1	A	131	VAL	CA-C	-5.37	1.48	1.53
1	A	241	ILE	CB-CG1	5.37	1.64	1.53
2	B	22	MET	C-O	-5.37	1.19	1.24
2	B	182	GLU	CD-OE2	5.37	1.35	1.25
1	A	100	LEU	C-N	-5.37	1.25	1.33
1	A	163	LEU	CG-CD1	5.36	1.70	1.52
2	B	58	ALA	C-O	-5.36	1.16	1.23
2	B	338	THR	C-N	5.36	1.41	1.33
2	B	367	GLU	CG-CD	-5.36	1.38	1.52
1	A	109	ASN	C-O	5.36	1.31	1.23
1	A	167	ALA	C-N	-5.36	1.26	1.33
2	B	71	THR	CB-OG1	5.36	1.52	1.43
2	B	88	THR	CB-OG1	-5.36	1.35	1.43
2	B	372	LEU	CG-CD2	5.36	1.70	1.52
1	A	194	HIS	CA-CB	5.35	1.62	1.53
1	A	8	PHE	CD2-CE2	5.35	1.54	1.38
2	B	378	GLY	C-O	5.35	1.29	1.23
1	A	78	PRO	C-O	5.34	1.31	1.24
2	B	185	HIS	C-N	5.34	1.41	1.33
2	B	287	MET	C-N	-5.34	1.26	1.33
2	B	278	ILE	CB-CG1	-5.34	1.42	1.53
2	B	342	HIS	CA-CB	5.33	1.62	1.53
2	B	12	PHE	CE2-CZ	-5.33	1.22	1.38
2	B	264	THR	CA-CB	5.32	1.62	1.53
2	B	167	LYS	CA-CB	5.32	1.62	1.53
2	B	23	PRO	CA-CB	5.32	1.61	1.53
2	B	133	TYR	N-CA	5.32	1.52	1.46
1	A	29	GLY	C-O	5.31	1.29	1.23
2	B	384	ILE	N-CA	-5.31	1.39	1.46
2	B	3	THR	N-CA	5.31	1.52	1.45
1	A	221	SER	C-O	5.30	1.30	1.24
2	B	347	PRO	N-CD	5.30	1.55	1.47
2	B	22	MET	CA-C	5.30	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	37	LYS	N-CA	-5.30	1.39	1.46
1	A	108	ASN	CA-C	-5.30	1.45	1.52
1	A	101	MET	SD-CE	5.29	1.92	1.79
1	A	41	ILE	C-N	-5.29	1.26	1.34
2	B	380	GLY	CA-C	-5.29	1.44	1.51
2	B	38	ASP	C-O	-5.29	1.17	1.24
1	A	212	PHE	CB-CG	5.28	1.62	1.50
2	B	48	LEU	CB-CG	5.28	1.64	1.53
2	B	52	TYR	C-O	-5.28	1.16	1.23
1	A	261	ALA	C-N	5.26	1.41	1.34
2	B	38	ASP	CB-CG	5.26	1.65	1.52
2	B	155	GLU	N-CA	5.26	1.52	1.46
1	A	119	GLU	C-O	5.25	1.30	1.24
2	B	338	THR	C-O	-5.25	1.18	1.24
1	A	107	PHE	CG-CD2	5.25	1.49	1.38
1	A	139	PHE	CD1-CE1	5.25	1.54	1.38
2	B	104	SER	N-CA	5.25	1.53	1.45
2	B	215	GLN	CD-NE2	5.25	1.44	1.33
1	A	134	GLU	CA-CB	5.24	1.62	1.53
2	B	394	ARG	CD-NE	5.24	1.53	1.46
2	B	271	LEU	CB-CG	-5.24	1.43	1.53
1	A	152	PHE	CD2-CE2	5.24	1.54	1.38
2	B	64	ASN	CG-ND2	5.23	1.44	1.33
2	B	296	GLU	CD-OE2	5.22	1.35	1.25
2	B	388	HIS	N-CA	5.22	1.52	1.46
1	A	117	ARG	C-N	5.21	1.40	1.33
2	B	19	GLN	C-O	-5.21	1.17	1.24
2	B	86	HIS	C-O	-5.21	1.17	1.24
1	A	171	ARG	C-O	5.20	1.30	1.23
2	B	169	ALA	C-O	5.20	1.30	1.24
2	B	139	VAL	C-O	5.19	1.30	1.24
2	B	383	ASP	CA-CB	5.19	1.62	1.53
2	B	74	TYR	CA-CB	-5.18	1.44	1.53
1	A	77	THR	CB-OG1	5.18	1.52	1.43
1	A	120	GLN	C-O	5.18	1.30	1.24
2	B	70	ARG	NE-CZ	5.17	1.38	1.33
2	B	295	GLU	CA-CB	-5.17	1.45	1.53
2	B	134	MET	N-CA	5.17	1.52	1.46
2	B	134	MET	CG-SD	5.17	1.93	1.80
2	B	357	HIS	CA-CB	5.17	1.61	1.53
1	A	55	SER	C-O	5.16	1.30	1.24
1	A	55	SER	CA-C	5.16	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	366	PRO	N-CA	5.16	1.54	1.47
1	A	205	ALA	CA-C	-5.15	1.46	1.53
2	B	377	SER	N-CA	5.15	1.52	1.46
2	B	39	PRO	N-CA	5.15	1.54	1.47
2	B	151	LEU	CG-CD2	5.15	1.69	1.52
2	B	216	ILE	C-O	5.15	1.30	1.24
2	B	96	LEU	CG-CD2	5.14	1.69	1.52
2	B	133	TYR	C-N	-5.14	1.26	1.33
2	B	181	TYR	N-CA	-5.14	1.39	1.46
2	B	55	ARG	CZ-NH1	-5.14	1.25	1.32
2	B	263	GLU	CG-CD	5.14	1.64	1.52
2	B	359	LEU	CA-C	5.13	1.59	1.52
2	B	311	PRO	CG-CD	5.13	1.68	1.50
1	A	163	LEU	C-N	-5.13	1.26	1.33
2	B	21	LEU	CB-CG	-5.13	1.43	1.53
1	A	220	VAL	C-N	5.13	1.40	1.33
2	B	125	LEU	CG-CD1	5.13	1.69	1.52
1	A	2	GLU	N-CA	5.12	1.52	1.46
2	B	215	GLN	CG-CD	-5.12	1.39	1.52
2	B	211	GLU	CB-CG	5.12	1.67	1.52
2	B	82	HIS	C-N	-5.12	1.25	1.33
2	B	90	GLN	N-CA	5.12	1.52	1.46
2	B	33	VAL	C-O	-5.11	1.18	1.24
2	B	358	ALA	C-N	-5.11	1.26	1.33
1	A	50	LEU	C-O	-5.10	1.18	1.23
1	A	201	LYS	CE-NZ	5.10	1.64	1.49
2	B	234	GLY	N-CA	-5.10	1.38	1.45
2	B	160	HIS	C-O	-5.09	1.17	1.24
2	B	181	TYR	CD1-CE1	5.09	1.53	1.38
1	A	19	PHE	N-CA	5.08	1.52	1.46
1	A	134	GLU	CA-C	5.08	1.59	1.52
2	B	16	TYR	N-CA	-5.08	1.40	1.46
1	A	209	LEU	CA-CB	5.08	1.61	1.53
2	B	122	ALA	N-CA	-5.08	1.39	1.46
1	A	135	GLU	CD-OE2	5.07	1.34	1.25
2	B	36	GLN	CD-NE2	5.07	1.43	1.33
2	B	385	PHE	CA-C	5.07	1.59	1.52
1	A	170	GLY	N-CA	-5.06	1.38	1.45
2	B	108	ALA	CA-C	-5.06	1.46	1.52
1	A	171	ARG	C-N	5.06	1.40	1.33
2	B	124	ALA	CA-C	-5.06	1.46	1.52
1	A	172	GLY	N-CA	-5.06	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	345	ILE	CB-CG2	5.05	1.69	1.52
1	A	169	TYR	C-O	5.05	1.30	1.24
2	B	316	LEU	N-CA	5.05	1.52	1.46
2	B	246	ASN	CG-ND2	-5.04	1.22	1.33
2	B	11	GLU	C-O	-5.04	1.17	1.24
1	A	78	PRO	CA-C	-5.03	1.44	1.52
2	B	152	MET	CB-CG	5.03	1.67	1.52
2	B	8	TYR	CG-CD2	5.03	1.50	1.39
1	A	41	ILE	CA-C	5.03	1.59	1.52
2	B	309	VAL	C-O	5.03	1.29	1.23
1	A	36	ILE	CB-CG1	5.02	1.63	1.53
2	B	270	PRO	N-CD	5.02	1.54	1.47
2	B	52	TYR	CG-CD2	5.02	1.49	1.39
2	B	25	LEU	CA-CB	5.01	1.61	1.53
2	B	122	ALA	C-O	5.01	1.30	1.24
1	A	96	PRO	N-CA	-5.01	1.41	1.47
1	A	160	ASP	CA-C	5.01	1.59	1.52
1	A	234	GLY	C-O	-5.00	1.17	1.23
1	A	256	ARG	CZ-NH2	5.00	1.40	1.33
1	A	199	LYS	CA-CB	-5.00	1.45	1.53
2	B	206[A]	ARG	CB-CG	-5.00	1.37	1.52
2	B	206[B]	ARG	CB-CG	-5.00	1.37	1.52

All (1376) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	254	GLY	O-C-N	-23.61	105.43	123.61
2	B	375	ASN	CA-C-O	20.99	143.04	120.58
2	B	368	LYS	O-C-N	20.15	148.35	122.96
2	B	328	THR	O-C-N	20.00	145.34	122.94
2	B	353	HIS	O-C-N	-19.79	99.59	122.15
2	B	321	ARG	CA-C-O	-19.71	96.20	119.27
2	B	49	LEU	CA-C-O	-19.57	99.68	120.42
2	B	106	ILE	CA-C-O	19.42	140.94	120.36
2	B	379	ARG	CD-NE-CZ	-19.18	97.55	124.40
2	B	6	ASN	CA-C-O	-19.11	100.78	119.51
2	B	29	GLU	CA-C-O	19.11	140.81	120.55
2	B	70	ARG	O-C-N	18.57	145.97	122.20
2	B	316	LEU	CA-C-O	-18.40	98.81	119.97
2	B	348	ALA	O-C-N	17.85	143.92	122.86
2	B	18	PRO	CA-C-O	17.74	142.14	121.56
2	B	54	GLY	O-C-N	-17.74	102.68	122.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	59	LEU	CA-C-O	-17.71	101.80	120.40
2	B	368	LYS	CA-C-O	-17.47	100.31	120.58
2	B	17	VAL	O-C-N	17.22	136.90	121.57
1	A	127	LEU	O-C-N	17.19	143.75	123.30
2	B	351	SER	O-C-N	17.16	143.37	122.27
1	A	125	SER	O-C-N	17.09	142.73	123.25
2	B	55	ARG	NE-CZ-NH1	16.77	138.27	121.50
2	B	375	ASN	O-C-N	-16.73	102.85	122.93
2	B	193	GLY	O-C-N	-16.67	105.10	121.77
2	B	29	GLU	O-C-N	-16.66	104.46	122.12
2	B	231	VAL	CA-C-O	16.59	134.99	120.22
2	B	348	ALA	CA-C-O	-16.34	103.75	121.56
2	B	281	GLY	CA-C-O	16.25	136.81	119.10
2	B	367	GLU	N-CA-C	16.20	131.19	112.72
2	B	23	PRO	O-C-N	16.17	143.07	122.22
2	B	55	ARG	O-C-N	-15.94	104.00	121.53
2	B	231	VAL	O-C-N	-15.72	108.82	122.97
2	B	106	ILE	O-C-N	-15.53	106.43	123.20
2	B	55	ARG	NE-CZ-NH2	-15.31	105.42	119.20
2	B	241	PHE	CA-C-O	15.28	138.25	119.31
1	A	140	ARG	NE-CZ-NH1	-15.24	106.26	121.50
2	B	353	HIS	CA-C-N	15.23	140.24	120.44
2	B	353	HIS	C-N-CA	15.23	140.24	120.44
2	B	86	HIS	O-C-N	15.18	142.62	122.43
2	B	93	GLY	CA-C-O	-15.14	103.64	120.30
2	B	328	THR	CA-C-O	-15.02	104.00	121.72
2	B	252	LEU	O-C-N	-14.95	104.29	123.13
2	B	60	THR	O-C-N	14.82	140.01	123.27
2	B	19	GLN	O-C-N	14.80	139.53	122.22
2	B	76	LYS	CA-C-O	14.74	137.19	120.54
1	A	121	VAL	O-C-N	14.56	136.26	122.14
2	B	18	PRO	O-C-N	-14.45	105.09	123.01
1	A	97	ILE	O-C-N	-14.44	107.53	122.99
2	B	242	ALA	N-CA-C	14.41	128.40	111.11
1	A	120	GLN	N-CA-C	14.40	126.98	111.28
2	B	286	MET	CA-CB-CG	14.38	142.85	114.10
2	B	30	GLU	O-C-N	14.34	138.49	122.15
2	B	90	GLN	OE1-CD-NE2	14.26	136.86	122.60
2	B	203	GLU	CA-C-O	-14.20	101.71	119.31
1	A	92	HIS	O-C-N	-14.11	109.18	121.17
2	B	321	ARG	N-CA-C	-14.10	95.74	113.23
2	B	336	PHE	O-C-N	14.02	138.14	122.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	360	LYS	CA-C-N	13.97	139.40	120.54
2	B	360	LYS	C-N-CA	13.97	139.40	120.54
2	B	203	GLU	O-C-N	13.97	141.74	122.46
2	B	284	ALA	CA-C-O	13.91	139.21	120.16
2	B	297	SER	N-CA-CB	-13.80	91.48	110.25
2	B	71	THR	CA-C-O	-13.78	105.08	120.92
2	B	362	MET	CA-C-O	-13.76	106.52	120.70
2	B	70	ARG	CA-C-O	-13.73	103.94	120.55
2	B	6	ASN	N-CA-C	13.72	133.59	109.58
1	A	48	LEU	CA-C-O	13.68	137.12	121.11
2	B	59	LEU	O-C-N	13.68	141.18	123.12
1	A	116	ALA	N-CA-C	13.68	126.19	111.28
2	B	105	GLU	O-C-N	13.67	140.06	123.24
2	B	222	ARG	NE-CZ-NH2	-13.63	106.93	119.20
2	B	339	LEU	O-C-N	13.62	140.58	122.33
2	B	291	ASP	CB-CG-OD1	-13.60	87.12	118.40
2	B	45	PHE	CA-C-O	-13.58	106.02	120.42
2	B	261	GLY	O-C-N	13.54	140.30	122.70
2	B	169	ALA	N-CA-C	13.53	127.34	111.11
1	A	153	ILE	CA-C-O	13.49	137.16	121.11
2	B	243	ASP	O-C-N	13.35	140.88	122.46
1	A	229	ALA	N-CA-C	13.34	129.32	113.18
2	B	212	THR	CA-CB-OG1	13.32	129.58	109.60
2	B	194	PRO	O-C-N	-13.30	106.70	123.06
2	B	6	ASN	CA-C-N	13.24	134.34	120.04
2	B	6	ASN	C-N-CA	13.24	134.34	120.04
2	B	314	ALA	O-C-N	-13.24	108.09	122.12
2	B	128	LEU	O-C-N	-13.21	107.91	123.10
2	B	360	LYS	O-C-N	-13.15	106.09	122.27
2	B	3	THR	O-C-N	-13.14	107.27	123.17
2	B	343	GLU	O-C-N	13.13	135.85	121.93
2	B	347	PRO	CA-C-O	13.12	144.48	120.60
2	B	7	PRO	O-C-N	13.08	140.29	122.37
2	B	56	PRO	CA-C-N	13.07	141.43	122.09
2	B	56	PRO	C-N-CA	13.07	141.43	122.09
2	B	204	PHE	CE1-CZ-CE2	13.05	143.50	120.00
2	B	339	LEU	CA-C-O	-12.98	104.47	119.79
2	B	241	PHE	N-CA-C	12.97	128.98	112.89
2	B	202	ARG	O-C-N	-12.96	108.39	122.12
2	B	285	PRO	CA-C-O	-12.93	107.40	121.23
1	A	210	GLN	CA-C-O	12.89	135.74	120.92
2	B	281	GLY	N-CA-C	12.87	131.94	115.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	200	ILE	O-C-N	12.72	134.21	121.87
2	B	230	CYS	O-C-N	12.69	137.32	122.85
1	A	98	GLY	O-C-N	12.67	134.66	123.25
2	B	267	HIS	CA-C-O	-12.67	107.93	121.36
2	B	5	LEU	CA-C-O	12.67	136.26	121.44
2	B	86	HIS	CA-C-O	-12.66	103.14	119.10
2	B	332	ALA	CA-C-O	-12.58	107.08	120.42
2	B	272	LYS	CB-CG-CD	12.55	140.16	111.30
1	A	141	GLN	O-C-N	-12.52	108.85	122.12
2	B	233	GLY	O-C-N	-12.47	106.50	122.70
2	B	372	LEU	N-CA-CB	12.43	131.57	110.68
2	B	327	ILE	O-C-N	-12.43	109.80	123.10
2	B	330	ASP	N-CA-C	12.32	124.71	111.28
2	B	82	HIS	CA-C-O	-12.24	107.62	120.96
2	B	379	ARG	O-C-N	-12.21	108.39	122.68
1	A	191	LEU	N-CA-C	12.18	136.72	109.81
2	B	351	SER	CA-C-O	-12.14	106.01	119.97
1	A	52	VAL	O-C-N	12.06	132.27	121.41
2	B	122	ALA	O-C-N	12.05	138.48	122.33
2	B	256	GLU	CA-C-O	-12.05	108.22	120.64
2	B	278	ILE	CA-C-O	11.95	133.02	120.36
2	B	350	GLU	O-C-N	-11.94	109.31	122.08
1	A	126	VAL	CA-C-O	11.90	133.37	120.64
2	B	134	MET	CA-C-N	-11.80	108.59	119.92
2	B	134	MET	C-N-CA	-11.80	108.59	119.92
2	B	242	ALA	O-C-N	-11.78	109.84	122.09
2	B	9	PHE	O-C-N	11.77	140.88	122.99
2	B	67	ALA	O-C-N	11.77	136.75	122.86
2	B	207	MET	CA-C-O	-11.77	104.91	119.38
2	B	373	VAL	O-C-N	-11.76	110.56	123.26
2	B	158	PRO	CB-CA-C	-11.75	94.28	110.85
1	A	97	ILE	CA-C-O	11.67	133.32	120.48
2	B	222	ARG	NE-CZ-NH1	11.66	133.16	121.50
