



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 05:48 PM UTC

PDB ID : 1TWA / pdb_00001twa
Title : RNA polymerase II complexed with ATP
Authors : Westover, K.D.; Bushnell, D.A.; Kornberg, R.D.
Deposited on : 2004-06-30
Resolution : 3.20 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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

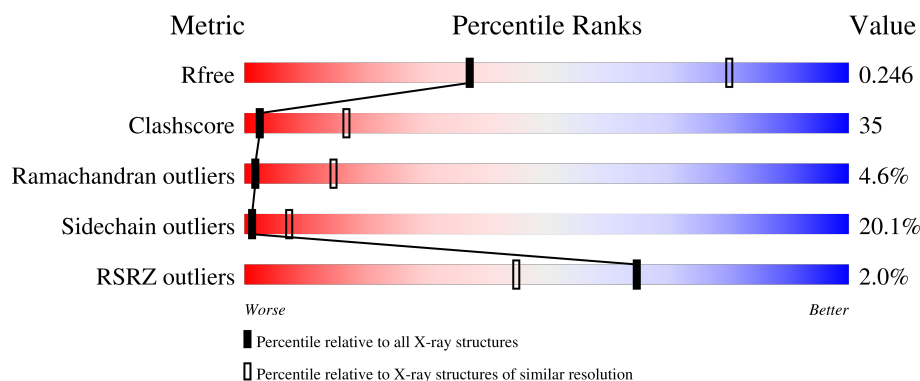
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	1733	5% 39% 25% 9% 22%
2	B	1224	2% 8% 42% 29% 10% 11%
3	C	318	5% 39% 30% 9% 16%
4	E	215	7% 40% 36% 16%
5	F	155	• 26% 16% 8% 46%

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Mol	Chain	Length	Quality of chain
6	H	146	
7	I	122	
8	J	70	
9	K	120	
10	L	70	

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
12	ZN	C	3002	-	-	X	-
12	ZN	J	3001	-	-	X	-
12	ZN	L	3005	-	-	X	-

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 27757 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 DNA-directed RNA polymerase II largest subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1352	Total	C	N	O	S	0	0	0
			10635	6711	1842	2024	58			

- Molecule 2 is a protein called DNA-directed RNA polymerase II 140 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1091	Total	C	N	O	S	0	0	0
			8690	5511	1516	1610	53			

- Molecule 3 is a protein called DNA-directed RNA polymerase II 45 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	266	Total	C	N	O	S	0	0	0
			2095	1317	348	417	13			

- Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	215	Total	C	N	O	S	0	0	0
			1760	1116	310	322	12			

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	83	Total	C	N	O	S	0	0	0
			670	428	114	125	3			

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	133	Total	C	N	O	S	0	0	0
			1068	673	180	211	4			

- Molecule 7 is a protein called DNA-directed RNA polymerase II 14.2 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	121	Total	C	N	O	S	0	0	0
			990	610	181	188	11			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III 8.3 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	J	64	Total	C	N	O	S	0	0	0
			525	334	92	93	6			

- Molecule 9 is a protein called DNA-directed RNA polymerase II 13.6 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	K	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	L	46	Total	C	N	O	S	0	0	0
			364	224	72	64	4			

- Molecule 11 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	2	Total	Mn	0	0
			2	2		

- Molecule 12 is ZINC ION (CCD ID: ZN) (formula: Zn).

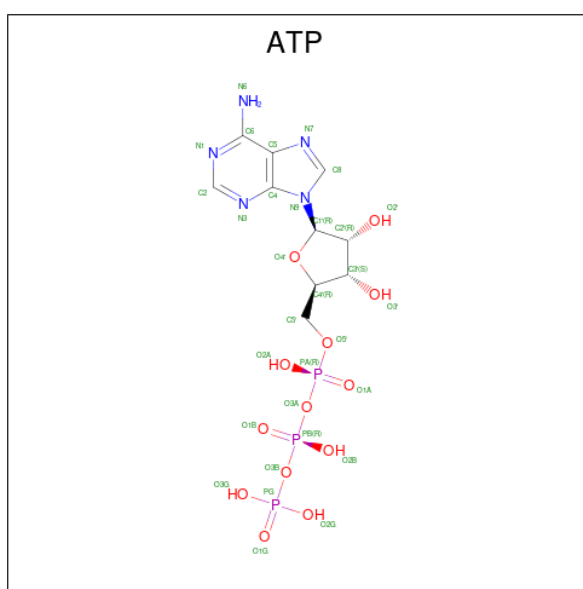
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	2	Total	Zn	0	0
			2	2		
12	B	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	C	1	Total	Zn	0	0
			1	1		
12	I	2	Total	Zn	0	0
			2	2		
12	J	1	Total	Zn	0	0
			1	1		
12	L	1	Total	Zn	0	0
			1	1		

- Molecule 13 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

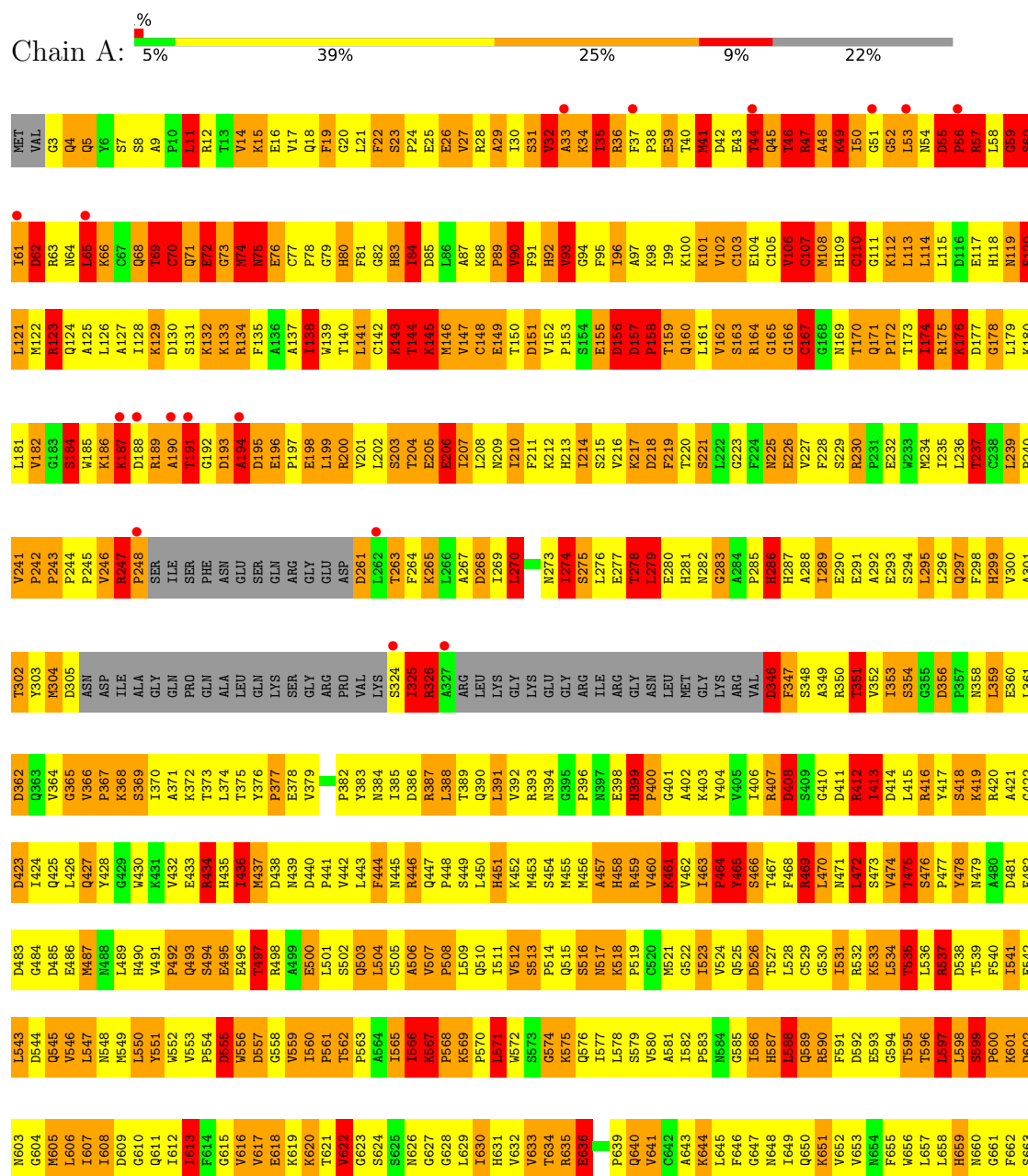


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

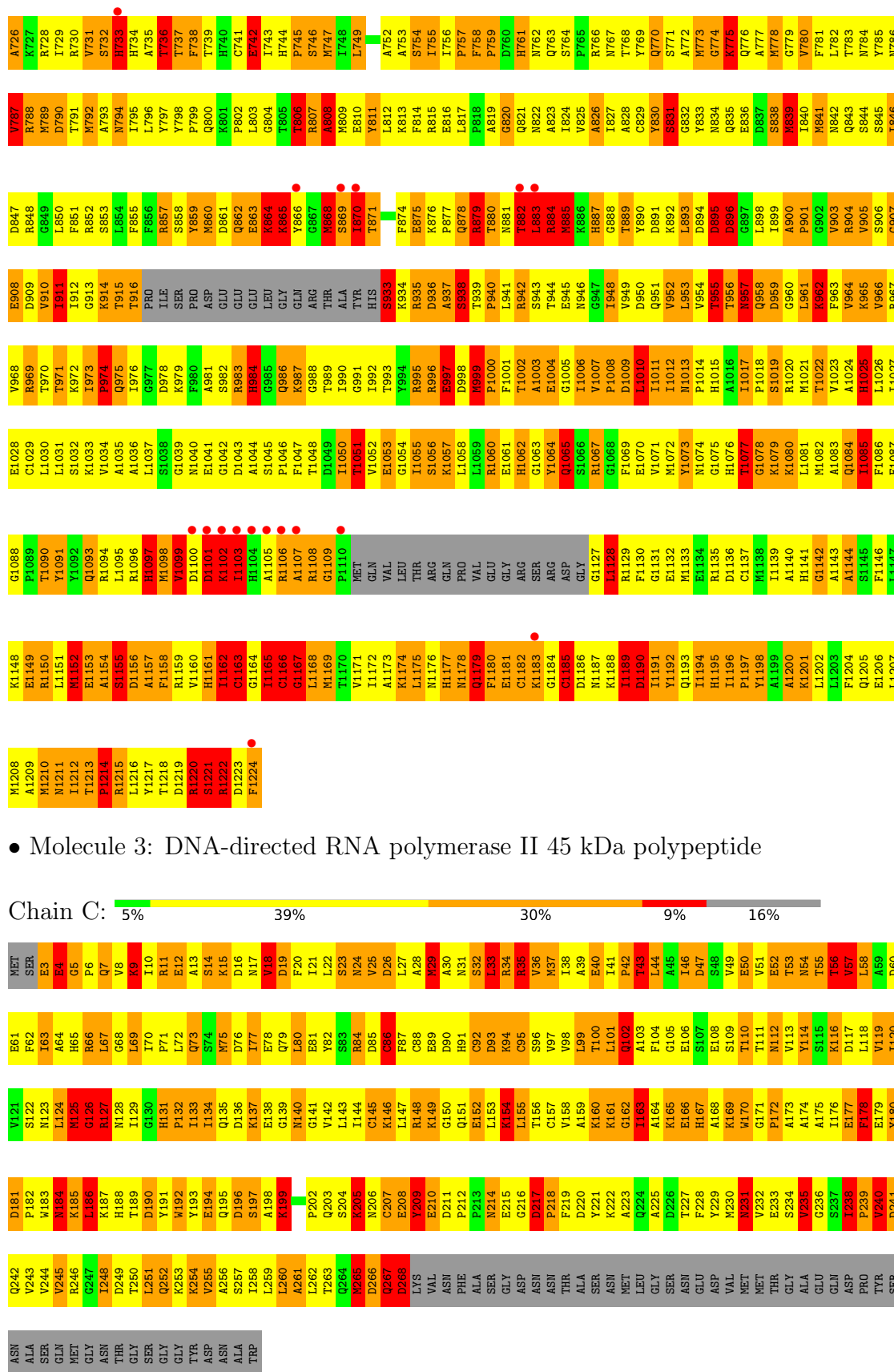
3 Residue-property plots

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: DNA-directed RNA polymerase II largest subunit



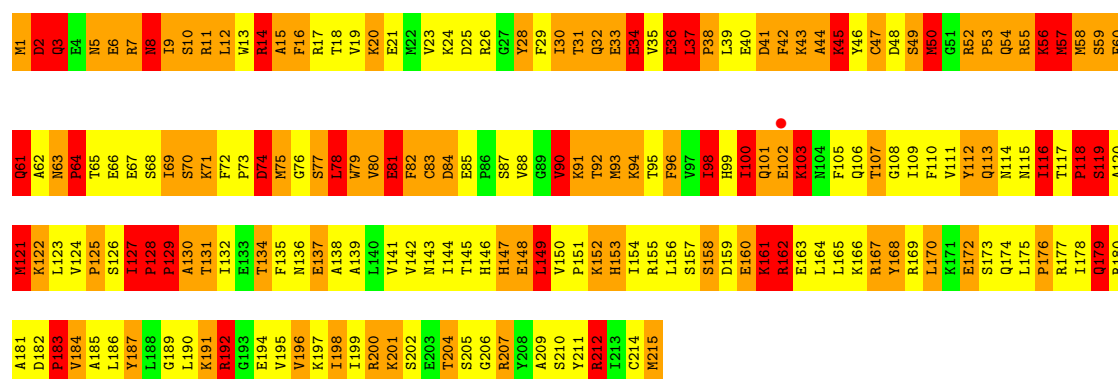




• Molecule 3: DNA-directed RNA polymerase II 45 kDa polypeptide

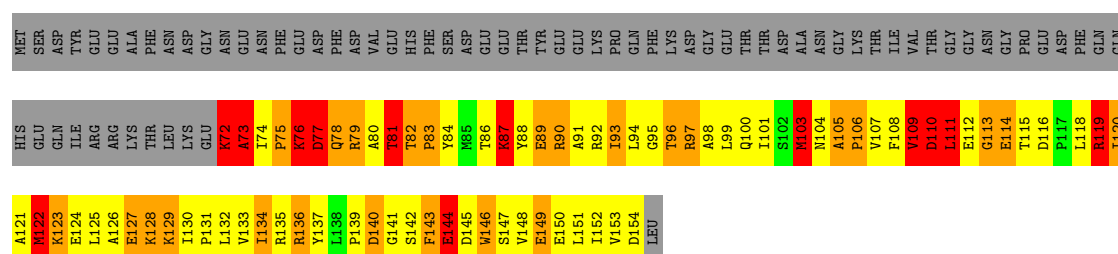
• Molecule 4: DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide

Chain E:



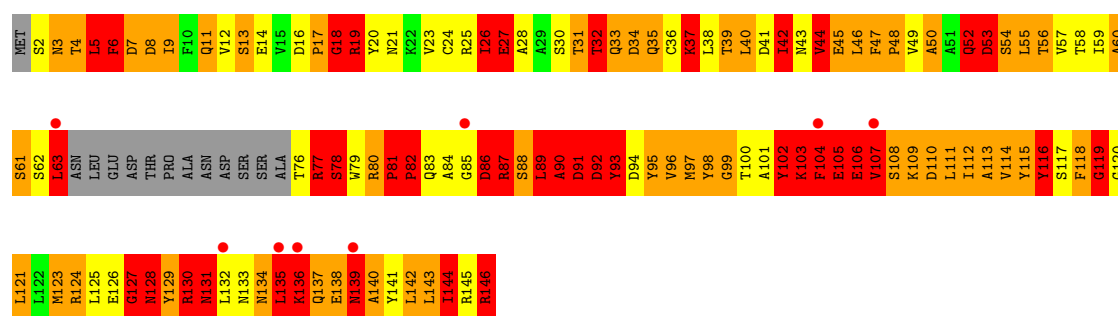
- Molecule 5: DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide

Chain F:



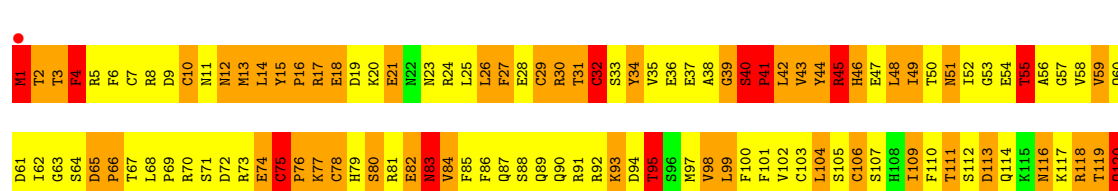
- Molecule 6: DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide

Chain H:



- Molecule 7: DNA-directed RNA polymerase II 14.2 kDa polypeptide

Chain I:



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	123.00Å 223.00Å 374.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.20 40.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.20) 97.9 (40.00-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 3.12Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.227 , 0.246 0.205 , 0.246	Depositor DCC
R_{free} test set	2779 reflections (2.97%)	wwPDB-VP
Wilson B-factor (Å ²)	55.9	Xtriage
Anisotropy	0.349	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 43.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	27757	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.89% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, MN, ZN

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	4.28	2326/10822 (21.5%)	2.86	1142/14641 (7.8%)
2	B	4.27	1874/8860 (21.2%)	2.77	855/11945 (7.2%)
3	C	4.40	461/2133 (21.6%)	2.88	204/2891 (7.1%)
4	E	4.24	333/1796 (18.5%)	2.77	183/2416 (7.6%)
5	F	3.95	131/682 (19.2%)	2.69	53/922 (5.7%)
6	H	4.22	216/1086 (19.9%)	2.73	119/1470 (8.1%)
7	I	4.27	226/1009 (22.4%)	3.00	137/1357 (10.1%)
8	J	4.08	109/533 (20.5%)	3.11	76/715 (10.6%)
9	K	4.10	188/937 (20.1%)	2.86	111/1265 (8.8%)
10	L	4.78	89/366 (24.3%)	3.04	41/485 (8.5%)
All	All	4.27	5953/28224 (21.1%)	2.83	2921/38107 (7.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	41
2	B	0	40
3	C	0	13
4	E	1	6
5	F	0	2
6	H	0	12
7	I	0	6
8	J	0	1
9	K	0	1
10	L	0	2
All	All	1	124