2	B	341	ARG	O-C-N	-11.61	106.78	122.33
1	A	92	HIS	CA-C-N	11.60	131.27	119.56
1	A	92	HIS	C-N-CA	11.60	131.27	119.56
1	A	139	PHE	O-C-N	11.58	136.18	122.17
2	B	66	THR	CA-CB-OG1	11.57	126.96	109.60
2	B	49	LEU	O-C-N	11.55	135.32	122.15
1	A	121	VAL	CA-C-N	-11.55	104.43	122.10
1	A	121	VAL	C-N-CA	-11.55	104.43	122.10
2	B	205	GLN	OE1-CD-NE2	11.54	134.14	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	79	ASP	O-C-N	11.54	137.40	122.39
1	A	243	LYS	N-CA-C	11.50	126.41	112.38
2	B	355	LEU	CA-C-O	-11.46	108.27	120.42
2	B	100	ARG	NE-CZ-NH1	11.46	132.96	121.50
2	B	196	PRO	O-C-N	11.43	142.81	121.10
2	B	12	PHE	O-C-N	11.35	137.46	123.16
2	B	271	LEU	N-CA-CB	11.32	126.42	110.01
2	B	332	ALA	O-C-N	11.28	135.01	122.15
2	B	204	PHE	CD1-CE1-CZ	-11.24	99.76	120.00
2	B	117	VAL	O-C-N	-11.09	108.71	122.57
2	B	22	MET	CA-C-O	11.09	128.83	118.63
2	B	85	ALA	O-C-N	-11.09	111.56	123.42
2	B	32	PHE	O-C-N	-11.02	110.72	122.07
2	B	215	GLN	N-CA-C	-11.00	98.17	111.69
2	B	255	VAL	CG1-CB-CG2	10.93	134.84	110.80
2	B	51	ASN	N-CA-C	10.92	126.39	113.18
2	B	87	LYS	N-CA-C	-10.91	99.16	111.71
2	B	370	GLN	O-C-N	10.88	135.63	123.33
1	A	136	SER	CA-C-O	-10.87	106.13	119.28
1	A	96	PRO	N-CA-CB	10.85	113.43	103.34
2	B	334	GLU	N-CA-C	10.84	123.10	111.28
2	B	282	MET	O-C-N	10.80	136.23	123.17
2	B	194	PRO	CA-C-N	10.78	136.25	120.83
2	B	194	PRO	C-N-CA	10.78	136.25	120.83
2	B	227	VAL	O-C-N	-10.77	112.15	123.14
2	B	347	PRO	O-C-N	-10.77	108.10	122.64
2	B	284	ALA	O-C-N	-10.69	109.03	121.32
2	B	256	GLU	N-CA-C	10.68	125.83	110.24
2	B	331	GLU	N-CA-CB	10.66	125.47	110.01
2	B	112	ALA	N-CA-C	-10.65	99.69	112.89
2	B	394	ARG	NE-CZ-NH1	-10.65	110.85	121.50
2	B	308	SER	CA-C-N	10.64	136.22	121.96
2	B	308	SER	C-N-CA	10.64	136.22	121.96
2	B	202	ARG	CA-C-O	10.63	132.11	120.63
1	A	194	HIS	N-CA-C	-10.63	99.49	111.82
1	A	169	TYR	N-CA-C	10.58	125.56	112.23
1	A	77	THR	O-C-N	10.57	129.79	121.55
2	B	202	ARG	NE-CZ-NH1	-10.57	110.93	121.50
2	B	384	ILE	N-CA-C	10.53	124.25	111.09
2	B	119	SER	N-CA-C	-10.52	98.98	112.23
2	B	357	HIS	CB-CG-ND1	-10.48	106.98	122.70
2	B	357	HIS	O-C-N	-10.45	110.24	122.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	119	SER	N-CA-CB	-10.45	94.21	110.30
2	B	354	ALA	N-CA-CB	10.44	125.15	110.01
2	B	30	GLU	CB-CG-CD	10.43	130.33	112.60
2	B	58	ALA	N-CA-CB	-10.42	96.10	110.38
2	B	370	GLN	CA-CB-CG	10.40	134.90	114.10
2	B	209	GLY	N-CA-C	10.39	125.51	112.83
2	B	236	ASN	O-C-N	10.36	135.02	122.27
2	B	106	ILE	CA-C-N	10.36	135.98	122.93
2	B	106	ILE	C-N-CA	10.36	135.98	122.93
2	B	255	VAL	N-CA-C	10.34	122.67	107.37
2	B	21	LEU	O-C-N	-10.31	107.77	122.41
2	B	181	TYR	N-CA-C	-10.24	100.80	113.18
2	B	358	ALA	O-C-N	10.22	134.17	122.22
2	B	254	GLY	CA-C-O	10.19	129.78	120.91
1	A	127	LEU	CA-C-O	-10.19	109.36	120.36
2	B	164	ALA	N-CA-C	-10.18	100.17	112.58
1	A	140	ARG	NE-CZ-NH2	10.17	128.35	119.20
2	B	71	THR	O-C-N	10.17	134.95	123.16
1	A	85	LEU	N-CA-C	-10.16	100.20	111.07
2	B	27	GLN	O-C-N	10.15	133.72	122.15
2	B	12	PHE	CA-C-N	-10.14	108.62	122.42
2	B	12	PHE	C-N-CA	-10.14	108.62	122.42
2	B	15	MET	CB-CG-SD	10.12	143.07	112.70
1	A	14	ARG	N-CA-C	-10.05	99.83	113.30
2	B	234	GLY	N-CA-C	10.04	129.11	114.95
1	A	49[A]	GLU	CA-C-N	-10.01	105.52	122.33
1	A	49[A]	GLU	C-N-CA	-10.01	105.52	122.33
1	A	49[B]	GLU	CA-C-N	-10.01	105.52	122.33
1	A	49[B]	GLU	C-N-CA	-10.01	105.52	122.33
2	B	188	LEU	CA-C-N	-10.00	107.11	122.30
2	B	188	LEU	C-N-CA	-10.00	107.11	122.30
2	B	311	PRO	O-C-N	-9.99	108.71	122.30
2	B	21	LEU	CA-C-O	9.97	131.05	119.18
2	B	98	ALA	N-CA-C	-9.95	100.42	111.07
2	B	52	TYR	CD1-CG-CD2	-9.94	103.18	118.10
1	A	219	GLN	N-CA-C	9.91	125.19	112.89
2	B	335	ALA	N-CA-C	-9.90	99.75	112.23
2	B	76	LYS	CA-C-N	-9.89	108.46	122.41
2	B	76	LYS	C-N-CA	-9.89	108.46	122.41
2	B	78	GLU	O-C-N	-9.89	108.00	122.43
2	B	357	HIS	ND1-CE1-NE2	9.89	118.29	108.40
2	B	58	ALA	O-C-N	9.88	134.70	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	193	GLY	CA-C-O	9.87	135.64	121.52
2	B	45	PHE	O-C-N	9.86	133.39	122.15
2	B	340	CYS	N-CA-C	-9.85	100.54	111.28
1	A	104	ASN	CA-CB-CG	-9.80	102.80	112.60
2	B	57	THR	CA-C-N	-9.78	102.67	121.06
2	B	57	THR	C-N-CA	-9.78	102.67	121.06
2	B	280	PHE	O-C-N	-9.78	109.58	122.59
1	A	52	VAL	N-CA-CB	-9.77	101.16	111.61
2	B	79	ASP	CA-C-O	-9.75	107.69	119.49
2	B	215	GLN	OE1-CD-NE2	-9.74	112.86	122.60
1	A	263	LYS	N-CA-C	-9.74	100.14	112.90
2	B	324	TYR	CZ-CE2-CD2	9.71	137.09	119.60
2	B	65	ILE	CA-C-O	-9.70	109.99	120.47
1	A	163	LEU	CA-C-O	-9.70	110.16	120.63
2	B	342	HIS	N-CA-C	9.68	125.24	113.23
2	B	258	GLY	CA-C-O	9.67	137.43	119.55
1	A	130	ASP	N-CA-C	9.66	123.48	112.57
1	A	47	ALA	N-CA-C	-9.63	94.05	108.79
2	B	61	LYS	N-CA-CB	-9.63	95.82	109.97
2	B	119	SER	O-C-N	9.62	135.22	122.33
2	B	204	PHE	CD1-CG-CD2	9.62	133.03	118.60
2	B	315	TYR	CE1-CZ-OH	9.61	148.74	119.90
2	B	298	TYR	CA-CB-CG	-9.60	96.61	113.90
2	B	275	ARG	O-C-N	9.60	134.95	123.33
2	B	316	LEU	N-CA-C	-9.59	100.69	111.82
2	B	223	LEU	N-CA-C	9.59	124.77	110.39
2	B	336	PHE	CA-C-O	-9.55	110.30	120.42
2	B	221	GLY	O-C-N	9.54	134.34	122.41
2	B	215	GLN	CG-CD-OE1	9.53	139.86	120.80
2	B	122	ALA	CA-C-O	-9.52	108.56	119.79
2	B	30	GLU	CA-C-O	-9.51	110.34	120.42
1	A	200	LEU	N-CA-C	-9.49	101.02	111.36
1	A	121	VAL	CA-C-O	-9.47	108.17	119.54
2	B	23	PRO	CA-C-O	-9.47	105.16	119.55
1	A	100	LEU	O-C-N	9.46	134.43	123.27
1	A	116	ALA	O-C-N	-9.46	112.10	122.12
2	B	345	ILE	CA-CB-CG1	9.43	126.43	110.40
2	B	264	THR	O-C-N	9.42	136.18	122.43
2	B	263	GLU	CG-CD-OE2	-9.40	96.79	118.40
2	B	54	GLY	CA-C-O	9.38	129.55	118.86
1	A	123	VAL	CA-C-O	9.37	131.24	121.59
2	B	121	LEU	O-C-N	-9.35	110.77	122.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	270	PRO	CA-C-N	9.34	132.59	120.44
2	B	270	PRO	C-N-CA	9.34	132.59	120.44
1	A	163	LEU	O-C-N	9.34	132.02	122.12
1	A	125	SER	CA-C-O	-9.33	111.25	121.33
2	B	98	ALA	N-CA-CB	9.32	123.53	110.01
2	B	337	LYS	O-C-N	-9.29	111.56	122.15
2	B	89	ASN	O-C-N	9.23	131.63	122.03
2	B	92	LEU	N-CA-C	-9.21	101.22	111.07
2	B	286	MET	CB-CG-SD	-9.18	85.15	112.70
2	B	312	GLN	O-C-N	9.18	132.62	122.15
2	B	12	PHE	CE1-CZ-CE2	9.16	136.49	120.00
1	A	139	PHE	CD1-CG-CD2	9.15	132.33	118.60
2	B	380	GLY	N-CA-C	9.15	134.86	113.18
2	B	72	THR	CA-C-O	-9.11	110.30	120.32
1	A	136	SER	O-C-N	9.10	134.93	122.37
2	B	207	MET	N-CA-C	-9.10	101.44	112.54
2	B	123	SER	N-CA-C	-9.09	101.45	111.36
2	B	264	THR	CA-C-O	-9.09	107.47	119.11
2	B	245	ILE	O-C-N	-9.06	113.08	121.87
2	B	203	GLU	N-CA-C	-9.05	101.66	112.89
1	A	77	THR	CB-CA-C	-9.04	95.48	109.22
2	B	93	GLY	O-C-N	9.04	132.14	122.28
2	B	370	GLN	CB-CG-CD	9.02	127.94	112.60
1	A	50	LEU	CA-C-N	-9.01	113.83	122.66
1	A	50	LEU	C-N-CA	-9.01	113.83	122.66
2	B	339	LEU	CB-CG-CD1	9.00	137.70	110.70
2	B	168	ASP	CA-C-N	-8.99	108.40	120.54
2	B	168	ASP	C-N-CA	-8.99	108.40	120.54
2	B	335	ALA	CA-C-O	-8.98	109.20	119.79
2	B	124	ALA	O-C-N	-8.97	112.83	122.07
2	B	335	ALA	O-C-N	8.97	134.35	122.33
2	B	28	LEU	CA-C-O	8.97	130.24	120.82
1	A	4	TYR	N-CA-C	-8.96	100.67	111.69
1	A	113	ALA	N-CA-C	8.95	122.00	111.71
2	B	97	LEU	CB-CG-CD2	8.94	137.51	110.70
1	A	210	GLN	O-C-N	-8.93	112.80	123.16
2	B	214	ALA	O-C-N	8.92	133.25	122.27
1	A	82	PHE	N-CA-C	-8.91	101.01	112.23
2	B	57	THR	N-CA-CB	8.91	124.66	110.23
2	B	269	ALA	CB-CA-C	-8.90	97.25	111.14
2	B	25	LEU	CA-C-O	8.90	129.85	120.42
2	B	261	GLY	CA-C-N	-8.90	109.12	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	261	GLY	C-N-CA	-8.90	109.12	120.60
2	B	315	TYR	CD1-CE1-CZ	8.89	135.61	119.60
2	B	223	LEU	CA-C-N	8.89	128.92	119.76
2	B	223	LEU	C-N-CA	8.89	128.92	119.76
2	B	12	PHE	CA-C-O	-8.89	111.12	121.16
1	A	139	PHE	CE1-CZ-CE2	8.88	135.99	120.00
1	A	230	GLY	O-C-N	8.86	132.42	123.92
1	A	47	ALA	N-CA-CB	8.86	125.29	111.56
1	A	141	GLN	CA-C-O	8.84	129.92	120.55
2	B	69	THR	O-C-N	-8.84	110.25	122.81
2	B	7	PRO	CA-C-N	-8.83	108.95	122.81
2	B	7	PRO	C-N-CA	-8.83	108.95	122.81
2	B	375	ASN	CA-CB-CG	-8.82	103.78	112.60
2	B	188	LEU	O-C-N	8.79	132.89	122.96
2	B	17	VAL	CA-CB-CG2	8.78	125.33	110.40
2	B	262	ILE	CA-C-O	8.78	130.40	121.27
2	B	91	VAL	CA-CB-CG1	8.78	125.33	110.40
2	B	49	LEU	N-CA-C	-8.77	101.80	111.36
2	B	209	GLY	O-C-N	-8.77	113.67	122.17
1	A	253	ALA	N-CA-C	8.76	120.44	111.07
2	B	236	ASN	CA-C-N	-8.76	107.86	120.29
2	B	236	ASN	C-N-CA	-8.76	107.86	120.29
1	A	225	ARG	NE-CZ-NH1	8.75	130.25	121.50
2	B	75	LEU	N-CA-CB	8.71	124.41	110.65
2	B	96	LEU	N-CA-CB	8.71	122.92	110.12
2	B	196	PRO	N-CD-CG	-8.69	93.37	103.80
2	B	252	LEU	CA-C-N	8.69	134.41	123.12
2	B	252	LEU	C-N-CA	8.69	134.41	123.12
2	B	253	ILE	N-CA-C	8.69	120.40	107.80
1	A	133	VAL	N-CA-C	8.67	123.14	111.17
2	B	262	ILE	O-C-N	-8.67	113.27	121.94
2	B	82	HIS	CA-C-N	8.66	135.98	122.20
2	B	82	HIS	C-N-CA	8.66	135.98	122.20
2	B	237	ALA	N-CA-C	8.65	120.79	111.36
2	B	257	PRO	N-CA-CB	8.65	110.22	103.30
2	B	183	THR	CA-CB-OG1	8.63	122.55	109.60
1	A	52	VAL	N-CA-C	-8.63	98.48	107.89
2	B	12	PHE	CD1-CG-CD2	8.60	131.50	118.60
2	B	371	LEU	CA-C-O	-8.60	111.16	120.36
1	A	142	ALA	O-C-N	-8.59	112.35	122.15
1	A	145	ARG	O-C-N	-8.59	112.17	122.22
2	B	283	LYS	O-C-N	8.59	133.01	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	240	MET	CA-C-N	-8.57	106.14	121.14
2	B	240	MET	C-N-CA	-8.57	106.14	121.14
2	B	69	THR	CA-CB-CG2	8.56	125.06	110.50
2	B	338	THR	CA-CB-OG1	-8.56	96.76	109.60
2	B	25	LEU	N-CA-C	8.55	120.68	111.36
2	B	291	ASP	CA-CB-CG	-8.55	104.05	112.60
2	B	149	MET	CA-C-O	-8.55	110.14	119.97
2	B	244	PHE	CA-C-N	-8.54	108.77	120.46
2	B	244	PHE	C-N-CA	-8.54	108.77	120.46
2	B	198	PRO	O-C-N	-8.53	112.00	122.23
1	A	80	GLN	O-C-N	8.51	132.74	122.27
2	B	55	ARG	CA-C-O	8.51	129.97	120.70
1	A	121	VAL	N-CA-C	-8.50	104.42	112.83
1	A	148	ILE	CB-CA-C	-8.50	97.41	110.50
2	B	214	ALA	CA-C-O	-8.47	110.22	119.97
1	A	150	PRO	O-C-N	8.45	131.13	122.93
1	A	51	GLY	CA-C-N	-8.45	114.13	123.43
1	A	51	GLY	C-N-CA	-8.45	114.13	123.43
2	B	119	SER	CA-C-O	-8.45	109.82	119.79
1	A	134	GLU	CA-C-O	-8.45	108.99	119.38
2	B	199	THR	O-C-N	8.45	131.21	122.09
2	B	222	ARG	O-C-N	-8.43	114.41	123.26
1	A	205	ALA	O-C-N	-8.41	113.20	122.79
2	B	256	GLU	CB-CG-CD	-8.41	98.30	112.60
2	B	310	GLY	O-C-N	-8.41	113.36	121.77
2	B	359	LEU	N-CA-C	-8.41	102.19	111.36
1	A	213	GLY	N-CA-C	-8.40	103.73	115.32
2	B	361	MET	N-CA-CB	8.40	122.45	109.94
2	B	394	ARG	NH1-CZ-NH2	8.40	130.21	119.30
2	B	314	ALA	CA-C-N	8.38	131.33	120.44
2	B	314	ALA	C-N-CA	8.38	131.33	120.44
1	A	62	PRO	N-CA-C	8.37	124.95	113.65
1	A	171	ARG	O-C-N	-8.37	113.47	123.10
1	A	256	ARG	N-CA-C	-8.37	102.11	111.07
2	B	31	ALA	N-CA-C	-8.37	102.11	111.07
2	B	235	SER	N-CA-C	8.35	122.75	112.23
2	B	290	ALA	CA-C-N	8.35	137.59	122.06
2	B	290	ALA	C-N-CA	8.35	137.59	122.06
2	B	373	VAL	CA-CB-CG2	8.34	124.58	110.40
2	B	122	ALA	N-CA-C	-8.33	101.73	112.23
2	B	3	THR	CA-C-O	8.33	130.81	121.40
1	A	37	ILE	N-CA-C	-8.32	101.93	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	345	ILE	O-C-N	-8.32	114.38	123.20
2	B	114	GLN	N-CA-CB	8.32	122.35	110.12
2	B	374	VAL	CA-CB-CG1	8.30	124.51	110.40
2	B	29	GLU	N-CA-C	8.27	120.30	111.28
2	B	80	LEU	N-CA-C	-8.27	103.19	113.28
2	B	230	CYS	CA-C-O	-8.27	112.06	121.81
2	B	267	HIS	O-C-N	8.26	132.59	122.92
2	B	355	LEU	O-C-N	8.26	131.57	122.15
2	B	303	GLY	N-CA-C	8.24	124.54	113.99
2	B	373	VAL	CA-C-N	8.24	133.41	123.19
2	B	373	VAL	C-N-CA	8.24	133.41	123.19
2	B	52	TYR	CA-C-N	-8.23	106.75	122.06
2	B	52	TYR	C-N-CA	-8.23	106.75	122.06
2	B	194	PRO	N-CA-C	8.23	124.46	111.38
2	B	380	GLY	CA-C-O	8.22	134.87	120.57
2	B	60	THR	CA-C-N	-8.22	109.20	120.87
2	B	60	THR	C-N-CA	-8.22	109.20	120.87
2	B	64	ASN	N-CA-CB	8.20	122.30	110.16
1	A	112	ASP	O-C-N	-8.20	113.56	122.09
2	B	149	MET	O-C-N	8.19	132.34	122.27
2	B	350	GLU	CA-C-N	8.19	132.75	120.31
2	B	350	GLU	C-N-CA	8.19	132.75	120.31
2	B	28	LEU	O-C-N	-8.18	113.65	122.07
2	B	103	LYS	O-C-N	8.17	132.17	122.85
2	B	234	GLY	CA-C-N	-8.17	106.79	120.68
2	B	234	GLY	C-N-CA	-8.17	106.79	120.68
1	A	84	MET	CA-C-O	-8.17	111.76	120.42
2	B	94	GLN	OE1-CD-NE2	-8.16	114.44	122.60
1	A	140	ARG	CD-NE-CZ	-8.15	112.98	124.40
1	A	3	ARG	N-CA-C	-8.15	102.36	111.82
2	B	243	ASP	N-CA-C	8.14	122.77	113.01
2	B	324	TYR	CG-CD1-CE1	8.13	133.40	121.20
2	B	17	VAL	N-CA-CB	-8.13	104.76	111.67
2	B	251	GLY	CA-C-O	-8.12	106.44	120.57
2	B	379	ARG	CA-C-O	8.11	131.38	121.89
2	B	9	PHE	CD1-CG-CD2	8.11	130.76	118.60
2	B	365	GLN	O-C-N	8.11	128.06	121.17
2	B	308	SER	CA-C-O	-8.11	110.06	121.98
2	B	161	SER	CB-CA-C	-8.10	95.12	109.62
2	B	183	THR	CA-CB-CG2	-8.10	96.73	110.50
1	A	130	ASP	CA-C-O	8.10	130.59	120.15
2	B	228	ILE	CA-CB-CG1	-8.10	96.64	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	325	VAL	O-C-N	-8.09	112.45	122.57
1	A	143	ALA	N-CA-C	-8.09	102.15	110.97
1	A	107	PHE	CG-CD1-CE1	8.06	134.40	120.70
2	B	204	PHE	CB-CG-CD2	-8.06	107.00	120.70
2	B	152	MET	CG-SD-CE	-8.05	83.18	100.90
2	B	152	MET	O-C-N	8.04	131.99	122.34
2	B	53	ALA	O-C-N	8.04	133.83	122.41
2	B	105	GLU	N-CA-CB	8.04	126.00	111.37
2	B	205	GLN	O-C-N	-8.04	112.71	122.20
2	B	26	ASN	N-CA-C	8.03	121.13	111.82
2	B	105	GLU	CA-C-O	-8.03	111.72	121.11
2	B	212	THR	O-C-N	-8.03	113.74	122.09
1	A	96	PRO	O-C-N	8.02	132.72	123.10
2	B	242	ALA	CA-C-O	8.00	129.46	120.90
1	A	125	SER	CA-C-N	-7.99	109.55	122.33
1	A	125	SER	C-N-CA	-7.99	109.55	122.33
2	B	22	MET	N-CA-C	7.97	123.62	113.25
1	A	105	LEU	N-CA-CB	7.96	122.61	110.28
1	A	138	PRO	O-C-N	-7.94	111.98	122.22
2	B	26	ASN	O-C-N	7.93	132.03	122.27
2	B	103	LYS	CA-C-O	-7.93	112.45	121.81
2	B	9	PHE	CB-CG-CD2	-7.90	107.27	120.70
1	A	95	ILE	CB-CA-C	7.90	119.77	110.68
2	B	316	LEU	CB-CG-CD2	7.89	134.36	110.70
2	B	338	THR	CA-C-O	7.89	129.15	120.63
2	B	117	VAL	N-CA-C	7.88	125.74	109.34
2	B	321	ARG	NE-CZ-NH2	-7.88	112.11	119.20
2	B	316	LEU	N-CA-CB	-7.87	98.08	110.28
1	A	153	ILE	O-C-N	-7.87	113.43	122.72
2	B	41	PHE	N-CA-C	-7.85	102.81	111.36
2	B	81	LEU	N-CA-CB	-7.85	98.36	110.29
2	B	338	THR	N-CA-C	7.84	120.82	111.33
2	B	210	GLU	CA-C-O	-7.83	110.55	119.79
2	B	320	GLY	O-C-N	-7.83	112.60	122.32
2	B	334	GLU	O-C-N	-7.83	113.81	122.12
1	A	98	GLY	CA-C-N	-7.82	110.28	122.87
1	A	98	GLY	C-N-CA	-7.82	110.28	122.87
1	A	225	ARG	NE-CZ-NH2	-7.80	112.18	119.20
2	B	182	GLU	CA-C-N	-7.80	110.12	122.29
2	B	182	GLU	C-N-CA	-7.80	110.12	122.29
2	B	298	TYR	N-CA-C	-7.79	94.45	108.48
2	B	202	ARG	NH1-CZ-NH2	7.75	129.38	119.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	13	ASP	CA-CB-CG	7.75	120.35	112.60
2	B	51	ASN	O-C-N	-7.75	111.12	122.43
2	B	60	THR	CA-C-O	-7.74	111.99	120.43
2	B	40	GLU	O-C-N	-7.74	113.92	122.12
2	B	61	LYS	CB-CA-C	7.74	122.88	109.65
2	B	17	VAL	CA-C-O	-7.73	110.44	120.95
2	B	123	SER	CA-CB-OG	-7.73	95.65	111.10
2	B	51	ASN	OD1-CG-ND2	-7.72	114.88	122.60
2	B	315	TYR	CB-CG-CD2	7.72	132.38	120.80
2	B	228	ILE	N-CA-CB	7.71	122.05	111.41
1	A	222	ALA	CA-C-N	-7.71	108.59	120.31
1	A	222	ALA	C-N-CA	-7.71	108.59	120.31
2	B	203	GLU	CA-C-N	-7.70	109.32	122.56
2	B	203	GLU	C-N-CA	-7.70	109.32	122.56
1	A	67	ALA	N-CA-C	-7.69	102.97	111.36
2	B	6	ASN	O-C-N	-7.69	114.62	121.31
1	A	139	PHE	CA-C-O	-7.69	112.32	120.55
2	B	53	ALA	CA-C-N	-7.69	111.62	122.00
2	B	53	ALA	C-N-CA	-7.69	111.62	122.00
1	A	176	LEU	CA-C-O	7.68	128.46	120.40
2	B	34	SER	O-C-N	7.67	130.90	122.15
2	B	229	ALA	N-CA-C	7.67	121.03	108.99
2	B	363	ARG	N-CA-C	-7.67	103.00	111.36
2	B	107	ILE	O-C-N	7.67	131.54	123.03
2	B	240	MET	O-C-N	7.67	130.37	122.09
2	B	375	ASN	CB-CA-C	-7.66	98.17	110.81
2	B	304	LEU	CB-CG-CD2	7.65	133.66	110.70
2	B	224	PRO	N-CA-CB	7.65	110.12	103.31
2	B	277	GLY	CA-C-N	-7.64	112.37	122.99
2	B	277	GLY	C-N-CA	-7.64	112.37	122.99
2	B	217	LEU	N-CA-CB	7.64	121.35	110.12
2	B	31	ALA	CA-C-N	-7.63	110.52	120.44
2	B	31	ALA	C-N-CA	-7.63	110.52	120.44
2	B	100	ARG	N-CA-C	-7.62	102.98	111.82
2	B	8	TYR	CG-CD1-CE1	7.62	132.62	121.20
2	B	211	GLU	CG-CD-OE1	7.61	135.90	118.40
2	B	357	HIS	ND1-CG-CD2	7.60	113.70	106.10
2	B	391	LEU	N-CA-C	-7.59	103.08	111.36
1	A	219	GLN	O-C-N	7.59	132.93	122.46
2	B	372	LEU	CD1-CG-CD2	7.59	127.49	110.80
2	B	356	ALA	N-CA-C	-7.58	102.01	111.11
2	B	295	GLU	CG-CD-OE2	7.58	135.84	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	52	TYR	CB-CG-CD1	7.58	132.17	120.80
2	B	270	PRO	O-C-N	-7.57	112.05	122.27
2	B	223	LEU	CA-C-O	-7.57	112.41	120.88
2	B	200	ILE	CA-C-O	-7.57	113.08	120.95
2	B	47	ASP	O-C-N	-7.56	113.53	122.15
2	B	78	GLU	N-CA-C	-7.56	104.03	113.18
1	A	216	SER	CA-C-O	7.55	127.28	120.34
2	B	350	GLU	CB-CG-CD	7.54	125.42	112.60
2	B	365	GLN	CB-CG-CD	-7.54	99.79	112.60
2	B	235	SER	CA-C-N	-7.53	108.86	120.31
2	B	235	SER	C-N-CA	-7.53	108.86	120.31
2	B	278	ILE	N-CA-CB	-7.53	100.53	111.52
1	A	107	PHE	CB-CG-CD1	7.52	133.49	120.70
2	B	168	ASP	N-CA-C	-7.52	103.17	111.36
2	B	306	PHE	N-CA-C	-7.52	94.72	108.85
2	B	352	SER	CA-C-N	-7.51	109.62	120.29
2	B	352	SER	C-N-CA	-7.51	109.62	120.29
2	B	59	LEU	N-CA-CB	-7.51	98.79	110.65
2	B	238	ILE	CB-CG1-CD1	-7.51	98.03	113.80
2	B	302	ALA	N-CA-C	7.50	123.75	111.37
2	B	94	GLN	CA-CB-CG	-7.49	99.12	114.10
2	B	204	PHE	CG-CD2-CE2	-7.48	107.98	120.70
2	B	210	GLU	CA-C-N	-7.48	108.94	120.31
2	B	210	GLU	C-N-CA	-7.48	108.94	120.31
2	B	287	MET	CB-CA-C	-7.48	98.46	110.81
1	A	115	TYR	CA-C-N	-7.48	110.26	120.28
1	A	115	TYR	C-N-CA	-7.48	110.26	120.28
2	B	258	GLY	O-C-N	-7.48	110.89	122.18
2	B	346	ILE	N-CA-C	-7.47	100.15	107.55
2	B	231	VAL	CB-CA-C	7.46	118.91	110.41
1	A	218	GLU	N-CA-C	7.45	121.63	112.54
2	B	207	MET	O-C-N	7.45	132.42	122.43
2	B	9	PHE	CA-C-N	-7.45	108.08	120.07
2	B	9	PHE	C-N-CA	-7.45	108.08	120.07
2	B	102	GLY	N-CA-C	7.44	125.70	114.61
2	B	104	SER	O-C-N	-7.44	114.12	122.23
2	B	200	ILE	CB-CG1-CD1	-7.44	98.17	113.80
2	B	158	PRO	CA-C-N	-7.43	113.46	123.12
2	B	158	PRO	C-N-CA	-7.43	113.46	123.12
2	B	97	LEU	CB-CA-C	-7.41	98.49	110.79
2	B	221	GLY	CA-C-N	-7.40	109.15	121.80
2	B	221	GLY	C-N-CA	-7.40	109.15	121.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	106	ILE	CB-CG1-CD1	7.38	129.29	113.80
1	A	23	VAL	N-CA-CB	7.37	125.70	111.92
1	A	63	THR	OG1-CB-CG2	-7.37	94.56	109.30
2	B	48	LEU	CA-C-N	-7.37	109.83	120.29
2	B	48	LEU	C-N-CA	-7.37	109.83	120.29
2	B	17	VAL	CB-CA-C	-7.36	100.52	110.97
1	A	33	SER	O-C-N	7.36	129.92	122.12
2	B	329	ASP	N-CA-C	-7.35	102.29	111.11
2	B	239	GLY	O-C-N	7.35	129.32	122.19
1	A	4	TYR	CB-CA-C	-7.35	97.26	110.70
2	B	273	HIS	CA-CB-CG	-7.35	106.45	113.80
2	B	248	THR	CA-C-O	-7.34	109.50	119.05
1	A	208	ALA	N-CA-C	7.34	121.42	109.76
1	A	155	PRO	CB-CA-C	-7.33	101.97	110.92
2	B	12	PHE	CG-CD2-CE2	-7.33	108.24	120.70
1	A	221	SER	O-C-N	-7.32	114.36	122.12
2	B	225	ASP	CA-C-O	-7.32	111.56	119.97
2	B	357	HIS	CA-C-O	7.32	128.18	120.42
2	B	327	ILE	CA-CB-CG1	7.31	122.83	110.40
2	B	365	GLN	CA-C-N	-7.30	112.18	119.56
2	B	365	GLN	C-N-CA	-7.30	112.18	119.56
2	B	191	ALA	N-CA-C	-7.30	101.30	111.81
2	B	354	ALA	CA-C-O	7.30	128.48	120.82
2	B	313	HIS	CA-CB-CG	-7.30	106.50	113.80
1	A	112	ASP	N-CA-C	7.29	119.86	111.11
2	B	85	ALA	CA-C-O	7.29	129.03	121.23
1	A	77	THR	CA-C-O	-7.28	113.43	120.64
2	B	194	PRO	CA-N-CD	7.27	122.18	112.00
2	B	291	ASP	CB-CG-OD2	7.27	135.12	118.40
1	A	103	ALA	CA-C-N	-7.26	109.27	120.31
1	A	103	ALA	C-N-CA	-7.26	109.27	120.31
1	A	95	ILE	CB-CG1-CD1	-7.26	98.56	113.80
1	A	260	SER	CA-CB-OG	-7.26	96.59	111.10
1	A	214	ILE	CB-CA-C	-7.25	104.11	111.80
2	B	59	LEU	CA-C-N	-7.24	112.72	122.72
2	B	59	LEU	C-N-CA	-7.24	112.72	122.72
2	B	372	LEU	CA-C-N	-7.24	113.66	123.14
2	B	372	LEU	C-N-CA	-7.24	113.66	123.14
2	B	183	THR	CB-CA-C	-7.24	97.40	109.99
2	B	289	THR	N-CA-C	7.24	119.31	110.41
1	A	56	ASP	N-CA-C	7.23	121.67	108.94
1	A	143	ALA	CB-CA-C	-7.23	99.83	110.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	122	GLY	N-CA-C	7.22	126.19	115.64
1	A	115	TYR	N-CA-C	-7.22	103.13	112.23
2	B	342	HIS	CA-C-O	7.21	127.71	119.27
1	A	102	TYR	CA-C-O	-7.21	112.71	121.36
2	B	100	ARG	CD-NE-CZ	7.21	134.49	124.40
2	B	227	VAL	CA-C-N	7.20	132.57	123.14
2	B	227	VAL	C-N-CA	7.20	132.57	123.14
2	B	323	ASP	N-CA-C	7.19	121.17	109.59
2	B	268	GLY	CA-C-N	-7.19	114.45	123.15
2	B	268	GLY	C-N-CA	-7.19	114.45	123.15
2	B	207	MET	CB-CG-SD	7.18	134.24	112.70
2	B	196	PRO	CA-CB-CG	-7.15	90.41	104.00
2	B	185	HIS	N-CA-C	-7.15	98.08	109.59
2	B	89	ASN	CA-C-O	-7.14	113.51	121.00
1	A	94	THR	O-C-N	7.13	131.11	122.48
1	A	40	LEU	N-CA-C	-7.12	103.52	111.28
2	B	370	GLN	CA-C-O	-7.12	113.02	120.99
1	A	73	ALA	N-CA-C	-7.11	103.53	111.71
2	B	255	VAL	O-C-N	-7.11	113.57	122.88
2	B	334	GLU	OE1-CD-OE2	-7.09	105.89	122.90
1	A	7	LEU	N-CA-C	-7.07	103.66	111.36
1	A	218	GLU	CA-C-O	7.07	128.07	119.38
1	A	220	VAL	O-C-N	-7.06	114.99	121.91
2	B	316	LEU	O-C-N	7.05	130.94	122.27
2	B	66	THR	CA-C-N	-7.04	109.89	120.94
2	B	66	THR	C-N-CA	-7.04	109.89	120.94
2	B	330	ASP	CA-C-N	7.04	129.59	120.44
2	B	330	ASP	C-N-CA	7.04	129.59	120.44
1	A	215	SER	N-CA-C	7.03	123.49	113.02
1	A	218	GLU	CA-C-N	-7.02	108.85	121.14
1	A	218	GLU	C-N-CA	-7.02	108.85	121.14
1	A	24	THR	CA-C-O	7.02	128.47	120.54