All (5953) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	50	MET	SD-CE	35.44	2.68	1.79
1	A	487	MET	SD-CE	-32.42	0.98	1.79
4	E	57	MET	SD-CE	32.19	2.60	1.79
3	C	181	ASP	C-O	-29.25	1.09	1.23
2	B	885	MET	SD-CE	29.19	2.52	1.79
2	B	552	MET	CG-SD	27.30	2.49	1.80
3	C	181	ASP	CA-C	-26.80	1.36	1.53
1	A	1285	MET	SD-CE	26.67	2.46	1.79
1	A	304	MET	SD-CE	26.16	2.44	1.79
2	B	101	MET	SD-CE	25.77	2.44	1.79
6	H	104	PHE	CA-C	25.22	1.86	1.52
2	B	552	MET	SD-CE	24.52	2.40	1.79
9	K	1	MET	SD-CE	24.41	2.40	1.79
3	C	125	MET	SD-CE	24.20	2.40	1.79
2	B	999	MET	SD-CE	-23.66	1.20	1.79
4	E	162	ARG	NE-CZ	22.78	1.58	1.33
1	A	549	MET	SD-CE	-22.69	1.22	1.79
1	A	464	PRO	C-O	-22.36	0.94	1.24
2	B	705	MET	SD-CE	-22.34	1.23	1.79
2	B	542	MET	SD-CE	-21.64	1.25	1.79
2	B	1097	HIS	CA-C	21.50	1.81	1.52
1	A	708	MET	SD-CE	21.46	2.33	1.79
10	L	26	THR	CA-CB	21.01	1.89	1.53
2	B	246	LYS	CA-C	20.78	1.79	1.52
5	F	103	MET	SD-CE	20.62	2.31	1.79
1	A	274	ILE	CA-CB	20.57	1.80	1.54
2	B	662	MET	SD-CE	20.56	2.31	1.79
10	L	48	CYS	CA-C	20.45	1.78	1.52
2	B	870	ILE	CA-CB	20.16	1.81	1.54
2	B	747	MET	SD-CE	-20.04	1.29	1.79
2	B	792	MET	SD-CE	19.78	2.29	1.79
3	C	75	MET	SD-CE	19.68	2.28	1.79
1	A	728	LYS	CD-CE	19.63	2.11	1.52
6	H	91	ASP	CA-C	19.54	1.75	1.52
1	A	437	MET	SD-CE	19.49	2.28	1.79
4	E	98	ILE	CA-CB	19.46	1.81	1.54
7	I	29	CYS	C-O	19.30	1.46	1.23
1	A	1259	MET	SD-CE	19.30	2.27	1.79
1	A	1145	SER	C-O	-19.23	0.99	1.24
3	C	165	LYS	CE-NZ	19.18	2.06	1.49
2	B	381	MET	SD-CE	-19.11	1.31	1.79
1	A	69	THR	CA-C	19.07	1.78	1.52
3	C	89	GLU	C-O	19.02	1.47	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	593	GLU	C-O	18.77	1.47	1.24
2	B	27	ALA	CA-CB	-18.68	1.23	1.53
1	A	849	MET	SD-CE	-18.67	1.32	1.79
2	B	1097	HIS	ND1-CE1	18.56	1.51	1.32
6	H	9	ILE	CA-CB	18.48	1.78	1.54
1	A	521	MET	SD-CE	-18.46	1.33	1.79
2	B	1154	ALA	CA-CB	18.12	1.83	1.53
4	E	162	ARG	CG-CD	18.09	2.06	1.52
3	C	97	VAL	C-O	-17.84	1.00	1.24
1	A	610	GLY	C-O	17.84	1.49	1.24
10	L	28	LYS	CA-C	17.77	1.76	1.52
7	I	50	THR	CA-C	-17.76	1.31	1.52
1	A	227	VAL	C-O	17.73	1.41	1.23
4	E	1	MET	SD-CE	17.61	2.23	1.79
2	B	1097	HIS	CD2-NE2	17.58	1.57	1.37
1	A	1111	MET	SD-CE	-17.54	1.35	1.79
2	B	1191	ILE	CA-CB	-17.45	1.37	1.55
4	E	93	MET	SD-CE	17.39	2.23	1.79
1	A	498	ARG	NE-CZ	-17.29	1.14	1.33
9	K	94	ILE	CA-CB	17.27	1.73	1.54
1	A	174	ILE	CA-CB	17.24	1.75	1.54
1	A	733	ALA	C-O	-17.21	1.03	1.24
6	H	136	LYS	CA-C	17.14	1.75	1.52
3	C	49	VAL	C-O	-17.11	1.06	1.24
1	A	1135	ARG	CZ-NH2	17.07	1.55	1.33
2	B	1050	ILE	C-O	-17.05	1.03	1.24
7	I	55	THR	CB-CG2	17.02	2.08	1.52
5	F	122	MET	SD-CE	-16.95	1.37	1.79
1	A	1149	ALA	C-O	16.93	1.44	1.23
1	A	673	GLY	C-O	-16.92	1.06	1.24
2	B	1097	HIS	CA-CB	16.89	1.82	1.53
1	A	44	THR	CA-CB	16.85	1.81	1.53
1	A	115	LEU	C-O	16.82	1.45	1.23
1	A	61	ILE	CA-CB	16.79	1.77	1.54
2	B	1150	ARG	CZ-NH2	16.79	1.55	1.33
1	A	880	LYS	C-O	-16.78	1.03	1.24
2	B	523	CYS	CA-C	-16.77	1.35	1.53
10	L	45	ALA	CA-CB	16.76	1.81	1.53
2	B	1083	ALA	CA-CB	-16.69	1.24	1.53
3	C	267	GLN	CA-C	16.65	1.75	1.52
8	J	1	MET	SD-CE	16.62	2.21	1.79
1	A	14	VAL	C-O	-16.60	1.04	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	39	ARG	NE-CZ	16.58	1.51	1.33
9	K	17	SER	C-O	-16.56	1.02	1.23
1	A	1045	VAL	CA-CB	-16.52	1.36	1.54
1	A	752	LYS	CE-NZ	16.34	1.98	1.49
4	E	30	ILE	C-O	-16.33	1.07	1.24
2	B	436	VAL	CA-CB	16.26	1.76	1.54
1	A	1232	ASN	CB-CG	16.19	1.92	1.52
6	H	107	VAL	CA-CB	16.17	1.76	1.54
3	C	28	ALA	C-O	16.15	1.42	1.24
2	B	986	GLN	CG-CD	16.12	1.92	1.52
1	A	1152	ILE	CA-CB	-16.08	1.35	1.54
2	B	448	ILE	CA-CB	15.96	1.73	1.54
1	A	843	LYS	C-O	-15.96	1.05	1.24
3	C	265	MET	SD-CE	15.95	2.19	1.79
1	A	677	ARG	NE-CZ	15.93	1.50	1.33
7	I	3	THR	CA-C	-15.82	1.34	1.53
2	B	60	GLN	C-O	-15.79	1.05	1.24
2	B	1106	ARG	CA-C	15.76	1.74	1.52
4	E	201	LYS	CG-CD	15.72	1.99	1.52
8	J	22	LEU	CA-C	15.70	1.72	1.52
9	K	111	LEU	C-O	15.70	1.43	1.24
1	A	1284	MET	CA-C	-15.66	1.32	1.52
2	B	723	VAL	CA-CB	15.60	1.74	1.54
2	B	812	LEU	C-O	-15.53	1.03	1.24
1	A	1349	TYR	C-O	-15.48	1.05	1.24
3	C	261	ALA	C-O	-15.44	1.03	1.24
2	B	104	GLU	CA-C	15.43	1.73	1.52
1	A	1227	ILE	C-O	-15.32	1.05	1.23
4	E	47	CYS	CA-C	15.15	1.70	1.52
1	A	31	SER	C-O	15.12	1.43	1.23
1	A	1105	LEU	CA-C	-15.11	1.32	1.52
1	A	1202	MET	SD-CE	15.11	2.17	1.79
2	B	556	THR	C-O	15.08	1.41	1.24
1	A	836	TYR	CA-C	15.02	1.71	1.52
2	B	1102	LYS	N-CA	15.02	1.63	1.46
1	A	1001	ARG	C-O	14.93	1.43	1.24
2	B	1002	THR	CA-C	14.90	1.72	1.52
5	F	93	ILE	C-O	-14.88	1.07	1.24
3	C	207	CYS	CA-C	14.84	1.71	1.52
2	B	1168	LEU	CA-C	-14.71	1.34	1.52
2	B	899	ILE	CA-CB	-14.66	1.38	1.54
1	A	1138	ILE	C-O	14.65	1.38	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	347	LYS	CG-CD	14.65	1.96	1.52
3	C	127	ARG	N-CA	14.59	1.63	1.46
2	B	458	LYS	C-O	-14.53	1.07	1.24
1	A	990	VAL	CA-CB	-14.51	1.34	1.54
2	B	883	LEU	CA-CB	14.50	1.75	1.53
2	B	246	LYS	N-CA	14.50	1.64	1.46
2	B	313	MET	SD-CE	-14.45	1.43	1.79
1	A	1302	PRO	C-O	14.45	1.40	1.23
1	A	670	ILE	CA-CB	-14.45	1.37	1.54
2	B	703	ILE	C-O	14.45	1.38	1.24
1	A	1080	THR	CA-C	14.43	1.72	1.52
3	C	154	LYS	CD-CE	14.38	1.95	1.52
2	B	321	GLY	C-O	-14.37	1.14	1.24
2	B	184	ALA	C-O	-14.36	1.06	1.23
1	A	1280	GLU	C-O	-14.35	1.05	1.24
2	B	598	GLU	CG-CD	14.34	1.88	1.52
6	H	103	LYS	CA-C	-14.33	1.33	1.52
1	A	1141	THR	C-O	14.31	1.40	1.23
1	A	434	ARG	CD-NE	-14.21	1.26	1.46
1	A	885	THR	N-CA	-14.17	1.27	1.46
2	B	957	ASN	CA-C	14.16	1.71	1.52
2	B	108	VAL	CA-CB	14.14	1.73	1.54
8	J	49	MET	SD-CE	-14.14	1.44	1.79
2	B	626	ILE	C-O	-14.12	1.09	1.24
3	C	113	VAL	C-O	-14.10	1.08	1.24
1	A	1433	MET	SD-CE	-14.06	1.44	1.79
7	I	17	ARG	CG-CD	14.06	1.94	1.52
2	B	172	ILE	C-O	14.05	1.38	1.24
1	A	1347	ALA	C-O	-14.05	1.07	1.24
2	B	169	ARG	NE-CZ	14.00	1.48	1.33
1	A	419	LYS	C-O	-13.99	1.06	1.24
1	A	821	ARG	CD-NE	-13.95	1.26	1.46
2	B	733	HIS	CA-C	13.80	1.71	1.52
1	A	728	LYS	CG-CD	13.79	1.93	1.52
2	B	1150	ARG	CZ-NH1	13.79	1.52	1.32
1	A	771	GLU	CD-OE2	13.78	1.51	1.25
1	A	1299	VAL	C-O	13.76	1.38	1.23
2	B	975	GLN	CD-NE2	13.71	1.62	1.33
2	B	620	ARG	CZ-NH2	13.70	1.51	1.33
1	A	752	LYS	CD-CE	13.69	1.93	1.52
2	B	1027	ILE	N-CA	-13.68	1.29	1.46
6	H	132	LEU	CA-CB	13.63	1.69	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	152	LYS	CD-CE	13.62	1.93	1.52
2	B	123	THR	CA-CB	-13.61	1.33	1.52
3	C	172	PRO	CA-C	-13.58	1.33	1.52
6	H	6	PHE	CA-C	-13.55	1.35	1.52
6	H	111	LEU	CA-C	13.55	1.70	1.52
10	L	68	GLU	CG-CD	13.53	1.85	1.52
2	B	1155	SER	N-CA	13.50	1.63	1.46
1	A	198	GLU	C-O	-13.49	1.08	1.24
7	I	75	CYS	CA-C	-13.46	1.36	1.53
1	A	1439	GLY	C-O	-13.44	1.11	1.24
1	A	620	LYS	CD-CE	13.42	1.92	1.52
1	A	191	THR	CA-C	13.41	1.70	1.52
2	B	525	ALA	C-O	13.40	1.42	1.23
2	B	1077	THR	C-O	-13.39	1.06	1.24
1	A	1443	VAL	C-O	-13.37	1.09	1.24
1	A	225	ASN	C-O	13.34	1.38	1.23
1	A	673	GLY	CA-C	-13.34	1.42	1.51
2	B	995	ARG	NE-CZ	-13.31	1.18	1.33
3	C	78	GLU	C-O	-13.30	1.07	1.24
3	C	16	ASP	C-O	-13.28	1.07	1.23
3	C	163	ILE	CA-CB	-13.28	1.32	1.55
1	A	1226	VAL	CA-CB	-13.28	1.37	1.54
1	A	1381	LEU	C-O	-13.27	1.07	1.23
4	E	162	ARG	CB-CG	13.27	1.92	1.52
1	A	671	ALA	CA-CB	-13.27	1.32	1.53
6	H	56	THR	CA-CB	13.26	1.70	1.53
2	B	502	ILE	CA-CB	13.25	1.90	1.54
1	A	839	ARG	NE-CZ	13.21	1.47	1.33
7	I	103	CYS	C-O	-13.19	1.08	1.24
2	B	962	LYS	CG-CD	13.16	1.92	1.52
6	H	23	VAL	CA-CB	-13.16	1.36	1.54
2	B	1101	ASP	CA-C	13.16	1.71	1.52
2	B	1082	MET	CA-C	-13.12	1.35	1.52
1	A	191	THR	CA-CB	13.10	1.75	1.53
8	J	3	VAL	CA-CB	-13.07	1.37	1.54
1	A	934	LYS	CD-CE	13.06	1.91	1.52
9	K	64	GLU	C-O	-13.04	1.07	1.24
2	B	529	GLU	CD-OE2	13.02	1.50	1.25
3	C	225	ALA	CA-CB	-13.01	1.35	1.53
2	B	608	ASP	C-O	-12.96	1.08	1.24
1	A	464	PRO	C-N	-12.95	1.15	1.33
2	B	531	GLN	CG-CD	12.94	1.84	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	466	TRP	CA-C	12.94	1.70	1.52
6	H	81	PRO	CA-C	12.94	1.64	1.52
4	E	179	GLN	CD-OE1	12.93	1.48	1.23
1	A	347	PHE	N-CA	12.92	1.65	1.46
2	B	106	ASP	CA-C	12.90	1.70	1.52
3	C	102	GLN	C-O	12.90	1.39	1.23
2	B	1154	ALA	CA-C	12.90	1.70	1.52
2	B	582	VAL	CA-C	-12.88	1.37	1.52
2	B	194	GLU	CD-OE1	12.86	1.49	1.25
2	B	212	LEU	C-O	-12.85	1.08	1.23
3	C	70	ILE	N-CA	12.84	1.62	1.46
2	B	1163	CYS	CA-CB	12.84	1.74	1.53
2	B	436	VAL	CA-C	12.82	1.69	1.52
1	A	782	ARG	C-O	-12.82	1.08	1.23
2	B	908	GLU	CA-CB	12.81	1.70	1.53
2	B	661	LEU	C-O	-12.81	1.09	1.24
2	B	63	ILE	CA-C	12.81	1.70	1.52
1	A	52	GLY	C-O	-12.79	1.06	1.23
7	I	56	ALA	C-O	-12.79	1.08	1.23
2	B	245	GLU	CA-C	12.78	1.69	1.52
2	B	310	MET	SD-CE	-12.77	1.47	1.79
1	A	1108	ALA	N-CA	-12.77	1.30	1.46
3	C	155	LEU	C-O	12.77	1.39	1.23
2	B	174	LEU	CA-C	-12.76	1.36	1.52
2	B	1143	ALA	CA-CB	-12.75	1.36	1.52
1	A	291	GLU	C-O	-12.75	1.08	1.24
6	H	37	LYS	C-O	12.74	1.40	1.23
1	A	217	LYS	CD-CE	12.73	1.90	1.52
2	B	709	ASP	CA-C	-12.73	1.35	1.52
1	A	750	GLY	C-O	-12.72	1.06	1.24
4	E	142	VAL	C-O	12.72	1.38	1.24
1	A	390	GLN	C-O	12.69	1.39	1.24
3	C	255	VAL	CA-CB	-12.68	1.36	1.54
1	A	1012	ARG	C-O	12.67	1.39	1.24
7	I	28	GLU	C-O	-12.66	1.07	1.23
7	I	83	ASN	CB-CG	-12.66	1.20	1.52
1	A	1214	GLU	C-O	12.65	1.40	1.24
2	B	735	ALA	N-CA	12.64	1.61	1.46
1	A	326	ARG	CA-C	12.63	1.69	1.52
4	E	121	MET	SD-CE	12.63	2.11	1.79
9	K	92	ASN	N-CA	12.62	1.60	1.46
5	F	148	VAL	C-O	12.61	1.39	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	15	LYS	CG-CD	12.61	1.90	1.52
1	A	1118	VAL	C-O	-12.59	1.10	1.24
1	A	15	LYS	C-O	-12.58	1.07	1.24
3	C	174	ALA	N-CA	-12.56	1.36	1.46
2	B	1165	ILE	CA-CB	12.53	1.68	1.55
1	A	1049	ILE	CA-CB	-12.51	1.40	1.54
1	A	1259	MET	CG-SD	12.48	2.12	1.80
2	B	848	ARG	NE-CZ	-12.47	1.19	1.33
3	C	186	LEU	CA-C	12.47	1.70	1.52
5	F	121	ALA	C-O	-12.46	1.08	1.24
1	A	597	LEU	CG-CD1	12.45	1.93	1.52
1	A	1288	ASP	N-CA	12.45	1.62	1.46
2	B	733	HIS	N-CA	12.44	1.62	1.46
1	A	1149	ALA	CA-CB	-12.44	1.31	1.53
2	B	448	ILE	N-CA	12.43	1.61	1.46
1	A	41	MET	SD-CE	12.42	2.10	1.79
1	A	1355	VAL	C-O	-12.42	1.09	1.24
2	B	784	ASN	N-CA	-12.41	1.32	1.46
1	A	420	ARG	CZ-NH2	-12.40	1.17	1.33
2	B	1189	ILE	CG1-CD1	12.40	2.00	1.51
1	A	1268	LEU	N-CA	-12.39	1.30	1.46
1	A	1277	GLU	CD-OE2	12.39	1.48	1.25
4	E	31	THR	CA-CB	12.38	1.71	1.53
2	B	488	TYR	C-O	12.37	1.38	1.24
1	A	392	VAL	CA-CB	-12.34	1.39	1.54
7	I	111	THR	C-O	-12.33	1.07	1.23
7	I	1	MET	CG-SD	12.33	2.11	1.80
1	A	446	ARG	CZ-NH1	12.32	1.50	1.32
2	B	949	VAL	CA-CB	-12.31	1.39	1.54
1	A	1228	TRP	CA-C	-12.30	1.38	1.52
2	B	773	MET	CG-SD	-12.29	1.50	1.80
7	I	17	ARG	CA-C	-12.29	1.37	1.52
3	C	168	ALA	C-O	-12.24	1.08	1.24
2	B	846	ILE	C-O	12.23	1.38	1.24
2	B	613	VAL	CA-C	-12.22	1.38	1.52
2	B	974	PRO	C-O	-12.22	1.08	1.23
1	A	1444	MET	SD-CE	12.22	2.10	1.79
3	C	158	VAL	C-O	-12.21	1.10	1.24
6	H	50	ALA	N-CA	12.20	1.60	1.45
2	B	787	VAL	N-CA	-12.17	1.33	1.46
1	A	109	HIS	C-O	-12.17	1.13	1.23
2	B	25	ILE	CA-C	-12.15	1.40	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	873	MET	SD-CE	-12.13	1.49	1.79
1	A	956	LEU	C-O	-12.13	1.11	1.24
2	B	1036	ALA	CA-CB	12.12	1.72	1.53
1	A	1120	LEU	C-O	-12.11	1.08	1.23
9	K	86	ALA	CA-CB	-12.10	1.33	1.53
6	H	131	ASN	CA-CB	12.10	1.72	1.53
1	A	1326	ARG	C-O	-12.10	1.08	1.24
1	A	174	ILE	C-O	-12.09	1.11	1.24
2	B	699	GLU	N-CA	-12.08	1.30	1.46
3	C	134	ILE	CA-CB	-12.07	1.38	1.54
1	A	776	ALA	C-O	-12.06	1.07	1.23
1	A	69	THR	CA-CB	12.05	1.73	1.53
1	A	1064	VAL	CA-C	-12.05	1.38	1.52
9	K	2	ASN	C-O	12.04	1.40	1.24
2	B	597	MET	SD-CE	-12.02	1.49	1.79
1	A	1339	LEU	CA-CB	-12.01	1.35	1.54
1	A	1448	GLU	CA-C	12.00	1.68	1.52
2	B	497	ARG	CZ-NH1	12.00	1.49	1.32
3	C	30	ALA	CA-CB	-12.00	1.34	1.53
2	B	1018	PRO	CA-C	-11.97	1.33	1.52
4	E	99	HIS	N-CA	11.96	1.60	1.46
10	L	27	LEU	CA-CB	11.96	1.73	1.53
1	A	1080	THR	CA-CB	11.92	1.73	1.53
2	B	1108	ARG	CA-C	11.92	1.68	1.52
7	I	91	ARG	CA-C	-11.92	1.34	1.53
4	E	195	VAL	CA-CB	-11.91	1.40	1.54
3	C	29	MET	SD-CE	11.88	2.09	1.79
1	A	346	ASP	CB-CG	11.87	1.81	1.52
2	B	729	ILE	C-O	-11.87	1.12	1.24
1	A	1038	THR	CA-C	-11.87	1.37	1.53
1	A	1095	THR	CA-C	-11.87	1.37	1.52
1	A	1075	PRO	C-O	-11.86	1.10	1.24
1	A	356	ASP	CA-C	-11.85	1.38	1.52
4	E	128	PRO	CA-C	11.85	1.63	1.52
1	A	938	LYS	CD-CE	11.83	1.88	1.52
1	A	643	ALA	CA-CB	-11.83	1.34	1.53
3	C	13	ALA	CA-C	-11.82	1.38	1.52
1	A	555	ASP	CB-CG	11.81	1.81	1.52
2	B	791	THR	N-CA	-11.81	1.32	1.46
9	K	81	TYR	C-O	-11.80	1.10	1.24
2	B	39	ARG	C-O	-11.79	1.10	1.24
2	B	204	ILE	CA-CB	-11.79	1.39	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1221	SER	N-CA	11.79	1.61	1.46
1	A	622	VAL	CA-CB	-11.78	1.42	1.54
7	I	44	TYR	N-CA	11.78	1.59	1.46
4	E	20	LYS	CE-NZ	11.77	1.84	1.49
1	A	1239	ARG	N-CA	-11.77	1.31	1.46
1	A	1209	MET	N-CA	-11.77	1.32	1.46
3	C	81	GLU	C-O	11.74	1.38	1.23
2	B	826	ALA	C-O	-11.74	1.09	1.23
7	I	42	LEU	C-O	-11.72	1.10	1.24
10	L	63	ARG	NE-CZ	11.72	1.46	1.33
1	A	198	GLU	CA-C	-11.71	1.38	1.52
1	A	874	ASP	CG-OD2	11.70	1.47	1.25
1	A	705	LYS	CB-CG	11.70	1.87	1.52
1	A	423	ASP	CB-CG	11.69	1.81	1.52
1	A	491	VAL	CA-CB	-11.69	1.41	1.53
1	A	1419	ASP	CG-OD1	11.69	1.47	1.25
3	C	66	ARG	NE-CZ	-11.69	1.20	1.33
2	B	531	GLN	CD-NE2	11.68	1.57	1.33
2	B	945	GLU	CD-OE1	11.68	1.47	1.25
2	B	996	ARG	CZ-NH1	11.68	1.49	1.32
1	A	45	GLN	CA-C	11.67	1.68	1.52
2	B	895	ASP	CB-CG	11.66	1.81	1.52
6	H	139	ASN	CB-CG	11.66	1.81	1.52
2	B	1017	ILE	CG1-CD1	-11.65	1.06	1.51
2	B	1158	PHE	C-O	-11.65	1.09	1.24
1	A	1005	GLU	CD-OE1	11.64	1.47	1.25
3	C	212	PRO	C-O	-11.64	1.11	1.24
3	C	18	VAL	CA-C	-11.61	1.38	1.52
2	B	1183	LYS	CA-CB	11.60	1.73	1.53
1	A	797	LYS	CA-C	-11.60	1.38	1.52
1	A	585	GLY	C-O	11.60	1.38	1.24
3	C	119	VAL	CA-CB	11.60	1.67	1.54
2	B	738	PHE	N-CA	-11.59	1.31	1.46
2	B	479	VAL	C-O	-11.58	1.08	1.24
3	C	84	ARG	C-O	-11.57	1.08	1.24
2	B	173	MET	C-O	-11.57	1.09	1.24
1	A	895	LYS	CD-CE	11.56	1.87	1.52
2	B	324	ILE	C-O	-11.56	1.11	1.24
1	A	301	ALA	C-O	-11.56	1.10	1.24
3	C	67	LEU	C-O	11.55	1.37	1.24
1	A	188	ASP	CA-C	11.54	1.68	1.52
1	A	974	ASP	N-CA	11.53	1.60	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	150	VAL	CA-CB	-11.53	1.41	1.53
2	B	1083	ALA	N-CA	11.53	1.59	1.45
2	B	840	ILE	CA-CB	-11.52	1.40	1.54
9	K	30	ALA	CA-C	-11.51	1.38	1.52
1	A	432	VAL	C-O	-11.51	1.11	1.24
1	A	1109	LYS	CG-CD	11.51	1.86	1.52
1	A	676	MET	CG-SD	11.50	2.09	1.80
2	B	1137	CYS	C-O	-11.49	1.10	1.24
7	I	92	ARG	C-O	11.48	1.38	1.23
3	C	159	ALA	C-O	-11.47	1.09	1.23
2	B	582	VAL	C-O	-11.45	1.12	1.24
8	J	5	VAL	CA-CB	11.45	1.67	1.54
1	A	1428	VAL	C-O	-11.45	1.11	1.24
4	E	54	GLN	CA-CB	11.45	1.67	1.53
1	A	578	LEU	N-CA	11.44	1.60	1.46
5	F	105	ALA	CA-CB	-11.43	1.33	1.53
3	C	102	GLN	CB-CG	11.43	1.86	1.52
10	L	66	GLN	C-O	-11.43	1.09	1.23
2	B	215	GLN	N-CA	-11.42	1.32	1.46
2	B	546	SER	C-O	-11.42	1.09	1.23
1	A	1232	ASN	C-O	11.41	1.38	1.24
2	B	1149	GLU	C-O	-11.41	1.10	1.24
1	A	995	GLU	C-O	-11.40	1.09	1.24
1	A	1225	PHE	CD1-CE1	11.40	1.72	1.38
1	A	377	PRO	C-O	-11.39	1.15	1.24
4	E	150	VAL	N-CA	-11.39	1.37	1.46
6	H	87	ARG	CA-C	11.38	1.63	1.52
1	A	1118	VAL	N-CA	-11.38	1.32	1.46
1	A	677	ARG	CZ-NH2	11.36	1.48	1.33
4	E	191	LYS	C-O	-11.36	1.09	1.23
8	J	48	ARG	CZ-NH2	-11.36	1.18	1.33
2	B	19	GLU	N-CA	11.36	1.60	1.46
3	C	10	ILE	CG1-CD1	-11.35	1.07	1.51
1	A	775	ILE	CA-CB	-11.35	1.40	1.54
1	A	641	VAL	C-O	-11.35	1.10	1.24
1	A	1119	TYR	CE2-CZ	-11.35	1.11	1.38
2	B	772	ALA	CA-C	11.35	1.67	1.52
1	A	1203	ASN	CA-C	11.34	1.67	1.52
1	A	1038	THR	C-O	-11.33	1.09	1.23
4	E	143	ASN	C-O	-11.30	1.09	1.23
2	B	265	SER	CA-C	11.28	1.66	1.52
1	A	1447	GLU	CA-C	11.28	1.67	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	229	TYR	CA-C	11.28	1.66	1.53
2	B	663	ALA	CA-CB	11.28	1.71	1.53
1	A	960	ILE	CA-CB	11.27	1.68	1.54