1	A	118	CYS	O-C-N	7.02	129.56	122.12
2	B	27	GLN	CA-C-O	-7.02	112.98	120.42
2	B	303	GLY	CA-C-O	7.02	127.93	119.65
2	B	78	GLU	CA-C-O	7.00	128.08	119.11
2	B	373	VAL	CA-CB-CG1	-7.00	98.50	110.40
2	B	247	ASP	CA-C-O	7.00	129.23	121.39
1	A	96	PRO	CA-C-N	-6.99	113.76	123.13
1	A	96	PRO	C-N-CA	-6.99	113.76	123.13
2	B	118	ALA	CA-C-N	-6.98	108.81	120.68
2	B	118	ALA	C-N-CA	-6.98	108.81	120.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	62	CYS	CA-CB-SG	-6.98	98.34	114.40
2	B	243	ASP	OD1-CG-OD2	-6.98	106.15	122.90
2	B	97	LEU	CA-CB-CG	-6.97	91.89	116.30
2	B	100	ARG	CA-C-O	-6.96	111.97	119.97
1	A	126	VAL	N-CA-CB	-6.96	99.38	111.63
1	A	254	GLU	N-CA-C	6.96	119.71	111.71
1	A	134	GLU	O-C-N	6.96	131.75	122.43
2	B	130	CYS	CA-C-O	6.94	127.95	120.38
1	A	164	ARG	N-CA-C	-6.94	103.80	111.36
2	B	12	PHE	CD1-CE1-CZ	-6.93	107.52	120.00
2	B	130	CYS	O-C-N	-6.93	115.11	123.29
2	B	300	ILE	CA-C-O	-6.93	113.15	120.57
2	B	65	ILE	N-CA-CB	-6.93	98.22	110.77
2	B	379	ARG	NE-CZ-NH2	6.93	125.44	119.20
1	A	171	ARG	CA-C-O	6.92	128.85	121.45
2	B	262	ILE	CA-CB-CG1	6.90	122.14	110.40
1	A	142	ALA	CB-CA-C	-6.90	99.12	110.85
1	A	234	GLY	CA-C-N	-6.90	111.23	120.54
1	A	234	GLY	C-N-CA	-6.90	111.23	120.54
2	B	226	ALA	N-CA-CB	6.89	123.61	111.13
1	A	93	PRO	N-CD-CG	-6.89	92.86	103.20
2	B	190	THR	CA-C-O	-6.89	113.75	121.40
2	B	213	LYS	CD-CE-NZ	-6.89	89.84	111.90
2	B	49	LEU	N-CA-CB	-6.88	99.97	110.16
2	B	28	LEU	CB-CA-C	6.88	121.69	110.88
2	B	356	ALA	O-C-N	-6.88	114.94	122.09
2	B	38	ASP	CA-C-O	-6.87	110.75	120.16
2	B	358	ALA	CA-C-O	-6.87	112.34	120.10
1	A	138	PRO	N-CA-C	6.86	122.92	113.65
2	B	79	ASP	CB-CG-OD1	6.84	134.12	118.40
2	B	57	THR	CA-CB-OG1	-6.83	99.35	109.60
2	B	241	PHE	CA-CB-CG	6.83	120.63	113.80
1	A	7	LEU	CB-CA-C	-6.83	99.25	110.85
2	B	121	LEU	N-CA-C	6.83	119.74	111.82
2	B	90	GLN	CG-CD-OE1	-6.82	107.16	120.80
2	B	206[A]	ARG	N-CA-CB	6.81	121.84	110.41
2	B	206[B]	ARG	N-CA-CB	6.81	121.84	110.41
1	A	44	GLY	CA-C-O	6.80	125.75	118.95
2	B	25	LEU	O-C-N	-6.80	114.40	122.15
1	A	3	ARG	CA-C-O	-6.79	112.16	119.97
2	B	25	LEU	CD1-CG-CD2	-6.79	95.86	110.80
2	B	364	GLU	CA-CB-CG	6.79	127.67	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	222	ARG	CA-C-O	6.78	128.57	121.38
2	B	53	ALA	CA-C-O	-6.78	111.12	119.18
2	B	201	VAL	N-CA-C	-6.77	103.88	110.72
2	B	237	ALA	CA-C-O	6.77	127.59	120.42
1	A	209	LEU	CA-C-N	-6.76	112.08	122.09
1	A	209	LEU	C-N-CA	-6.76	112.08	122.09
2	B	151	LEU	O-C-N	-6.76	113.60	122.59
1	A	100	LEU	CB-CG-CD2	6.75	130.96	110.70
2	B	231	VAL	CA-CB-CG1	-6.75	98.92	110.40
2	B	154	ALA	O-C-N	-6.75	115.33	122.96
2	B	159	VAL	CA-CB-CG1	6.74	121.86	110.40
1	A	257	SER	CB-CA-C	-6.74	100.30	110.88
2	B	11	GLU	CA-C-O	6.74	127.81	119.05
2	B	104	SER	CA-C-O	6.74	126.64	119.03
2	B	13	GLY	O-C-N	6.73	133.04	123.56
2	B	188	LEU	N-CA-CB	-6.72	100.07	110.29
2	B	228	ILE	CA-CB-CG2	6.72	121.93	110.50
2	B	78	GLU	CG-CD-OE1	-6.72	102.95	118.40
2	B	282	MET	CA-CB-CG	-6.71	100.67	114.10
2	B	362	MET	CA-CB-CG	-6.71	100.69	114.10
2	B	368	LYS	CG-CD-CE	-6.71	95.87	111.30
2	B	367	GLU	CA-C-O	6.71	127.76	119.78
2	B	86	HIS	CB-CG-CD2	-6.70	122.49	131.20
1	A	24	THR	CA-CB-OG1	-6.70	99.55	109.60
2	B	100	ARG	NH1-CZ-NH2	-6.69	110.60	119.30
2	B	328	THR	N-CA-CB	6.68	121.15	110.46
1	A	263	LYS	CA-C-O	-6.68	111.78	119.60
2	B	146	VAL	N-CA-CB	6.68	117.92	110.51
2	B	114	GLN	N-CA-C	6.67	118.56	111.28
2	B	229	ALA	O-C-N	-6.67	115.79	123.33
2	B	381	ASP	N-CA-C	6.67	119.40	111.33
1	A	140	ARG	CB-CA-C	6.66	121.34	110.88
1	A	221	SER	CA-CB-OG	-6.66	97.78	111.10
1	A	127	LEU	N-CA-CB	-6.65	99.50	110.68
1	A	222	ALA	N-CA-C	6.64	118.52	111.28
2	B	73	LEU	O-C-N	6.64	131.21	123.30
2	B	252	LEU	CD1-CG-CD2	-6.64	96.18	110.80
2	B	339	LEU	N-CA-C	-6.64	103.86	112.23
2	B	121	LEU	CA-C-O	6.64	127.61	119.97
1	A	84	MET	N-CA-C	-6.64	104.13	111.36
2	B	312	GLN	N-CA-CB	6.64	119.98	110.16
1	A	232	ILE	CA-C-O	-6.63	113.43	120.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	349	LEU	N-CA-C	-6.63	104.05	111.28
2	B	157	ILE	N-CA-CB	-6.63	103.04	111.39
2	B	244	PHE	O-C-N	6.63	130.63	122.34
2	B	319	ILE	CG1-CB-CG2	-6.63	90.82	110.70
2	B	330	ASP	CB-CG-OD1	6.62	133.64	118.40
1	A	11	LEU	CA-C-O	-6.62	112.35	119.97
2	B	229	ALA	CA-C-O	-6.62	113.57	120.99
1	A	263	LYS	CA-C-N	-6.62	111.41	120.28
1	A	263	LYS	C-N-CA	-6.62	111.41	120.28
1	A	219	GLN	CG-CD-OE1	-6.62	107.57	120.80
2	B	80	LEU	CD1-CG-CD2	6.61	125.35	110.80
1	A	140	ARG	CG-CD-NE	-6.61	97.45	112.00
2	B	48	LEU	O-C-N	6.60	128.87	122.07
2	B	77	ARG	CB-CA-C	-6.60	102.02	112.05
2	B	94	GLN	N-CA-C	-6.60	103.91	112.23
2	B	296	GLU	O-C-N	6.60	130.46	123.06
1	A	111	ILE	N-CA-C	-6.60	104.42	110.82
1	A	37	ILE	CA-C-O	-6.60	113.65	120.71
1	A	128	VAL	O-C-N	6.60	132.46	122.76
2	B	283	LYS	CG-CD-CE	-6.59	96.13	111.30
2	B	278	ILE	CA-CB-CG2	-6.59	99.30	110.50
2	B	78	GLU	N-CA-CB	-6.59	99.34	110.41
2	B	361	MET	CA-CB-CG	-6.59	100.92	114.10
2	B	188	LEU	CD1-CG-CD2	-6.58	96.33	110.80
2	B	280	PHE	CA-C-O	6.58	129.92	120.51
2	B	202	ARG	N-CA-C	6.58	119.29	111.33
2	B	243	ASP	CA-C-N	-6.57	111.69	122.54
2	B	243	ASP	C-N-CA	-6.57	111.69	122.54
1	A	132	PRO	CA-C-N	-6.57	109.85	120.62
1	A	132	PRO	C-N-CA	-6.57	109.85	120.62
2	B	212	THR	CB-CA-C	6.56	121.31	110.81
2	B	72	THR	N-CA-C	-6.55	97.84	108.52
2	B	296	GLU	CA-CB-CG	6.55	127.21	114.10
2	B	132	ILE	O-C-N	6.54	129.90	123.03
1	A	142	ALA	CA-C-O	6.54	127.36	120.42
2	B	350	GLU	N-CA-CB	6.54	119.76	109.82
1	A	76	VAL	CA-CB-CG2	-6.54	99.29	110.40
1	A	134	GLU	CG-CD-OE1	6.54	133.43	118.40
2	B	200	ILE	CA-CB-CG1	-6.54	99.29	110.40
2	B	316	LEU	CB-CG-CD1	-6.54	91.09	110.70
2	B	196	PRO	CA-C-O	-6.53	104.53	120.20
1	A	107	PHE	O-C-N	6.52	131.39	122.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	196	LEU	N-CA-C	-6.52	104.10	111.14
1	A	107	PHE	CE1-CZ-CE2	-6.51	108.28	120.00
2	B	244	PHE	CA-C-O	-6.50	111.74	119.35
2	B	365	GLN	CA-CB-CG	-6.50	101.09	114.10
1	A	35	LYS	N-CA-C	-6.50	104.04	112.23
2	B	343	GLU	CG-CD-OE1	6.49	133.34	118.40
2	B	88	THR	O-C-N	-6.49	114.62	122.22
2	B	91	VAL	CA-CB-CG2	-6.49	99.36	110.40
1	A	261	ALA	O-C-N	-6.49	115.24	122.12
1	A	107	PHE	CA-CB-CG	6.49	120.28	113.80
1	A	219	GLN	CG-CD-NE2	6.48	126.12	116.40
2	B	268	GLY	O-C-N	-6.48	114.27	122.70
2	B	286	MET	CA-C-N	6.48	131.03	122.42
2	B	286	MET	C-N-CA	6.48	131.03	122.42
2	B	33	VAL	CG1-CB-CG2	6.47	125.03	110.80
2	B	373	VAL	N-CA-CB	-6.46	102.49	111.41
2	B	287	MET	O-C-N	6.46	130.69	122.93
1	A	149	ALA	O-C-N	6.46	130.91	121.54
1	A	42	ASP	N-CA-C	-6.46	104.33	111.82
2	B	215	GLN	CA-CB-CG	-6.46	101.19	114.10
1	A	166	VAL	CB-CA-C	-6.45	103.44	112.14
1	A	176	LEU	N-CA-C	-6.44	96.74	108.02
2	B	225	ASP	CA-CB-CG	-6.44	106.16	112.60
1	A	139	PHE	CA-CB-CG	-6.44	107.36	113.80
2	B	205	GLN	CG-CD-OE1	-6.44	107.92	120.80
2	B	280	PHE	N-CA-CB	-6.44	99.61	110.49
2	B	91	VAL	CB-CA-C	6.43	120.81	112.14
2	B	234	GLY	CA-C-O	6.42	125.73	118.86
2	B	209	GLY	CA-C-O	6.41	127.08	120.80
2	B	186	TYR	CA-C-N	-6.40	113.18	123.23
2	B	186	TYR	C-N-CA	-6.40	113.18	123.23
2	B	146	VAL	CA-C-O	6.39	127.92	121.27
2	B	33	VAL	CA-C-O	6.38	127.69	121.05
1	A	32	GLN	CB-CG-CD	6.34	123.39	112.60
2	B	215	GLN	CA-C-N	-6.34	109.90	120.30
2	B	215	GLN	C-N-CA	-6.34	109.90	120.30
2	B	336	PHE	N-CA-C	-6.34	104.45	111.36
2	B	215	GLN	CG-CD-NE2	-6.33	106.90	116.40
2	B	322	ALA	O-C-N	-6.33	114.92	123.15
2	B	27	GLN	N-CA-C	-6.33	104.46	111.36
1	A	148	ILE	CG1-CB-CG2	-6.31	91.78	110.70
2	B	78	GLU	CG-CD-OE2	6.31	132.91	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	233	GLY	CA-C-N	6.31	132.33	122.30
2	B	233	GLY	C-N-CA	6.31	132.33	122.30
1	A	194	HIS	CB-CA-C	6.30	122.78	110.67
2	B	271	LEU	N-CA-C	-6.30	104.33	111.07
2	B	47	ASP	CA-C-N	6.30	128.63	120.44
2	B	47	ASP	C-N-CA	6.30	128.63	120.44
2	B	385	PHE	CB-CA-C	-6.30	100.34	110.79
2	B	353	HIS	CA-C-O	6.29	127.09	120.42
2	B	34	SER	CA-CB-OG	-6.27	98.56	111.10
1	A	94	THR	CB-CA-C	-6.27	98.54	109.07
2	B	128	LEU	CA-C-O	6.26	128.67	121.28
2	B	15	MET	CA-CB-CG	6.26	126.63	114.10
2	B	56	PRO	CB-CG-CD	-6.26	91.01	105.40
2	B	235	SER	O-C-N	6.26	130.71	122.33
2	B	346	ILE	O-C-N	-6.25	117.43	121.37
2	B	5	LEU	O-C-N	-6.25	115.03	123.15
2	B	33	VAL	N-CA-C	6.25	117.74	110.62
1	A	157	ASN	N-CA-C	-6.25	104.29	112.41
1	A	204	HIS	CB-CA-C	-6.24	103.50	111.86
2	B	222	ARG	CD-NE-CZ	6.23	133.13	124.40
1	A	261	ALA	N-CA-C	6.23	118.07	111.28
2	B	149	MET	CA-CB-CG	-6.23	101.64	114.10
2	B	195	HIS	O-C-N	6.23	126.49	121.38
2	B	341	ARG	CA-C-N	6.23	132.62	121.66
2	B	341	ARG	C-N-CA	6.23	132.62	121.66
2	B	99	LYS	CD-CE-NZ	-6.22	91.99	111.90
1	A	102	TYR	CA-C-N	6.22	128.61	120.28
1	A	102	TYR	C-N-CA	6.22	128.61	120.28
2	B	326	SER	N-CA-CB	6.21	123.08	111.53
2	B	59	LEU	N-CA-C	-6.21	97.16	108.02
2	B	92	LEU	O-C-N	-6.21	115.67	122.07
2	B	326	SER	O-C-N	6.21	130.47	123.27
1	A	88	ILE	CA-CB-CG1	-6.21	99.85	110.40
1	A	25	LEU	CA-C-O	-6.20	113.68	120.81
2	B	61	LYS	CA-CB-CG	-6.20	101.70	114.10
2	B	135	GLY	CA-C-O	-6.20	115.96	121.41
1	A	131	VAL	CA-CB-CG2	-6.20	99.87	110.40
2	B	206[A]	ARG	CD-NE-CZ	6.20	133.07	124.40
2	B	206[B]	ARG	CD-NE-CZ	6.20	133.07	124.40
2	B	5	LEU	CA-C-N	-6.19	110.64	121.35
2	B	5	LEU	C-N-CA	-6.19	110.64	121.35
2	B	291	ASP	OD1-CG-OD2	6.19	137.75	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	61	LYS	O-C-N	-6.19	115.34	122.89
2	B	65	ILE	CA-CB-CG1	-6.18	99.89	110.40
1	A	150	PRO	N-CD-CG	6.18	112.47	103.20
2	B	210	GLU	N-CA-C	-6.18	104.45	112.23
2	B	278	ILE	O-C-N	-6.17	116.53	123.20
2	B	256	GLU	CA-C-N	6.17	127.82	120.23
2	B	256	GLU	C-N-CA	6.17	127.82	120.23
1	A	207	PRO	CB-CA-C	-6.17	103.51	111.46
2	B	368	LYS	CD-CE-NZ	-6.17	92.17	111.90
2	B	88	THR	CA-C-N	6.16	128.78	120.65
2	B	88	THR	C-N-CA	6.16	128.78	120.65
2	B	9	PHE	CE1-CZ-CE2	6.16	131.09	120.00
2	B	4	LEU	N-CA-C	6.16	119.99	112.23
2	B	354	ALA	CA-C-N	-6.16	111.55	120.29
2	B	354	ALA	C-N-CA	-6.16	111.55	120.29
1	A	11	LEU	CB-CG-CD2	6.15	129.16	110.70
2	B	6	ASN	N-CA-CB	-6.15	96.72	109.45
1	A	60	ASP	CA-CB-CG	-6.14	106.46	112.60
2	B	43	ALA	CA-C-N	6.14	128.42	120.44
2	B	43	ALA	C-N-CA	6.14	128.42	120.44
2	B	77	ARG	CG-CD-NE	6.13	125.50	112.00
2	B	86	HIS	CG-CD2-NE2	-6.13	101.06	107.20
2	B	241	PHE	CA-C-N	-6.13	112.26	120.54
2	B	241	PHE	C-N-CA	-6.13	112.26	120.54
1	A	54	PHE	N-CA-C	-6.13	99.00	109.24
1	A	18	ALA	N-CA-CB	-6.13	100.41	110.41
2	B	51	ASN	N-CA-CB	-6.13	100.12	110.41
2	B	112	ALA	CA-C-N	-6.13	113.99	122.63
2	B	112	ALA	C-N-CA	-6.13	113.99	122.63
1	A	38	ASP	N-CA-C	-6.12	104.72	111.82
2	B	309	VAL	CA-C-N	6.12	131.48	121.87
2	B	309	VAL	C-N-CA	6.12	131.48	121.87
2	B	40	GLU	CA-C-O	6.12	127.03	120.55
1	A	259	VAL	O-C-N	6.11	127.80	121.87
1	A	89	ARG	CA-C-O	-6.11	113.94	120.42
1	A	265	ALA	CA-C-O	6.11	126.88	119.49
1	A	110	GLY	O-C-N	6.10	130.63	122.70
1	A	88	ILE	CB-CG1-CD1	-6.10	100.99	113.80
2	B	43	ALA	O-C-N	-6.10	114.30	122.23
2	B	161	SER	N-CA-C	6.10	118.64	110.35
2	B	59	LEU	CB-CA-C	6.10	120.55	110.74
1	A	17	GLY	N-CA-C	-6.09	103.33	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	317	ASN	CB-CG-ND2	6.09	125.54	116.40
2	B	69	THR	CA-C-O	6.09	128.97	121.60
2	B	113	GLY	CA-C-O	-6.08	112.17	119.04
1	A	259	VAL	CA-CB-CG2	-6.08	100.07	110.40
2	B	46	ALA	CA-C-O	6.08	126.99	120.55
1	A	24	THR	CA-CB-CG2	-6.08	100.17	110.50
1	A	84	MET	CA-C-N	6.07	128.33	120.44
1	A	84	MET	C-N-CA	6.07	128.33	120.44
2	B	250	VAL	CA-C-N	6.06	133.29	121.41
2	B	250	VAL	C-N-CA	6.06	133.29	121.41
2	B	345	ILE	CB-CG1-CD1	6.06	126.53	113.80
2	B	61	LYS	CA-C-N	6.06	130.91	122.79
2	B	61	LYS	C-N-CA	6.06	130.91	122.79
2	B	291	ASP	N-CA-CB	-6.05	100.95	110.46
1	A	139	PHE	CA-C-N	-6.05	112.57	120.44
1	A	139	PHE	C-N-CA	-6.05	112.57	120.44
2	B	103	LYS	CD-CE-NZ	-6.05	92.55	111.90
1	A	263	LYS	O-C-N	6.05	130.94	122.36
2	B	208	ILE	CA-CB-CG1	6.05	120.68	110.40
2	B	352	SER	N-CA-C	-6.04	104.76	111.71
1	A	60	ASP	N-CA-C	6.04	119.31	109.59
2	B	55	ARG	CD-NE-CZ	-6.04	115.94	124.40
2	B	97	LEU	CA-C-N	6.04	128.29	120.44
2	B	97	LEU	C-N-CA	6.04	128.29	120.44
1	A	209	LEU	N-CA-CB	6.04	120.05	110.57
1	A	3	ARG	O-C-N	6.03	129.69	122.27
1	A	80	GLN	CA-C-O	-6.03	113.04	119.97
2	B	237	ALA	O-C-N	-6.03	115.28	122.15
2	B	67	ALA	N-CA-CB	-6.02	101.50	110.17
1	A	205	ALA	CA-C-O	6.02	128.85	121.87
1	A	236	ALA	N-CA-C	6.02	117.84	111.28
1	A	150	PRO	CA-C-O	-6.01	113.39	120.85
2	B	77	ARG	NE-CZ-NH1	-6.01	115.49	121.50
2	B	56	PRO	O-C-N	-6.01	109.69	121.10
2	B	383	ASP	CA-C-N	-6.01	110.45	120.30
2	B	383	ASP	C-N-CA	-6.01	110.45	120.30
2	B	311	PRO	CA-C-N	6.00	128.80	120.29
2	B	311	PRO	C-N-CA	6.00	128.80	120.29
2	B	147	PHE	N-CA-C	5.99	117.89	111.36
2	B	162	GLY	N-CA-C	-5.99	99.88	111.02
2	B	278	ILE	N-CA-C	-5.98	99.51	108.12
2	B	336	PHE	CA-C-N	-5.98	111.80	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	336	PHE	C-N-CA	-5.98	111.80	120.29
1	A	151	ILE	CA-CB-CG1	5.97	120.56	110.40
1	A	232	ILE	CA-CB-CG2	-5.97	100.35	110.50
2	B	359	LEU	CA-C-N	-5.97	111.23	120.31
2	B	359	LEU	C-N-CA	-5.97	111.23	120.31
2	B	77	ARG	NH1-CZ-NH2	5.97	127.06	119.30
2	B	323	ASP	CB-CG-OD2	5.97	132.13	118.40
2	B	13	GLY	N-CA-C	-5.96	105.54	111.56
2	B	73	LEU	CA-C-O	-5.96	113.92	120.36
2	B	324	TYR	OH-CZ-CE2	5.96	137.78	119.90
2	B	283	LYS	CA-CB-CG	-5.96	102.19	114.10
2	B	330	ASP	OD1-CG-OD2	-5.95	108.61	122.90
2	B	219	LYS	N-CA-CB	5.95	119.25	110.33
2	B	289	THR	CA-C-O	-5.94	115.22	121.99
2	B	340	CYS	CB-CA-C	-5.94	100.93	110.79
1	A	213	GLY	CA-C-N	-5.94	112.77	122.33
1	A	213	GLY	C-N-CA	-5.94	112.77	122.33
2	B	182	GLU	CG-CD-OE2	5.94	132.05	118.40
2	B	161	SER	CA-CB-OG	5.93	122.97	111.10
2	B	314	ALA	N-CA-C	-5.93	104.81	111.28
2	B	376	LEU	CD1-CG-CD2	-5.93	97.75	110.80
2	B	118	ALA	O-C-N	5.92	128.40	122.12
2	B	8	TYR	CZ-CE2-CD2	5.92	130.25	119.60
2	B	315	TYR	N-CA-C	5.92	117.40	111.07
2	B	377	SER	N-CA-CB	-5.92	100.75	110.40
2	B	224	PRO	CA-C-O	-5.92	114.60	121.34
1	A	241	ILE	O-C-N	5.91	127.70	121.91
2	B	99	LYS	CB-CG-CD	-5.91	97.70	111.30
1	A	237	ILE	N-CA-C	-5.91	104.56	111.00
2	B	90	GLN	CA-C-O	-5.91	112.82	119.79
2	B	132	ILE	CA-CB-CG1	-5.90	100.37	110.40
2	B	295	GLU	N-CA-C	5.90	118.44	109.95
2	B	52	TYR	CE1-CZ-CE2	-5.90	108.51	120.30
2	B	48	LEU	CD1-CG-CD2	-5.89	97.84	110.80
2	B	76	LYS	O-C-N	-5.89	116.51	123.22
2	B	89	ASN	CA-C-N	-5.89	110.67	120.68
2	B	89	ASN	C-N-CA	-5.89	110.67	120.68
2	B	233	GLY	CA-C-O	5.88	130.80	120.57
2	B	246	ASN	N-CA-CB	5.88	120.28	110.41
1	A	127	LEU	CA-C-N	-5.87	115.24	122.93
1	A	127	LEU	C-N-CA	-5.87	115.24	122.93
1	A	10	GLN	N-CA-CB	5.87	118.85	110.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	257	PRO	CB-CA-C	-5.87	105.16	111.56
2	B	357	HIS	CB-CG-CD2	5.87	138.83	131.20
2	B	78	GLU	CB-CG-CD	5.87	122.58	112.60
1	A	88	ILE	CB-CA-C	-5.87	104.33	112.02
2	B	2	THR	OG1-CB-CG2	-5.87	97.57	109.30
2	B	187	MET	CB-CA-C	-5.86	101.44	111.41
2	B	368	LYS	CA-CB-CG	-5.86	102.38	114.10
2	B	285	PRO	CA-N-CD	5.85	120.20	112.00
2	B	27	GLN	CG-CD-NE2	-5.85	107.63	116.40
1	A	99	LEU	CA-C-O	5.85	127.77	121.16
1	A	219	GLN	CB-CG-CD	-5.85	102.66	112.60
2	B	366	PRO	O-C-N	-5.85	114.35	122.30
2	B	315	TYR	OH-CZ-CE2	-5.84	102.37	119.90
2	B	123	SER	O-C-N	5.84	128.81	122.15
1	A	130	ASP	O-C-N	-5.84	114.66	122.19
2	B	290	ALA	O-C-N	5.84	128.86	122.20
1	A	107	PHE	N-CA-C	-5.83	106.00	113.23
2	B	367	GLU	N-CA-CB	-5.83	102.01	110.70
1	A	136	SER	N-CA-C	-5.82	105.94	113.16
2	B	208	ILE	CB-CA-C	5.82	119.15	111.70
2	B	322	ALA	CA-C-O	5.82	128.25	121.44
2	B	350	GLU	CA-CB-CG	-5.82	102.47	114.10
2	B	323	ASP	OD1-CG-OD2	-5.82	108.94	122.90
1	A	228	ALA	N-CA-C	-5.81	101.92	110.52
2	B	56	PRO	N-CD-CG	5.81	110.77	103.80
1	A	206	ALA	CA-C-O	-5.81	114.13	120.69
2	B	203	GLU	CB-CA-C	-5.81	97.85	109.99
1	A	100	LEU	CA-C-O	-5.80	113.94	120.32
1	A	117	ARG	CA-C-N	-5.80	112.51	120.28
1	A	117	ARG	C-N-CA	-5.80	112.51	120.28
2	B	16	TYR	N-CA-C	5.80	118.32	109.62
2	B	282	MET	CA-C-O	-5.80	114.84	121.40
2	B	288	GLN	OE1-CD-NE2	5.80	128.40	122.60
2	B	198	PRO	CA-C-N	5.80	128.32	120.44
2	B	198	PRO	C-N-CA	5.80	128.32	120.44
1	A	30	ILE	N-CA-C	-5.79	105.08	110.53
1	A	121	VAL	CB-CA-C	-5.78	101.66	111.37
1	A	243	LYS	CA-C-N	-5.78	113.36	122.79
1	A	243	LYS	C-N-CA	-5.78	113.36	122.79
1	A	40	LEU	CA-C-O	5.78	126.68	120.55
1	A	28	PRO	N-CD-CG	5.78	110.74	103.80
2	B	206[A]	ARG	CA-C-N	-5.77	111.08	120.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	206[A]	ARG	C-N-CA	-5.77	111.08	120.72
2	B	206[B]	ARG	CA-C-N	-5.77	111.08	120.72
2	B	206[B]	ARG	C-N-CA	-5.77	111.08	120.72
1	A	122	GLY	CA-C-O	5.77	125.19	118.96
2	B	238	ILE	CA-C-N	-5.77	113.66	120.00
2	B	238	ILE	C-N-CA	-5.77	113.66	120.00
2	B	232	GLY	N-CA-C	-5.76	99.52	113.18
2	B	95	ALA	CA-C-O	-5.76	114.31	120.42
2	B	122	ALA	CA-C-N	-5.76	112.11	120.29
2	B	122	ALA	C-N-CA	-5.76	112.11	120.29
2	B	258	GLY	N-CA-C	5.76	125.46	115.62
1	A	65	GLN	O-C-N	-5.75	116.11	122.09
2	B	230	CYS	N-CA-CB	5.75	119.19	110.45
1	A	128	VAL	N-CA-C	-5.74	98.95	107.51
2	B	123	SER	CB-CA-C	-5.74	101.09	110.85
2	B	54	GLY	CA-C-N	5.72	129.38	120.68
2	B	54	GLY	C-N-CA	5.72	129.38	120.68
2	B	95	ALA	CA-C-N	5.72	127.95	120.28
2	B	95	ALA	C-N-CA	5.72	127.95	120.28
2	B	142	GLN	CA-C-N	5.72	126.87	120.06
2	B	142	GLN	C-N-CA	5.72	126.87	120.06
2	B	315	TYR	CE1-CZ-CE2	-5.72	108.86	120.30
1	A	2	GLU	N-CA-C	5.72	122.98	110.80
1	A	55	SER	N-CA-C	-5.72	105.13	111.71
2	B	32	PHE	N-CA-CB	-5.72	101.72	110.01
2	B	337	LYS	N-CA-C	-5.72	105.12	111.36
2	B	264	THR	CA-CB-CG2	-5.72	100.78	110.50
1	A	50	LEU	O-C-N	-5.71	116.39	123.36
2	B	30	GLU	CG-CD-OE2	5.71	131.53	118.40
1	A	137	ALA	O-C-N	-5.71	114.76	121.32
2	B	173	ALA	O-C-N	5.71	127.95	122.07
2	B	97	LEU	CD1-CG-CD2	-5.70	98.25	110.80
2	B	315	TYR	CG-CD2-CE2	5.70	129.75	121.20
2	B	114	GLN	CA-C-N	-5.69	111.65	120.31
2	B	114	GLN	C-N-CA	-5.69	111.65	120.31
2	B	51	ASN	CA-C-N	5.69	132.46	122.79
2	B	51	ASN	C-N-CA	5.69	132.46	122.79
2	B	213	LYS	N-CA-C	5.69	117.16	111.07
2	B	306	PHE	CA-CB-CG	5.69	119.49	113.80
2	B	336	PHE	CG-CD2-CE2	-5.69	111.03	120.70
2	B	275	ARG	CA-C-O	-5.68	113.78	120.60
1	A	131	VAL	N-CA-C	5.68	113.68	107.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	42	GLN	CA-C-O	-5.68	113.68	120.10
2	B	275	ARG	N-CA-CB	-5.67	100.97	111.13
2	B	333	LEU	CB-CG-CD2	-5.67	93.68	110.70
1	A	154	CYS	CB-CA-C	-5.66	103.89	110.17
2	B	3	THR	CA-CB-CG2	5.66	120.11	110.50
2	B	211	GLU	CB-CA-C	-5.65	99.81	110.67
2	B	55	ARG	CA-CB-CG	-5.65	102.80	114.10
2	B	32	PHE	CG-CD1-CE1	-5.65	111.10	120.70
1	A	163	LEU	CB-CG-CD2	5.64	127.63	110.70
1	A	145	ARG	CA-C-N	5.64	131.64	122.67
1	A	145	ARG	C-N-CA	5.64	131.64	122.67
2	B	125	LEU	CA-C-O	5.64	126.53	120.55
2	B	117	VAL	CA-C-O	5.63	127.82	120.78
2	B	315	TYR	CA-C-O	5.63	126.73	120.82
1	A	171	ARG	CD-NE-CZ	5.63	132.28	124.40
1	A	199	LYS	O-C-N	5.63	128.57	122.15
1	A	266	SER	O-C-N	5.63	130.40	122.41
2	B	364	GLU	O-C-N	5.63	128.09	122.12
1	A	265	ALA	O-C-N	-5.62	115.08	122.39
2	B	143	SER	CA-CB-OG	-5.62	99.86	111.10
2	B	321	ARG	O-C-N	5.62	130.16	122.46
1	A	140	ARG	O-C-N	5.62	127.86	122.07
2	B	83	GLY	CA-C-O	5.62	125.22	119.10
1	A	41	ILE	CG1-CB-CG2	-5.62	93.86	110.70
2	B	207	MET	CG-SD-CE	-5.61	88.57	100.90
2	B	241	PHE	O-C-N	-5.59	114.74	122.46
2	B	343	GLU	CA-C-O	-5.59	111.44	118.43
1	A	85	LEU	CA-C-N	-5.59	112.79	120.28
1	A	85	LEU	C-N-CA	-5.59	112.79	120.28
2	B	263	GLU	OE1-CD-OE2	5.59	136.31	122.90
2	B	243	ASP	CB-CG-OD2	5.58	131.25	118.40
2	B	45	PHE	CD1-CE1-CZ	-5.58	109.96	120.00
2	B	313	HIS	O-C-N	5.58	127.81	122.07
2	B	324	TYR	CD1-CE1-CZ	-5.58	109.56	119.60
2	B	71	THR	CB-CA-C	5.57	118.72	109.53
1	A	149	ALA	CA-C-O	-5.57	115.09	119.66
1	A	64	ILE	CB-CA-C	5.57	119.90	112.22
2	B	210	GLU	O-C-N	5.57	129.79	122.33
2	B	154	ALA	CA-C-O	5.56	127.87	121.47
2	B	350	GLU	CA-C-O	5.56	127.18	121.07
1	A	7	LEU	CA-C-O	-5.55	114.53	120.42
2	B	211	GLU	N-CA-CB	-5.55	101.67	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	11	GLU	CA-C-N	-5.55	113.93	122.87
2	B	11	GLU	C-N-CA	-5.55	113.93	122.87
2	B	119	SER	CA-CB-OG	-5.55	100.00	111.10
2	B	285	PRO	CA-C-N	5.55	131.31	122.59
2	B	285	PRO	C-N-CA	5.55	131.31	122.59
2	B	212	THR	OG1-CB-CG2	-5.55	98.20	109.30
1	A	223	ALA	O-C-N	5.54	129.09	122.27
1	A	165	GLN	O-C-N	-5.54	116.11	122.09
1	A	176	LEU	CB-CA-C	-5.54	101.82	110.74
2	B	47	ASP	CB-CG-OD2	5.54	131.14	118.40
2	B	186	TYR	CZ-CE2-CD2	5.53	129.56	119.60
2	B	248	THR	CA-C-N	-5.53	110.80	121.58
2	B	248	THR	C-N-CA	-5.53	110.80	121.58
1	A	114	PHE	CA-C-O	-5.52	114.57	120.42
2	B	287	MET	N-CA-C	-5.52	99.52	108.41
1	A	54	PHE	O-C-N	5.51	130.00	123.27
1	A	94	THR	CA-C-O	-5.51	113.07	118.97
2	B	52	TYR	CG-CD1-CE1	5.51	129.47	121.20
2	B	132	ILE	CB-CG1-CD1	-5.51	102.22	113.80
1	A	214	ILE	O-C-N	-5.51	116.55	122.45
2	B	203	GLU	CA-CB-CG	-5.51	103.08	114.10
1	A	3	ARG	CA-C-N	-5.50	111.17	120.58
1	A	3	ARG	C-N-CA	-5.50	111.17	120.58
2	B	276	VAL	CA-C-O	5.50	127.65	120.78
2	B	283	LYS	CB-CG-CD	-5.50	98.66	111.30
2	B	151	LEU	CA-C-O	5.49	128.36	120.51
2	B	349	LEU	CA-C-O	-5.49	114.73	120.55
2	B	59	LEU	CA-CB-CG	-5.48	97.12	116.30