2	B	230	ALA	CA-CB	11.27	1.71	1.53
2	B	700	SER	C-O	-11.27	1.08	1.24
4	E	52	ARG	C-O	11.27	1.38	1.23
2	B	364	ILE	CA-CB	-11.27	1.39	1.54
2	B	972	LYS	C-O	-11.27	1.10	1.24
1	A	1264	GLU	CA-C	-11.26	1.38	1.52
1	A	1359	ASP	N-CA	11.26	1.60	1.46
2	B	271	ALA	C-O	-11.26	1.09	1.23
1	A	1308	THR	N-CA	-11.24	1.32	1.45
1	A	729	ALA	CA-CB	-11.24	1.33	1.53
1	A	895	LYS	N-CA	11.23	1.60	1.46
4	E	103	LYS	N-CA	11.23	1.59	1.46
2	B	1140	ALA	CA-CB	-11.22	1.35	1.53
2	B	1135	ARG	NE-CZ	-11.22	1.20	1.33
1	A	288	ALA	CA-CB	11.21	1.71	1.53
1	A	801	GLU	CD-OE1	11.21	1.46	1.25
1	A	1283	VAL	CA-C	11.21	1.66	1.52
1	A	464	PRO	CA-C	-11.21	1.36	1.52
1	A	44	THR	N-CA	11.20	1.60	1.46
2	B	736	THR	CB-CG2	11.20	1.89	1.52
1	A	795	GLU	C-O	-11.20	1.10	1.24
2	B	259	TYR	C-O	-11.19	1.09	1.23
1	A	738	LYS	C-O	-11.17	1.09	1.23
1	A	1232	ASN	CG-OD1	11.17	1.44	1.23
1	A	966	ASN	N-CA	-11.16	1.33	1.46
2	B	1164	GLY	C-O	11.16	1.37	1.23
4	E	162	ARG	CD-NE	11.16	1.61	1.46
8	J	2	ILE	C-O	-11.14	1.11	1.23
1	A	1135	ARG	CG-CD	11.13	1.85	1.52
1	A	1309	ASP	CA-C	-11.13	1.38	1.52
4	E	131	THR	CB-CG2	11.12	1.89	1.52
6	H	104	PHE	C-O	11.12	1.38	1.24
1	A	462	VAL	CA-CB	-11.12	1.40	1.54
1	A	1292	PRO	C-O	11.12	1.36	1.23
2	B	1070	GLU	C-O	-11.12	1.10	1.23
2	B	1221	SER	CA-C	11.12	1.67	1.52
6	H	121	LEU	C-O	11.10	1.37	1.24
1	A	1281	ARG	NE-CZ	11.10	1.45	1.33
2	B	223	VAL	C-O	-11.10	1.10	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	731	ARG	C-O	-11.09	1.11	1.24
7	I	118	ARG	CA-C	11.09	1.68	1.52
2	B	130	VAL	CA-C	11.09	1.66	1.52
2	B	175	ARG	C-O	-11.09	1.06	1.24
1	A	471	ASN	CA-C	-11.08	1.38	1.52
1	A	209	ASN	CG-ND2	11.07	1.56	1.33
2	B	477	ALA	CA-CB	11.07	1.89	1.52
3	C	143	LEU	C-O	-11.07	1.11	1.24
6	H	139	ASN	CA-CB	11.07	1.72	1.53
2	B	1097	HIS	CE1-NE2	11.06	1.43	1.32
4	E	131	THR	CA-CB	11.06	1.71	1.53
1	A	599	SER	CA-C	-11.05	1.39	1.52
4	E	79	TRP	CA-C	-11.05	1.39	1.52
1	A	1195	LEU	C-N	-11.05	1.19	1.33
2	B	808	ALA	CA-CB	-11.05	1.34	1.53
1	A	209	ASN	CG-OD1	11.03	1.44	1.23
1	A	1282	VAL	CA-CB	-11.02	1.40	1.54
2	B	975	GLN	C-O	-11.02	1.10	1.23
1	A	966	ASN	CA-C	-11.02	1.39	1.52
2	B	1183	LYS	CA-C	11.01	1.67	1.52
2	B	1128	LEU	CA-C	10.99	1.67	1.52
2	B	828	ALA	C-O	-10.99	1.10	1.23
1	A	466	SER	CB-OG	-10.99	1.20	1.42
2	B	1042	GLY	CA-C	-10.98	1.44	1.52
9	K	20	LYS	CG-CD	10.98	1.85	1.52
3	C	154	LYS	CG-CD	10.98	1.85	1.52
1	A	677	ARG	CZ-NH1	10.97	1.48	1.32
2	B	641	GLU	CG-CD	10.96	1.79	1.52
2	B	619	ILE	CA-CB	-10.96	1.39	1.54
2	B	646	LEU	CG-CD2	10.96	1.88	1.52
4	E	192	ARG	NE-CZ	10.96	1.45	1.33
1	A	601	LYS	CD-CE	10.95	1.85	1.52
1	A	162	VAL	C-O	-10.94	1.12	1.23
1	A	830	LYS	CG-CD	10.94	1.85	1.52
2	B	346	GLU	CG-CD	10.94	1.79	1.52
2	B	272	THR	CA-C	-10.93	1.39	1.52
1	A	35	ILE	CA-C	10.93	1.66	1.52
2	B	915	THR	CA-CB	10.93	1.74	1.54
6	H	139	ASN	C-O	10.93	1.37	1.24
1	A	1442	ASP	CA-C	-10.93	1.39	1.52
2	B	962	LYS	CD-CE	10.93	1.85	1.52
9	K	99	GLY	C-O	10.92	1.38	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	557	PHE	N-CA	-10.91	1.33	1.46
3	C	253	LYS	C-O	10.90	1.37	1.24
1	A	734	GLU	CA-C	-10.90	1.39	1.52
1	A	1238	ILE	C-O	-10.88	1.12	1.24
3	C	25	VAL	N-CA	10.89	1.58	1.46
7	I	120	GLN	CA-C	10.88	1.67	1.52
6	H	136	LYS	N-CA	10.88	1.60	1.46
7	I	45	ARG	CG-CD	10.88	1.85	1.52
2	B	184	ALA	CA-CB	-10.88	1.34	1.53
1	A	795	GLU	CG-CD	10.87	1.79	1.52
1	A	189	ARG	N-CA	10.87	1.58	1.46
1	A	188	ASP	N-CA	10.84	1.60	1.46
2	B	240	ILE	C-O	-10.83	1.13	1.24
2	B	30	SER	C-O	-10.83	1.11	1.24
2	B	352	ALA	CA-CB	-10.83	1.36	1.53
1	A	1275	GLY	C-O	10.83	1.33	1.23
7	I	90	GLN	C-O	-10.83	1.08	1.23
1	A	695	LYS	CD-CE	10.82	1.84	1.52
2	B	230	ALA	CA-C	10.82	1.66	1.52
1	A	434	ARG	C-O	-10.82	1.10	1.23
2	B	257	LYS	N-CA	-10.82	1.33	1.46
1	A	1422	ARG	NE-CZ	10.81	1.45	1.33
4	E	162	ARG	CZ-NH1	10.79	1.47	1.32
1	A	368	LYS	CG-CD	10.78	1.84	1.52
6	H	37	LYS	CA-C	10.78	1.65	1.52
6	H	27	GLU	CA-C	10.77	1.66	1.52
2	B	607	GLY	C-O	-10.77	1.10	1.24
7	I	14	LEU	C-O	-10.76	1.11	1.23
2	B	112	LEU	C-O	-10.76	1.11	1.24
1	A	652	VAL	CA-C	-10.75	1.39	1.52
1	A	787	PHE	CG-CD1	-10.75	1.16	1.38
9	K	91	CYS	CA-C	10.75	1.67	1.52
3	C	63	ILE	CA-CB	10.73	1.66	1.54
8	J	47	ARG	NE-CZ	-10.73	1.21	1.33
1	A	523	ILE	N-CA	-10.73	1.33	1.46
2	B	226	PHE	CA-C	-10.72	1.39	1.52
2	B	531	GLN	CD-OE1	10.72	1.44	1.23
1	A	1338	VAL	CA-CB	-10.72	1.42	1.54
9	K	17	SER	CA-C	-10.72	1.40	1.52
1	A	1222	ASN	CA-C	10.72	1.66	1.52
2	B	509	ALA	CA-CB	10.71	1.87	1.52
1	A	1212	VAL	CA-CB	-10.70	1.40	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1181	GLU	N-CA	10.70	1.59	1.46
4	E	135	PHE	C-O	-10.70	1.11	1.24
1	A	808	LEU	N-CA	-10.68	1.32	1.45
2	B	822	ASN	CA-C	-10.68	1.39	1.52
1	A	1446	ASP	CA-CB	10.67	1.67	1.52
4	E	204	THR	CA-CB	-10.67	1.38	1.53
2	B	825	VAL	CA-CB	-10.66	1.40	1.54
1	A	23	SER	CA-C	10.66	1.66	1.52
1	A	1303	GLU	C-O	-10.66	1.11	1.23
2	B	1186	ASP	CA-CB	10.66	1.69	1.53
2	B	361	LEU	C-N	-10.66	1.22	1.34
10	L	41	SER	N-CA	10.65	1.59	1.46
2	B	594	ALA	CA-CB	-10.65	1.35	1.53
1	A	957	PRO	CA-CB	-10.64	1.39	1.53
1	A	1195	LEU	N-CA	10.64	1.59	1.46
1	A	366	VAL	C-N	-10.64	1.19	1.33
1	A	476	SER	C-O	-10.64	1.10	1.24
2	B	25	ILE	C-O	-10.64	1.08	1.23
1	A	896	ARG	N-CA	-10.63	1.32	1.46
1	A	1318	THR	C-O	-10.63	1.09	1.24
9	K	14	GLU	CA-C	10.63	1.66	1.52
2	B	542	MET	CA-CB	10.62	1.69	1.53
2	B	734	HIS	C-N	10.61	1.47	1.33
7	I	92	ARG	CA-C	10.61	1.65	1.52
2	B	650	GLU	CD-OE2	10.61	1.45	1.25
1	A	787	PHE	N-CA	-10.60	1.32	1.45
2	B	1101	ASP	CB-CG	10.59	1.78	1.52
10	L	65	VAL	CA-C	-10.59	1.39	1.52
1	A	1333	ILE	CA-CB	-10.58	1.41	1.54
6	H	19	ARG	CG-CD	10.58	1.84	1.52
4	E	74	ASP	CA-C	10.58	1.67	1.52
2	B	355	ILE	C-O	-10.58	1.12	1.24
2	B	1103	ILE	N-CA	10.58	1.59	1.46
1	A	941	LYS	CD-CE	10.56	1.84	1.52
2	B	1041	GLU	CD-OE2	10.56	1.45	1.25
6	H	48	PRO	C-O	10.56	1.37	1.23
3	C	23	SER	CB-OG	10.55	1.63	1.42
2	B	772	ALA	CA-CB	-10.54	1.37	1.53
2	B	882	THR	CA-C	10.54	1.66	1.52
7	I	70	ARG	NE-CZ	-10.53	1.21	1.33
1	A	180	LYS	C-O	-10.53	1.11	1.24
2	B	945	GLU	C-O	10.53	1.36	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	211	VAL	CB-CG1	-10.53	1.17	1.52
2	B	706	GLN	CB-CG	10.52	1.84	1.52
2	B	904	ARG	C-O	-10.52	1.11	1.23
1	A	213	HIS	CA-CB	10.51	1.72	1.53
1	A	129	LYS	C-O	10.51	1.39	1.23
1	A	1080	THR	N-CA	10.50	1.59	1.46
2	B	165	VAL	CA-CB	10.50	1.68	1.54
1	A	699	ALA	C-O	-10.50	1.09	1.24
1	A	801	GLU	CD-OE2	10.50	1.45	1.25
1	A	1103	GLU	C-O	10.50	1.36	1.24
1	A	917	SER	C-O	-10.49	1.12	1.24
2	B	959	ASP	CA-CB	10.49	1.72	1.53
2	B	531	GLN	CB-CG	10.48	1.83	1.52
2	B	1102	LYS	CB-CG	10.47	1.83	1.52
2	B	1140	ALA	C-O	10.47	1.36	1.24
3	C	248	ILE	CA-CB	-10.47	1.42	1.54
1	A	190	ALA	CA-CB	10.46	1.71	1.53
2	B	1219	ASP	N-CA	10.46	1.58	1.46
1	A	1131	ALA	CA-CB	-10.46	1.36	1.53
6	H	9	ILE	C-O	10.46	1.34	1.24
3	C	148	ARG	N-CA	-10.46	1.33	1.45
1	A	279	LEU	CA-C	-10.45	1.38	1.52
1	A	661	GLY	CA-C	10.45	1.63	1.52
6	H	77	ARG	NE-CZ	10.45	1.44	1.33
2	B	224	GLN	N-CA	-10.45	1.33	1.46
1	A	912	LEU	CA-C	-10.44	1.38	1.52
1	A	603	ASN	N-CA	-10.44	1.33	1.45
1	A	962	ARG	C-O	-10.44	1.10	1.24
8	J	7	CYS	CA-CB	10.44	1.69	1.53
8	J	31	ASP	C-O	10.43	1.36	1.23
1	A	491	VAL	C-O	-10.43	1.12	1.24
1	A	620	LYS	CE-NZ	10.43	1.80	1.49
1	A	1061	GLY	CA-C	10.43	1.65	1.51
1	A	993	LEU	CA-C	-10.43	1.39	1.52
3	C	249	ASP	CA-C	10.42	1.66	1.52
1	A	1263	ILE	CG1-CD1	10.42	1.92	1.51
2	B	959	ASP	CB-CG	10.41	1.78	1.52
3	C	228	PHE	N-CA	-10.41	1.33	1.46
2	B	865	LYS	CA-C	10.40	1.66	1.52
2	B	112	LEU	CA-C	-10.40	1.40	1.52
1	A	762	SER	C-O	-10.40	1.09	1.23
2	B	434	ARG	CG-CD	10.40	1.83	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	580	VAL	C-O	10.39	1.38	1.24
2	B	1190	ASP	C-O	-10.39	1.10	1.24
2	B	344	LYS	CB-CG	10.39	1.83	1.52
6	H	136	LYS	CA-CB	10.39	1.71	1.53
2	B	598	GLU	N-CA	10.38	1.58	1.46
1	A	1286	LYS	C-O	-10.38	1.11	1.24
3	C	26	ASP	CG-OD1	10.38	1.45	1.25
4	E	155	ARG	CD-NE	10.37	1.60	1.46
10	L	59	ALA	N-CA	10.37	1.59	1.46
1	A	974	ASP	CA-C	-10.36	1.40	1.52
1	A	157	ASP	CB-CG	10.35	1.77	1.52
9	K	48	ALA	CA-CB	-10.35	1.36	1.53
2	B	732	SER	CA-C	10.35	1.66	1.52
1	A	686	ALA	C-N	-10.35	1.20	1.34
7	I	37	GLU	CD-OE1	10.35	1.45	1.25
2	B	357	GLN	C-O	-10.35	1.10	1.24
2	B	869	SER	CA-C	10.35	1.66	1.52
3	C	260	LEU	CG-CD2	10.34	1.86	1.52
1	A	1277	GLU	CA-C	-10.34	1.39	1.52
1	A	516	SER	CB-OG	10.34	1.62	1.42
1	A	1280	GLU	CD-OE2	10.34	1.45	1.25
2	B	136	THR	C-O	10.34	1.36	1.24
6	H	11	GLN	CA-C	-10.33	1.40	1.52
1	A	959	ASN	CA-CB	-10.33	1.38	1.52
3	C	84	ARG	NE-CZ	10.33	1.44	1.33
2	B	592	ASN	CG-OD1	10.32	1.43	1.23
2	B	1055	ILE	CA-CB	10.32	1.68	1.54
1	A	1198	ASP	N-CA	10.31	1.58	1.46
2	B	1096	ARG	C-O	-10.31	1.09	1.23
1	A	422	GLY	C-O	-10.31	1.10	1.23
1	A	1446	ASP	CB-CG	10.31	1.77	1.52
3	C	61	GLU	N-CA	10.31	1.59	1.46
2	B	415	GLN	CB-CG	10.30	1.83	1.52
1	A	911	SER	C-O	10.30	1.37	1.24
9	K	46	ILE	CA-CB	-10.30	1.42	1.54
1	A	193	ASP	N-CA	10.29	1.59	1.46
2	B	100	PRO	CA-C	10.29	1.63	1.52
2	B	164	LYS	CD-CE	10.28	1.83	1.52
1	A	496	GLU	CD-OE1	10.27	1.44	1.25
1	A	1144	LYS	CA-C	-10.27	1.39	1.52
8	J	1	MET	CG-SD	-10.26	1.55	1.80
1	A	771	GLU	CA-C	-10.26	1.40	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	929	LEU	N-CA	-10.26	1.33	1.46
1	A	800	VAL	CA-CB	-10.25	1.41	1.53
8	J	22	LEU	N-CA	-10.25	1.34	1.46
1	A	976	THR	CA-CB	10.25	1.69	1.53
1	A	1027	ALA	C-O	10.25	1.36	1.23
3	C	139	GLY	CA-C	10.25	1.62	1.51
4	E	56	LYS	N-CA	-10.25	1.32	1.46
1	A	1331	SER	C-O	10.24	1.37	1.23
1	A	36	ARG	CA-C	-10.24	1.39	1.52
3	C	10	ILE	CA-CB	-10.24	1.40	1.54
2	B	209	GLU	C-O	-10.24	1.12	1.24
2	B	365	THR	C-O	10.24	1.36	1.23
1	A	826	ASP	CG-OD2	10.23	1.44	1.25
2	B	1008	PRO	CA-CB	-10.23	1.40	1.53
6	H	116	TYR	N-CA	10.23	1.59	1.46
1	A	23	SER	C-O	10.23	1.37	1.24
2	B	643	ASP	CA-C	-10.23	1.39	1.52
2	B	695	ALA	CA-C	-10.22	1.39	1.52
1	A	811	GLN	N-CA	-10.22	1.33	1.46
9	K	72	LYS	C-O	-10.22	1.12	1.23
3	C	57	VAL	CA-CB	-10.21	1.40	1.54
2	B	1156	ASP	CA-CB	10.21	1.70	1.53
1	A	1123	GLY	CA-C	10.20	1.66	1.51
3	C	4	GLU	CA-C	-10.20	1.39	1.52
2	B	660	LYS	N-CA	-10.19	1.33	1.46
1	A	1015	VAL	CB-CG2	-10.19	1.19	1.52
2	B	95	ILE	CA-C	-10.19	1.40	1.52
1	A	187	LYS	CA-C	10.19	1.66	1.52
2	B	651	LEU	CG-CD2	-10.18	1.19	1.52
1	A	576	GLN	CA-C	-10.18	1.39	1.52
2	B	1149	GLU	CA-C	-10.18	1.39	1.52
1	A	1116	LEU	C-O	-10.17	1.10	1.24
7	I	59	VAL	C-O	-10.17	1.13	1.24
4	E	66	GLU	CA-CB	10.17	1.69	1.53
2	B	995	ARG	CD-NE	-10.16	1.32	1.46
10	L	26	THR	N-CA	10.16	1.59	1.46
1	A	367	PRO	N-CA	-10.16	1.34	1.47
2	B	370	PHE	N-CA	10.16	1.59	1.46
1	A	297	GLN	C-O	-10.15	1.12	1.24
1	A	171	GLN	C-O	-10.15	1.12	1.24
1	A	647	GLY	C-O	-10.15	1.11	1.23
2	B	90	ILE	N-CA	10.14	1.59	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1155	ASP	CA-CB	-10.14	1.40	1.53
1	A	240	PRO	C-O	10.14	1.35	1.23
1	A	1109	LYS	CB-CG	10.14	1.82	1.52
3	C	26	ASP	C-O	10.14	1.36	1.23
1	A	918	GLU	CA-C	-10.14	1.38	1.52
2	B	999	MET	CG-SD	10.13	2.06	1.80
4	E	200	ARG	NE-CZ	-10.12	1.22	1.33
2	B	1210	MET	SD-CE	10.12	2.04	1.79
1	A	1287	TYR	C-O	10.11	1.36	1.23
1	A	400	PRO	C-O	-10.11	1.10	1.24
4	E	44	ALA	CA-CB	10.10	1.70	1.53
2	B	218	SER	C-O	-10.10	1.11	1.23
2	B	742	GLU	N-CA	-10.10	1.33	1.46
1	A	1010	ALA	CA-C	-10.09	1.39	1.52
2	B	987	LYS	CE-NZ	10.09	1.79	1.49
4	E	162	ARG	CA-CB	10.09	1.69	1.53
9	K	28	PRO	C-O	-10.09	1.12	1.23
1	A	144	THR	C-O	-10.08	1.11	1.24
1	A	873	MET	C-O	-10.08	1.10	1.23
1	A	598	LEU	CA-C	10.08	1.66	1.53
2	B	871	THR	CA-CB	10.07	1.69	1.53
2	B	1041	GLU	N-CA	10.07	1.58	1.46
1	A	895	LYS	CG-CD	10.06	1.82	1.52
1	A	1429	ILE	CA-C	-10.06	1.40	1.52
2	B	1212	ILE	N-CA	10.05	1.58	1.46
1	A	241	VAL	CA-CB	10.05	1.64	1.53
1	A	662	PHE	CA-C	-10.05	1.39	1.52
1	A	875	ALA	CA-CB	-10.05	1.35	1.53
1	A	17	VAL	CA-CB	-10.04	1.41	1.54
2	B	227	LYS	CG-CD	10.04	1.82	1.52
4	E	138	ALA	C-O	-10.04	1.12	1.24
2	B	598	GLU	CD-OE2	10.04	1.44	1.25
2	B	1097	HIS	CG-ND1	10.04	1.49	1.38
1	A	681	GLU	CD-OE1	10.04	1.44	1.25
1	A	925	LEU	C-O	-10.03	1.12	1.24
1	A	411	ASP	CA-C	-10.03	1.39	1.52
1	A	1304	TRP	CE2-CZ2	-10.03	1.18	1.39
3	C	21	ILE	CA-CB	-10.03	1.41	1.54
2	B	561	TRP	CA-C	-10.02	1.40	1.52
1	A	1188	GLN	C-O	10.01	1.36	1.24
1	A	536	LEU	CA-C	10.01	1.67	1.53
4	E	23	VAL	C-O	9.99	1.35	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	153	VAL	CA-C	-9.99	1.42	1.52
6	H	127	GLY	CA-C	9.98	1.66	1.51
7	I	48	LEU	C-O	-9.98	1.11	1.24
1	A	998	LEU	C-O	-9.97	1.12	1.23
3	C	43	THR	N-CA	-9.97	1.34	1.46
1	A	247	ARG	CA-C	9.96	1.63	1.52
2	B	595	ARG	CG-CD	9.96	1.82	1.52
3	C	179	GLU	C-O	-9.96	1.11	1.23
1	A	32	VAL	C-O	9.96	1.35	1.24
1	A	769	SER	CA-C	9.96	1.64	1.52
1	A	1145	SER	CA-C	9.96	1.66	1.52
9	K	18	LYS	C-O	-9.96	1.12	1.24
2	B	242	SER	C-O	-9.95	1.11	1.23
6	H	83	GLN	CA-C	9.95	1.66	1.52
2	B	564	GLU	CD-OE1	9.94	1.44	1.25
1	A	1237	ILE	N-CA	-9.94	1.34	1.46
1	A	93	VAL	CA-C	-9.93	1.40	1.52
1	A	558	GLY	C-O	-9.93	1.10	1.23
1	A	1144	LYS	CD-CE	9.93	1.82	1.52
1	A	1368	MET	SD-CE	-9.93	1.54	1.79
10	L	33	GLU	CA-C	9.92	1.66	1.52
2	B	595	ARG	C-O	-9.92	1.12	1.24
4	E	182	ASP	CA-C	-9.92	1.43	1.53
2	B	1100	ASP	CA-C	9.91	1.66	1.52
1	A	666	ILE	CA-CB	-9.90	1.40	1.54
3	C	190	ASP	C-O	-9.90	1.12	1.24
1	A	148	CYS	CA-CB	9.90	1.66	1.52
2	B	723	VAL	CB-CG1	9.89	1.85	1.52
1	A	220	THR	N-CA	9.89	1.58	1.46
2	B	841	MET	CA-C	9.89	1.64	1.52
9	K	46	ILE	C-N	-9.89	1.21	1.33
1	A	299	HIS	C-O	-9.88	1.11	1.24
2	B	646	LEU	CB-CG	9.88	1.73	1.53
1	A	479	ASN	C-O	-9.88	1.10	1.23
1	A	39	GLU	CA-C	9.87	1.64	1.52
1	A	844	ALA	CA-C	-9.86	1.39	1.52
1	A	1211	GLN	CA-C	-9.86	1.40	1.52
2	B	255	GLN	N-CA	-9.86	1.33	1.46
2	B	1155	SER	CA-CB	9.85	1.70	1.53
1	A	375	THR	C-O	-9.85	1.11	1.23
3	C	125	MET	CA-C	9.85	1.66	1.52
6	H	111	LEU	N-CA	9.85	1.58	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	744	LYS	CA-C	-9.84	1.39	1.52
1	A	1117	THR	N-CA	9.84	1.58	1.46
1	A	1277	GLU	N-CA	9.84	1.58	1.46
4	E	215	MET	SD-CE	9.84	2.04	1.79
4	E	161	LYS	CD-CE	9.84	1.81	1.52
2	B	573	GLN	C-O	-9.83	1.11	1.24
1	A	518	LYS	CD-CE	9.83	1.81	1.52
2	B	1030	LEU	CA-C	-9.82	1.40	1.52
9	K	26	LYS	CA-C	9.82	1.66	1.52
2	B	198	ASP	C-O	-9.82	1.11	1.23
2	B	823	ALA	CA-C	-9.82	1.40	1.52
1	A	1073	GLY	C-O	-9.81	1.11	1.23
1	A	1068	ALA	CA-C	-9.81	1.40	1.52
2	B	89	GLU	CA-C	9.81	1.73	1.52
1	A	722	LEU	C-O	-9.81	1.11	1.24
9	K	2	ASN	CA-C	9.81	1.67	1.52
1	A	469	ARG	NE-CZ	-9.80	1.22	1.33
1	A	1187	GLN	CB-CG	9.80	1.81	1.52
2	B	1087	PHE	C-O	-9.80	1.12	1.23
9	K	97	LYS	C-O	-9.80	1.11	1.24
2	B	368	GLU	CA-CB	9.80	1.68	1.53
1	A	1438	THR	CB-CG2	-9.79	1.20	1.52
1	A	1385	THR	CA-C	9.78	1.73	1.52
8	J	54	VAL	N-CA	-9.78	1.33	1.46
7	I	82	GLU	CD-OE1	9.78	1.44	1.25
2	B	231	PRO	CA-C	9.78	1.69	1.52
2	B	865	LYS	CA-CB	9.78	1.70	1.53
2	B	481	GLN	C-O	9.77	1.35	1.23
10	L	50	ASP	CA-C	9.77	1.65	1.52
2	B	958	GLN	N-CA	9.77	1.58	1.46
1	A	1020	CYS	C-O	9.76	1.36	1.24
1	A	1222	ASN	CA-CB	9.76	1.68	1.53
2	B	308	TRP	CA-C	-9.76	1.39	1.52
2	B	213	ILE	N-CA	-9.76	1.33	1.46
1	A	443	LEU	CA-C	-9.75	1.40	1.52
1	A	1217	LYS	C-O	9.75	1.36	1.24
2	B	737	THR	C-O	-9.75	1.11	1.24
3	C	55	THR	CB-OG1	-9.75	1.28	1.43
1	A	450	LEU	N-CA	-9.75	1.32	1.46
6	H	77	ARG	CB-CG	9.74	1.81	1.52
2	B	870	ILE	N-CA	9.74	1.58	1.46
1	A	43	GLU	CA-C	9.74	1.65	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	190	LEU	C-O	9.74	1.36	1.23
1	A	734	GLU	CD-OE2	9.72	1.43	1.25
2	B	620	ARG	CG-CD	9.72	1.81	1.52
1	A	1311	VAL	N-CA	-9.72	1.34	1.46
2	B	864	LYS	CA-C	9.72	1.65	1.52
1	A	590	ARG	CZ-NH2	-9.71	1.20	1.33
1	A	1003	LYS	CD-CE	9.71	1.81	1.52
9	K	67	PHE	C-O	-9.71	1.11	1.24
4	E	52	ARG	CA-C	9.71	1.64	1.53
1	A	854	ASN	CA-CB	-9.70	1.39	1.53
1	A	980	ASP	C-O	9.70	1.36	1.24
2	B	1129	ARG	NE-CZ	9.70	1.43	1.33