2	B	120	ALA	CA-C-N	-5.48	111.98	120.31
2	B	120	ALA	C-N-CA	-5.48	111.98	120.31
1	A	261	ALA	CA-C-O	5.48	126.36	120.55
2	B	138	ASP	N-CA-CB	-5.47	102.06	110.16
2	B	376	LEU	CA-CB-CG	-5.47	97.14	116.30
2	B	379	ARG	NE-CZ-NH1	-5.47	116.03	121.50
2	B	270	PRO	CB-CA-C	-5.47	104.12	112.11
1	A	193	LEU	CA-C-O	5.47	126.53	120.63
1	A	7	LEU	CB-CG-CD2	-5.47	94.30	110.70
1	A	51	GLY	O-C-N	5.47	129.36	123.18
2	B	231	VAL	N-CA-CB	-5.47	105.23	112.34
1	A	196	LEU	CB-CG-CD1	5.46	127.06	110.70
2	B	272	LYS	CA-CB-CG	-5.45	103.21	114.10
2	B	356	ALA	CB-CA-C	5.45	119.52	110.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	4	LEU	O-C-N	5.44	129.62	122.33
2	B	22	MET	N-CA-CB	5.44	120.37	110.08
2	B	376	LEU	CB-CG-CD2	-5.44	94.37	110.70
2	B	2	THR	CA-CB-OG1	-5.44	101.44	109.60
2	B	213	LYS	N-CA-CB	-5.44	102.13	110.01
1	A	120	GLN	CB-CG-CD	-5.43	103.36	112.60
1	A	126	VAL	N-CA-C	-5.43	100.83	108.27
1	A	216	SER	N-CA-CB	-5.43	103.59	111.25
2	B	70	ARG	CA-C-N	-5.43	114.05	122.09
2	B	70	ARG	C-N-CA	-5.43	114.05	122.09
1	A	36	ILE	CA-CB-CG1	-5.43	101.17	110.40
2	B	228	ILE	N-CA-C	5.43	115.71	108.11
1	A	11	LEU	CA-CB-CG	-5.42	97.31	116.30
1	A	257	SER	N-CA-C	5.42	116.87	111.07
2	B	66	THR	OG1-CB-CG2	-5.42	98.46	109.30
1	A	265	ALA	N-CA-C	5.40	118.97	112.38
2	B	41	PHE	CD1-CG-CD2	-5.40	110.51	118.60
1	A	131	VAL	CB-CA-C	-5.39	104.98	111.18
2	B	137	LYS	N-CA-CB	5.39	118.04	110.12
1	A	147	ASN	CA-C-N	-5.39	115.45	122.94
1	A	147	ASN	C-N-CA	-5.39	115.45	122.94
2	B	334	GLU	CA-CB-CG	-5.39	103.33	114.10
2	B	11	GLU	N-CA-C	5.38	119.47	113.01
2	B	80	LEU	CA-C-N	-5.38	112.45	121.39
2	B	80	LEU	C-N-CA	-5.38	112.45	121.39
1	A	266	SER	CB-CA-C	-5.38	99.39	109.72
2	B	302	ALA	O-C-N	-5.38	115.92	122.11
1	A	99	LEU	N-CA-C	-5.38	101.40	109.95
1	A	44	GLY	N-CA-C	5.37	123.64	115.63
2	B	85	ALA	N-CA-CB	-5.37	103.24	111.56
2	B	238	ILE	CA-CB-CG2	-5.37	101.37	110.50
2	B	199	THR	CA-CB-OG1	-5.37	101.55	109.60
2	B	216	ILE	CB-CG1-CD1	-5.37	102.53	113.80
2	B	21	LEU	N-CA-C	5.36	119.82	113.28
2	B	330	ASP	O-C-N	-5.36	116.44	122.12
1	A	206	ALA	O-C-N	5.36	127.43	121.43
2	B	322	ALA	N-CA-CB	-5.36	102.23	111.55
2	B	385	PHE	CA-C-N	-5.36	112.68	120.29
2	B	385	PHE	C-N-CA	-5.36	112.68	120.29
2	B	191	ALA	CA-C-O	-5.36	112.21	121.53
2	B	236	ASN	N-CA-C	5.35	118.03	111.82
1	A	86	ALA	N-CA-C	5.35	117.11	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	27	GLN	CG-CD-OE1	5.35	131.50	120.80
2	B	102	GLY	O-C-N	-5.34	116.22	122.31
1	A	98	GLY	CA-C-O	-5.34	116.30	121.11
2	B	298	TYR	CA-C-O	5.34	127.42	120.21
2	B	302	ALA	CA-C-N	5.34	129.93	120.74
2	B	302	ALA	C-N-CA	5.34	129.93	120.74
2	B	126	LEU	O-C-N	5.34	129.01	122.34
1	A	220	VAL	CA-C-O	5.34	126.83	121.17
2	B	23	PRO	CA-CB-CG	-5.33	94.37	104.50
2	B	345	ILE	CA-CB-CG2	-5.33	101.44	110.50
1	A	58	LEU	N-CA-C	5.33	122.16	110.80
1	A	259	VAL	CA-C-O	-5.33	115.41	120.95
1	A	91	LYS	N-CA-C	5.33	119.84	113.23
2	B	280	PHE	N-CA-C	5.33	122.15	110.80
2	B	99	LYS	O-C-N	-5.33	116.47	122.12
2	B	143	SER	CB-CA-C	-5.33	101.73	111.64
2	B	86	HIS	CE1-NE2-CD2	5.32	114.32	109.00
2	B	191	ALA	O-C-N	5.32	129.85	122.08
1	A	102	TYR	N-CA-C	5.32	118.77	110.32
2	B	231	VAL	CA-CB-CG2	5.32	119.44	110.40
2	B	170	CYS	N-CA-C	-5.31	104.90	111.33
2	B	103	LYS	N-CA-CB	5.31	118.52	110.45
2	B	32	PHE	CB-CG-CD1	-5.31	111.68	120.70
2	B	299	SER	O-C-N	5.30	129.42	123.48
2	B	117	VAL	N-CA-CB	-5.30	102.49	111.23
2	B	383	ASP	N-CA-C	5.30	119.84	113.17
2	B	3	THR	CA-CB-OG1	-5.29	101.67	109.60
2	B	86	HIS	CB-CG-ND1	5.29	130.63	122.70
2	B	365	GLN	OE1-CD-NE2	-5.29	117.31	122.60
2	B	338	THR	OG1-CB-CG2	5.28	119.86	109.30
1	A	36	ILE	CB-CA-C	-5.28	105.01	112.14
2	B	250	VAL	O-C-N	-5.28	116.50	122.94
1	A	107	PHE	CB-CG-CD2	-5.28	111.73	120.70
2	B	123	SER	CA-C-N	-5.28	113.58	120.44
2	B	123	SER	C-N-CA	-5.28	113.58	120.44
2	B	195	HIS	ND1-CG-CD2	-5.28	100.82	106.10
2	B	362	MET	O-C-N	5.28	127.79	122.09
2	B	382	LYS	CA-C-N	-5.28	113.84	122.54
2	B	382	LYS	C-N-CA	-5.28	113.84	122.54
2	B	361	MET	CG-SD-CE	5.27	112.50	100.90
1	A	139	PHE	CB-CA-C	-5.27	101.93	110.79
2	B	312	GLN	N-CA-C	-5.27	105.62	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	327	ILE	CB-CA-C	5.27	118.62	110.50
2	B	157	ILE	CA-C-N	5.26	125.67	119.99
2	B	157	ILE	C-N-CA	5.26	125.67	119.99
2	B	304	LEU	CA-C-O	-5.26	113.74	119.95
2	B	368	LYS	CA-C-N	-5.26	113.67	121.24
2	B	368	LYS	C-N-CA	-5.26	113.67	121.24
2	B	81	LEU	CA-C-N	-5.26	113.53	121.05
2	B	81	LEU	C-N-CA	-5.26	113.53	121.05
2	B	134	MET	CA-C-O	5.26	126.75	120.28
2	B	344	GLY	CA-C-O	5.26	126.13	119.72
2	B	89	ASN	N-CA-C	-5.25	105.25	110.97
2	B	318	SER	N-CA-C	5.25	118.47	111.75
1	A	139	PHE	CD1-CE1-CZ	-5.25	110.56	120.00
2	B	92	LEU	CB-CA-C	5.25	119.12	110.88
2	B	72	THR	OG1-CB-CG2	-5.25	98.81	109.30
2	B	132	ILE	CB-CA-C	-5.25	102.74	110.82
2	B	320	GLY	CA-C-O	5.24	126.26	119.44
1	A	221	SER	CA-C-O	5.24	126.10	120.55
2	B	387	VAL	CA-CB-CG1	5.23	119.30	110.40
2	B	57	THR	N-CA-C	-5.23	101.17	109.96
1	A	126	VAL	CB-CA-C	-5.22	101.47	110.65
2	B	220	GLU	CA-CB-CG	5.21	124.53	114.10
1	A	46	ASP	N-CA-CB	5.21	118.57	110.44
1	A	262	MET	CA-C-N	-5.21	111.94	121.52
1	A	262	MET	C-N-CA	-5.21	111.94	121.52
2	B	217	LEU	CA-C-N	-5.21	111.83	120.68
2	B	217	LEU	C-N-CA	-5.21	111.83	120.68
2	B	244	PHE	CD1-CG-CD2	5.21	126.41	118.60
2	B	70	ARG	CG-CD-NE	5.21	123.45	112.00
2	B	36	GLN	O-C-N	-5.20	115.46	122.43
2	B	197	TYR	N-CA-C	-5.20	105.77	113.16
2	B	261	GLY	CA-C-O	-5.20	111.53	120.57
2	B	357	HIS	CG-ND1-CE1	-5.20	100.47	109.30
2	B	247	ASP	CA-C-N	-5.19	110.90	121.18
2	B	247	ASP	C-N-CA	-5.19	110.90	121.18
1	A	232	ILE	N-CA-CB	-5.19	104.25	111.41
2	B	211	GLU	OE1-CD-OE2	-5.19	110.45	122.90
2	B	272	LYS	N-CA-CB	-5.18	102.91	110.53
1	A	4	TYR	CA-CB-CG	-5.18	104.57	113.90
2	B	340	CYS	CA-C-N	-5.18	111.88	120.68
2	B	340	CYS	C-N-CA	-5.18	111.88	120.68
1	A	13	ASP	CA-C-O	-5.18	114.40	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	149	ALA	N-CA-CB	-5.18	102.66	110.32
2	B	157	ILE	N-CA-C	5.17	113.63	107.73
2	B	64	ASN	CA-C-O	5.17	125.90	120.42
1	A	144	LEU	CB-CA-C	5.17	120.70	110.42
2	B	300	ILE	CB-CG1-CD1	-5.17	102.95	113.80
2	B	363	ARG	N-CA-CB	5.16	117.80	110.16
2	B	208	ILE	N-CA-C	-5.16	104.87	110.23
2	B	19	GLN	CA-C-N	-5.16	112.08	120.64
2	B	19	GLN	C-N-CA	-5.16	112.08	120.64
2	B	49	LEU	CB-CA-C	-5.16	102.08	110.85
2	B	288	GLN	CG-CD-OE1	-5.15	110.50	120.80
1	A	239	LYS	CB-CG-CD	-5.15	99.46	111.30
1	A	220	VAL	CA-CB-CG2	5.15	119.15	110.40
2	B	266	GLU	CA-C-N	5.14	130.29	122.11
2	B	266	GLU	C-N-CA	5.14	130.29	122.11
1	A	197	ILE	CG1-CB-CG2	-5.14	95.28	110.70
1	A	239	LYS	N-CA-C	5.14	117.62	111.71
2	B	7	PRO	N-CD-CG	-5.14	95.49	103.20
2	B	45	PHE	N-CA-C	-5.14	105.76	111.36
2	B	177	TRP	CE3-CZ3-CH2	5.14	127.78	121.10
2	B	226	ALA	O-C-N	5.14	129.42	123.41
2	B	199	THR	CA-C-O	-5.13	115.41	120.70
2	B	251	GLY	CA-C-N	-5.13	115.82	123.11
2	B	251	GLY	C-N-CA	-5.13	115.82	123.11
2	B	216	ILE	N-CA-C	5.13	117.51	111.09
1	A	167	ALA	CA-C-O	-5.12	114.99	120.42
2	B	149	MET	N-CA-C	-5.12	105.88	111.82
1	A	81	CYS	N-CA-C	-5.12	105.70	111.28
1	A	235	SER	CA-CB-OG	-5.11	100.88	111.10
2	B	296	GLU	N-CA-C	-5.11	102.19	110.32
2	B	324	TYR	CA-CB-CG	-5.11	104.70	113.90
2	B	371	LEU	N-CA-CB	-5.11	102.10	110.42
2	B	74	TYR	CZ-CE2-CD2	5.10	128.78	119.60
1	A	96	PRO	CA-CB-CG	-5.10	94.81	104.50
2	B	214	ALA	N-CA-C	-5.10	105.91	111.82
1	A	105	LEU	N-CA-C	-5.09	105.91	111.82
2	B	20	ILE	N-CA-C	-5.09	104.91	112.04
2	B	88	THR	N-CA-C	5.09	117.57	111.71
2	B	9	PHE	CG-CD2-CE2	-5.09	112.04	120.70
1	A	138	PRO	CA-CB-CG	-5.09	94.83	104.50
2	B	60	THR	CA-CB-OG1	-5.09	101.97	109.60
1	A	54	PHE	CA-C-O	-5.09	114.81	120.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111	ILE	CA-C-O	-5.09	114.91	120.96
2	B	359	LEU	CD1-CG-CD2	5.08	121.99	110.80
1	A	131	VAL	CG1-CB-CG2	-5.08	99.61	110.80
2	B	39	PRO	N-CD-CG	-5.08	95.58	103.20
2	B	313	HIS	CA-C-N	-5.08	113.47	120.28
2	B	313	HIS	C-N-CA	-5.08	113.47	120.28
2	B	187	MET	CB-CG-SD	-5.08	97.46	112.70
2	B	195	HIS	CB-CG-ND1	5.08	130.31	122.70
1	A	108	ASN	CA-C-N	-5.07	114.52	122.79
1	A	108	ASN	C-N-CA	-5.07	114.52	122.79
2	B	9	PHE	N-CA-CB	-5.07	102.60	110.87
2	B	91	VAL	N-CA-C	5.07	115.80	110.62
1	A	63	THR	O-C-N	5.07	127.57	122.09
1	A	237	ILE	N-CA-CB	-5.07	102.09	110.56
1	A	145	ARG	CD-NE-CZ	-5.07	117.30	124.40
2	B	210	GLU	N-CA-CB	-5.07	102.49	110.30
2	B	124	ALA	CA-C-N	5.07	127.07	120.28
2	B	124	ALA	C-N-CA	5.07	127.07	120.28
2	B	85	ALA	CB-CA-C	5.07	120.04	110.62
2	B	99	LYS	CA-CB-CG	-5.07	103.97	114.10
2	B	244	PHE	CB-CA-C	-5.06	101.64	110.09
2	B	275	ARG	CA-CB-CG	5.06	124.22	114.10
2	B	59	LEU	CD1-CG-CD2	5.05	121.92	110.80
2	B	338	THR	O-C-N	-5.05	116.77	122.12
2	B	212	THR	N-CA-C	-5.05	105.05	111.11
1	A	37	ILE	CB-CA-C	-5.05	105.48	112.24
1	A	48	LEU	CA-C-N	-5.05	115.87	122.99
1	A	48	LEU	C-N-CA	-5.05	115.87	122.99
2	B	351	SER	N-CA-C	-5.04	105.97	111.82
1	A	88	ILE	N-CA-C	-5.04	105.79	110.53
2	B	110	THR	CA-C-N	-5.04	111.53	121.41
2	B	110	THR	C-N-CA	-5.04	111.53	121.41
2	B	148	ARG	CB-CA-C	-5.04	102.42	110.79
2	B	195	HIS	CG-ND1-CE1	5.04	117.87	109.30
2	B	384	ILE	CA-CB-CG1	-5.04	101.84	110.40
1	A	169	TYR	CB-CG-CD1	5.04	128.36	120.80
2	B	331	GLU	CA-C-N	-5.04	113.14	120.29
2	B	331	GLU	C-N-CA	-5.04	113.14	120.29
2	B	113	GLY	N-CA-C	-5.03	108.06	114.85
1	A	159	ASP	N-CA-CB	5.03	117.27	110.38
2	B	114	GLN	CB-CA-C	-5.03	102.44	110.79
2	B	250	VAL	N-CA-C	5.03	115.92	108.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	22	MET	CA-C-N	-5.03	113.75	119.28
2	B	22	MET	C-N-CA	-5.03	113.75	119.28
2	B	372	LEU	N-CA-C	-5.03	100.71	108.90
1	A	104	ASN	CA-C-N	5.02	127.94	120.31
1	A	104	ASN	C-N-CA	5.02	127.94	120.31
2	B	46	ALA	N-CA-C	-5.02	105.81	111.28
2	B	38	ASP	N-CA-CB	5.02	119.31	110.37
2	B	78	GLU	CA-CB-CG	-5.02	104.06	114.10
2	B	74	TYR	CG-CD1-CE1	5.01	128.72	121.20
2	B	245	ILE	CA-C-O	-5.01	115.74	120.95
2	B	272	LYS	CG-CD-CE	-5.01	99.78	111.30
1	A	175	TYR	CA-C-N	-5.00	115.77	123.07
1	A	175	TYR	C-N-CA	-5.00	115.77	123.07
2	B	141	ARG	N-CA-CB	5.00	117.72	110.47
2	B	211	GLU	O-C-N	5.00	128.42	122.27
2	B	317	ASN	CB-CG-OD1	-5.00	110.80	120.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	267	ARG	Peptide
2	B	54	GLY	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1955	0	1961	89	0
2	B	2987	0	2964	252	0
3	A	17	0	11	1	0
4	B	1	0	0	0	0
5	B	15	0	7	1	0
6	A	129	0	0	2	0
6	B	248	0	0	2	0
All	All	5352	0	4943	339	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 34.