1	A	1227	ILE	N-CA	-9.70	1.34	1.46
2	B	896	ASP	CA-C	-9.70	1.39	1.52
5	F	129	LYS	CE-NZ	9.70	1.78	1.49
3	C	113	VAL	CA-CB	-9.70	1.42	1.54
1	A	107	CYS	CA-CB	9.69	1.67	1.53
7	I	61	ASP	C-O	-9.69	1.11	1.24
8	J	24	LEU	C-O	-9.69	1.11	1.24
1	A	1066	VAL	CA-C	-9.68	1.41	1.52
1	A	1115	SER	CA-C	9.67	1.64	1.52
1	A	74	MET	SD-CE	9.67	2.03	1.79
1	A	961	ARG	NE-CZ	9.67	1.43	1.33
1	A	1056	SER	C-O	-9.67	1.11	1.24
2	B	822	ASN	C-O	-9.67	1.12	1.24
1	A	1171	GLN	CG-CD	9.66	1.76	1.52
1	A	24	PRO	CA-C	9.66	1.66	1.52
8	J	13	VAL	C-O	-9.66	1.12	1.24
1	A	761	MET	CA-C	-9.65	1.40	1.52
1	A	940	ARG	CD-NE	-9.65	1.32	1.46
1	A	901	LEU	C-O	9.65	1.36	1.24
1	A	137	ALA	C-O	9.64	1.35	1.24
1	A	1256	GLU	CA-C	9.64	1.65	1.52
1	A	1077	THR	CA-C	9.64	1.65	1.52
1	A	1032	LEU	CA-C	-9.63	1.41	1.52
2	B	1169	MET	SD-CE	9.63	2.03	1.79
1	A	1132	LYS	CD-CE	9.63	1.81	1.52
2	B	482	VAL	CA-C	-9.63	1.42	1.52
2	B	297	ILE	CG1-CD1	-9.63	1.14	1.51
2	B	304	ASP	N-CA	9.63	1.58	1.46
2	B	911	ILE	CA-CB	9.63	1.67	1.54
4	E	41	ASP	CB-CG	9.63	1.76	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	459	ARG	CD-NE	-9.62	1.32	1.46
1	A	225	ASN	CA-C	9.62	1.64	1.52
8	J	8	PHE	C-O	-9.62	1.12	1.24
1	A	566	ILE	CB-CG2	9.62	1.84	1.52
1	A	1222	ASN	CB-CG	9.61	1.76	1.52
4	E	42	PHE	C-O	9.61	1.36	1.24
2	B	554	ILE	CG1-CD1	-9.61	1.14	1.51
6	H	131	ASN	CA-C	9.60	1.65	1.52
1	A	1057	VAL	CA-CB	9.60	1.65	1.54
2	B	1019	SER	CB-OG	-9.60	1.23	1.42
1	A	1157	ASP	C-O	9.59	1.35	1.24
4	E	152	LYS	CG-CD	9.59	1.81	1.52
1	A	1426	GLU	C-O	9.59	1.35	1.24
2	B	115	GLN	CG-CD	9.59	1.76	1.52
1	A	1349	TYR	CG-CD2	-9.58	1.19	1.39
1	A	85	ASP	C-O	9.57	1.35	1.23
1	A	967	ALA	CA-CB	-9.57	1.37	1.53
3	C	166	GLU	CD-OE2	9.57	1.43	1.25
7	I	52	ILE	CA-C	-9.57	1.41	1.52
1	A	219	PHE	C-O	-9.57	1.11	1.24
1	A	864	ILE	C-O	9.57	1.33	1.23
2	B	1001	PHE	CA-C	-9.57	1.41	1.52
6	H	52	GLN	CG-CD	9.57	1.75	1.52
2	B	1072	MET	SD-CE	-9.56	1.55	1.79
4	E	14	ARG	CZ-NH2	-9.56	1.21	1.33
1	A	125	ALA	CA-CB	-9.56	1.37	1.53
1	A	975	HIS	CA-C	9.56	1.65	1.52
2	B	285	ILE	CA-CB	-9.55	1.42	1.54
1	A	713	SER	N-CA	-9.55	1.34	1.46
2	B	484	ASN	CB-CG	-9.55	1.28	1.52
1	A	1144	LYS	N-CA	-9.55	1.35	1.46
2	B	802	PRO	C-O	-9.55	1.13	1.23
2	B	945	GLU	CA-C	9.55	1.65	1.52
2	B	1182	CYS	CA-C	9.54	1.65	1.52
10	L	27	LEU	CB-CG	9.54	1.72	1.53
1	A	449	SER	C-O	-9.54	1.10	1.23
1	A	1241	ARG	CA-C	-9.54	1.40	1.52
6	H	19	ARG	NE-CZ	9.53	1.43	1.33
3	C	232	VAL	CA-CB	-9.53	1.42	1.54
3	C	97	VAL	CA-CB	-9.53	1.42	1.54
1	A	270	LEU	CA-C	9.52	1.65	1.52
2	B	986	GLN	CA-C	9.52	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1326	ARG	CA-C	9.51	1.65	1.52
2	B	704	ALA	C-O	-9.51	1.12	1.23
1	A	919	ILE	N-CA	9.51	1.56	1.46
2	B	1079	LYS	CA-C	-9.51	1.40	1.52
3	C	35	ARG	CZ-NH2	-9.51	1.21	1.33
2	B	657	HIS	C-N	-9.50	1.22	1.33
6	H	35	GLN	CA-C	9.49	1.63	1.52
6	H	90	ALA	CA-CB	-9.49	1.37	1.53
2	B	420	LEU	CA-C	-9.49	1.39	1.52
7	I	99	LEU	C-O	-9.49	1.12	1.23
10	L	62	LYS	CD-CE	9.48	1.80	1.52
1	A	837	ILE	N-CA	-9.48	1.35	1.46
1	A	644	LYS	C-O	-9.48	1.12	1.24
2	B	695	ALA	N-CA	-9.47	1.34	1.46
1	A	1305	VAL	C-O	-9.47	1.14	1.24
1	A	1148	ILE	C-O	-9.46	1.13	1.24
9	K	8	GLU	C-O	9.46	1.36	1.24
1	A	32	VAL	CA-C	9.45	1.64	1.52
2	B	529	GLU	CD-OE1	9.45	1.43	1.25
3	C	198	ALA	CA-CB	-9.45	1.38	1.53
9	K	40	HIS	CA-C	9.45	1.65	1.52
1	A	192	GLY	C-O	9.44	1.32	1.23
1	A	1415	SER	C-O	-9.44	1.11	1.24
6	H	131	ASN	N-CA	9.44	1.57	1.46
1	A	563	PRO	CA-C	-9.43	1.40	1.52
4	E	155	ARG	NE-CZ	9.43	1.43	1.33
2	B	1193	GLN	C-O	-9.43	1.11	1.23
1	A	645	LEU	C-O	-9.43	1.13	1.24
2	B	557	PHE	C-O	9.43	1.35	1.24
2	B	40	GLU	CA-C	-9.43	1.40	1.52
2	B	866	TYR	N-CA	9.42	1.59	1.46
1	A	169	ASN	CA-C	-9.42	1.40	1.52
2	B	730	ARG	C-O	-9.42	1.12	1.23
7	I	83	ASN	C-O	9.42	1.35	1.23
3	C	47	ASP	C-O	-9.41	1.10	1.24
1	A	605	MET	SD-CE	-9.41	1.56	1.79
1	A	742	ASN	CB-CG	-9.41	1.28	1.52
1	A	813	PHE	N-CA	-9.41	1.34	1.46
3	C	175	ALA	CA-C	-9.41	1.40	1.53
3	C	252	GLN	C-O	-9.41	1.13	1.24
2	B	371	GLU	C-O	-9.41	1.11	1.24
1	A	557	ASP	CA-C	9.40	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	662	MET	CG-SD	-9.40	1.57	1.80
6	H	21	ASN	CA-C	-9.40	1.40	1.52
9	K	26	LYS	CG-CD	9.40	1.80	1.52
4	E	7	ARG	NE-CZ	9.40	1.43	1.33
1	A	459	ARG	C-O	-9.40	1.12	1.24
1	A	1234	GLU	CD-OE1	9.40	1.43	1.25
4	E	136	ASN	C-O	-9.40	1.12	1.23
6	H	28	ALA	CA-C	9.40	1.64	1.52
3	C	241	ASP	CA-CB	9.39	1.69	1.53
1	A	860	LEU	C-O	-9.39	1.11	1.24
8	J	30	LEU	CA-C	-9.39	1.40	1.52
2	B	345	LYS	C-O	-9.39	1.12	1.24
1	A	843	LYS	CD-CE	9.38	1.80	1.52
2	B	211	VAL	N-CA	-9.38	1.35	1.46
2	B	970	THR	CA-CB	-9.38	1.30	1.54
2	B	1057	LYS	CG-CD	9.38	1.80	1.52
2	B	105	SER	CA-C	9.38	1.65	1.52
2	B	200	GLY	C-O	-9.38	1.08	1.23
4	E	66	GLU	CD-OE2	9.38	1.43	1.25
1	A	917	SER	CA-C	-9.37	1.41	1.52
1	A	47	ARG	CA-C	9.37	1.65	1.52
1	A	191	THR	N-CA	9.37	1.58	1.46
5	F	122	MET	CA-C	-9.37	1.40	1.52
6	H	86	ASP	CA-C	9.37	1.65	1.52
4	E	9	ILE	CA-CB	9.36	1.67	1.54
4	E	207	ARG	NE-CZ	9.37	1.43	1.33
1	A	295	LEU	CG-CD2	9.36	1.83	1.52
1	A	1280	GLU	CG-CD	9.36	1.75	1.52
8	J	56	LEU	N-CA	-9.36	1.33	1.46
2	B	385	LEU	CA-C	-9.36	1.41	1.52
7	I	51	ASN	C-O	-9.35	1.11	1.24
1	A	416	ARG	C-O	-9.35	1.11	1.24
10	L	56	LEU	C-O	-9.35	1.12	1.24
2	B	940	PRO	C-O	-9.35	1.11	1.24
10	L	61	THR	CB-CG2	9.35	1.83	1.52
2	B	1215	ARG	C-O	-9.35	1.12	1.24
1	A	1384	VAL	CA-CB	-9.34	1.44	1.54
1	A	902	LEU	N-CA	-9.34	1.35	1.46
1	A	1169	ILE	CA-CB	9.33	1.67	1.54
7	I	119	THR	N-CA	9.33	1.57	1.46
1	A	1264	GLU	CD-OE1	-9.33	1.07	1.25
2	B	55	VAL	C-O	9.33	1.35	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	39	ARG	N-CA	9.32	1.57	1.46
5	F	116	ASP	C-O	-9.32	1.12	1.24
1	A	580	VAL	CA-CB	-9.32	1.41	1.54
2	B	1041	GLU	CD-OE1	9.31	1.43	1.25
1	A	1225	PHE	CA-CB	9.31	1.67	1.53
10	L	42	ARG	CA-C	9.31	1.63	1.52
3	C	104	PHE	CA-C	-9.30	1.41	1.52
1	A	1119	TYR	C-O	9.30	1.35	1.23
3	C	174	ALA	C-O	-9.30	1.12	1.24
1	A	603	ASN	CB-CG	-9.30	1.28	1.52
2	B	399	ASP	CB-CG	9.30	1.75	1.52
4	E	199	ILE	CA-C	-9.30	1.40	1.52
2	B	263	GLY	C-O	9.29	1.36	1.23
3	C	234	SER	CA-C	-9.29	1.41	1.52
1	A	195	ASP	CA-C	9.29	1.66	1.53
1	A	577	ILE	CA-CB	-9.29	1.42	1.54
2	B	234	ILE	N-CA	-9.29	1.35	1.46
1	A	781	ASP	C-O	9.29	1.39	1.24
2	B	367	LEU	CA-CB	9.29	1.67	1.53
2	B	793	ALA	N-CA	-9.28	1.34	1.46
10	L	37	LYS	C-O	-9.29	1.12	1.24
1	A	367	PRO	CA-C	-9.28	1.42	1.52
1	A	689	LYS	C-O	-9.28	1.13	1.24
1	A	843	LYS	CA-CB	9.28	1.67	1.53
2	B	24	PRO	CA-CB	-9.28	1.42	1.53
2	B	1185	CYS	CA-CB	9.28	1.69	1.53
1	A	167	CYS	CA-C	9.27	1.65	1.52
1	A	1223	ASP	CB-CG	9.27	1.75	1.52
2	B	249	ARG	NE-CZ	9.27	1.43	1.33
3	C	199	LYS	CD-CE	9.27	1.80	1.52
9	K	78	THR	CA-CB	-9.26	1.38	1.53
2	B	45	SER	CA-C	-9.26	1.39	1.52
10	L	27	LEU	CA-C	9.26	1.65	1.52
2	B	1135	ARG	C-O	-9.26	1.13	1.24
2	B	706	GLN	CG-CD	9.25	1.75	1.52
2	B	682	SER	CA-C	-9.25	1.40	1.52
9	K	111	LEU	CA-C	9.25	1.65	1.52
1	A	34	LYS	C-O	-9.24	1.11	1.24
1	A	109	HIS	CA-C	9.24	1.61	1.53
9	K	5	ASP	CG-OD2	9.24	1.43	1.25
1	A	367	PRO	CA-CB	-9.24	1.41	1.53
5	F	121	ALA	C-N	-9.24	1.21	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	65	LEU	CA-C	9.24	1.65	1.52
3	C	252	GLN	CD-OE1	9.24	1.41	1.23
6	H	55	LEU	CA-C	-9.24	1.41	1.52
1	A	822	GLU	C-O	-9.24	1.13	1.24
1	A	803	SER	C-O	-9.23	1.11	1.23
2	B	1075	GLY	C-O	9.23	1.34	1.23
3	C	43	THR	C-O	9.23	1.34	1.23
2	B	432	MET	SD-CE	9.23	2.02	1.79
2	B	946	ASN	C-O	-9.23	1.12	1.23
2	B	1011	ILE	CA-CB	9.22	1.66	1.54
2	B	618	ASP	C-O	9.22	1.34	1.24
1	A	537	ARG	CZ-NH2	9.22	1.45	1.33
4	E	129	PRO	CG-CD	9.22	1.76	1.51
2	B	1214	PRO	C-O	9.21	1.35	1.24
1	A	438	ASP	CA-C	-9.21	1.40	1.52
1	A	1265	ASN	CA-C	9.21	1.65	1.52
4	E	50	MET	CA-C	9.20	1.65	1.52
2	B	266	ALA	C-O	9.20	1.35	1.24
7	I	31	THR	CA-C	9.20	1.64	1.52
1	A	606	LEU	N-CA	-9.20	1.34	1.46
4	E	166	LYS	C-O	9.20	1.34	1.24
1	A	53	LEU	N-CA	9.19	1.59	1.46
2	B	1067	ARG	CZ-NH2	-9.19	1.21	1.33
7	I	18	GLU	CA-C	9.19	1.64	1.52
10	L	44	ASP	C-O	9.19	1.35	1.24
6	H	135	LEU	CA-C	9.19	1.65	1.52
1	A	469	ARG	CD-NE	-9.19	1.33	1.46
2	B	217	ARG	CZ-NH1	-9.19	1.19	1.32
8	J	62	ARG	C-O	-9.19	1.11	1.24
10	L	46	VAL	C-O	-9.19	1.13	1.24
1	A	27	VAL	CA-CB	-9.18	1.43	1.54
1	A	1064	VAL	C-N	-9.18	1.20	1.33
2	B	1085	ILE	CG1-CD1	-9.18	1.16	1.51
2	B	1097	HIS	CB-CG	-9.18	1.37	1.50
1	A	941	LYS	CE-NZ	9.18	1.76	1.49
2	B	136	THR	CA-C	9.18	1.64	1.52
5	F	148	VAL	CA-C	-9.18	1.41	1.52
1	A	734	GLU	CD-OE1	9.18	1.42	1.25
1	A	74	MET	CB-CG	9.18	1.79	1.52
1	A	111	GLY	C-O	9.18	1.36	1.24
1	A	1424	VAL	CA-CB	-9.18	1.42	1.54
1	A	217	LYS	CG-CD	9.17	1.79	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	749	LEU	C-O	9.17	1.35	1.23
2	B	224	GLN	C-O	-9.17	1.13	1.24
2	B	595	ARG	CD-NE	9.17	1.59	1.46
1	A	301	ALA	N-CA	9.17	1.57	1.46
2	B	895	ASP	CA-CB	9.17	1.68	1.53
9	K	103	THR	C-O	9.17	1.35	1.24
2	B	883	LEU	CB-CG	9.16	1.71	1.53
1	A	624	SER	N-CA	9.16	1.58	1.46
3	C	23	SER	CA-CB	9.16	1.68	1.53
3	C	208	GLU	CA-C	9.16	1.65	1.52
1	A	358	ASN	CA-C	-9.15	1.40	1.52
1	A	229	SER	CA-C	9.15	1.64	1.53
1	A	612	ILE	CA-C	-9.15	1.42	1.52
1	A	671	ALA	C-O	-9.15	1.12	1.23
1	A	792	TYR	CA-C	-9.15	1.39	1.52
3	C	209	TYR	CE2-CZ	9.15	1.60	1.38
5	F	146	TRP	CA-C	9.15	1.63	1.52
2	B	18	PHE	CB-CG	9.15	1.71	1.50
2	B	589	VAL	CA-CB	-9.15	1.41	1.54
7	I	36	GLU	CA-CB	-9.15	1.37	1.53
1	A	181	LEU	C-O	9.14	1.34	1.23
2	B	136	THR	CA-CB	9.14	1.66	1.53
1	A	406	ILE	CA-CB	-9.14	1.42	1.54
6	H	131	ASN	CB-CG	9.13	1.74	1.52
1	A	1235	LYS	CD-CE	9.13	1.79	1.52
2	B	1069	PHE	C-O	9.13	1.35	1.23
9	K	54	ARG	NE-CZ	9.13	1.43	1.33
10	L	42	ARG	NE-CZ	9.12	1.43	1.33
2	B	367	LEU	CA-C	9.12	1.64	1.52
2	B	556	THR	CA-C	9.12	1.64	1.52
1	A	958	VAL	CA-CB	-9.12	1.42	1.54
2	B	758	PHE	CE2-CZ	-9.12	1.11	1.38
2	B	1146	PHE	C-O	-9.12	1.13	1.24
1	A	184	SER	CA-C	9.12	1.62	1.53
3	C	239	PRO	C-N	-9.11	1.23	1.33
2	B	709	ASP	C-O	-9.10	1.12	1.24
1	A	171	GLN	CD-NE2	9.10	1.52	1.33
1	A	515	GLN	CA-C	-9.10	1.41	1.52
2	B	1012	ILE	CA-CB	-9.10	1.42	1.54
1	A	1336	MET	SD-CE	-9.09	1.56	1.79
2	B	394	ASP	CG-OD2	9.09	1.42	1.25
6	H	19	ARG	N-CA	9.09	1.57	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	728	ARG	CZ-NH1	-9.09	1.20	1.32
1	A	497	THR	CB-CG2	-9.09	1.22	1.52
2	B	351	TYR	C-O	9.09	1.34	1.24
2	B	645	SER	CA-C	9.09	1.65	1.52
1	A	858	ASN	CB-CG	-9.09	1.29	1.52
3	C	34	ARG	CD-NE	-9.09	1.33	1.46
1	A	982	THR	CB-OG1	-9.08	1.29	1.43
1	A	1064	VAL	N-CA	-9.08	1.36	1.46
8	J	31	ASP	CA-C	9.08	1.64	1.52
10	L	67	PHE	C-O	-9.07	1.12	1.23
1	A	1216	ILE	CA-CB	-9.07	1.43	1.54
4	E	9	ILE	CA-C	-9.07	1.40	1.52
2	B	30	SER	N-CA	9.06	1.57	1.46
2	B	1021	MET	CG-SD	-9.06	1.58	1.80
2	B	459	TYR	CG-CD2	9.06	1.58	1.39
1	A	795	GLU	CA-C	-9.06	1.41	1.52
1	A	886	ILE	CA-CB	9.06	1.66	1.54
2	B	1081	LEU	CA-C	-9.05	1.41	1.52
2	B	209	GLU	CA-CB	-9.04	1.40	1.53
1	A	896	ARG	CZ-NH1	9.04	1.45	1.32
2	B	118	ARG	CD-NE	-9.04	1.33	1.46
1	A	741	ASN	C-O	-9.04	1.13	1.24
4	E	122	LYS	CA-CB	9.04	1.68	1.53
2	B	479	VAL	CA-CB	-9.03	1.41	1.54
4	E	186	LEU	CA-C	-9.03	1.41	1.52
2	B	787	VAL	CA-CB	-9.03	1.45	1.54
2	B	581	PHE	C-O	9.03	1.35	1.23
7	I	25	LEU	CA-C	9.03	1.63	1.52
1	A	1027	ALA	N-CA	-9.02	1.34	1.45
7	I	74	GLU	CA-C	-9.02	1.42	1.52
1	A	1354	ASN	C-O	-9.02	1.13	1.24
6	H	123	MET	CG-SD	9.02	2.03	1.80
1	A	730	GLY	CA-C	-9.02	1.39	1.51
1	A	548	ASN	CA-C	9.01	1.64	1.52
2	B	937	ALA	N-CA	9.01	1.57	1.46
7	I	46	HIS	CA-C	-9.01	1.42	1.52
2	B	838	SER	CB-OG	-9.01	1.24	1.42
1	A	9	ALA	CA-C	-9.00	1.42	1.52
1	A	49	LYS	CD-CE	9.00	1.79	1.52
3	C	185	LYS	CA-C	-9.00	1.40	1.52
2	B	328	GLU	CD-OE2	9.00	1.42	1.25
1	A	1278	ASN	CG-OD1	9.00	1.40	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	364	ILE	N-CA	-9.00	1.35	1.46
2	B	657	HIS	C-O	-9.00	1.13	1.24
1	A	1191	TRP	C-O	8.99	1.34	1.24
2	B	198	ASP	CB-CG	-8.99	1.29	1.52
2	B	249	ARG	CA-C	8.99	1.64	1.52
1	A	808	LEU	C-O	-8.99	1.12	1.23
1	A	1215	ARG	CA-C	-8.99	1.41	1.52
1	A	1320	PRO	CA-C	-8.99	1.41	1.52
1	A	269	ILE	C-O	-8.98	1.13	1.24
1	A	123	ARG	NE-CZ	8.98	1.43	1.33
2	B	1012	ILE	C-O	-8.97	1.13	1.24
2	B	227	LYS	CD-CE	8.97	1.79	1.52
2	B	499	ASN	CA-C	-8.97	1.41	1.52
2	B	1171	VAL	C-O	8.97	1.32	1.24
4	E	164	LEU	CA-CB	-8.97	1.39	1.53
2	B	870	ILE	CG1-CD1	8.96	1.86	1.51
2	B	256	VAL	C-O	-8.96	1.14	1.24
2	B	55	VAL	N-CA	-8.95	1.35	1.46
2	B	735	ALA	CA-CB	-8.95	1.39	1.53
2	B	951	GLN	N-CA	-8.95	1.34	1.46
3	C	205	LYS	N-CA	8.95	1.57	1.46
1	A	462	VAL	CA-C	-8.95	1.42	1.52
1	A	108	MET	SD-CE	-8.94	1.57	1.79
1	A	1419	ASP	CA-C	-8.94	1.41	1.52
1	A	892	ALA	C-O	-8.94	1.12	1.24
1	A	1110	ASN	CB-CG	8.94	1.74	1.52
4	E	134	THR	C-O	-8.94	1.12	1.24
1	A	684	ALA	CA-C	8.93	1.64	1.52
2	B	124	TYR	CA-CB	-8.93	1.38	1.53
1	A	384	ASN	CA-C	8.93	1.64	1.52
1	A	1209	MET	SD-CE	-8.93	1.57	1.79
2	B	337	ARG	CD-NE	-8.93	1.33	1.46
1	A	1039	LYS	CA-C	8.93	1.64	1.52
1	A	1126	ALA	CA-CB	-8.92	1.38	1.53
1	A	1230	GLU	CD-OE1	8.92	1.42	1.25
2	B	188	ASP	C-O	8.92	1.34	1.24
1	A	414	ASP	C-O	-8.92	1.13	1.24
1	A	455	MET	N-CA	8.92	1.57	1.46
3	C	174	ALA	CA-CB	-8.92	1.39	1.52
1	A	1193	LEU	C-N	-8.92	1.22	1.33
1	A	1256	GLU	N-CA	8.92	1.57	1.46
2	B	31	TRP	CZ3-CH2	-8.92	1.18	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	163	GLU	CA-CB	8.92	1.67	1.53
1	A	110	CYS	CA-CB	8.91	1.67	1.53
1	A	995	GLU	CD-OE2	8.90	1.42	1.25
4	E	63	ASN	CA-C	8.90	1.64	1.52
1	A	302	THR	CA-CB	8.89	1.67	1.53
1	A	985	ASP	CG-OD2	8.89	1.42	1.25
9	K	9	LEU	C-O	8.89	1.35	1.24
10	L	63	ARG	CD-NE	8.89	1.58	1.46
1	A	66	LYS	CA-C	8.89	1.62	1.52
2	B	451	LYS	CA-C	8.89	1.64	1.52
2	B	494	HIS	C-O	-8.89	1.13	1.24
9	K	102	LYS	CA-C	8.89	1.64	1.52
1	A	151	ASP	C-O	-8.88	1.11	1.23
1	A	1346	ALA	CA-C	8.88	1.64	1.52
2	B	697	GLU	C-O	-8.88	1.12	1.24
1	A	770	VAL	C-O	-8.88	1.14	1.24
1	A	1372	VAL	CB-CG1	-8.88	1.23	1.52
2	B	233	PRO	CA-C	8.88	1.65	1.52
9	K	61	TYR	C-O	-8.87	1.12	1.23
2	B	1060	ARG	CZ-NH2	-8.86	1.22	1.33
2	B	1128	LEU	N-CA	8.86	1.57	1.46
1	A	387	ARG	CG-CD	8.86	1.79	1.52
2	B	1069	PHE	CA-C	8.86	1.64	1.52
7	I	120	GLN	CB-CG	8.86	1.79	1.52
1	A	1011	GLN	CD-OE1	-8.85	1.06	1.23
4	E	92	THR	N-CA	8.85	1.56	1.46
3	C	240	VAL	CA-C	-8.85	1.42	1.52
5	F	126	ALA	C-O	-8.85	1.13	1.24
9	K	93	SER	C-O	8.85	1.35	1.24
1	A	16	GLU	CD-OE1	8.84	1.42	1.25
7	I	105	SER	N-CA	8.84	1.57	1.46
9	K	36	GLU	CA-CB	-8.84	1.39	1.53
1	A	1348	LEU	C-O	-8.84	1.13	1.24
3	C	184	ASN	N-CA	8.84	1.58	1.46
1	A	613	ILE	CA-CB	8.83	1.62	1.55
3	C	90	ASP	N-CA	8.83	1.57	1.46
1	A	579	SER	C-O	8.83	1.35	1.24
2	B	1071	VAL	C-O	8.83	1.35	1.24
2	B	643	ASP	CA-CB	8.83	1.68	1.53
1	A	406	ILE	CA-C	-8.83	1.41	1.52
6	H	57	VAL	CA-C	8.83	1.62	1.52
2	B	973	ILE	N-CA	-8.82	1.35	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	85	PHE	C-O	-8.82	1.13	1.23
3	C	173	ALA	C-O	-8.82	1.12	1.23
2	B	538	ASN	CA-CB	-8.82	1.38	1.53
1	A	720	ARG	CG-CD	8.81	1.78	1.52
2	B	191	LYS	CA-C	-8.81	1.41	1.52
2	B	690	VAL	C-O	-8.81	1.15	1.24
4	E	28	TYR	CA-C	-8.81	1.41	1.52
2	B	241	ARG	NE-CZ	8.81	1.42	1.33
1	A	1111	MET	CG-SD	8.80	2.02	1.80
2	B	267	ARG	C-O	-8.80	1.13	1.23
5	F	110	ASP	C-O	8.80	1.34	1.24
2	B	459	TYR	C-O	-8.80	1.14	1.24
1	A	163	SER	N-CA	8.80	1.57	1.45
1	A	1225	PHE	C-O	-8.80	1.14	1.24
6	H	58	THR	CA-C	8.80	1.64	1.52
7	I	1	MET	SD-CE	8.80	2.01	1.79
3	C	62	PHE	C-O	-8.79	1.14	1.24
1	A	545	GLN	C-O	-8.79	1.13	1.24
1	A	1436	ILE	CA-C	8.79	1.63	1.52
2	B	325	GLN	CD-OE1	8.79	1.40	1.23
2	B	764	SER	CB-OG	-8.79	1.24	1.42
1	A	1147	THR	C-O	-8.79	1.13	1.24
2	B	643	ASP	C-O	-8.79	1.12	1.24
4	E	137	GLU	CD-OE1	8.79	1.42	1.25
7	I	30	ARG	CA-CB	-8.78	1.39	1.53
9	K	111	LEU	CG-CD1	8.78	1.81	1.52
2	B	882	THR	N-CA	8.78	1.57	1.46
2	B	1180	PHE	C-O	8.78	1.33	1.24
9	K	61	TYR	CE1-CZ	-8.78	1.17	1.38
1	A	199	LEU	CG-CD1	8.77	1.81	1.52
1	A	841	LEU	CA-C	8.77	1.64	1.52
1	A	1237	ILE	CA-CB	-8.77	1.42	1.54
1	A	842	VAL	C-O	-8.77	1.14	1.24
2	B	1216	LEU	C-O	8.77	1.34	1.24
1	A	664	THR	CA-C	-8.76	1.41	1.52
2	B	605	ARG	NE-CZ	-8.76	1.23	1.33
10	L	55	ILE	CA-CB	8.76	1.65	1.54
1	A	1341	ILE	CA-CB	-8.76	1.43	1.54
8	J	29	GLU	CA-C	8.76	1.65	1.53
2	B	580	VAL	CA-CB	-8.76	1.43	1.54
7	I	28	GLU	CD-OE2	8.76	1.42	1.25
1	A	167	CYS	N-CA	8.75	1.57	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	12	ARG	C-O	-8.75	1.12	1.23
1	A	1314	SER	C-O	8.75	1.35	1.24
2	B	244	LEU	CA-C	8.75	1.62	1.52
6	H	132	LEU	CA-C	8.75	1.63	1.53
9	K	26	LYS	CB-CG	8.75	1.78	1.52
4	E	50	MET	CG-SD	8.74	2.02	1.80
2	B	240	ILE	CA-C	-8.74	1.42	1.52
1	A	117	GLU	CD-OE1	8.74	1.42	1.25
1	A	1224	LEU	CA-CB	-8.74	1.40	1.53
7	I	45	ARG	CD-NE	8.74	1.58	1.46
1	A	346	ASP	CA-CB	8.74	1.71	1.53
1	A	1187	GLN	CG-CD	8.74	1.73	1.52
2	B	110	HIS	CA-C	8.74	1.62	1.52
2	B	586	TRP	C-O	-8.74	1.13	1.24
2	B	604	ARG	N-CA	8.74	1.57	1.46
4	E	62	ALA	CA-C	-8.74	1.41	1.52
2	B	820	GLY	N-CA	-8.73	1.34	1.45
3	C	204	SER	C-O	8.73	1.34	1.23
1	A	1196	GLU	CA-C	8.73	1.62	1.52
3	C	79	GLN	N-CA	-8.73	1.36	1.46
2	B	1195	HIS	CA-C	8.73	1.63	1.52
1	A	280	GLU	N-CA	-8.72	1.35	1.46
7	I	84	VAL	CB-CG2	-8.72	1.23	1.52
1	A	285	PRO	C-O	-8.72	1.12	1.23
1	A	697	ALA	CA-CB	-8.72	1.39	1.53
4	E	211	TYR	CE1-CZ	-8.72	1.17	1.38
3	C	123	ASN	CA-CB	8.71	1.64	1.53
1	A	107	CYS	CA-C	-8.71	1.42	1.52
3	C	176	ILE	C-O	-8.71	1.14	1.24
7	I	111	THR	CA-CB	-8.71	1.33	1.53
4	E	54	GLN	CB-CG	8.71	1.78	1.52
1	A	113	LEU	C-O	8.70	1.34	1.23
1	A	718	VAL	CA-CB	-8.70	1.42	1.54
1	A	193	ASP	CA-CB	8.69	1.68	1.53
1	A	1291	VAL	CA-CB	-8.69	1.40	1.54
1	A	1362	TYR	C-O	-8.68	1.14	1.23
1	A	549	MET	CA-C	-8.67	1.41	1.52
1	A	437	MET	C-O	-8.66	1.12	1.23
7	I	6	PHE	C-O	-8.66	1.12	1.23
1	A	656	TRP	CG-CD2	-8.66	1.28	1.43
3	C	37	MET	CA-C	-8.66	1.42	1.52
1	A	305	ASP	N-CA	8.66	1.62	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	K	76	GLN	CA-C	8.65	1.62	1.52
1	A	105	CYS	N-CA	8.65	1.57	1.45
1	A	226	GLU	CD-OE2	8.65	1.41	1.25
1	A	913	LEU	CA-CB	8.65	1.68	1.53
2	B	204	ILE	CG1-CD1	-8.65	1.18	1.51
2	B	973	ILE	C-O	8.65	1.35	1.24
3	C	249	ASP	CA-CB	8.65	1.66	1.53
1	A	1200	ALA	C-O	8.65	1.34	1.24
3	C	15	LYS	C-O	-8.65	1.12	1.24
3	C	22	LEU	C-O	-8.65	1.13	1.23
1	A	1226	VAL	C-O	8.64	1.32	1.24
2	B	591	ARG	CA-C	-8.64	1.41	1.52
3	C	188	HIS	CA-C	8.64	1.64	1.52
1	A	696	GLU	N-CA	-8.64	1.36	1.46
2	B	371	GLU	CD-OE1	8.63	1.41	1.25
9	K	54	ARG	CD-NE	8.63	1.58	1.46
2	B	729	ILE	CA-CB	-8.63	1.43	1.53
3	C	16	ASP	CA-C	8.63	1.63	1.52
2	B	208	SER	C-O	8.62	1.34	1.24
2	B	1102	LYS	CA-CB	8.62	1.69	1.54
4	E	75	MET	C-O	8.62	1.34	1.24
5	F	78	GLN	C-O	-8.62	1.13	1.24
2	B	358	LYS	CA-C	-8.62	1.41	1.52
2	B	706	GLN	CA-C	-8.61	1.42	1.52
1	A	737	LEU	C-O	8.61	1.33	1.23
2	B	337	ARG	NE-CZ	-8.61	1.23	1.33
2	B	916	THR	CA-C	8.61	1.71	1.52
2	B	970	THR	C-O	-8.61	1.13	1.23
7	I	21	GLU	C-O	-8.61	1.13	1.24
1	A	264	PHE	CB-CG	8.60	1.70	1.50
4	E	127	ILE	CA-C	-8.60	1.43	1.52
1	A	1336	MET	C-O	-8.60	1.13	1.24
4	E	106	GLN	CG-CD	8.60	1.73	1.52
5	F	129	LYS	CD-CE	8.60	1.78	1.52
1	A	931	GLU	CD-OE2	8.60	1.41	1.25
1	A	1418	LEU	C-O	-8.59	1.13	1.23
2	B	782	LEU	CG-CD1	-8.59	1.24	1.52
2	B	1098	MET	C-O	-8.59	1.12	1.23
7	I	45	ARG	CZ-NH2	-8.59	1.22	1.33
7	I	50	THR	C-O	-8.59	1.12	1.23
2	B	331	LEU	CA-C	-8.59	1.41	1.52
1	A	883	LEU	N-CA	-8.58	1.35	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	348	ARG	C-O	-8.58	1.14	1.24
1	A	207	ILE	CG1-CD1	-8.58	1.18	1.51
1	A	1163	ILE	C-O	8.58	1.34	1.24
1	A	1132	LYS	CG-CD	8.58	1.78	1.52
1	A	1203	ASN	C-O	8.58	1.34	1.24
1	A	1345	ARG	NE-CZ	-8.57	1.23	1.33
2	B	708	GLU	N-CA	-8.57	1.34	1.46
2	B	948	ILE	C-O	-8.57	1.13	1.24
1	A	881	GLN	N-CA	-8.57	1.35	1.45
7	I	82	GLU	CA-C	8.57	1.64	1.53
1	A	356	ASP	C-N	-8.57	1.24	1.34
1	A	705	LYS	CA-CB	8.57	1.74	1.53
1	A	11	LEU	C-O	-8.56	1.13	1.24
1	A	985	ASP	C-O	-8.56	1.14	1.24
1	A	160	GLN	CA-C	-8.56	1.42	1.52
1	A	681	GLU	CD-OE2	8.56	1.41	1.25
2	B	39	ARG	CZ-NH2	8.55	1.44	1.33
2	B	479	VAL	CA-C	-8.55	1.39	1.52
2	B	1103	ILE	C-O	8.55	1.34	1.24
1	A	1322	ILE	CB-CG2	-8.55	1.24	1.52
3	C	65	HIS	N-CA	-8.55	1.35	1.46
6	H	91	ASP	C-O	8.55	1.33	1.24
2	B	951	GLN	CG-CD	8.55	1.73	1.52
2	B	976	ILE	CA-C	-8.55	1.40	1.52
2	B	1148	LYS	C-O	-8.54	1.14	1.24
3	C	110	THR	CA-C	-8.54	1.42	1.52
1	A	1448	GLU	N-CA	8.54	1.57	1.46
1	A	446	ARG	NE-CZ	-8.54	1.23	1.33
2	B	660	LYS	CD-CE	-8.54	1.26	1.52
1	A	668	ASP	N-CA	-8.54	1.35	1.46
2	B	1212	ILE	CA-CB	-8.54	1.44	1.54
2	B	982	SER	C-O	-8.53	1.12	1.23
1	A	49	LYS	N-CA	8.53	1.57	1.46
1	A	144	THR	CA-CB	8.53	1.67	1.53
3	C	42	PRO	CA-CB	-8.53	1.41	1.53
5	F	144	GLU	N-CA	-8.53	1.35	1.45
1	A	1315	GLU	CA-C	-8.53	1.41	1.52
2	B	634	TYR	CA-C	-8.53	1.42	1.52
6	H	82	PRO	CA-C	8.53	1.64	1.52
1	A	1289	ARG	CZ-NH2	-8.53	1.22	1.33
2	B	692	TYR	C-O	-8.53	1.13	1.24
2	B	1101	ASP	CA-CB	8.53	1.68	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	846	ILE	CA-CB	8.52	1.65	1.54
2	B	1106	ARG	N-CA	8.52	1.57	1.46
1	A	515	GLN	C-O	8.52	1.33	1.24
2	B	857	ARG	C-O	-8.52	1.13	1.24
1	A	921	GLY	C-N	-8.51	1.21	1.33
1	A	264	PHE	CA-C	8.50	1.64	1.52
2	B	694	ASP	CG-OD2	8.50	1.41	1.25
3	C	167	HIS	CA-C	-8.50	1.41	1.52
8	J	28	ASP	CA-C	-8.50	1.42	1.52
2	B	583	ASN	CG-OD1	-8.50	1.07	1.23
7	I	48	LEU	CG-CD2	-8.49	1.24	1.52
7	I	72	ASP	CB-CG	8.49	1.73	1.52
3	C	159	ALA	N-CA	-8.49	1.35	1.45
4	E	70	SER	C-N	8.49	1.45	1.33
1	A	506	ALA	CA-C	-8.49	1.41	1.52
7	I	118	ARG	NE-CZ	8.49	1.42	1.33
1	A	684	ALA	CA-CB	8.48	1.67	1.53
2	B	453	ILE	CA-CB	8.48	1.66	1.54
2	B	955	THR	CA-C	-8.48	1.42	1.53
1	A	53	LEU	CA-CB	8.48	1.66	1.53
2	B	987	LYS	CA-CB	-8.47	1.39	1.53
1	A	1036	ARG	CA-C	-8.46	1.42	1.53
1	A	1278	ASN	CA-C	-8.46	1.41	1.52
2	B	127	GLY	C-O	-8.47	1.12	1.23
2	B	664	THR	C-O	-8.47	1.14	1.24
2	B	1135	ARG	CA-C	-8.46	1.42	1.52
1	A	425	GLN	C-O	8.46	1.33	1.24
2	B	1019	SER	C-N	-8.45	1.21	1.33
6	H	19	ARG	CB-CG	8.46	1.77	1.52
7	I	84	VAL	CB-CG1	-8.46	1.24	1.52
2	B	174	LEU	C-O	-8.45	1.13	1.23
4	E	7	ARG	CD-NE	8.45	1.58	1.46
9	K	21	ILE	C-O	-8.45	1.15	1.24
1	A	1303	GLU	N-CA	-8.45	1.35	1.46
7	I	28	GLU	CD-OE1	8.45	1.41	1.25
2	B	376	PHE	C-O	-8.45	1.14	1.24
5	F	95	GLY	C-O	-8.45	1.12	1.23
1	A	747	VAL	CA-CB	-8.45	1.44	1.54
1	A	1193	LEU	N-CA	8.44	1.56	1.46
3	C	162	GLY	C-O	8.44	1.33	1.24
1	A	1384	VAL	CA-C	-8.44	1.43	1.52
1	A	171	GLN	CD-OE1	8.43	1.39	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	587	HIS	C-O	-8.43	1.12	1.24
2	B	786	ASN	CG-OD1	-8.43	1.07	1.23
4	E	178	ILE	CA-C	8.43	1.63	1.52
2	B	1149	GLU	C-N	-8.43	1.22	1.34
4	E	121	MET	CG-SD	8.43	2.01	1.80
2	B	372	SER	C-O	8.43	1.33	1.24
1	A	247	ARG	C-O	8.43	1.35	1.24
10	L	26	THR	C-O	8.43	1.34	1.24
1	A	826	ASP	CA-C	-8.42	1.42	1.52
2	B	661	LEU	CA-C	-8.42	1.42	1.52
1	A	1068	ALA	CA-CB	-8.42	1.40	1.53
4	E	102	GLU	N-CA	-8.42	1.35	1.46
5	F	145	ASP	C-O	8.42	1.34	1.24
1	A	943	LEU	C-O	-8.41	1.13	1.24
2	B	1035	ALA	CA-C	-8.41	1.42	1.52
4	E	79	TRP	C-O	-8.41	1.13	1.24
1	A	189	ARG	CA-C	8.41	1.64	1.52
2	B	1154	ALA	N-CA	8.41	1.57	1.46
7	I	8	ARG	CZ-NH1	8.41	1.44	1.32
2	B	316	PRO	C-O	8.41	1.35	1.24
1	A	804	TYR	N-CA	-8.41	1.35	1.46
3	C	11	ARG	C-O	8.41	1.34	1.24
6	H	3	ASN	CB-CG	8.41	1.73	1.52
9	K	73	LEU	C-O	8.41	1.34	1.24
9	K	74	ARG	NE-CZ	-8.41	1.23	1.33
10	L	70	ARG	NE-CZ	8.41	1.42	1.33
2	B	90	ILE	C-O	8.40	1.34	1.24
2	B	347	LYS	CD-CE	8.40	1.77	1.52
2	B	411	PRO	C-O	8.40	1.35	1.24
2	B	265	SER	CA-CB	8.40	1.65	1.53
1	A	371	ALA	CA-CB	-8.40	1.39	1.53
2	B	775	LYS	CB-CG	8.40	1.77	1.52
2	B	138	GLU	N-CA	8.39	1.62	1.46
2	B	222	ILE	CA-CB	-8.39	1.44	1.54
2	B	790	ASP	CA-CB	8.39	1.67	1.53
2	B	1011	ILE	C-O	-8.39	1.14	1.24
3	C	57	VAL	CA-C	8.39	1.64	1.52
10	L	68	GLU	CD-OE1	8.39	1.41	1.25
2	B	103	ASN	CA-CB	8.39	1.67	1.53
1	A	349	ALA	CA-C	-8.38	1.42	1.52
2	B	934	LYS	CA-CB	8.38	1.63	1.52
3	C	154	LYS	CB-CG	8.38	1.77	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	969	GLN	CD-OE1	8.38	1.39	1.23
6	H	9	ILE	CG1-CD1	8.38	1.84	1.51
1	A	907	THR	CA-CB	8.38	1.65	1.53
1	A	1273	LEU	C-O	8.38	1.33	1.24
1	A	1127	ASP	CA-CB	8.38	1.65	1.52
1	A	1268	LEU	CA-CB	-8.37	1.39	1.53
1	A	635	ARG	CZ-NH2	8.37	1.44	1.33
1	A	348	SER	C-O	-8.37	1.13	1.23
2	B	791	THR	CA-CB	-8.36	1.40	1.53
2	B	803	LEU	CA-CB	-8.36	1.39	1.53
1	A	677	ARG	CD-NE	8.36	1.57	1.46
2	B	981	ALA	CA-CB	-8.36	1.39	1.53
2	B	190	TYR	CA-CB	-8.36	1.40	1.53
5	F	101	ILE	CG1-CD1	-8.36	1.19	1.51
9	K	92	ASN	C-O	-8.36	1.14	1.24
4	E	74	ASP	CB-CG	-8.35	1.31	1.52
1	A	351	THR	C-O	-8.35	1.13	1.24
3	C	100	THR	C-O	8.35	1.34	1.23
2	B	239	GLU	CG-CD	8.34	1.73	1.52
1	A	1214	GLU	CD-OE1	8.34	1.41	1.25
2	B	118	ARG	CZ-NH1	-8.34	1.21	1.32
2	B	1037	LEU	C-O	-8.34	1.14	1.24
2	B	785	TYR	CA-C	-8.33	1.41	1.52
1	A	994	GLN	CA-C	-8.33	1.42	1.52
2	B	935	ARG	NE-CZ	8.33	1.42	1.33
1	A	899	VAL	CA-C	8.32	1.63	1.52
1	A	1071	SER	C-N	-8.32	1.23	1.33
1	A	1025	ARG	NE-CZ	-8.32	1.23	1.33
2	B	692	TYR	CG-CD2	-8.32	1.21	1.39
2	B	1106	ARG	NE-CZ	8.32	1.42	1.33
4	E	202	SER	C-O	-8.32	1.13	1.23
7	I	75	CYS	C-O	-8.31	1.12	1.24
2	B	948	ILE	CA-C	-8.31	1.42	1.52
2	B	343	ILE	C-O	-8.31	1.16	1.24
2	B	668	ASP	CB-CG	8.31	1.72	1.52
2	B	340	ALA	CA-CB	-8.30	1.40	1.53
2	B	638	PHE	CA-C	-8.30	1.42	1.52
2	B	769	TYR	N-CA	-8.31	1.35	1.46
1	A	1264	GLU	CD-OE2	-8.30	1.09	1.25
2	B	1022	THR	CA-CB	-8.30	1.40	1.53
3	C	54	ASN	C-O	-8.30	1.13	1.23
3	C	169	LYS	CA-C	-8.30	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	20	LYS	N-CA	-8.30	1.36	1.46
1	A	1309	ASP	CA-CB	-8.30	1.42	1.53
3	C	22	LEU	CA-C	-8.30	1.41	1.52
9	K	13	GLY	C-O	8.30	1.33	1.23
5	F	106	PRO	C-O	-8.30	1.13	1.23
1	A	172	PRO	C-O	-8.30	1.14	1.23
1	A	286	HIS	CB-CG	8.29	1.61	1.50
1	A	920	LEU	CA-CB	-8.29	1.39	1.53
2	B	235	SER	CA-C	-8.29	1.40	1.52
2	B	824	ILE	C-O	-8.29	1.15	1.24
1	A	100	LYS	CE-NZ	-8.29	1.24	1.49
1	A	618	GLU	CD-OE2	8.29	1.41	1.25
4	E	170	LEU	N-CA	8.29	1.55	1.45
3	C	254	LYS	CA-C	-8.29	1.42	1.52
9	K	83	PRO	CA-CB	-8.29	1.41	1.53
3	C	145	CYS	N-CA	-8.29	1.35	1.46
3	C	148	ARG	CA-C	8.28	1.64	1.53
3	C	159	ALA	CA-C	-8.28	1.41	1.53
2	B	711	GLU	CA-CB	-8.28	1.40	1.53
2	B	1223	ASP	CA-C	8.28	1.63	1.52
6	H	130	ARG	CA-C	8.28	1.65	1.52
1	A	1102	LYS	CG-CD	8.28	1.77	1.52
2	B	1182	CYS	CA-CB	8.28	1.64	1.52
3	C	50	GLU	CG-CD	8.28	1.72	1.52
5	F	149	GLU	N-CA	8.28	1.56	1.46
2	B	1139	ILE	C-O	-8.28	1.14	1.24
3	C	203	GLN	CG-CD	-8.27	1.31	1.52
1	A	1056	SER	CA-CB	-8.27	1.39	1.53
2	B	1022	THR	CB-OG1	-8.27	1.30	1.43
1	A	37	PHE	CA-C	8.27	1.61	1.53
4	E	74	ASP	C-O	8.27	1.34	1.24
6	H	12	VAL	CA-C	8.27	1.62	1.52
1	A	1261	LYS	CD-CE	8.26	1.77	1.52
1	A	1093	LYS	N-CA	8.26	1.56	1.46
7	I	84	VAL	CA-CB	-8.26	1.41	1.54
1	A	1277	GLU	CA-CB	8.26	1.67	1.53
2	B	759	PRO	C-O	8.26	1.34	1.24
2	B	958	GLN	CG-CD	8.26	1.72	1.52
5	F	137	TYR	CA-CB	-8.26	1.41	1.53
6	H	11	GLN	CA-CB	8.26	1.64	1.53
7	I	49	ILE	CG1-CD1	8.26	1.83	1.51
1	A	33	ALA	C-O	-8.25	1.13	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	174	ALA	CA-C	-8.25	1.49	1.53
1	A	648	ASN	CB-CG	-8.25	1.31	1.52
1	A	985	ASP	CA-C	8.25	1.63	1.52
2	B	706	GLN	CD-NE2	8.25	1.50	1.33
7	I	83	ASN	CG-OD1	8.25	1.39	1.23
1	A	1411	GLU	CG-CD	8.25	1.72	1.52
3	C	82	TYR	N-CA	8.25	1.56	1.46
4	E	90	VAL	CA-CB	8.25	1.65	1.54
1	A	784	LEU	CA-CB	-8.24	1.42	1.53
6	H	32	THR	CA-CB	8.24	1.67	1.53
2	B	1172	ILE	C-O	8.24	1.32	1.23
4	E	178	ILE	C-O	-8.24	1.15	1.24
1	A	971	PHE	CA-C	8.24	1.65	1.52
1	A	1420	ASP	CG-OD2	8.24	1.41	1.25
2	B	1133	MET	SD-CE	-8.24	1.58	1.79
9	K	107	THR	C-O	8.24	1.33	1.24
2	B	579	ARG	NE-CZ	-8.24	1.24	1.33
1	A	84	ILE	C-O	-8.24	1.14	1.24
2	B	788	ARG	CD-NE	-8.24	1.34	1.46
1	A	1414	ALA	N-CA	-8.23	1.35	1.46
1	A	1040	GLN	C-O	-8.23	1.14	1.24
1	A	433	GLU	CA-CB	-8.23	1.42	1.52
7	I	39	GLY	C-O	-8.22	1.14	1.23
2	B	568	ASP	C-O	-8.22	1.13	1.24
2	B	743	ILE	CG1-CD1	-8.22	1.19	1.51
1	A	772	GLY	C-O	-8.22	1.12	1.24
1	A	1289	ARG	CA-C	-8.22	1.43	1.52
1	A	1204	ASP	CB-CG	8.21	1.72	1.52
1	A	1344	GLY	C-O	-8.22	1.13	1.23
1	A	37	PHE	CG-CD2	8.21	1.56	1.38
1	A	1236	LEU	N-CA	8.21	1.56	1.46
2	B	561	TRP	C-N	-8.21	1.22	1.33
1	A	882	SER	C-O	-8.20	1.13	1.23
3	C	223	ALA	CA-CB	-8.20	1.39	1.53
2	B	407	ASP	C-O	-8.20	1.14	1.24
2	B	1156	ASP	CB-CG	8.20	1.72	1.52
5	F	109	VAL	CA-CB	-8.20	1.42	1.54
2	B	434	ARG	CB-CG	8.20	1.77	1.52
2	B	815	ARG	C-O	-8.20	1.13	1.24
1	A	1130	GLN	CG-CD	8.20	1.72	1.52
1	A	1289	ARG	NE-CZ	-8.19	1.24	1.33
2	B	299	GLU	C-O	-8.19	1.13	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	709	THR	CA-C	-8.19	1.42	1.52
2	B	268	THR	N-CA	-8.19	1.35	1.45
1	A	1164	PRO	CA-C	8.19	1.64	1.52
2	B	305	VAL	CB-CG1	8.19	1.79	1.52
2	B	984	HIS	C-O	-8.19	1.11	1.23
1	A	588	LEU	C-O	-8.18	1.13	1.23
1	A	1297	GLU	N-CA	-8.18	1.35	1.45
2	B	193	LYS	CA-C	8.18	1.65	1.52
2	B	315	LYS	CA-CB	-8.18	1.42	1.53
1	A	1170	ILE	CA-CB	8.18	1.65	1.54
7	I	65	ASP	N-CA	8.18	1.57	1.46
2	B	401	PHE	C-O	-8.18	1.13	1.24
1	A	718	VAL	C-O	-8.17	1.13	1.24
10	L	54	ARG	CG-CD	8.17	1.76	1.52
6	H	60	ALA	CA-C	-8.17	1.42	1.52
2	B	943	SER	CA-C	8.17	1.63	1.52
1	A	511	ILE	C-O	-8.17	1.14	1.24
1	A	702	LEU	N-CA	-8.17	1.36	1.46
3	C	128	ASN	CA-C	8.17	1.63	1.52
5	F	97	ARG	N-CA	-8.17	1.36	1.46
2	B	1189	ILE	CA-C	8.16	1.63	1.52
7	I	28	GLU	CA-C	-8.16	1.42	1.52
1	A	840	ARG	CG-CD	8.16	1.76	1.52
1	A	898	ARG	NE-CZ	8.16	1.42	1.33
2	B	646	LEU	CG-CD1	8.16	1.79	1.52
6	H	56	THR	N-CA	-8.16	1.35	1.46
1	A	509	LEU	C-O	-8.16	1.12	1.24
6	H	127	GLY	N-CA	8.16	1.57	1.45
1	A	537	ARG	CZ-NH1	8.16	1.44	1.32
1	A	940	ARG	CZ-NH1	-8.16	1.21	1.32
1	A	1155	ASP	N-CA	8.16	1.54	1.46
2	B	136	THR	N-CA	8.16	1.56	1.46
7	I	93	LYS	CG-CD	8.16	1.76	1.52
9	K	63	VAL	CA-CB	8.16	1.64	1.53
1	A	176	LYS	C-O	-8.15	1.14	1.23
2	B	52	ASN	C-N	-8.15	1.22	1.34
2	B	1155	SER	CA-C	8.15	1.63	1.52
1	A	56	PRO	C-O	8.15	1.34	1.24
1	A	738	LYS	CA-C	-8.15	1.41	1.53
2	B	282	ILE	CA-C	-8.15	1.40	1.52
9	K	65	HIS	CA-C	-8.15	1.43	1.52
10	L	26	THR	CB-CG2	8.15	1.79	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	121	LEU	CB-CG	8.15	1.69	1.53
1	A	1302	PRO	CB-CG	8.14	1.90	1.49
2	B	68	THR	CA-CB	8.14	1.66	1.53
3	C	64	ALA	CA-CB	-8.14	1.39	1.53
2	B	783	THR	C-O	-8.14	1.13	1.24
1	A	964	ILE	CA-CB	8.14	1.65	1.54
1	A	1137	ALA	C-O	8.14	1.34	1.24
1	A	955	PRO	CA-CB	-8.13	1.43	1.53
2	B	813	LYS	CA-C	-8.13	1.41	1.53
1	A	496	GLU	CG-CD	8.13	1.72	1.52
1	A	1196	GLU	CD-OE1	8.13	1.40	1.25
2	B	350	GLN	C-O	-8.13	1.13	1.24
2	B	937	ALA	CA-CB	8.13	1.67	1.53
5	F	152	ILE	N-CA	-8.13	1.36	1.46
6	H	78	SER	C-O	-8.13	1.13	1.24
2	B	789	MET	CA-C	-8.13	1.43	1.53
2	B	1185	CYS	CA-C	8.13	1.63	1.52
4	E	186	LEU	N-CA	-8.13	1.36	1.46
1	A	177	ASP	CG-OD2	8.12	1.40	1.25
1	A	188	ASP	CA-CB	8.12	1.67	1.53
1	A	418	SER	C-O	-8.12	1.13	1.24
2	B	487	THR	C-O	-8.12	1.14	1.23
5	F	94	LEU	CA-C	-8.12	1.41	1.52
5	F	98	ALA	CA-CB	-8.12	1.40	1.53
1	A	529	CYS	C-O	-8.12	1.14	1.24
1	A	961	ARG	CZ-NH2	8.12	1.44	1.33
2	B	1210	MET	CA-C	-8.12	1.41	1.52
2	B	118	ARG	CG-CD	8.11	1.76	1.52
1	A	362	ASP	CB-CG	-8.11	1.31	1.52
1	A	104	GLU	C-O	8.11	1.34	1.24
2	B	479	VAL	CB-CG1	-8.10	1.25	1.52
3	C	209	TYR	CA-C	-8.10	1.42	1.52
1	A	1438	THR	CA-CB	-8.10	1.38	1.53
2	B	987	LYS	C-O	-8.10	1.13	1.23
1	A	408	ASP	C-O	8.10	1.34	1.24
1	A	706	HIS	CA-C	-8.10	1.42	1.52
4	E	200	ARG	CB-CG	-8.09	1.28	1.52
1	A	827	THR	CA-CB	8.09	1.65	1.53
1	A	1058	VAL	C-O	-8.09	1.13	1.24
2	B	397	ASP	CA-CB	8.09	1.63	1.52
2	B	604	ARG	C-O	-8.09	1.13	1.24
1	A	1035	TYR	CA-CB	8.09	1.66	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	46	GLN	N-CA	8.09	1.56	1.46
1	A	66	LYS	CB-CG	8.08	1.76	1.52
1	A	502	SER	C-O	-8.08	1.13	1.24
4	E	1	MET	CG-SD	8.08	2.00	1.80
4	E	46	TYR	CA-C	-8.08	1.42	1.52
7	I	98	VAL	CB-CG2	-8.08	1.25	1.52