All (339) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:235:SER:CA	2:B:235:SER:CB	1.74	1.64
2:B:278:ILE:CG1	2:B:278:ILE:CD1	1.74	1.64
2:B:129:LYS:CD	2:B:129:LYS:CG	1.75	1.63
1:A:52:VAL:CB	1:A:52:VAL:CG1	1.75	1.63
1:A:126:VAL:CB	1:A:126:VAL:CG1	1.75	1.63
2:B:71:THR:CB	2:B:71:THR:CG2	1.77	1.63
2:B:37:LYS:CD	2:B:37:LYS:CG	1.75	1.62
1:A:87:LEU:CG	1:A:87:LEU:CD1	1.74	1.61
2:B:58:ALA:CA	2:B:58:ALA:CB	1.75	1.61
2:B:183:THR:CB	2:B:183:THR:CG2	1.74	1.61
1:A:140:ARG:CD	1:A:140:ARG:CG	1.76	1.60
2:B:231:VAL:CB	2:B:231:VAL:CG1	1.79	1.60
1:A:54:PHE:C	1:A:54:PHE:CA	1.75	1.59
2:B:117:VAL:CA	2:B:117:VAL:CB	1.75	1.59
2:B:66:THR:CB	2:B:66:THR:CG2	1.75	1.58
2:B:212:THR:CB	2:B:212:THR:CG2	1.77	1.58
1:A:13:ASP:CG	1:A:13:ASP:CB	1.76	1.58
2:B:25:LEU:CD2	2:B:25:LEU:CG	1.75	1.58
2:B:319:ILE:CB	2:B:319:ILE:CG2	1.75	1.58
2:B:353:HIS:CB	2:B:353:HIS:CA	1.77	1.58
2:B:49:LEU:CD2	2:B:49:LEU:CG	1.80	1.57
2:B:286:MET:CA	2:B:286:MET:CB	1.77	1.57
2:B:55:ARG:CD	2:B:55:ARG:CG	1.75	1.57
2:B:333:LEU:CD2	2:B:333:LEU:CG	1.75	1.57
2:B:351:SER:CA	2:B:351:SER:C	1.76	1.57
1:A:94:THR:CB	1:A:94:THR:CA	1.75	1.57
2:B:196:PRO:C	2:B:196:PRO:CA	1.77	1.57
2:B:282:MET:CB	2:B:282:MET:CA	1.77	1.57
2:B:59:LEU:C	2:B:59:LEU:CA	1.77	1.57
2:B:76:LYS:CE	2:B:76:LYS:CD	1.77	1.57
2:B:287:MET:CG	2:B:287:MET:CB	1.76	1.57
1:A:101:MET:CG	1:A:101:MET:CB	1.76	1.56
2:B:61:LYS:CG	2:B:61:LYS:CB	1.84	1.56
2:B:339:LEU:CD2	2:B:339:LEU:CG	1.80	1.56
2:B:150:ARG:CG	2:B:150:ARG:CB	1.74	1.56
2:B:264:THR:CB	2:B:264:THR:CG2	1.75	1.56
1:A:123:VAL:CB	1:A:123:VAL:CA	1.76	1.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:VAL:CG2	1:A:166:VAL:CB	1.77	1.55
2:B:139:VAL:CB	2:B:139:VAL:CG2	1.79	1.55
2:B:205:GLN:CD	2:B:205:GLN:CG	1.80	1.55
1:A:7:LEU:CD2	1:A:7:LEU:CG	1.78	1.54
1:A:219:GLN:CG	1:A:219:GLN:CB	1.82	1.54
2:B:203:GLU:CA	2:B:203:GLU:C	1.77	1.54
2:B:59:LEU:CA	2:B:59:LEU:N	1.71	1.54
2:B:108:ALA:CB	2:B:108:ALA:CA	1.78	1.54
2:B:256:GLU:CG	2:B:256:GLU:CD	1.76	1.54
2:B:373:VAL:CB	2:B:373:VAL:CG1	1.82	1.53
2:B:23:PRO:CG	2:B:23:PRO:CB	1.80	1.53
2:B:328:THR:C	2:B:328:THR:CA	1.77	1.53
2:B:368:LYS:C	2:B:368:LYS:CA	1.75	1.53
1:A:117:ARG:CG	1:A:117:ARG:CD	1.82	1.52
1:A:24:THR:CB	1:A:24:THR:CA	1.75	1.52
2:B:304:LEU:CD1	2:B:304:LEU:CG	1.83	1.52
2:B:255:VAL:CA	2:B:255:VAL:CB	1.80	1.52
2:B:70:ARG:C	2:B:70:ARG:CA	1.81	1.51
2:B:61:LYS:N	2:B:61:LYS:CA	1.72	1.50
2:B:167:LYS:CE	2:B:167:LYS:NZ	1.71	1.50
2:B:376:LEU:CG	2:B:376:LEU:CD2	1.84	1.49
2:B:362:MET:SD	2:B:362:MET:CG	2.01	1.49
2:B:15:MET:CE	2:B:15:MET:SD	2.02	1.47
2:B:282:MET:CG	2:B:282:MET:SD	2.02	1.45
2:B:149:MET:SD	2:B:149:MET:CG	2.07	1.40
2:B:286:MET:CB	2:B:286:MET:CG	2.04	1.35
1:A:191:LEU:HD12	1:A:192:PRO:CD	1.85	1.06
1:A:191:LEU:CD1	1:A:192:PRO:HD2	1.86	1.04
1:A:243:LYS:HD2	1:A:243:LYS:N	1.74	1.03
2:B:134:MET:CE	2:B:139:VAL:HG22	1.89	1.02
2:B:134:MET:HE3	2:B:139:VAL:CG2	1.88	1.02
1:A:194:HIS:O	1:A:198:GLU:HG2	1.63	0.98
2:B:376:LEU:CD2	2:B:376:LEU:CB	2.43	0.97
2:B:183:THR:CG2	2:B:183:THR:CA	2.41	0.97
2:B:71:THR:CG2	2:B:71:THR:CA	2.44	0.95
2:B:333:LEU:CD2	2:B:333:LEU:CB	2.46	0.94
1:A:7:LEU:CD2	1:A:7:LEU:CB	2.46	0.94
1:A:243:LYS:HD2	1:A:243:LYS:H	1.27	0.94
2:B:282:MET:CG	2:B:282:MET:CE	2.47	0.93
1:A:126:VAL:CG1	1:A:126:VAL:CG2	2.47	0.92
2:B:134:MET:HE3	2:B:139:VAL:HG22	0.95	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:282:MET:CA	2:B:282:MET:CG	2.46	0.92
2:B:319:ILE:CG2	2:B:319:ILE:CG1	2.46	0.92
2:B:59:LEU:N	2:B:59:LEU:CB	2.33	0.90
1:A:54:PHE:C	1:A:54:PHE:CB	2.46	0.89
2:B:333:LEU:CD2	2:B:333:LEU:CD1	2.50	0.89
1:A:24:THR:CA	1:A:24:THR:CG2	2.49	0.89
2:B:61:LYS:CB	2:B:61:LYS:N	2.36	0.88
2:B:256:GLU:CD	2:B:256:GLU:CB	2.47	0.87
2:B:25:LEU:CD2	2:B:25:LEU:CD1	2.52	0.87
1:A:215:SER:H	1:A:219:GLN:HE22	1.17	0.86
2:B:373:VAL:CG1	2:B:373:VAL:CG2	2.54	0.86
1:A:52:VAL:CG1	1:A:52:VAL:CG2	2.54	0.86
2:B:373:VAL:CG1	2:B:373:VAL:CA	2.53	0.86
1:A:140:ARG:CD	1:A:140:ARG:CB	2.54	0.84
1:A:215:SER:H	1:A:219:GLN:NE2	1.74	0.84
2:B:297:SER:HB3	2:B:305:ASP:OD1	1.78	0.84
2:B:304:LEU:CD1	2:B:304:LEU:CD2	2.54	0.84
1:A:156:PRO:O	1:A:191:LEU:HB3	1.78	0.84
2:B:339:LEU:CD2	2:B:339:LEU:CD1	2.56	0.84
1:A:94:THR:CB	1:A:94:THR:C	2.51	0.84
1:A:140:ARG:CG	1:A:140:ARG:NE	2.40	0.83
2:B:112:ALA:HB2	2:B:302:ALA:HB1	1.60	0.83
2:B:282:MET:CB	2:B:282:MET:SD	2.66	0.83
2:B:55:ARG:CD	2:B:55:ARG:CB	2.57	0.83
2:B:61:LYS:CG	2:B:61:LYS:CA	2.56	0.83
2:B:286:MET:CB	2:B:286:MET:SD	2.66	0.83
2:B:212:THR:CG2	2:B:212:THR:CA	2.57	0.82
2:B:255:VAL:CA	2:B:255:VAL:CG1	2.58	0.82
2:B:222:ARG:NH2	6:B:736:HOH:O	2.13	0.81
2:B:353:HIS:CB	2:B:353:HIS:C	2.53	0.81
2:B:203:GLU:C	2:B:203:GLU:CB	2.53	0.81
1:A:7:LEU:CD2	1:A:7:LEU:CD1	2.58	0.81
2:B:60:THR:C	2:B:61:LYS:CA	2.53	0.81
1:A:191:LEU:HD12	1:A:192:PRO:HD2	0.91	0.81
2:B:58:ALA:CB	2:B:58:ALA:N	2.45	0.80
2:B:368:LYS:CA	2:B:369:GLU:N	2.44	0.80
1:A:123:VAL:CA	1:A:123:VAL:CG1	2.59	0.80
2:B:362:MET:CG	2:B:362:MET:CE	2.59	0.79
2:B:264:THR:CG2	2:B:264:THR:CA	2.60	0.79
2:B:134:MET:HE1	2:B:146:VAL:HG22	1.65	0.78
1:A:87:LEU:CD1	1:A:87:LEU:CD2	2.61	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:368:LYS:CA	2:B:368:LYS:O	2.32	0.78
1:A:126:VAL:CG1	1:A:126:VAL:CA	2.62	0.78
2:B:362:MET:SD	2:B:362:MET:CB	2.71	0.78
1:A:52:VAL:CG1	1:A:52:VAL:CA	2.62	0.78
2:B:66:THR:CG2	2:B:66:THR:CA	2.62	0.78
2:B:353:HIS:CA	2:B:353:HIS:CG	2.66	0.78
2:B:328:THR:C	2:B:328:THR:CB	2.57	0.78
2:B:203:GLU:C	2:B:203:GLU:N	2.39	0.77
2:B:231:VAL:CG1	2:B:231:VAL:CA	2.62	0.77
2:B:339:LEU:CD2	2:B:339:LEU:CB	2.61	0.77
2:B:231:VAL:CG1	2:B:231:VAL:CG2	2.60	0.77
1:A:239:LYS:O	1:A:243:LYS:HD3	1.85	0.77
2:B:297:SER:C	2:B:305:ASP:OD1	2.28	0.76
2:B:287:MET:HG3	2:B:307:PRO:CB	2.16	0.75
1:A:54:PHE:C	1:A:54:PHE:N	2.44	0.74
2:B:351:SER:CA	2:B:352:SER:N	2.48	0.74
2:B:58:ALA:C	2:B:59:LEU:CA	2.59	0.74
1:A:101:MET:CG	1:A:101:MET:CA	2.64	0.74
1:A:239:LYS:O	1:A:243:LYS:CD	2.36	0.74
2:B:70:ARG:CA	2:B:71:THR:N	2.49	0.74
2:B:76:LYS:CE	2:B:76:LYS:CG	2.64	0.74
1:A:94:THR:CA	1:A:94:THR:CG2	2.64	0.73
2:B:117:VAL:CA	2:B:117:VAL:CG2	2.64	0.73
2:B:255:VAL:CA	2:B:255:VAL:CG2	2.67	0.73
2:B:15:MET:CE	2:B:15:MET:CG	2.66	0.73
2:B:49:LEU:CD2	2:B:49:LEU:CD1	2.66	0.73
1:A:123:VAL:CB	1:A:123:VAL:N	2.53	0.72
2:B:139:VAL:CG2	2:B:139:VAL:CG1	2.64	0.72
2:B:149:MET:SD	2:B:149:MET:CB	2.77	0.72
2:B:255:VAL:CB	2:B:255:VAL:C	2.62	0.72
2:B:278:ILE:CD1	2:B:278:ILE:CB	2.66	0.72
2:B:37:LYS:CD	2:B:37:LYS:CB	2.68	0.72
1:A:24:THR:CB	1:A:24:THR:C	2.62	0.72
2:B:54:GLY:O	6:B:735:HOH:O	2.06	0.72
2:B:61:LYS:CB	2:B:61:LYS:CD	2.68	0.72
1:A:166:VAL:CG2	1:A:166:VAL:CG1	2.66	0.72
2:B:376:LEU:CD2	2:B:376:LEU:CD1	2.68	0.72
2:B:328:THR:CA	2:B:329:ASP:N	2.49	0.71
1:A:166:VAL:CG2	1:A:166:VAL:CA	2.68	0.71
2:B:235:SER:CB	2:B:235:SER:C	2.64	0.70
2:B:235:SER:CB	2:B:235:SER:N	2.53	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:212:THR:CG2	2:B:212:THR:OG1	2.39	0.70
2:B:150:ARG:CG	2:B:150:ARG:CA	2.69	0.69
2:B:255:VAL:CB	2:B:255:VAL:N	2.52	0.69
2:B:286:MET:CB	2:B:286:MET:N	2.55	0.69
2:B:304:LEU:CD1	2:B:304:LEU:CB	2.69	0.69
1:A:24:THR:CA	1:A:24:THR:OG1	2.41	0.69
1:A:219:GLN:CB	1:A:219:GLN:CD	2.67	0.68
2:B:134:MET:HE1	2:B:146:VAL:CG2	2.23	0.68
2:B:282:MET:CB	2:B:282:MET:C	2.66	0.68
2:B:196:PRO:CA	2:B:197:TYR:N	2.52	0.68
2:B:203:GLU:CA	2:B:203:GLU:O	2.41	0.67
2:B:351:SER:CA	2:B:351:SER:O	2.38	0.67
2:B:287:MET:CG	2:B:307:PRO:CB	2.72	0.67
2:B:70:ARG:CA	2:B:70:ARG:O	2.38	0.67
1:A:123:VAL:CA	1:A:123:VAL:CG2	2.70	0.67
2:B:59:LEU:CA	2:B:59:LEU:O	2.42	0.66
2:B:386:THR:O	2:B:390:ILE:HD12	1.95	0.66
2:B:206[B]:ARG:NH2	2:B:243:ASP:OD1	2.28	0.66
2:B:117:VAL:CB	2:B:117:VAL:N	2.57	0.66
2:B:351:SER:C	2:B:351:SER:N	2.51	0.65
2:B:11:GLU:HG2	2:B:11:GLU:O	1.94	0.65
1:A:60:ASP:OD1	3:A:501:IAG:N1	2.29	0.65
2:B:177:TRP:N	2:B:178:PRO:CD	2.59	0.65
2:B:328:THR:CA	2:B:328:THR:O	2.40	0.65
1:A:58:LEU:C	1:A:58:LEU:HD12	2.23	0.64
2:B:353:HIS:CB	2:B:353:HIS:N	2.60	0.64
2:B:319:ILE:HD13	2:B:319:ILE:HG21	1.80	0.64
2:B:143:SER:N	2:B:144:PRO:CD	2.61	0.64
2:B:286:MET:CB	2:B:286:MET:C	2.69	0.63
2:B:66:THR:CG2	2:B:66:THR:OG1	2.45	0.63
2:B:70:ARG:C	2:B:70:ARG:CB	2.71	0.63
2:B:327:ILE:HG23	2:B:331:GLU:HB2	1.80	0.63
2:B:206[A]:ARG:HD2	2:B:210:GLU:OE2	1.99	0.63
2:B:58:ALA:CB	2:B:58:ALA:C	2.73	0.62
2:B:55:ARG:CG	2:B:55:ARG:NE	2.63	0.62
2:B:196:PRO:CA	2:B:196:PRO:O	2.45	0.62
2:B:117:VAL:CB	2:B:117:VAL:C	2.62	0.62
2:B:38:ASP:OD1	2:B:38:ASP:C	2.40	0.61
2:B:287:MET:CG	2:B:307:PRO:HA	2.30	0.61
1:A:24:THR:CB	1:A:24:THR:N	2.62	0.61
2:B:25:LEU:CD2	2:B:25:LEU:CB	2.69	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:76:LYS:CD	2:B:76:LYS:NZ	2.61	0.60
1:A:123:VAL:CB	1:A:123:VAL:C	2.68	0.60
2:B:134:MET:O	2:B:158:PRO:HA	2.02	0.60
2:B:287:MET:CB	2:B:287:MET:SD	2.88	0.60
1:A:194:HIS:O	1:A:198:GLU:CG	2.47	0.59
2:B:287:MET:CG	2:B:307:PRO:CA	2.80	0.59
2:B:264:THR:CG2	2:B:264:THR:OG1	2.46	0.58
1:A:177:LEU:HD11	1:A:212:PHE:CD2	2.38	0.58
2:B:287:MET:HG3	2:B:307:PRO:HB3	1.86	0.58
1:A:87:LEU:CD1	1:A:87:LEU:CB	2.78	0.58
1:A:239:LYS:O	1:A:243:LYS:HD2	2.04	0.58
1:A:54:PHE:CA	1:A:55:SER:N	2.62	0.58
1:A:234:GLY:O	1:A:235:SER:C	2.42	0.57
2:B:112:ALA:CB	2:B:302:ALA:HB1	2.32	0.57
1:A:16:GLU:HG3	6:A:566:HOH:O	2.05	0.57
2:B:59:LEU:C	2:B:59:LEU:N	2.61	0.57
2:B:59:LEU:CA	2:B:60:THR:N	2.56	0.57
2:B:139:VAL:CG2	2:B:139:VAL:CA	2.78	0.57
1:A:117:ARG:CD	1:A:117:ARG:CB	2.74	0.56
1:A:211:GLY:O	1:A:212:PHE:HB2	2.04	0.56
2:B:87:LYS:HD2	2:B:114:GLN:HG3	1.87	0.56
2:B:108:ALA:CB	2:B:108:ALA:C	2.71	0.56
2:B:255:VAL:CG1	2:B:255:VAL:C	2.78	0.56
2:B:287:MET:HG3	2:B:307:PRO:CA	2.36	0.56
2:B:333:LEU:CD2	2:B:333:LEU:HB3	2.36	0.55
1:A:100:LEU:C	1:A:100:LEU:HD13	2.31	0.55