2	B	176	SER	C-O	-8.08	1.11	1.23
1	A	187	LYS	N-CA	8.07	1.56	1.45
1	A	962	ARG	C-N	-8.07	1.24	1.34
1	A	463	ILE	CA-C	8.07	1.61	1.52
2	B	103	ASN	CB-CG	8.07	1.72	1.52
2	B	1182	CYS	N-CA	8.07	1.57	1.46
6	H	115	TYR	C-O	-8.07	1.12	1.23
4	E	87	SER	CA-C	8.06	1.62	1.52
1	A	190	ALA	CA-C	8.06	1.63	1.52
4	E	108	GLY	C-O	-8.06	1.13	1.23
7	I	47	GLU	C-O	-8.06	1.14	1.24
1	A	1282	VAL	C-O	-8.06	1.15	1.24
6	H	37	LYS	N-CA	8.06	1.55	1.45
2	B	635	ARG	CZ-NH2	-8.06	1.23	1.33
2	B	889	THR	N-CA	8.05	1.56	1.46
4	E	197	LYS	N-CA	-8.05	1.36	1.46
2	B	640	VAL	C-O	-8.05	1.15	1.24
3	C	40	GLU	CA-C	8.05	1.63	1.52
9	K	88	LYS	CG-CD	8.04	1.76	1.52
10	L	50	ASP	CB-CG	8.04	1.72	1.52
2	B	731	VAL	CA-C	-8.04	1.42	1.52
7	I	63	GLY	C-O	-8.04	1.13	1.23
1	A	505	CYS	C-O	-8.03	1.12	1.23
1	A	1208	THR	CA-C	8.03	1.62	1.52
2	B	565	PRO	CA-C	-8.03	1.43	1.52
6	H	25	ARG	CA-C	8.03	1.63	1.53
1	A	626	ASN	CG-ND2	8.03	1.50	1.33
2	B	652	LYS	CE-NZ	8.03	1.73	1.49
5	F	73	ALA	N-CA	8.03	1.56	1.46
1	A	92	HIS	CA-CB	8.02	1.64	1.53
1	A	751	SER	C-O	-8.02	1.13	1.24
1	A	1279	ILE	N-CA	-8.02	1.36	1.46
7	I	31	THR	CA-CB	-8.02	1.42	1.53
1	A	269	ILE	CA-C	-8.02	1.42	1.52
1	A	358	ASN	C-O	-8.02	1.12	1.24
1	A	681	GLU	C-O	8.02	1.33	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	767	GLN	CD-OE1	-8.01	1.08	1.23
2	B	372	SER	CA-C	8.01	1.63	1.52
1	A	438	ASP	CA-CB	-8.01	1.40	1.53
2	B	833	TYR	CE1-CZ	-8.01	1.19	1.38
9	K	35	PHE	C-O	-8.01	1.14	1.24
1	A	70	CYS	N-CA	8.01	1.56	1.46
1	A	587	HIS	N-CA	-8.01	1.36	1.46
9	K	35	PHE	CE1-CZ	-8.01	1.14	1.38
9	K	69	ALA	N-CA	8.01	1.56	1.46
2	B	850	LEU	C-O	-8.01	1.14	1.23
2	B	986	GLN	C-O	8.01	1.33	1.24
5	F	100	GLN	CD-OE1	8.01	1.38	1.23
1	A	445	ASN	C-O	8.00	1.33	1.23
1	A	483	ASP	CG-OD1	8.00	1.40	1.25
1	A	1036	ARG	C-N	-8.00	1.22	1.33
1	A	678	GLU	N-CA	-8.00	1.36	1.46
3	C	63	ILE	CA-C	8.00	1.62	1.52
3	C	20	PHE	C-O	-8.00	1.13	1.24
1	A	411	ASP	N-CA	8.00	1.56	1.46
1	A	1118	VAL	CA-CB	8.00	1.64	1.54
2	B	120	ARG	CZ-NH2	8.00	1.43	1.33
2	B	137	TYR	CB-CG	8.00	1.69	1.51
2	B	486	TYR	C-O	-8.00	1.14	1.24
3	C	6	PRO	C-O	7.99	1.33	1.23
8	J	54	VAL	CA-CB	-7.99	1.44	1.54
9	K	46	ILE	CG1-CD1	-7.99	1.20	1.51
1	A	1355	VAL	CA-CB	-7.99	1.45	1.54
1	A	217	LYS	CA-C	7.99	1.63	1.52
1	A	848	ILE	C-O	-7.99	1.15	1.24
2	B	694	ASP	CB-CG	7.99	1.72	1.52
3	C	256	ALA	CA-CB	-7.99	1.41	1.53
2	B	46	GLN	CA-C	7.98	1.63	1.52
1	A	293	GLU	N-CA	7.98	1.56	1.46
1	A	913	LEU	CA-C	7.98	1.62	1.52
1	A	1014	ALA	C-N	-7.98	1.24	1.33
3	C	55	THR	CA-C	7.98	1.63	1.52
4	E	145	THR	CA-CB	-7.98	1.40	1.53
1	A	1003	LYS	CG-CD	7.98	1.76	1.52
1	A	1383	SER	C-O	-7.98	1.13	1.23
4	E	34	GLU	CD-OE2	7.98	1.40	1.25
1	A	1218	GLN	CD-OE1	7.98	1.38	1.23
2	B	92	PHE	CA-CB	7.97	1.65	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	239	GLU	CD-OE2	7.97	1.40	1.25
1	A	1237	ILE	CA-C	-7.97	1.42	1.52
1	A	1350	LYS	CG-CD	7.97	1.76	1.52
2	B	792	MET	CA-CB	-7.97	1.39	1.53
7	I	52	ILE	C-O	-7.97	1.16	1.24
1	A	659	HIS	CA-CB	-7.97	1.41	1.53
1	A	412	ARG	NE-CZ	-7.96	1.24	1.33
6	H	118	PHE	CA-CB	7.96	1.65	1.53
4	E	62	ALA	CA-CB	-7.96	1.40	1.53
1	A	16	GLU	CD-OE2	7.95	1.40	1.25
3	C	152	GLU	C-O	-7.95	1.14	1.23
6	H	21	ASN	C-O	-7.95	1.12	1.23
1	A	71	GLN	CG-CD	7.95	1.72	1.52
1	A	639	PRO	CA-C	7.95	1.64	1.52
1	A	44	THR	CA-C	7.95	1.63	1.52
7	I	24	ARG	C-O	7.95	1.33	1.23
8	J	21	TYR	CA-CB	7.95	1.66	1.53
7	I	118	ARG	CD-NE	7.95	1.57	1.46
2	B	572	HIS	C-O	-7.94	1.14	1.24
10	L	65	VAL	CB-CG2	7.94	1.78	1.52
1	A	541	ILE	CG1-CD1	-7.94	1.20	1.51
2	B	698	GLU	C-O	7.94	1.34	1.24
2	B	838	SER	CA-C	-7.94	1.42	1.52
1	A	163	SER	CA-CB	7.94	1.65	1.53
2	B	887	HIS	CA-C	7.94	1.63	1.52
1	A	123	ARG	CG-CD	7.93	1.76	1.52
3	C	9	LYS	CG-CD	7.93	1.76	1.52
1	A	159	THR	C-O	-7.93	1.14	1.24
1	A	975	HIS	CA-CB	7.93	1.66	1.53
2	B	95	ILE	N-CA	7.93	1.55	1.46
2	B	827	ILE	C-O	-7.93	1.15	1.24
3	C	84	ARG	N-CA	-7.93	1.35	1.46
2	B	992	ILE	CA-C	-7.92	1.44	1.52
1	A	1362	TYR	CG-CD2	-7.92	1.22	1.39
7	I	38	ALA	CA-C	-7.92	1.42	1.52
7	I	19	ASP	C-O	7.92	1.34	1.23
2	B	1132	GLU	C-O	7.92	1.33	1.24
2	B	227	LYS	C-O	-7.92	1.12	1.23
2	B	434	ARG	NE-CZ	7.92	1.41	1.33
4	E	90	VAL	CA-C	7.92	1.62	1.52
2	B	595	ARG	NE-CZ	7.92	1.41	1.33
9	K	92	ASN	CA-CB	7.92	1.66	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	478	GLY	N-CA	7.91	1.57	1.45
1	A	740	LEU	N-CA	-7.91	1.35	1.46
2	B	55	VAL	CA-C	-7.91	1.42	1.52
2	B	1080	LYS	CA-C	7.91	1.63	1.52
8	J	54	VAL	CA-C	7.91	1.62	1.52
1	A	138	ILE	N-CA	-7.91	1.37	1.46
2	B	1162	ILE	CA-CB	7.91	1.65	1.54
4	E	71	LYS	N-CA	7.91	1.56	1.46
1	A	207	ILE	CA-CB	7.91	1.63	1.54
2	B	643	ASP	CB-CG	7.91	1.71	1.52
6	H	3	ASN	CA-C	7.91	1.62	1.53
2	B	390	LEU	CB-CG	-7.90	1.37	1.53
4	E	103	LYS	CA-CB	7.90	1.64	1.53
4	E	212	ARG	CZ-NH1	-7.90	1.21	1.32
1	A	1224	LEU	C-O	-7.90	1.13	1.23
2	B	252	SER	N-CA	7.90	1.56	1.46
3	C	68	GLY	N-CA	7.90	1.56	1.45
2	B	390	LEU	CA-C	7.90	1.63	1.52
4	E	122	LYS	N-CA	7.90	1.56	1.46
6	H	55	LEU	C-O	-7.90	1.15	1.24
1	A	595	THR	C-O	-7.89	1.14	1.23
1	A	5	GLN	CB-CG	7.89	1.76	1.52
2	B	693	ILE	CA-CB	7.89	1.64	1.54
4	E	184	VAL	CA-CB	7.89	1.65	1.54
1	A	291	GLU	CG-CD	7.88	1.71	1.52
1	A	434	ARG	CA-C	-7.88	1.42	1.52
1	A	1022	LEU	N-CA	7.88	1.55	1.46
1	A	1077	THR	C-O	-7.88	1.14	1.24
5	F	96	THR	N-CA	-7.88	1.36	1.46
1	A	109	HIS	CG-ND1	7.88	1.47	1.38
1	A	1156	PRO	C-O	7.88	1.34	1.24
1	A	956	LEU	N-CA	7.88	1.53	1.45
3	C	214	ASN	N-CA	7.87	1.55	1.46
1	A	938	LYS	CA-C	-7.87	1.42	1.52
1	A	802	ASN	CA-C	-7.87	1.42	1.52
1	A	908	LEU	CA-C	-7.87	1.43	1.52
8	J	24	LEU	CA-C	-7.87	1.42	1.52
10	L	50	ASP	CA-CB	7.87	1.66	1.53
2	B	523	CYS	C-O	-7.86	1.13	1.24
1	A	138	ILE	C-O	7.86	1.32	1.24
1	A	460	VAL	N-CA	-7.86	1.36	1.46
1	A	764	CYS	CA-CB	-7.86	1.41	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	617	VAL	CA-CB	-7.86	1.44	1.54
1	A	787	PHE	CE2-CZ	-7.86	1.15	1.38
1	A	813	PHE	C-O	-7.86	1.15	1.24
1	A	892	ALA	CA-CB	-7.86	1.40	1.53
2	B	667	GLN	C-O	7.86	1.32	1.23
3	C	218	PRO	C-O	7.86	1.32	1.23
1	A	149	GLU	CA-CB	-7.85	1.40	1.53
2	B	57	TYR	CA-CB	7.85	1.66	1.53
3	C	186	LEU	C-O	7.85	1.34	1.24
7	I	30	ARG	CG-CD	7.85	1.76	1.52
9	K	11	LEU	C-O	-7.85	1.15	1.24
1	A	1236	LEU	CG-CD2	7.85	1.78	1.52
2	B	618	ASP	CG-OD1	7.85	1.40	1.25
1	A	506	ALA	C-O	-7.85	1.13	1.23
1	A	1161	THR	C-O	7.85	1.33	1.23
2	B	434	ARG	CA-C	7.85	1.64	1.52
8	J	47	ARG	CZ-NH1	-7.85	1.21	1.32
2	B	371	GLU	CA-C	-7.85	1.41	1.52
1	A	402	ALA	CA-CB	-7.84	1.40	1.53
1	A	1136	SER	N-CA	-7.84	1.35	1.46
9	K	74	ARG	C-O	7.84	1.32	1.24
1	A	1224	LEU	CA-C	-7.84	1.42	1.52
1	A	1349	TYR	CA-C	-7.84	1.42	1.52
3	C	218	PRO	CA-C	7.84	1.62	1.52
4	E	124	VAL	C-N	7.84	1.40	1.33
7	I	1	MET	CB-CG	7.84	1.75	1.52
1	A	843	LYS	CG-CD	7.83	1.75	1.52
1	A	242	PRO	CA-C	7.83	1.56	1.51
1	A	484	GLY	C-O	-7.83	1.13	1.23
1	A	562	THR	CA-CB	7.83	1.66	1.52
6	H	103	LYS	C-O	-7.83	1.14	1.24
1	A	96	ILE	CG1-CD1	-7.83	1.21	1.51
2	B	366	GLN	C-O	-7.83	1.13	1.24
2	B	827	ILE	N-CA	-7.83	1.36	1.46
2	B	406	LEU	CG-CD2	-7.83	1.26	1.52
1	A	213	HIS	CB-CG	7.83	1.61	1.50
7	I	34	TYR	CG-CD2	-7.83	1.23	1.39
1	A	941	LYS	CG-CD	7.82	1.75	1.52
9	K	93	SER	CA-CB	7.82	1.66	1.53
3	C	41	ILE	CA-C	7.82	1.59	1.53
1	A	175	ARG	CD-NE	7.82	1.57	1.46
2	B	852	ARG	CZ-NH1	-7.82	1.21	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1232	ASN	CA-C	7.82	1.63	1.52
1	A	1359	ASP	CB-CG	7.82	1.71	1.52
2	B	1219	ASP	CB-CG	7.82	1.71	1.52
3	C	263	THR	CA-CB	-7.82	1.40	1.53
4	E	149	LEU	CG-CD1	-7.82	1.26	1.52
2	B	183	GLU	CA-C	7.81	1.63	1.52
1	A	969	GLN	CA-C	-7.81	1.43	1.52
1	A	649	ILE	CG1-CD1	-7.81	1.21	1.51
5	F	106	PRO	CA-CB	-7.81	1.42	1.53
1	A	144	THR	CB-CG2	7.81	1.78	1.52
2	B	255	GLN	CA-C	-7.81	1.43	1.52
2	B	641	GLU	CD-OE1	7.81	1.40	1.25
3	C	267	GLN	N-CA	7.81	1.56	1.46
1	A	777	PHE	CA-CB	7.81	1.63	1.52
2	B	518	HIS	CE1-NE2	-7.81	1.24	1.32
8	J	38	ARG	CB-CG	7.81	1.75	1.52
1	A	1445	ILE	CG1-CD1	7.80	1.82	1.51
2	B	644	GLU	N-CA	-7.80	1.36	1.46
2	B	135	ARG	C-O	7.80	1.33	1.23
2	B	642	ASP	CA-CB	7.80	1.62	1.52
4	E	110	PHE	N-CA	-7.80	1.36	1.46
3	C	116	LYS	CD-CE	7.80	1.75	1.52
1	A	205	GLU	CD-OE1	7.79	1.40	1.25
1	A	205	GLU	CA-C	7.79	1.63	1.52
1	A	200	ARG	C-O	-7.79	1.14	1.24
1	A	571	LEU	CG-CD2	7.79	1.78	1.52
1	A	1004	ASN	CA-C	7.79	1.64	1.53
3	C	15	LYS	CB-CG	7.79	1.75	1.52
4	E	45	LYS	CD-CE	7.79	1.75	1.52
9	K	55	LYS	C-O	7.79	1.34	1.24
1	A	65	LEU	CA-CB	7.79	1.66	1.53
1	A	751	SER	CB-OG	7.79	1.57	1.42
1	A	724	GLU	CA-C	-7.79	1.42	1.52
3	C	210	GLU	CA-C	7.79	1.62	1.52
2	B	284	ILE	CG1-CD1	-7.78	1.21	1.51
1	A	199	LEU	C-O	-7.78	1.14	1.23
1	A	151	ASP	N-CA	-7.78	1.37	1.46
2	B	284	ILE	N-CA	-7.78	1.37	1.46
2	B	879	ARG	N-CA	7.78	1.56	1.46
2	B	1012	ILE	CB-CG1	-7.78	1.37	1.53
4	E	154	ILE	C-O	7.78	1.32	1.24
1	A	653	VAL	C-O	-7.78	1.14	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	797	TYR	CA-C	-7.78	1.43	1.52
2	B	1025	HIS	CA-CB	7.78	1.65	1.53
6	H	96	VAL	N-CA	-7.78	1.37	1.46
3	C	21	ILE	CA-C	-7.78	1.43	1.52
2	B	636	PRO	N-CA	-7.77	1.37	1.47
2	B	1012	ILE	CA-C	-7.77	1.42	1.52
1	A	978	PRO	CB-CG	7.77	1.88	1.49
7	I	79	HIS	C-O	7.77	1.33	1.24
1	A	1240	CYS	CA-C	7.77	1.62	1.52
4	E	57	MET	CA-CB	7.76	1.66	1.53
1	A	815	PHE	C-O	-7.76	1.14	1.24
2	B	216	GLU	CD-OE2	7.76	1.40	1.25
2	B	887	HIS	CA-CB	7.76	1.66	1.53
6	H	104	PHE	N-CA	7.76	1.56	1.46
2	B	1027	ILE	CA-CB	-7.76	1.43	1.54
2	B	1154	ALA	C-N	7.76	1.44	1.33
1	A	973	ILE	C-O	7.75	1.33	1.24
1	A	1269	GLU	C-O	-7.75	1.13	1.23
2	B	707	PRO	N-CD	-7.75	1.36	1.47
2	B	1094	ARG	CA-CB	-7.75	1.42	1.53
10	L	40	LEU	CB-CG	7.75	1.69	1.53
3	C	18	VAL	N-CA	-7.75	1.36	1.46
7	I	94	ASP	CA-CB	7.75	1.65	1.53
1	A	1262	LYS	CA-CB	7.75	1.65	1.53
5	F	72	LYS	CD-CE	7.75	1.75	1.52
1	A	417	TYR	C-O	-7.75	1.14	1.24
2	B	1194	ILE	CA-C	-7.75	1.43	1.52
4	E	191	LYS	CD-CE	7.75	1.75	1.52
1	A	1355	VAL	CA-C	-7.74	1.43	1.52
2	B	1017	ILE	N-CA	-7.74	1.37	1.46
3	C	86	CYS	CA-CB	7.74	1.65	1.53
2	B	815	ARG	CZ-NH2	7.74	1.43	1.33
2	B	92	PHE	N-CA	7.73	1.55	1.46
1	A	897	TYR	C-O	-7.73	1.13	1.24
10	L	69	ALA	CA-C	-7.73	1.43	1.53
1	A	162	VAL	N-CA	-7.73	1.37	1.46
5	F	100	GLN	N-CA	-7.72	1.37	1.46
8	J	36	LEU	CA-C	-7.72	1.42	1.52
2	B	983	ARG	N-CA	-7.72	1.37	1.46
1	A	950	GLY	C-O	-7.72	1.13	1.24
1	A	1215	ARG	CB-CG	7.72	1.75	1.52
8	J	14	VAL	CA-CB	-7.72	1.44	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1023	ARG	CZ-NH2	-7.72	1.23	1.33
2	B	701	ILE	N-CA	-7.72	1.36	1.46
2	B	109	THR	CA-CB	7.71	1.66	1.53
3	C	196	ASP	CB-CG	7.71	1.71	1.52
2	B	324	ILE	N-CA	-7.71	1.36	1.46
1	A	858	ASN	C-O	-7.71	1.13	1.23
1	A	1133	LEU	CA-C	-7.71	1.42	1.52
2	B	137	TYR	N-CA	7.71	1.56	1.46
2	B	1210	MET	N-CA	-7.71	1.37	1.46
5	F	152	ILE	CA-CB	7.71	1.62	1.54
4	E	114	ASN	CA-C	-7.71	1.43	1.52
9	K	32	VAL	CB-CG2	-7.71	1.27	1.52
2	B	1046	PRO	C-O	7.71	1.32	1.23
3	C	92	CYS	CA-CB	7.71	1.66	1.53
3	C	26	ASP	N-CA	7.71	1.55	1.46
1	A	726	ARG	N-CA	-7.70	1.37	1.46
3	C	120	ILE	CA-CB	-7.70	1.46	1.54
7	I	88	SER	CA-C	-7.70	1.42	1.52
8	J	26	GLN	CB-CG	7.70	1.75	1.52
1	A	1071	SER	CA-C	-7.70	1.42	1.52
1	A	850	VAL	CA-CB	7.70	1.64	1.54
1	A	1152	ILE	N-CA	-7.69	1.37	1.46
1	A	1239	ARG	CG-CD	7.69	1.75	1.52
5	F	90	ARG	NE-CZ	-7.69	1.24	1.33
5	F	106	PRO	CG-CD	-7.69	1.24	1.50
1	A	1194	ARG	CD-NE	-7.69	1.35	1.46
2	B	659	ALA	CA-CB	7.69	1.65	1.53
2	B	1063	GLY	CA-C	-7.69	1.40	1.51
4	E	191	LYS	CE-NZ	7.69	1.72	1.49
7	I	87	GLN	CA-C	-7.69	1.42	1.53
5	F	143	PHE	C-O	-7.68	1.14	1.23
1	A	432	VAL	N-CA	-7.68	1.36	1.46
1	A	697	ALA	CA-C	-7.68	1.42	1.52
3	C	82	TYR	CG-CD2	-7.68	1.23	1.39
3	C	219	PHE	C-O	7.68	1.32	1.23
4	E	153	HIS	CA-CB	-7.68	1.41	1.53
9	K	113	THR	CA-C	7.68	1.61	1.52
1	A	840	ARG	NE-CZ	7.68	1.41	1.33
3	C	70	ILE	C-N	-7.68	1.23	1.33
3	C	127	ARG	C-O	7.68	1.33	1.23
1	A	962	ARG	NE-CZ	-7.68	1.24	1.33
4	E	200	ARG	CA-C	-7.68	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	923	LEU	CA-C	-7.67	1.42	1.52
1	A	1163	ILE	CA-C	-7.67	1.46	1.53
2	B	585	VAL	CA-C	7.67	1.61	1.52
1	A	1345	ARG	C-O	-7.67	1.15	1.24
2	B	1144	ALA	CA-CB	-7.67	1.40	1.53
1	A	792	TYR	C-O	-7.67	1.14	1.24
1	A	1103	GLU	CD-OE2	7.67	1.40	1.25
2	B	893	LEU	CG-CD2	-7.67	1.27	1.52
2	B	1091	TYR	CA-C	-7.67	1.43	1.52
3	C	211	ASP	CA-C	7.67	1.63	1.52
1	A	368	LYS	CD-CE	7.67	1.75	1.52
2	B	604	ARG	NE-CZ	-7.67	1.24	1.33
6	H	110	ASP	N-CA	7.67	1.55	1.46
1	A	1415	SER	CB-OG	-7.66	1.26	1.42
2	B	1019	SER	CA-C	-7.66	1.42	1.52
2	B	612	GLU	CA-CB	-7.66	1.40	1.53
4	E	164	LEU	CA-C	-7.66	1.42	1.52
3	C	144	ILE	CG1-CD1	-7.66	1.21	1.51
3	C	169	LYS	CD-CE	7.66	1.75	1.52
1	A	675	THR	C-O	-7.65	1.15	1.24
1	A	732	LEU	N-CA	-7.65	1.37	1.46
2	B	706	GLN	N-CA	7.65	1.55	1.46
7	I	44	TYR	C-O	7.65	1.33	1.23
1	A	565	ILE	CG1-CD1	-7.65	1.22	1.51
1	A	1102	LYS	CD-CE	7.65	1.75	1.52
2	B	1152	MET	SD-CE	7.65	1.98	1.79
2	B	653	VAL	CB-CG2	-7.65	1.27	1.52
1	A	423	ASP	CG-OD1	7.65	1.39	1.25
1	A	302	THR	N-CA	-7.65	1.36	1.46
2	B	1223	ASP	N-CA	7.65	1.56	1.46
1	A	391	LEU	N-CA	7.64	1.55	1.46
1	A	1094	VAL	CA-C	7.64	1.61	1.52
1	A	1242	VAL	N-CA	-7.64	1.36	1.46
2	B	1086	PHE	CG-CD1	-7.64	1.22	1.38
4	E	109	ILE	C-O	7.64	1.31	1.24
6	H	12	VAL	CA-CB	7.64	1.62	1.53
8	J	48	ARG	CA-C	-7.64	1.42	1.52
7	I	54	GLU	C-O	-7.64	1.15	1.24
1	A	482	PHE	CA-CB	-7.64	1.43	1.53
1	A	1308	THR	CA-CB	-7.64	1.41	1.53
1	A	226	GLU	CA-C	-7.63	1.42	1.52
2	B	737	THR	CA-CB	-7.63	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	71	LYS	CG-CD	7.63	1.75	1.52
5	F	80	ALA	CA-CB	7.63	1.64	1.54
1	A	681	GLU	C-N	7.63	1.43	1.33
7	I	70	ARG	N-CA	7.63	1.55	1.45
6	H	88	SER	N-CA	7.62	1.56	1.46
2	B	1094	ARG	NE-CZ	-7.62	1.24	1.33
3	C	209	TYR	N-CA	-7.62	1.36	1.46
3	C	47	ASP	CG-OD2	7.62	1.39	1.25
6	H	126	GLU	N-CA	7.62	1.55	1.45
3	C	95	CYS	CA-C	7.62	1.62	1.52
2	B	358	LYS	CB-CG	7.62	1.75	1.52
2	B	1051	THR	C-N	-7.62	1.24	1.34
1	A	456	MET	SD-CE	-7.61	1.60	1.79
2	B	639	ILE	CA-CB	-7.61	1.44	1.54
1	A	438	ASP	N-CA	-7.61	1.36	1.46
1	A	1270	ASN	C-O	7.61	1.34	1.24
7	I	70	ARG	CZ-NH2	-7.61	1.23	1.33
2	B	829	CYS	CA-CB	7.61	1.63	1.53
1	A	618	GLU	CA-C	7.60	1.61	1.53
1	A	745	GLN	CD-OE1	7.60	1.38	1.23
1	A	769	SER	N-CA	-7.60	1.36	1.45
1	A	1011	GLN	N-CA	7.60	1.55	1.46
1	A	1308	THR	C-N	7.60	1.46	1.33
3	C	39	ALA	CA-CB	-7.60	1.42	1.53
1	A	987	VAL	CA-CB	-7.60	1.45	1.54
1	A	1288	ASP	CG-OD1	7.60	1.39	1.25
4	E	11	ARG	C-O	7.60	1.32	1.24
7	I	5	ARG	NE-CZ	7.60	1.41	1.33
2	B	457	LEU	C-O	-7.60	1.16	1.23
1	A	1140	HIS	C-O	-7.59	1.14	1.23
5	F	79	ARG	CA-C	7.59	1.62	1.52
2	B	815	ARG	N-CA	7.59	1.56	1.46
2	B	617	ARG	C-O	-7.59	1.14	1.24
3	C	9	LYS	CD-CE	7.59	1.75	1.52
1	A	944	ARG	CZ-NH2	-7.59	1.23	1.33
2	B	89	GLU	C-O	7.59	1.38	1.23
6	H	117	SER	CA-C	-7.59	1.43	1.52
2	B	126	SER	CA-C	-7.59	1.43	1.52
2	B	989	THR	C-O	-7.59	1.14	1.23
2	B	1057	LYS	CD-CE	7.59	1.75	1.52
4	E	200	ARG	C-O	-7.58	1.14	1.23
1	A	4	GLN	CA-C	7.58	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1205	LYS	C-O	7.58	1.35	1.24
2	B	325	GLN	CA-CB	-7.58	1.42	1.53
2	B	1052	VAL	C-O	-7.58	1.14	1.24
2	B	621	GLU	CD-OE2	7.58	1.39	1.25
2	B	712	PRO	CG-CD	7.58	1.76	1.50
4	E	52	ARG	CB-CG	7.58	1.75	1.52
6	H	31	THR	CA-C	7.58	1.62	1.52
1	A	371	ALA	C-O	-7.58	1.14	1.24
2	B	1216	LEU	N-CA	-7.58	1.36	1.46
9	K	98	LEU	N-CA	-7.58	1.36	1.46
2	B	961	LEU	CG-CD1	7.57	1.77	1.52
4	E	103	LYS	CD-CE	7.57	1.75	1.52
2	B	774	GLY	CA-C	7.57	1.61	1.51
1	A	1208	THR	CA-CB	7.57	1.65	1.53
1	A	1318	THR	CA-CB	-7.57	1.40	1.53
1	A	1154	TYR	CA-CB	7.57	1.63	1.53
2	B	52	ASN	N-CA	-7.57	1.37	1.46
2	B	968	VAL	N-CA	-7.57	1.36	1.46
2	B	1130	PHE	CA-C	-7.57	1.44	1.53
10	L	40	LEU	CA-CB	7.57	1.63	1.54
8	J	32	GLU	CA-C	-7.56	1.42	1.52
1	A	750	GLY	CA-C	-7.56	1.40	1.51
1	A	1031	VAL	CA-CB	-7.56	1.45	1.54
2	B	958	GLN	CA-CB	7.56	1.65	1.53