2:B:287:MET:HB2	2:B:307:PRO:HB2	1.88	0.55
1:A:156:PRO:HA	1:A:196:LEU:HD21	1.89	0.55
2:B:319:ILE:CG2	2:B:319:ILE:CD1	2.84	0.55
2:B:203:GLU:CA	2:B:204:PHE:N	2.58	0.55
2:B:287:MET:HG3	2:B:307:PRO:HA	1.88	0.55
2:B:362:MET:HB3	2:B:362:MET:HE2	1.89	0.55
1:A:242:GLU:CD	1:A:243:LYS:HZ1	2.15	0.54
1:A:16:GLU:CG	6:A:566:HOH:O	2.56	0.54
2:B:134:MET:O	2:B:159:VAL:N	2.41	0.53
2:B:328:THR:C	2:B:328:THR:N	2.59	0.53
2:B:297:SER:CB	2:B:305:ASP:OD1	2.53	0.53
2:B:142:GLN:C	2:B:144:PRO:HD2	2.33	0.53
2:B:61:LYS:N	2:B:61:LYS:C	2.57	0.53
2:B:205:GLN:CG	2:B:205:GLN:OE1	2.51	0.53
2:B:129:LYS:CD	2:B:129:LYS:CB	2.77	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:32:PHE:CD1	2:B:200:ILE:HG12	2.44	0.52
2:B:373:VAL:CG1	2:B:373:VAL:C	2.82	0.52
2:B:287:MET:HG2	2:B:307:PRO:HA	1.91	0.52
2:B:287:MET:HG2	2:B:307:PRO:CA	2.39	0.51
2:B:286:MET:CA	2:B:286:MET:HB2	2.18	0.51
1:A:125:SER:HB2	1:A:151:ILE:HG12	1.91	0.51
2:B:111:GLY:O	2:B:138:ASP:HB3	2.10	0.51
2:B:117:VAL:HG23	2:B:117:VAL:H	1.76	0.51
2:B:319:ILE:CG2	2:B:319:ILE:CA	2.78	0.51
2:B:206[A]:ARG:CD	2:B:210:GLU:OE2	2.57	0.50
1:A:243:LYS:H	1:A:243:LYS:CD	2.11	0.50
2:B:143:SER:N	2:B:144:PRO:HD2	2.26	0.50
2:B:362:MET:CB	2:B:362:MET:HE2	2.42	0.50
1:A:220:VAL:CG2	1:A:262:MET:HE3	2.42	0.50
2:B:85:ALA:HA	2:B:377:SER:O	2.10	0.50
1:A:123:VAL:CG1	1:A:123:VAL:C	2.86	0.49
2:B:177:TRP:N	2:B:178:PRO:HD3	2.25	0.49
1:A:263:LYS:O	1:A:266:SER:OG	2.26	0.49
2:B:129:LYS:CG	2:B:129:LYS:CE	2.83	0.49
2:B:297:SER:O	2:B:305:ASP:OD1	2.31	0.49
2:B:150:ARG:CB	2:B:150:ARG:CD	2.81	0.49
2:B:205:GLN:CD	2:B:205:GLN:CB	2.75	0.48
2:B:255:VAL:C	2:B:255:VAL:HG12	2.39	0.48
2:B:319:ILE:CG2	2:B:319:ILE:HD13	2.40	0.48
1:A:125:SER:HB2	1:A:151:ILE:CG1	2.44	0.48
2:B:62:CYS:SG	2:B:75:LEU:HG	2.54	0.47
2:B:87:LYS:HD2	2:B:114:GLN:CG	2.44	0.47
2:B:286:MET:CA	2:B:286:MET:HB3	2.18	0.47
2:B:87:LYS:NZ	5:B:502:PLP:O3	2.47	0.47
2:B:70:ARG:C	2:B:70:ARG:N	2.57	0.47
1:A:148:ILE:HD12	1:A:148:ILE:HG23	1.54	0.47
2:B:59:LEU:HD12	2:B:59:LEU:HA	1.67	0.47
1:A:22:PHE:CD1	1:A:22:PHE:C	2.92	0.47
2:B:115:HIS:CE1	2:B:189:GLY:HA2	2.50	0.47
2:B:381:ASP:O	2:B:384:ILE:HG12	2.15	0.47
2:B:227:VAL:C	2:B:228:ILE:HG13	2.39	0.46
2:B:364:GLU:C	2:B:365:GLN:CG	2.88	0.46
1:A:127:LEU:HD23	1:A:128:VAL:N	2.30	0.46
2:B:203:GLU:N	2:B:204:PHE:N	2.64	0.46
1:A:132:PRO:HD3	2:B:17:VAL:O	2.15	0.46
2:B:300:ILE:HB	2:B:329:ASP:CG	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:333:LEU:CD2	2:B:333:LEU:HD13	2.44	0.46
1:A:76:VAL:HA	1:A:80:GLN:OE1	2.16	0.45
1:A:216:SER:H	1:A:219:GLN:HE21	1.63	0.45
2:B:279:TYR:CG	2:B:280:PHE:N	2.83	0.45
2:B:117:VAL:CA	2:B:117:VAL:CG1	2.85	0.45
2:B:362:MET:CE	2:B:362:MET:CB	2.91	0.45
2:B:22:MET:HB3	2:B:22:MET:HE3	1.66	0.45
2:B:368:LYS:C	2:B:368:LYS:N	2.66	0.45
2:B:255:VAL:CG2	2:B:255:VAL:N	2.78	0.45
2:B:112:ALA:HB2	2:B:302:ALA:CB	2.39	0.45
2:B:173:ALA:HB1	2:B:186:TYR:CE1	2.51	0.45
2:B:71:THR:CG2	2:B:71:THR:C	2.90	0.44
2:B:287:MET:CG	2:B:307:PRO:HB2	2.47	0.44
2:B:263:GLU:H	2:B:263:GLU:CD	2.26	0.44
2:B:319:ILE:HG21	2:B:319:ILE:CD1	2.43	0.44
1:A:55:SER:HB3	2:B:293:GLN:HB3	1.99	0.44
2:B:264:THR:CG2	2:B:264:THR:N	2.81	0.43
2:B:272:LYS:HD3	2:B:324:TYR:HB2	2.00	0.43
2:B:287:MET:HG2	2:B:307:PRO:O	2.18	0.43
2:B:279:TYR:CD1	2:B:280:PHE:N	2.84	0.43
2:B:364:GLU:C	2:B:365:GLN:HG3	2.43	0.43
1:A:95:ILE:HG21	1:A:95:ILE:HD13	1.64	0.43
2:B:157:ILE:HA	2:B:158:PRO:HD3	1.42	0.43
1:A:157:ASN:OD1	1:A:157:ASN:C	2.61	0.43
2:B:117:VAL:CG2	2:B:117:VAL:N	2.82	0.43
1:A:219:GLN:CG	1:A:219:GLN:CA	2.89	0.43
2:B:282:MET:CG	2:B:282:MET:C	2.90	0.43
2:B:349:LEU:HD23	2:B:349:LEU:HA	1.90	0.43
1:A:193:LEU:HA	1:A:193:LEU:HD23	1.51	0.42
2:B:176:ASP:C	2:B:178:PRO:HD2	2.44	0.42
2:B:231:VAL:CG1	2:B:231:VAL:C	2.92	0.42
2:B:176:ASP:C	2:B:176:ASP:OD1	2.63	0.42
1:A:54:PHE:C	1:A:54:PHE:CG	2.96	0.42
1:A:140:ARG:HH11	1:A:140:ARG:HD3	0.88	0.42
2:B:70:ARG:N	2:B:71:THR:N	2.67	0.42
2:B:301:SER:OG	2:B:350:GLU:HG3	2.19	0.42
2:B:80:LEU:HD23	2:B:80:LEU:HA	1.66	0.42
2:B:79:ASP:HB2	2:B:379:ARG:HB3	2.02	0.41
2:B:97:LEU:HD23	2:B:97:LEU:HA	2.00	0.41
1:A:85:LEU:HD23	1:A:85:LEU:HA	1.95	0.41
2:B:57:THR:OG1	2:B:76:LYS:HE3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:THR:CG2	1:A:24:THR:C	2.93	0.41
1:A:216:SER:HA	1:A:217:PRO:HD3	1.91	0.41
2:B:174:LEU:HA	2:B:174:LEU:HD23	1.73	0.41
1:A:126:VAL:CG1	1:A:126:VAL:C	2.94	0.41
1:A:30:ILE:HD11	1:A:76:VAL:HG22	2.03	0.41
2:B:282:MET:C	2:B:282:MET:HG3	2.46	0.41
2:B:368:LYS:C	2:B:368:LYS:CB	2.78	0.41
2:B:133:TYR:HA	2:B:157:ILE:O	2.21	0.41
2:B:373:VAL:C	2:B:373:VAL:HG12	2.46	0.41
2:B:167:LYS:O	2:B:170:CYS:HB2	2.21	0.41
2:B:71:THR:CG2	2:B:71:THR:OG1	2.61	0.40
2:B:202:ARG:HH11	2:B:202:ARG:HD3	1.48	0.40
2:B:66:THR:HA	2:B:362:MET:SD	2.61	0.40
2:B:351:SER:N	2:B:352:SER:N	2.65	0.40
2:B:59:LEU:C	2:B:59:LEU:CB	2.73	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	255/268 (95%)	250 (98%)	3 (1%)	2 (1%)	16	5
2	B	393/396 (99%)	371 (94%)	20 (5%)	2 (0%)	24	12
All	All	648/664 (98%)	621 (96%)	23 (4%)	4 (1%)	21	9

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	191	LEU
1	A	234	GLY
2	B	117	VAL

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Mol	Chain	Res	Type
2	B	139	VAL

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 X-ray entries followed by that with respect to entries of similar resolution.

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	203/208 (98%)	192 (95%)	11 (5%)	20	6
2	B	309/310 (100%)	294 (95%)	15 (5%)	22	8
All	All	512/518 (99%)	486 (95%)	26 (5%)	21	7

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	30	ILE
1	A	37	ILE
1	A	78	PRO
1	A	100	LEU
1	A	112	ASP
1	A	121	VAL
1	A	193	LEU
1	A	196	LEU
1	A	247	SER
1	A	248	PRO
2	B	2	THR
2	B	65	ILE
2	B	69	THR
2	B	141	ARG
2	B	143	SER
2	B	161	SER
2	B	176	ASP
2	B	207	MET
2	B	216	ILE
2	B	228	ILE
2	B	297	SER

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Mol	Chain	Res	Type
2	B	347	PRO
2	B	351	SER
2	B	390	ILE
2	B	394	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	109	ASN
1	A	165	GLN
1	A	204	HIS
1	A	219	GLN
2	B	246	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	IAG	A	501	-	18,18,18	2.63	9 (50%)	24,24,24	6.69	14 (58%)
5	PLP	B	502	2	15,15,16	3.71	12 (80%)	21,22,23	2.93	6 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	IAG	A	501	-	-	2/9/9/9	0/2/2/2
5	PLP	B	502	2	-	0/6/6/8	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	502	PLP	P-O4P	-6.92	1.38	1.60
5	B	502	PLP	C2A-C2	6.04	1.59	1.50
3	A	501	IAG	C7-C2	-5.66	1.34	1.44
5	B	502	PLP	C3-C2	-5.57	1.35	1.41
5	B	502	PLP	P-O3P	-4.47	1.38	1.54
3	A	501	IAG	O1-C10	4.18	1.31	1.23
3	A	501	IAG	C9-C2	-4.15	1.45	1.50
5	B	502	PLP	C5A-C5	4.10	1.61	1.50
5	B	502	PLP	C5-C4	3.96	1.45	1.40
3	A	501	IAG	O2-C12	3.73	1.34	1.22
3	A	501	IAG	C3-C7	-3.18	1.35	1.39
5	B	502	PLP	O4P-C5A	3.07	1.56	1.44
3	A	501	IAG	C1-C2	2.92	1.41	1.36
5	B	502	PLP	C2-N1	2.78	1.38	1.33
3	A	501	IAG	C9-C10	-2.42	1.48	1.51
5	B	502	PLP	C3-C4	-2.41	1.35	1.40
3	A	501	IAG	C6-C8	2.25	1.43	1.39
3	A	501	IAG	C8-N1	-2.17	1.34	1.37
5	B	502	PLP	P-O1P	2.08	1.56	1.50
5	B	502	PLP	C6-C5	-2.06	1.33	1.37
5	B	502	PLP	O3-C3	2.01	1.41	1.36

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	IAG	C8-N1-C1	18.16	125.24	109.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	IAG	C2-C1-N1	-15.45	93.35	110.31
3	A	501	IAG	C7-C8-N1	-11.99	97.53	107.52
3	A	501	IAG	C7-C2-C1	9.54	115.92	106.16
3	A	501	IAG	C6-C8-N1	9.16	145.41	130.74
5	B	502	PLP	O4P-C5A-C5	8.43	125.17	109.36
3	A	501	IAG	C9-C2-C1	-7.20	117.00	126.84
5	B	502	PLP	O3P-P-O4P	7.06	125.09	106.67
3	A	501	IAG	C6-C8-C7	-5.46	116.91	122.19
3	A	501	IAG	C11-N2-C10	-4.59	108.22	121.49
3	A	501	IAG	C4-C5-C6	-4.36	114.86	120.24
5	B	502	PLP	C4A-C4-C5	-4.30	116.50	120.94
3	A	501	IAG	C9-C10-N2	-3.78	111.29	116.25
3	A	501	IAG	O3-C12-O2	3.65	132.73	123.33
5	B	502	PLP	O4P-P-O1P	-3.64	96.60	106.44
3	A	501	IAG	C12-C11-N2	-3.54	102.06	113.06
3	A	501	IAG	C5-C4-C3	3.03	123.97	120.24
3	A	501	IAG	C5-C6-C8	2.61	124.00	118.69
5	B	502	PLP	C4A-C4-C3	2.47	124.64	120.52
5	B	502	PLP	O2P-P-O4P	-2.01	101.44	106.67

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	IAG	N2-C10-C9-C2
3	A	501	IAG	O1-C10-C9-C2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	IAG	1	0
5	B	502	PLP	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	6
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	65:ILE	C	66:THR	N	1.19
1	B	321:ARG	C	322:ALA	N	1.19
1	B	332:ALA	C	333:LEU	N	1.19
1	B	343:GLU	C	344:GLY	N	1.19
1	B	362:MET	C	363:ARG	N	1.19
1	B	368:LYS	C	369:GLU	N	1.19
1	A	232:ILE	C	233:SER	N	1.18

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	257/268 (95%)	0.26	10 (3%)	43 47	13, 26, 48, 78	2 (0%)
2	B	394/396 (99%)	0.15	22 (5%)	30 33	11, 19, 42, 73	1 (0%)
All	All	651/664 (98%)	0.19	32 (4%)	35 38	11, 22, 44, 78	3 (0%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	159	VAL	6.5
1	A	268	ALA	5.5
2	B	395	GLY	4.7
1	A	190	ALA	4.2
2	B	385	PHE	3.9
2	B	135	GLY	3.8
2	B	112	ALA	3.7
2	B	306	PHE	3.3
1	A	194	HIS	3.2
2	B	136	ALA	3.1
2	B	157	ILE	3.0
2	B	164	ALA	2.9
1	A	109	ASN	2.9
1	A	1	MET	2.9
1	A	192	PRO	2.9
2	B	165	THR	2.8
2	B	158	PRO	2.8
2	B	138	ASP	2.8
2	B	297	SER	2.8
2	B	62	CYS	2.7
1	A	191	LEU	2.6
1	A	212	PHE	2.6
2	B	160	HIS	2.6
2	B	169	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	393	ALA	2.5
2	B	142	GLN	2.5
1	A	246	ALA	2.4
1	A	156	PRO	2.4
2	B	139	VAL	2.3
2	B	133	TYR	2.2
2	B	145	ASN	2.1
2	B	111	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	IAG	A	501	17/17	0.84	0.10	22,35,50,52	0
5	PLP	B	502	15/16	0.98	0.06	15,18,28,30	0
4	NA	B	503	1/1	0.99	0.06	17,17,17,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.