2	B	167	ILE	CG1-CD1	7.56	1.81	1.51
2	B	238	ALA	CA-CB	7.56	1.71	1.53
3	C	95	CYS	C-O	-7.56	1.13	1.24
5	F	76	LYS	C-O	-7.56	1.14	1.24
5	F	137	TYR	C-O	-7.56	1.14	1.24
6	H	85	GLY	CA-C	7.56	1.62	1.51
6	H	38	LEU	CA-C	-7.56	1.43	1.52
4	E	17	ARG	NE-CZ	7.56	1.41	1.33
2	B	963	PHE	CA-C	-7.55	1.43	1.52
3	C	195	GLN	CD-OE1	7.55	1.38	1.23
1	A	677	ARG	C-O	-7.55	1.14	1.24
2	B	1108	ARG	N-CA	7.55	1.55	1.46
1	A	583	PRO	CA-C	7.55	1.61	1.52
1	A	836	TYR	CZ-OH	7.55	1.53	1.38
1	A	1419	ASP	CB-CG	7.55	1.71	1.52
1	A	287	HIS	CA-C	7.55	1.62	1.52
1	A	1117	THR	C-O	-7.55	1.15	1.24
2	B	766	ARG	CZ-NH2	7.55	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1030	LEU	C-O	-7.55	1.15	1.24
3	C	199	LYS	CG-CD	7.55	1.75	1.52
2	B	909	ASP	C-O	-7.54	1.14	1.23
3	C	267	GLN	C-O	7.54	1.33	1.24
2	B	183	GLU	CG-CD	7.54	1.71	1.52
2	B	745	PRO	C-O	-7.54	1.14	1.24
1	A	41	MET	CA-C	7.54	1.62	1.52
2	B	1219	ASP	CA-CB	7.53	1.66	1.53
1	A	1266	THR	CA-CB	7.53	1.65	1.53
1	A	548	ASN	C-O	-7.52	1.14	1.24
1	A	736	ASN	C-N	-7.52	1.22	1.33
8	J	53	HIS	CE1-NE2	-7.52	1.25	1.32
6	H	115	TYR	CA-CB	-7.52	1.42	1.53
1	A	45	GLN	N-CA	7.52	1.55	1.46
1	A	465	TYR	C-O	-7.52	1.14	1.24
1	A	889	SER	C-O	-7.52	1.13	1.23
1	A	1018	PHE	CA-C	7.52	1.62	1.52
6	H	80	ARG	CA-CB	7.52	1.63	1.53
8	J	33	GLY	N-CA	7.52	1.56	1.45
1	A	1327	ILE	CA-CB	7.52	1.62	1.54
2	B	370	PHE	CD1-CE1	7.52	1.61	1.38
3	C	94	LYS	CB-CG	7.52	1.75	1.52
2	B	755	ILE	C-O	7.51	1.33	1.24
4	E	149	LEU	C-N	7.51	1.39	1.33
6	H	79	TRP	CA-CB	-7.51	1.38	1.54
1	A	37	PHE	CD1-CE1	7.51	1.61	1.38
2	B	792	MET	C-O	-7.51	1.14	1.23
2	B	301	ILE	CA-C	7.50	1.63	1.52
3	C	5	GLY	CA-C	7.50	1.62	1.51
1	A	1112	LYS	CD-CE	7.50	1.75	1.52
2	B	983	ARG	CD-NE	-7.50	1.35	1.46
3	C	170	TRP	CA-C	-7.50	1.41	1.52
1	A	90	VAL	CA-CB	-7.50	1.42	1.54
1	A	1405	THR	N-CA	-7.49	1.36	1.46
1	A	959	ASN	C-O	-7.49	1.13	1.23
1	A	1208	THR	C-O	7.49	1.32	1.23
2	B	870	ILE	CB-CG1	7.49	1.68	1.53
1	A	578	LEU	CA-C	-7.49	1.43	1.52
1	A	1322	ILE	CG1-CD1	-7.49	1.22	1.51
2	B	685	LEU	C-O	-7.49	1.15	1.24
3	C	118	LEU	C-O	7.49	1.33	1.24
3	C	102	GLN	CA-C	-7.49	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	97	MET	CA-CB	-7.49	1.42	1.53
2	B	465	ASN	CB-CG	7.48	1.70	1.52
1	A	424	ILE	C-O	-7.48	1.15	1.24
1	A	135	PHE	N-CA	7.48	1.55	1.46
1	A	146	MET	CG-SD	7.48	1.99	1.80
3	C	205	LYS	CB-CG	7.48	1.74	1.52
2	B	1177	HIS	N-CA	7.48	1.56	1.46
1	A	446	ARG	C-O	-7.47	1.15	1.24
4	E	209	ALA	CA-C	-7.47	1.43	1.52
1	A	663	SER	N-CA	7.47	1.55	1.46
1	A	912	LEU	C-N	-7.47	1.24	1.33
1	A	1290	LYS	CE-NZ	7.47	1.71	1.49
1	A	800	VAL	N-CA	-7.46	1.37	1.46
1	A	923	LEU	CA-CB	7.46	1.65	1.53
1	A	986	ILE	C-O	-7.46	1.15	1.24
2	B	250	PHE	CA-CB	7.46	1.63	1.53
2	B	665	GLU	CD-OE2	7.46	1.39	1.25
2	B	876	LYS	C-O	-7.46	1.14	1.24
7	I	93	LYS	C-O	7.46	1.33	1.24
2	B	227	LYS	CE-NZ	7.46	1.71	1.49
4	E	186	LEU	C-N	-7.46	1.24	1.34
1	A	714	PHE	CA-C	-7.46	1.43	1.52
1	A	1162	VAL	CA-C	-7.45	1.41	1.52
1	A	1405	THR	C-N	-7.45	1.24	1.33
2	B	592	ASN	CB-CG	7.45	1.70	1.52
1	A	50	ILE	N-CA	7.45	1.55	1.46
4	E	24	LYS	CA-C	-7.45	1.43	1.52
6	H	83	GLN	N-CA	7.45	1.55	1.46
1	A	941	LYS	CA-CB	7.45	1.65	1.53
4	E	40	GLU	CA-CB	7.45	1.65	1.53
1	A	847	ASP	C-O	-7.44	1.14	1.24
1	A	1366	ARG	N-CA	-7.44	1.36	1.46
1	A	928	LEU	C-O	-7.44	1.15	1.24
2	B	604	ARG	CD-NE	-7.44	1.35	1.46
10	L	47	ARG	NE-CZ	7.44	1.41	1.33
6	H	24	CYS	C-O	-7.44	1.14	1.23
2	B	119	LEU	C-O	7.44	1.32	1.24
7	I	120	GLN	N-CA	7.44	1.55	1.46
2	B	870	ILE	C-O	7.43	1.32	1.24
2	B	972	LYS	CA-CB	-7.43	1.42	1.53
2	B	978	ASP	CG-OD2	7.43	1.39	1.25
1	A	1343	ALA	C-O	-7.43	1.14	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1001	ARG	CA-C	7.43	1.62	1.52
7	I	67	THR	C-O	-7.43	1.14	1.24
5	F	98	ALA	C-O	-7.43	1.15	1.24
4	E	72	PHE	CG-CD1	7.43	1.54	1.38
9	K	102	LYS	CD-CE	7.43	1.74	1.52
2	B	827	ILE	CA-CB	-7.42	1.45	1.53
6	H	27	GLU	C-O	-7.42	1.14	1.23
1	A	601	LYS	C-O	-7.42	1.14	1.24
1	A	1003	LYS	C-O	7.42	1.33	1.24
2	B	577	ALA	CA-C	-7.42	1.43	1.52
1	A	123	ARG	CD-NE	7.42	1.56	1.46
3	C	104	PHE	CD2-CE2	7.42	1.60	1.38
8	J	13	VAL	N-CA	-7.42	1.37	1.46
2	B	397	ASP	CG-OD1	7.42	1.39	1.25
1	A	1015	VAL	CA-C	7.42	1.62	1.52
1	A	1093	LYS	CA-C	7.42	1.62	1.52
2	B	293	PRO	C-O	7.41	1.31	1.23
2	B	788	ARG	C-O	-7.41	1.14	1.23
1	A	774	ARG	CD-NE	-7.41	1.35	1.46
2	B	1053	GLU	C-O	-7.41	1.15	1.24
1	A	175	ARG	CB-CG	7.41	1.74	1.52
6	H	6	PHE	CA-CB	-7.41	1.40	1.53
1	A	1159	ARG	C-O	-7.40	1.14	1.24
6	H	43	ASN	C-O	-7.40	1.14	1.24
2	B	246	LYS	CA-CB	7.40	1.64	1.53
9	K	63	VAL	N-CA	7.40	1.55	1.46
1	A	474	VAL	CA-CB	-7.40	1.44	1.54
5	F	134	ILE	N-CA	7.40	1.54	1.46
1	A	788	SER	CA-CB	7.40	1.65	1.53
1	A	905	ASP	N-CA	-7.40	1.36	1.46
10	L	26	THR	CA-C	7.40	1.62	1.52
1	A	662	PHE	CG-CD2	-7.39	1.23	1.38
1	A	902	LEU	CG-CD2	-7.39	1.28	1.52
4	E	114	ASN	CG-OD1	7.39	1.37	1.23
1	A	624	SER	CA-CB	7.39	1.62	1.52
2	B	1018	PRO	C-O	-7.39	1.15	1.24
3	C	21	ILE	C-O	7.39	1.31	1.24
1	A	871	ASP	C-O	-7.39	1.14	1.24
2	B	99	LYS	C-O	7.39	1.33	1.24
3	C	243	VAL	CA-CB	-7.39	1.44	1.54
1	A	946	VAL	C-N	-7.39	1.24	1.33
4	E	91	LYS	CA-CB	7.39	1.65	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	89	PRO	CA-C	-7.39	1.42	1.52
6	H	3	ASN	C-O	-7.39	1.17	1.24
1	A	689	LYS	CD-CE	7.38	1.74	1.52
1	A	945	GLU	N-CA	-7.38	1.36	1.46
3	C	117	ASP	C-O	7.38	1.34	1.24
1	A	407	ARG	CZ-NH1	7.38	1.43	1.32
4	E	111	VAL	C-O	-7.38	1.16	1.24
2	B	1100	ASP	CA-CB	7.38	1.65	1.53
2	B	353	LYS	CG-CD	7.38	1.74	1.52
2	B	428	ILE	CG1-CD1	7.38	1.80	1.51
2	B	1207	LEU	N-CA	-7.38	1.37	1.46
6	H	42	ILE	CA-CB	7.38	1.65	1.54
2	B	982	SER	CA-C	-7.37	1.43	1.53
1	A	185	TRP	C-O	-7.37	1.15	1.23
1	A	209	ASN	C-O	7.37	1.33	1.24
1	A	294	SER	N-CA	7.37	1.55	1.46
2	B	1030	LEU	CA-CB	-7.37	1.41	1.53
2	B	752	ALA	CA-CB	7.37	1.65	1.53
9	K	98	LEU	C-O	7.37	1.33	1.23
1	A	833	GLU	CG-CD	7.37	1.70	1.52
1	A	1128	GLN	CA-C	7.37	1.62	1.52
1	A	1425	SER	CB-OG	7.37	1.56	1.42
1	A	587	HIS	CA-CB	7.37	1.66	1.53
1	A	666	ILE	CG1-CD1	-7.37	1.23	1.51
1	A	810	PRO	CA-C	7.37	1.62	1.52
1	A	587	HIS	CA-C	-7.36	1.43	1.52
1	A	1329	THR	N-CA	-7.36	1.36	1.45
1	A	1434	ALA	CA-CB	-7.36	1.38	1.53
1	A	149	GLU	CD-OE1	7.36	1.39	1.25
2	B	370	PHE	CA-CB	7.36	1.66	1.53
1	A	656	TRP	CD2-CE3	-7.36	1.28	1.40
2	B	447	ALA	C-N	7.36	1.42	1.33
1	A	123	ARG	CB-CG	7.36	1.74	1.52
1	A	1277	GLU	CG-CD	7.36	1.70	1.52
1	A	1331	SER	N-CA	-7.36	1.37	1.46
2	B	874	PHE	CA-CB	7.36	1.62	1.53
10	L	42	ARG	N-CA	7.36	1.54	1.46
2	B	272	THR	N-CA	-7.35	1.37	1.46
2	B	346	GLU	N-CA	-7.35	1.37	1.46
2	B	711	GLU	CA-C	7.35	1.62	1.52
1	A	850	VAL	CA-C	-7.35	1.43	1.52
2	B	650	GLU	C-O	-7.35	1.14	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	80	LEU	CA-C	7.35	1.61	1.52
1	A	1381	LEU	C-N	-7.35	1.23	1.33
1	A	1359	ASP	CG-OD1	7.34	1.39	1.25
2	B	298	LEU	C-O	-7.34	1.14	1.24
4	E	192	ARG	CZ-NH2	7.34	1.43	1.33
2	B	512	ARG	CA-C	7.34	1.62	1.52
2	B	638	PHE	C-O	-7.34	1.14	1.23
2	B	882	THR	CA-CB	7.34	1.65	1.53
3	C	189	THR	CA-C	-7.34	1.43	1.52
8	J	38	ARG	N-CA	-7.34	1.36	1.46
2	B	418	LYS	CD-CE	7.34	1.74	1.52
4	E	207	ARG	N-CA	-7.34	1.36	1.45
1	A	416	ARG	CZ-NH2	-7.34	1.24	1.33
2	B	213	ILE	CA-CB	7.33	1.63	1.54
1	A	61	ILE	C-O	7.33	1.32	1.24
6	H	81	PRO	CA-CB	7.33	1.64	1.54
3	C	56	THR	CB-CG2	-7.33	1.28	1.52
5	F	101	ILE	CA-C	7.33	1.62	1.52
1	A	848	ILE	CA-C	-7.33	1.44	1.52
1	A	962	ARG	CG-CD	7.33	1.74	1.52
2	B	284	ILE	CA-CB	-7.33	1.45	1.54
2	B	222	ILE	C-O	-7.32	1.16	1.24
2	B	1088	GLY	C-O	-7.32	1.14	1.24
1	A	264	PHE	CA-CB	7.32	1.65	1.53
2	B	389	ALA	CA-CB	-7.32	1.41	1.53
3	C	228	PHE	CG-CD1	-7.32	1.23	1.38
1	A	709	THR	CB-CG2	-7.32	1.28	1.52
1	A	965	GLN	CG-CD	7.32	1.70	1.52
7	I	87	GLN	C-O	-7.32	1.14	1.23
1	A	954	TRP	C-O	-7.31	1.15	1.24
8	J	21	TYR	C-O	-7.31	1.15	1.24
4	E	80	VAL	C-O	7.31	1.31	1.23
9	K	42	LEU	CA-C	-7.31	1.42	1.52
10	L	41	SER	CA-C	7.31	1.62	1.52
2	B	624	LEU	CA-CB	-7.30	1.42	1.53
6	H	79	TRP	CA-C	-7.30	1.43	1.52
5	F	99	LEU	CB-CG	-7.30	1.38	1.53
8	J	62	ARG	CA-C	-7.30	1.42	1.52
2	B	106	ASP	CG-OD2	7.30	1.39	1.25
4	E	10	SER	N-CA	7.30	1.54	1.46
1	A	839	ARG	CZ-NH1	7.30	1.43	1.32
2	B	267	ARG	C-N	-7.30	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	732	LEU	C-O	7.30	1.32	1.24
1	A	1236	LEU	C-O	-7.30	1.15	1.24
1	A	1419	ASP	N-CA	7.30	1.55	1.46
6	H	24	CYS	CA-C	-7.30	1.43	1.52
1	A	795	GLU	C-N	-7.29	1.24	1.34
2	B	165	VAL	N-CA	7.29	1.55	1.46
2	B	203	PHE	C-O	7.29	1.32	1.23
7	I	13	MET	SD-CE	7.29	1.97	1.79
1	A	771	GLU	C-O	-7.29	1.14	1.23
2	B	811	TYR	CE2-CZ	-7.29	1.20	1.38
1	A	244	PRO	CA-C	7.29	1.58	1.52
1	A	721	PHE	C-O	7.29	1.32	1.24
2	B	695	ALA	CA-CB	-7.29	1.42	1.53
7	I	37	GLU	C-O	-7.29	1.14	1.23
9	K	47	ARG	N-CA	-7.29	1.37	1.46
2	B	1079	LYS	C-N	-7.28	1.23	1.33
4	E	155	ARG	C-O	7.28	1.32	1.24
1	A	1243	VAL	CA-CB	7.28	1.74	1.54
1	A	436	ILE	CA-CB	7.28	1.62	1.54
1	A	1041	ALA	C-O	-7.28	1.15	1.24
2	B	169	ARG	CZ-NH2	7.28	1.43	1.33
2	B	276	ILE	CG1-CD1	-7.28	1.23	1.51
2	B	1002	THR	CB-OG1	-7.28	1.32	1.43
2	B	769	TYR	CA-C	-7.28	1.43	1.52
4	E	46	TYR	C-O	7.28	1.34	1.24
2	B	312	GLU	CA-C	7.27	1.62	1.52
1	A	413	ILE	C-O	-7.27	1.15	1.23
1	A	867	ILE	CB-CG1	-7.27	1.39	1.53
2	B	743	ILE	CA-C	-7.27	1.44	1.52
1	A	206	GLU	CD-OE2	7.27	1.39	1.25
1	A	690	VAL	CA-C	-7.27	1.44	1.52
1	A	883	LEU	CA-CB	-7.27	1.43	1.53
1	A	1385	THR	CB-CG2	7.27	1.76	1.52
2	B	96	TYR	N-CA	7.27	1.54	1.45
1	A	940	ARG	CA-CB	-7.27	1.42	1.53
2	B	828	ALA	CA-CB	-7.27	1.41	1.53
2	B	963	PHE	CE1-CZ	7.27	1.60	1.38
3	C	180	TYR	C-O	-7.27	1.14	1.23
1	A	1235	LYS	CE-NZ	7.26	1.71	1.49
3	C	79	GLN	CD-OE1	7.26	1.37	1.23
2	B	793	ALA	CA-CB	-7.26	1.41	1.53
1	A	159	THR	CA-CB	7.26	1.65	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1205	GLN	CA-CB	-7.26	1.41	1.53
1	A	739	ASP	N-CA	-7.26	1.36	1.46
1	A	879	GLU	CD-OE1	7.26	1.39	1.25
1	A	944	ARG	N-CA	-7.26	1.36	1.46
1	A	1412	ALA	C-O	-7.26	1.15	1.24
6	H	130	ARG	NE-CZ	-7.26	1.25	1.33
7	I	62	ILE	C-O	-7.26	1.15	1.24
3	C	101	LEU	C-O	-7.25	1.15	1.23
1	A	112	LYS	N-CA	-7.25	1.37	1.46
2	B	1029	CYS	CA-C	7.25	1.62	1.52
1	A	390	GLN	CA-CB	7.25	1.64	1.53
7	I	111	THR	CA-C	-7.25	1.44	1.52
8	J	44	TYR	CE1-CZ	-7.25	1.20	1.38
2	B	219	ALA	CA-CB	7.25	1.65	1.53
3	C	97	VAL	CA-C	-7.25	1.43	1.52
2	B	1212	ILE	CG1-CD1	-7.25	1.23	1.51
1	A	461	LYS	CD-CE	7.25	1.74	1.52
1	A	1104	ILE	CB-CG2	-7.25	1.28	1.52
1	A	1433	MET	CA-C	-7.25	1.43	1.52
2	B	190	TYR	C-O	-7.25	1.15	1.24
2	B	1151	LEU	CA-C	7.25	1.63	1.52
3	C	142	VAL	CA-CB	-7.25	1.45	1.54
2	B	109	THR	N-CA	7.24	1.55	1.46
1	A	1303	GLU	CD-OE1	7.24	1.39	1.25
2	B	261	ARG	NE-CZ	7.24	1.41	1.33
1	A	87	ALA	CA-C	-7.24	1.43	1.52
2	B	115	GLN	CB-CG	7.24	1.74	1.52
5	F	147	SER	CA-C	7.24	1.62	1.53
9	K	97	LYS	C-N	-7.24	1.23	1.33
10	L	51	CYS	N-CA	7.24	1.55	1.46
1	A	983	ILE	C-N	-7.24	1.24	1.34
4	E	35	VAL	CB-CG1	-7.24	1.28	1.52
5	F	72	LYS	CG-CD	7.24	1.74	1.52
6	H	85	GLY	C-O	7.24	1.33	1.23
1	A	1108	ALA	CA-C	-7.23	1.43	1.52
2	B	179	CYS	C-O	-7.23	1.15	1.23
2	B	520	GLY	C-O	-7.23	1.13	1.24
6	H	95	TYR	C-O	-7.23	1.15	1.23
1	A	206	GLU	CA-C	-7.23	1.42	1.52
1	A	444	PHE	C-O	-7.23	1.15	1.23
2	B	25	ILE	CA-CB	7.23	1.64	1.54
6	H	27	GLU	N-CA	7.23	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1135	ARG	N-CA	-7.23	1.37	1.46
2	B	1012	ILE	CG1-CD1	-7.23	1.23	1.51
2	B	1057	LYS	N-CA	-7.23	1.37	1.46
3	C	103	ALA	N-CA	7.23	1.54	1.45
1	A	1093	LYS	CB-CG	7.22	1.74	1.52
2	B	369	GLY	CA-C	7.22	1.62	1.51
9	K	10	PHE	N-CA	7.22	1.55	1.45
10	L	43	THR	N-CA	7.22	1.56	1.46
2	B	533	CYS	N-CA	-7.22	1.36	1.46
2	B	612	GLU	CG-CD	7.22	1.70	1.52
6	H	80	ARG	NE-CZ	7.22	1.41	1.33
2	B	1198	TYR	CA-CB	7.22	1.64	1.53
4	E	43	LYS	CB-CG	7.22	1.74	1.52
8	J	62	ARG	CG-CD	-7.22	1.30	1.52
2	B	245	GLU	CG-CD	7.21	1.70	1.52
2	B	901	PRO	C-O	-7.21	1.14	1.23
3	C	68	GLY	C-O	7.21	1.33	1.24
1	A	652	VAL	CB-CG1	-7.21	1.28	1.52
5	F	93	ILE	CA-CB	-7.21	1.46	1.54
1	A	786	HIS	C-O	-7.21	1.14	1.24
2	B	485	ARG	CG-CD	-7.21	1.30	1.52
1	A	608	ILE	CB-CG1	7.21	1.67	1.53
2	B	1097	HIS	CG-CD2	7.21	1.43	1.35
2	B	106	ASP	CB-CG	7.21	1.70	1.52
1	A	368	LYS	CA-C	-7.20	1.43	1.52
1	A	424	ILE	CA-C	-7.20	1.44	1.52
2	B	832	GLY	C-O	-7.20	1.14	1.24
7	I	82	GLU	CG-CD	7.20	1.70	1.52
5	F	148	VAL	N-CA	-7.20	1.38	1.46
1	A	352	VAL	CA-CB	-7.20	1.45	1.54
1	A	603	ASN	CA-C	-7.20	1.43	1.52
2	B	241	ARG	CD-NE	7.20	1.56	1.46
4	E	152	LYS	CB-CG	7.20	1.74	1.52
4	E	152	LYS	N-CA	7.20	1.55	1.46
2	B	1139	ILE	CA-C	-7.20	1.43	1.52
1	A	969	GLN	CD-NE2	7.20	1.48	1.33
2	B	1033	LYS	CA-C	7.20	1.61	1.52
1	A	37	PHE	C-O	-7.19	1.14	1.24
1	A	1135	ARG	C-O	7.19	1.32	1.24
2	B	274	PRO	CA-C	7.19	1.60	1.52
2	B	344	LYS	CD-CE	7.19	1.74	1.52
2	B	658	ILE	CA-C	-7.19	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	816	GLU	N-CA	-7.19	1.36	1.46
1	A	850	VAL	CB-CG1	-7.19	1.28	1.52
2	B	577	ALA	C-O	-7.19	1.15	1.23
4	E	58	MET	N-CA	7.19	1.55	1.46
2	B	336	ARG	CB-CG	-7.18	1.30	1.52
2	B	327	ARG	CB-CG	-7.18	1.30	1.52
2	B	975	GLN	N-CA	7.18	1.55	1.45
10	L	50	ASP	N-CA	7.18	1.55	1.46
5	F	135	ARG	CD-NE	7.18	1.56	1.46
1	A	377	PRO	N-CA	-7.18	1.40	1.47
1	A	920	LEU	CG-CD2	-7.18	1.28	1.52
1	A	1142	THR	CA-C	7.18	1.61	1.52
4	E	74	ASP	CG-OD2	-7.17	1.11	1.25
9	K	54	ARG	CZ-NH2	7.17	1.42	1.33
2	B	348	ARG	NE-CZ	-7.17	1.25	1.33
1	A	510	GLN	C-N	7.17	1.42	1.33
1	A	1239	ARG	CD-NE	7.17	1.56	1.46
1	A	1109	LYS	CD-CE	7.17	1.74	1.52
2	B	1022	THR	CA-C	7.17	1.60	1.53
6	H	104	PHE	CA-CB	7.17	1.65	1.53
9	K	53	ASP	CA-CB	7.17	1.61	1.53
1	A	1062	GLU	CA-CB	-7.16	1.41	1.53
1	A	1438	THR	N-CA	-7.16	1.36	1.46
1	A	720	ARG	CA-CB	7.16	1.64	1.53
2	B	169	ARG	CZ-NH1	7.16	1.42	1.32
2	B	780	VAL	C-O	-7.16	1.16	1.24
9	K	70	ARG	N-CA	-7.16	1.36	1.45
1	A	359	LEU	CA-CB	-7.16	1.42	1.53
3	C	57	VAL	C-O	-7.16	1.16	1.24
5	F	86	THR	C-O	-7.16	1.14	1.23
1	A	510	GLN	CD-NE2	-7.15	1.18	1.33
1	A	589	GLN	CD-OE1	7.15	1.37	1.23
2	B	312	GLU	CD-OE1	7.15	1.39	1.25
2	B	763	GLN	C-N	-7.15	1.24	1.33
2	B	226	PHE	CD1-CE1	7.15	1.60	1.38
1	A	827	THR	C-N	-7.14	1.24	1.33
1	A	486	GLU	C-N	-7.14	1.24	1.33
2	B	310	MET	CA-C	7.14	1.61	1.52
2	B	385	LEU	N-CA	-7.14	1.37	1.46
3	C	192	TRP	CE3-CZ3	-7.14	1.17	1.38
1	A	412	ARG	CA-C	-7.14	1.43	1.52
6	H	13	SER	CA-CB	7.14	1.65	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	320	ASP	C-O	-7.13	1.14	1.24
2	B	430	ARG	NE-CZ	7.13	1.40	1.33
2	B	1048	THR	CA-C	-7.13	1.43	1.52
4	E	109	ILE	CA-CB	7.13	1.64	1.54
4	E	146	HIS	CA-C	-7.13	1.41	1.52
1	A	446	ARG	CZ-NH2	7.13	1.42	1.33
2	B	810	GLU	CA-C	7.13	1.62	1.52
2	B	27	ALA	N-CA	-7.13	1.37	1.46
2	B	191	LYS	CD-CE	7.13	1.73	1.52
1	A	235	ILE	CA-C	7.13	1.61	1.52
2	B	37	PHE	C-O	7.13	1.32	1.24
2	B	895	ASP	N-CA	7.13	1.55	1.46
7	I	58	VAL	CA-C	-7.12	1.44	1.52
6	H	41	ASP	CB-CG	7.12	1.69	1.52
1	A	420	ARG	CB-CG	-7.12	1.31	1.52
6	H	109	LYS	CA-C	7.12	1.62	1.52
2	B	914	LYS	C-O	7.12	1.32	1.23
1	A	396	PRO	CA-C	-7.12	1.40	1.52
1	A	611	GLN	CA-C	-7.12	1.44	1.52
1	A	1381	LEU	N-CA	7.12	1.55	1.46
2	B	1084	GLN	C-O	-7.12	1.14	1.23
6	H	113	ALA	CA-CB	-7.12	1.41	1.53
7	I	45	ARG	NE-CZ	-7.12	1.25	1.33
1	A	919	ILE	CA-CB	7.12	1.62	1.54
2	B	698	GLU	N-CA	-7.12	1.37	1.46
1	A	893	PHE	CG-CD1	-7.12	1.24	1.38
1	A	214	ILE	N-CA	7.11	1.55	1.46
1	A	932	GLU	C-O	-7.11	1.15	1.24
2	B	861	ASP	CA-C	-7.11	1.43	1.52
2	B	870	ILE	CA-C	7.11	1.61	1.52
1	A	12	ARG	CZ-NH1	7.11	1.42	1.32
2	B	615	MET	CA-C	-7.11	1.44	1.52
1	A	5	GLN	CA-CB	7.11	1.64	1.53
9	K	54	ARG	CG-CD	7.11	1.73	1.52
2	B	963	PHE	CB-CG	-7.11	1.34	1.50
3	C	230	MET	C-O	-7.11	1.14	1.23
1	A	1199	ARG	C-O	7.10	1.32	1.24
2	B	435	THR	N-CA	7.10	1.56	1.46
2	B	1221	SER	CA-CB	7.10	1.65	1.53
2	B	736	THR	CB-OG1	-7.10	1.32	1.43
4	E	174	GLN	CD-NE2	-7.10	1.18	1.33
7	I	66	PRO	C-O	7.10	1.33	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1211	ASN	CG-OD1	-7.10	1.10	1.23
2	B	815	ARG	CD-NE	-7.10	1.36	1.46
1	A	847	ASP	CG-OD1	7.09	1.38	1.25
2	B	1033	LYS	N-CA	7.09	1.54	1.46
3	C	13	ALA	C-N	-7.09	1.24	1.33
9	K	30	ALA	CA-CB	-7.09	1.39	1.53
2	B	199	MET	SD-CE	7.09	1.97	1.79
2	B	529	GLU	CG-CD	7.09	1.69	1.52
1	A	85	ASP	N-CA	7.09	1.54	1.46
4	E	41	ASP	CG-OD1	7.09	1.38	1.25
1	A	1270	ASN	CA-CB	7.09	1.62	1.53
2	B	965	LYS	C-O	-7.09	1.16	1.24
1	A	828	ALA	CA-CB	-7.09	1.42	1.53
1	A	838	GLN	CD-OE1	7.09	1.37	1.23
1	A	1135	ARG	NE-CZ	7.09	1.40	1.33
1	A	1210	GLY	CA-C	7.09	1.60	1.51
9	K	24	ASP	CA-C	-7.09	1.44	1.52
1	A	237	THR	CB-CG2	7.08	1.75	1.52
1	A	682	THR	CA-CB	-7.08	1.42	1.53
2	B	1218	THR	CA-CB	-7.08	1.41	1.53
3	C	268	ASP	CA-C	7.08	1.67	1.52
1	A	1435	PRO	C-O	-7.08	1.14	1.24
4	E	49	SER	CA-C	7.08	1.61	1.52
5	F	110	ASP	CG-OD1	7.08	1.38	1.25
1	A	1449	SER	CA-C	7.08	1.61	1.52
2	B	842	ASN	CG-ND2	-7.08	1.18	1.33
2	B	1210	MET	CG-SD	-7.08	1.63	1.80
2	B	723	VAL	N-CA	7.08	1.54	1.46
1	A	180	LYS	CD-CE	7.08	1.73	1.52
1	A	1160	SER	CA-C	7.08	1.61	1.52
2	B	609	ILE	N-CA	7.08	1.55	1.46
3	C	85	ASP	C-O	-7.08	1.14	1.24
4	E	78	LEU	N-CA	-7.08	1.37	1.46
1	A	1112	LYS	CE-NZ	7.07	1.70	1.49
10	L	32	ALA	C-O	7.07	1.32	1.24
1	A	1382	THR	N-CA	-7.07	1.37	1.46
1	A	700	ASN	CA-C	-7.07	1.43	1.52
2	B	813	LYS	C-N	-7.07	1.23	1.33
2	B	1047	PHE	CA-CB	-7.07	1.43	1.53
1	A	1294	PRO	CB-CG	7.07	1.84	1.49
2	B	435	THR	CA-C	7.07	1.60	1.53
2	B	547	VAL	CA-CB	-7.07	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	58	VAL	C-O	-7.06	1.15	1.23
2	B	1013	ASN	C-O	-7.06	1.14	1.24
2	B	267	ARG	CA-C	7.06	1.62	1.52
2	B	795	ILE	C-O	-7.06	1.17	1.24
1	A	74	MET	CG-SD	7.06	1.98	1.80
1	A	1327	ILE	C-O	-7.06	1.17	1.24
2	B	205	ILE	CA-CB	-7.06	1.44	1.53
1	A	651	LYS	CA-C	7.06	1.62	1.52
1	A	937	VAL	CA-C	-7.05	1.44	1.52
1	A	1334	ASP	CA-C	-7.05	1.43	1.52
2	B	315	LYS	CE-NZ	7.05	1.70	1.49
4	E	90	VAL	CB-CG1	7.05	1.75	1.52
1	A	514	PRO	CA-CB	-7.05	1.42	1.53
2	B	705	MET	CG-SD	7.05	1.98	1.80
2	B	824	ILE	N-CA	-7.05	1.38	1.46
1	A	589	GLN	CA-C	-7.05	1.44	1.52
2	B	882	THR	CB-CG2	7.05	1.75	1.52
1	A	1417	GLU	CA-CB	7.04	1.64	1.53
2	B	523	CYS	C-N	-7.04	1.26	1.34
4	E	192	ARG	N-CA	-7.04	1.37	1.46
1	A	1308	THR	CB-CG2	-7.04	1.29	1.52
2	B	183	GLU	CD-OE1	7.04	1.38	1.25
2	B	203	PHE	N-CA	7.04	1.54	1.45
3	C	75	MET	N-CA	7.04	1.54	1.46
9	K	34	THR	C-N	-7.04	1.23	1.33
1	A	393	ARG	CA-C	-7.04	1.43	1.52
2	B	1080	LYS	CD-CE	7.04	1.73	1.52
5	F	153	VAL	N-CA	-7.04	1.37	1.46
1	A	475	THR	N-CA	-7.04	1.37	1.46
1	A	510	GLN	C-O	7.04	1.33	1.24
10	L	47	ARG	CG-CD	7.04	1.73	1.52
1	A	806	ARG	N-CA	-7.03	1.37	1.46
3	C	177	GLU	CD-OE2	7.03	1.38	1.25
4	E	69	ILE	CA-CB	-7.03	1.44	1.54
4	E	68	SER	C-O	7.03	1.32	1.24
4	E	83	CYS	CA-C	-7.03	1.44	1.52
5	F	78	GLN	CA-C	7.03	1.62	1.52
2	B	323	VAL	N-CA	-7.03	1.36	1.46
1	A	572	TRP	CZ3-CH2	-7.03	1.22	1.40
1	A	1421	CYS	C-O	-7.03	1.14	1.23
7	I	55	THR	CA-CB	-7.03	1.42	1.53
1	A	1433	MET	N-CA	7.03	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	120	GLN	C-O	7.03	1.32	1.24
2	B	96	TYR	CG-CD1	7.03	1.54	1.39
2	B	351	TYR	CA-C	7.03	1.61	1.52
1	A	1366	ARG	CD-NE	-7.02	1.36	1.46
2	B	893	LEU	C-O	-7.02	1.15	1.23
3	C	238	ILE	CA-CB	-7.02	1.45	1.54
1	A	515	GLN	CG-CD	7.02	1.69	1.52
1	A	1221	LYS	CB-CG	7.02	1.73	1.52
6	H	23	VAL	C-N	7.02	1.42	1.33
2	B	283	VAL	C-O	-7.01	1.15	1.24
2	B	726	ALA	CA-CB	7.01	1.65	1.53
2	B	734	HIS	CA-C	7.01	1.62	1.52
1	A	1420	ASP	CG-OD1	7.01	1.38	1.25
2	B	616	ILE	CG1-CD1	7.01	1.79	1.51
9	K	114	LEU	CB-CG	7.01	1.67	1.53
1	A	1441	PHE	N-CA	-7.01	1.37	1.46
3	C	3	GLU	CD-OE2	7.01	1.38	1.25
1	A	31	SER	CA-C	7.01	1.62	1.52
1	A	466	SER	N-CA	7.01	1.54	1.46
2	B	705	MET	C-O	-7.01	1.14	1.24
7	I	110	PHE	CD1-CE1	7.01	1.59	1.38
1	A	187	LYS	C-O	7.00	1.33	1.24
1	A	1352	VAL	CA-CB	-7.00	1.46	1.54
1	A	940	ARG	CZ-NH2	-7.00	1.24	1.33
2	B	222	ILE	N-CA	-7.00	1.38	1.46
2	B	514	LEU	CA-C	-7.00	1.44	1.52
10	L	32	ALA	CA-CB	-7.00	1.42	1.53
1	A	65	LEU	C-O	7.00	1.32	1.24
1	A	157	ASP	CA-CB	7.00	1.64	1.53
1	A	751	SER	CA-C	-6.99	1.43	1.52
6	H	43	ASN	C-N	-6.99	1.27	1.34
1	A	1104	ILE	CA-CB	-6.99	1.46	1.54
4	E	192	ARG	CD-NE	6.99	1.56	1.46
7	I	52	ILE	C-N	-6.99	1.23	1.33
9	K	20	LYS	CB-CG	6.99	1.73	1.52
1	A	710	LEU	CG-CD2	6.99	1.75	1.52
1	A	806	ARG	CZ-NH2	6.99	1.42	1.33
1	A	1023	ARG	CA-CB	-6.99	1.41	1.53
2	B	814	PHE	CA-C	-6.99	1.43	1.52
1	A	1210	GLY	C-O	6.99	1.33	1.23
1	A	106	VAL	C-O	-6.99	1.14	1.24
1	A	685	GLU	CA-C	-6.99	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	233	PRO	C-O	-6.99	1.14	1.24
3	C	160	LYS	CG-CD	6.99	1.73	1.52
1	A	370	ILE	C-O	-6.98	1.15	1.24
2	B	510	LYS	N-CA	6.98	1.55	1.46
2	B	908	GLU	N-CA	6.98	1.54	1.46
2	B	18	PHE	CA-CB	6.98	1.67	1.53
5	F	89	GLU	CA-CB	6.98	1.64	1.53
1	A	954	TRP	C-N	6.97	1.41	1.33
2	B	894	ASP	CA-C	6.97	1.62	1.53
3	C	231	ASN	CB-CG	6.97	1.69	1.52
1	A	103	CYS	C-O	6.97	1.32	1.24
1	A	986	ILE	CA-C	-6.97	1.44	1.52
2	B	1188	LYS	CG-CD	6.97	1.73	1.52
1	A	1207	LEU	CA-C	6.97	1.60	1.52
2	B	1106	ARG	CA-CB	6.97	1.62	1.52
9	K	85	ASP	CA-CB	6.97	1.64	1.53
2	B	527	THR	CA-CB	-6.96	1.41	1.53
3	C	148	ARG	CD-NE	6.96	1.56	1.46
4	E	185	ALA	CA-CB	-6.96	1.42	1.53
1	A	508	PRO	CA-CB	6.96	1.64	1.53
2	B	450	ALA	CA-C	-6.96	1.45	1.53
2	B	966	VAL	C-O	-6.96	1.16	1.24
1	A	439	ASN	CG-ND2	-6.96	1.18	1.33
1	A	830	LYS	CD-CE	6.96	1.73	1.52
4	E	111	VAL	CA-CB	-6.96	1.46	1.54
9	K	96	ASN	CA-C	-6.96	1.43	1.52
1	A	498	ARG	CZ-NH2	-6.96	1.24	1.33
1	A	613	ILE	CA-C	-6.96	1.43	1.53
2	B	516	ASN	C-O	-6.96	1.16	1.24
2	B	813	LYS	C-O	-6.96	1.13	1.23
1	A	1026	LEU	C-O	-6.96	1.14	1.23
1	A	560	ILE	C-N	-6.96	1.24	1.33
2	B	241	ARG	C-O	-6.95	1.15	1.23
2	B	974	PRO	CA-CB	-6.95	1.44	1.53
4	E	36	GLU	C-O	-6.95	1.15	1.24
2	B	230	ALA	N-CA	6.95	1.55	1.46
5	F	142	SER	C-O	-6.95	1.14	1.23
10	L	64	LEU	C-O	6.95	1.31	1.23
3	C	180	TYR	CG-CD1	-6.95	1.24	1.39
2	B	425	THR	CB-CG2	6.95	1.75	1.52
7	I	30	ARG	CA-C	-6.94	1.42	1.52
1	A	681	GLU	CG-CD	6.94	1.69	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	910	VAL	CA-C	-6.94	1.44	1.52
1	A	1163	ILE	N-CA	6.94	1.51	1.46
2	B	435	THR	CA-CB	6.94	1.65	1.53
3	C	209	TYR	CG-CD2	6.94	1.53	1.39
1	A	455	MET	C-O	-6.94	1.16	1.23
1	A	510	GLN	CB-CG	6.94	1.73	1.52
1	A	1037	LEU	C-O	-6.94	1.15	1.23
2	B	70	ILE	CA-CB	6.93	1.73	1.54
1	A	4	GLN	CB-CG	6.93	1.73	1.52
1	A	493	GLN	CA-CB	-6.93	1.42	1.53
1	A	1326	ARG	CD-NE	-6.93	1.36	1.46
1	A	1341	ILE	CA-C	-6.93	1.44	1.52
2	B	1018	PRO	N-CA	-6.93	1.38	1.47
1	A	1427	ASN	CA-CB	-6.93	1.42	1.53
3	C	142	VAL	N-CA	-6.93	1.38	1.46
2	B	69	LEU	CA-C	6.93	1.63	1.53
1	A	601	LYS	CE-NZ	6.93	1.70	1.49
1	A	978	PRO	CA-C	6.93	1.60	1.52
1	A	616	VAL	CA-CB	-6.92	1.46	1.54
3	C	243	VAL	CA-C	-6.92	1.43	1.52
1	A	229	SER	CA-CB	-6.92	1.41	1.52
2	B	798	TYR	CA-CB	6.92	1.61	1.53
2	B	375	ALA	N-CA	-6.92	1.38	1.46
2	B	620	ARG	NE-CZ	-6.92	1.25	1.33
1	A	553	VAL	CA-CB	-6.92	1.45	1.54
2	B	434	ARG	CA-CB	6.92	1.62	1.53
5	F	94	LEU	C-N	-6.92	1.23	1.33
6	H	63	LEU	CA-C	6.92	1.67	1.52
9	K	50	LEU	CB-CG	-6.92	1.39	1.53
1	A	1202	MET	C-O	6.91	1.32	1.24
9	K	26	LYS	CA-CB	6.91	1.64	1.53
2	B	831	SER	C-O	-6.91	1.15	1.24
1	A	1100	ARG	CA-C	-6.91	1.43	1.52
2	B	184	ALA	CA-C	-6.91	1.44	1.52
4	E	160	GLU	N-CA	6.91	1.54	1.46
6	H	89	LEU	CA-CB	6.91	1.65	1.53
1	A	734	GLU	C-O	-6.91	1.16	1.24
4	E	95	THR	CA-CB	6.91	1.64	1.53
2	B	593	PRO	CB-CG	6.90	1.84	1.49
2	B	95	ILE	C-O	-6.90	1.16	1.24
2	B	302	CYS	C-O	6.90	1.31	1.24
3	C	160	LYS	CE-NZ	6.90	1.70	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	2	SER	CA-C	6.90	1.67	1.52
10	L	43	THR	CB-CG2	6.90	1.75	1.52
2	B	893	LEU	CA-CB	-6.89	1.42	1.53
2	B	933	SER	CA-C	6.89	1.67	1.52
2	B	1165	ILE	C-O	-6.89	1.15	1.23
3	C	252	GLN	CG-CD	6.89	1.69	1.52
7	I	86	PHE	CA-C	-6.89	1.44	1.52
1	A	660	ASN	CA-C	-6.89	1.43	1.52
1	A	1450	LEU	N-CA	6.89	1.59	1.46
4	E	204	THR	CB-CG2	-6.89	1.29	1.52
2	B	137	TYR	CG-CD1	6.89	1.53	1.39
1	A	524	VAL	C-O	-6.89	1.15	1.23
2	B	975	GLN	CB-CG	-6.89	1.31	1.52
9	K	25	THR	CB-CG2	6.89	1.75	1.52
1	A	460	VAL	C-O	-6.88	1.16	1.24
3	C	58	LEU	N-CA	-6.88	1.37	1.46
6	H	102	TYR	C-O	-6.88	1.15	1.24
8	J	8	PHE	N-CA	6.88	1.54	1.46
1	A	1383	SER	CA-CB	-6.88	1.42	1.53
2	B	528	PRO	CA-CB	-6.88	1.44	1.53
2	B	763	GLN	CB-CG	-6.88	1.31	1.52
9	K	77	THR	CB-OG1	6.88	1.54	1.43
1	A	485	ASP	C-O	-6.88	1.15	1.23
3	C	208	GLU	CD-OE2	6.88	1.38	1.25
6	H	109	LYS	CA-CB	6.88	1.65	1.53
5	F	139	PRO	C-O	-6.88	1.15	1.24
1	A	709	THR	CA-CB	-6.87	1.41	1.53
1	A	944	ARG	CA-CB	-6.87	1.41	1.53
2	B	196	PRO	CA-C	6.87	1.62	1.52
1	A	1194	ARG	N-CA	-6.87	1.38	1.46
5	F	151	LEU	CA-CB	-6.87	1.42	1.53
1	A	1309	ASP	C-O	6.87	1.32	1.24
2	B	480	SER	N-CA	6.87	1.54	1.46
2	B	1144	ALA	N-CA	-6.87	1.37	1.46
5	F	116	ASP	N-CA	6.87	1.56	1.46
1	A	818	MET	SD-CE	-6.86	1.62	1.79
2	B	596	LEU	CG-CD1	-6.86	1.29	1.52
2	B	482	VAL	C-O	-6.86	1.16	1.24
4	E	205	SER	C-O	-6.86	1.15	1.24
5	F	121	ALA	CA-CB	-6.86	1.42	1.53
1	A	82	GLY	C-O	-6.86	1.15	1.23
2	B	803	LEU	CA-C	-6.86	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	809	MET	CG-SD	6.86	1.97	1.80
7	I	23	ASN	CB-CG	6.86	1.69	1.52
1	A	379	VAL	N-CA	6.86	1.54	1.46
1	A	783	THR	C-O	-6.86	1.15	1.24
1	A	205	GLU	C-O	6.85	1.32	1.24
5	F	79	ARG	NE-CZ	-6.85	1.25	1.33
9	K	68	PHE	CG-CD1	-6.85	1.24	1.38
3	C	236	GLY	N-CA	-6.85	1.35	1.45
1	A	965	GLN	C-O	-6.85	1.15	1.24
4	E	65	THR	C-O	6.85	1.32	1.23
4	E	185	ALA	CA-C	6.85	1.61	1.52
7	I	65	ASP	C-O	6.85	1.32	1.24
1	A	924	LYS	CA-C	6.84	1.62	1.52
6	H	85	GLY	N-CA	6.84	1.55	1.45
1	A	1205	LYS	N-CA	6.84	1.53	1.46
1	A	186	LYS	CG-CD	6.84	1.73	1.52
1	A	832	ALA	CA-CB	-6.84	1.42	1.53
2	B	1017	ILE	C-O	-6.84	1.15	1.24
4	E	164	LEU	C-N	-6.84	1.24	1.34
8	J	41	LEU	CG-CD2	-6.84	1.29	1.52
10	L	53	HIS	N-CA	6.84	1.54	1.46
4	E	63	ASN	CG-OD1	6.84	1.36	1.23
1	A	909	ASP	CG-OD1	6.84	1.38	1.25
1	A	1154	TYR	C-N	6.83	1.41	1.33
1	A	178	GLY	CA-C	-6.83	1.46	1.53
1	A	1356	ILE	C-O	-6.83	1.16	1.24
1	A	1049	ILE	N-CA	-6.83	1.38	1.46
2	B	173	MET	CA-C	-6.83	1.43	1.52
10	L	64	LEU	CG-CD1	6.83	1.75	1.52
1	A	603	ASN	C-O	-6.83	1.15	1.23
1	A	1411	GLU	CD-OE1	6.83	1.38	1.25
3	C	158	VAL	N-CA	-6.83	1.38	1.46
3	C	183	TRP	N-CA	6.83	1.54	1.45
1	A	641	VAL	CA-C	-6.82	1.44	1.52
1	A	1030	ARG	CZ-NH2	-6.82	1.24	1.33
1	A	121	LEU	CG-CD1	6.82	1.75	1.52
1	A	1235	LYS	CA-C	6.82	1.60	1.52
1	A	1256	GLU	CA-CB	6.82	1.65	1.53
1	A	1366	ARG	CA-CB	-6.82	1.41	1.53
2	B	58	THR	CA-CB	-6.82	1.42	1.53
2	B	1186	ASP	CA-C	6.82	1.62	1.53
2	B	651	LEU	N-CA	-6.81	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	560	ILE	C-O	-6.81	1.15	1.24
1	A	186	LYS	CB-CG	6.81	1.72	1.52
2	B	1090	THR	CA-CB	-6.81	1.39	1.54
2	B	132	VAL	CA-CB	-6.81	1.45	1.54
2	B	346	GLU	CA-CB	6.81	1.64	1.53
6	H	86	ASP	CA-CB	6.81	1.65	1.53
1	A	567	LYS	CD-CE	6.81	1.72	1.52
1	A	1222	ASN	C-O	6.81	1.32	1.24
2	B	1078	GLY	C-N	-6.81	1.24	1.33
4	E	2	ASP	CA-C	6.81	1.61	1.52
4	E	37	LEU	CG-CD1	6.81	1.75	1.52
1	A	109	HIS	CB-CG	6.81	1.59	1.50
1	A	492	PRO	CA-C	-6.81	1.43	1.52
2	B	965	LYS	CA-C	-6.81	1.44	1.52
1	A	570	PRO	CA-C	6.80	1.62	1.52
1	A	1159	ARG	NE-CZ	6.80	1.40	1.33
1	A	896	ARG	NE-CZ	-6.80	1.25	1.33
1	A	1035	TYR	CG-CD1	-6.80	1.25	1.39
2	B	766	ARG	CZ-NH1	6.80	1.42	1.32
1	A	1371	LEU	C-O	6.80	1.31	1.24
2	B	465	ASN	CG-OD1	6.80	1.36	1.23
2	B	996	ARG	CA-CB	-6.80	1.42	1.53
2	B	1132	GLU	CG-CD	6.80	1.69	1.52
2	B	963	PHE	C-O	6.80	1.32	1.23
9	K	63	VAL	CB-CG1	-6.80	1.30	1.52
2	B	384	ARG	CA-C	6.79	1.61	1.52
2	B	518	HIS	CA-CB	-6.79	1.41	1.53
1	A	415	LEU	C-O	6.79	1.32	1.24
1	A	421	ALA	N-CA	-6.79	1.38	1.46
1	A	821	ARG	NE-CZ	-6.79	1.25	1.33
1	A	1157	ASP	CA-CB	6.79	1.62	1.53
2	B	373	ARG	C-O	-6.79	1.16	1.24
2	B	449	ASN	CA-C	6.79	1.61	1.52
3	C	140	ASN	N-CA	-6.79	1.37	1.46
2	B	368	GLU	N-CA	6.79	1.54	1.46
1	A	388	LEU	CB-CG	-6.79	1.39	1.53
1	A	505	CYS	C-N	-6.79	1.24	1.33
1	A	1188	GLN	N-CA	6.79	1.54	1.46
1	A	1411	GLU	C-O	6.79	1.32	1.24
6	H	121	LEU	N-CA	-6.79	1.37	1.46
7	I	20	LYS	CD-CE	6.79	1.72	1.52
9	K	9	LEU	CA-CB	-6.79	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	680	THR	N-CA	-6.79	1.37	1.46
2	B	489	SER	C-O	-6.79	1.15	1.24
8	J	29	GLU	CD-OE1	6.79	1.38	1.25
1	A	789	LYS	CG-CD	-6.78	1.32	1.52
1	A	813	PHE	CA-CB	-6.78	1.42	1.53
2	B	549	THR	C-O	6.78	1.31	1.23
2	B	766	ARG	N-CA	-6.78	1.37	1.46
2	B	18	PHE	C-N	6.78	1.43	1.33
1	A	1042	PHE	CA-C	-6.78	1.44	1.52
1	A	1290	LYS	CD-CE	6.78	1.72	1.52
2	B	608	ASP	CA-CB	6.78	1.64	1.53
1	A	750	GLY	C-N	-6.78	1.23	1.33
1	A	1198	ASP	C-O	6.78	1.32	1.24
1	A	994	GLN	C-O	-6.78	1.16	1.24
3	C	12	GLU	CD-OE2	6.78	1.38	1.25
3	C	145	CYS	CA-CB	-6.78	1.42	1.53
1	A	578	LEU	C-O	-6.77	1.16	1.24
2	B	1183	LYS	N-CA	6.77	1.54	1.46
10	L	41	SER	C-O	6.77	1.32	1.24
3	C	134	ILE	CG1-CD1	-6.77	1.25	1.51
1	A	672	ASP	CA-CB	6.77	1.65	1.53
2	B	284	ILE	CA-C	6.77	1.61	1.52
5	F	119	ARG	N-CA	-6.77	1.37	1.46
1	A	350	ARG	CZ-NH2	-6.76	1.24	1.33
2	B	417	PHE	CA-C	6.76	1.62	1.52
2	B	958	GLN	CB-CG	6.76	1.72	1.52
3	C	34	ARG	C-O	6.76	1.32	1.24
1	A	734	GLU	CA-CB	6.76	1.63	1.53
2	B	732	SER	CA-CB	6.76	1.64	1.53
2	B	274	PRO	C-O	6.76	1.31	1.23
3	C	172	PRO	C-O	6.76	1.32	1.24
5	F	146	TRP	CB-CG	-6.76	1.29	1.50
1	A	1255	GLU	CA-C	6.76	1.61	1.52
2	B	1131	GLY	C-O	6.76	1.29	1.23
1	A	462	VAL	N-CA	6.75	1.53	1.46
2	B	577	ALA	CA-CB	-6.75	1.43	1.53
1	A	19	PHE	C-O	-6.75	1.15	1.23
2	B	288	ALA	N-CA	6.75	1.55	1.46
3	C	12	GLU	N-CA	-6.75	1.37	1.46
5	F	124	GLU	N-CA	-6.75	1.38	1.46
1	A	107	CYS	N-CA	6.75	1.54	1.46
1	A	1037	LEU	CB-CG	6.75	1.67	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	724	GLU	CG-CD	6.75	1.69	1.52
2	B	178	ASN	CG-OD1	6.75	1.36	1.23
2	B	635	ARG	CA-CB	-6.75	1.44	1.53
1	A	373	THR	C-O	-6.75	1.15	1.24
1	A	394	ASN	C-O	6.75	1.32	1.24
3	C	126	GLY	C-O	6.75	1.33	1.23
4	E	19	VAL	N-CA	6.75	1.54	1.46
2	B	858	SER	CA-CB	-6.75	1.43	1.53
1	A	605	MET	N-CA	-6.74	1.38	1.46
2	B	320	ASP	CB-CG	6.74	1.69	1.52
2	B	102	VAL	CA-C	6.74	1.60	1.52
2	B	111	ALA	CA-CB	6.74	1.64	1.53
2	B	350	GLN	C-N	-6.74	1.25	1.33
1	A	755	PHE	C-O	6.74	1.31	1.24
6	H	42	ILE	N-CA	-6.74	1.38	1.46
9	K	16	GLU	C-O	-6.74	1.15	1.23
1	A	536	LEU	C-N	6.74	1.42	1.33
3	C	163	ILE	CB-CG2	6.74	1.74	1.52
1	A	448	PRO	CG-CD	-6.74	1.33	1.51
1	A	1052	GLN	CD-OE1	6.74	1.36	1.23
2	B	221	ASN	C-O	6.74	1.35	1.24
7	I	68	LEU	N-CA	-6.74	1.36	1.46
1	A	953	ASN	CG-OD1	6.73	1.36	1.23
2	B	962	LYS	C-O	6.73	1.32	1.23
2	B	1223	ASP	C-N	6.73	1.42	1.33
4	E	147	HIS	C-O	-6.73	1.15	1.23
5	F	74	ILE	CA-C	-6.73	1.45	1.52
1	A	915	SER	C-N	-6.73	1.25	1.33
2	B	1020	ARG	CZ-NH1	6.73	1.42	1.32
1	A	81	PHE	CE2-CZ	-6.73	1.18	1.38
1	A	1332	PHE	N-CA	-6.73	1.38	1.46
2	B	31	TRP	CD2-CE2	-6.73	1.29	1.41
2	B	904	ARG	CB-CG	-6.73	1.32	1.52
9	K	89	ASN	CB-CG	6.73	1.68	1.52
2	B	955	THR	CA-CB	6.72	1.62	1.53
7	I	93	LYS	CD-CE	6.72	1.72	1.52
1	A	348	SER	N-CA	-6.72	1.37	1.45
1	A	1214	GLU	CG-CD	6.72	1.68	1.52
2	B	552	MET	CA-CB	-6.72	1.44	1.53
3	C	110	THR	CA-CB	6.72	1.63	1.53
4	E	185	ALA	N-CA	-6.72	1.38	1.46
3	C	55	THR	C-O	6.72	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	163	SER	CA-C	-6.72	1.43	1.52
1	A	949	ASP	C-O	-6.72	1.15	1.24
4	E	173	SER	C-O	-6.72	1.15	1.24
1	A	1142	THR	C-O	6.72	1.32	1.23
9	K	110	ASN	CB-CG	6.71	1.68	1.52
1	A	196	GLU	C-O	-6.71	1.15	1.24
8	J	53	HIS	CG-ND1	-6.71	1.30	1.38
3	C	3	GLU	N-CA	6.71	1.58	1.46
1	A	510	GLN	CA-CB	-6.71	1.43	1.53
2	B	35	SER	CA-CB	-6.71	1.42	1.53
1	A	298	PHE	N-CA	6.71	1.54	1.46
2	B	114	PRO	CG-CD	-6.71	1.27	1.50
3	C	248	ILE	CA-C	6.71	1.60	1.52
2	B	396	ASP	C-O	6.70	1.32	1.23
1	A	1112	LYS	CB-CG	6.70	1.72	1.52
2	B	231	PRO	CB-CG	6.70	1.83	1.49
2	B	1178	ASN	N-CA	6.70	1.56	1.46
2	B	266	ALA	CA-C	6.70	1.61	1.52
2	B	482	VAL	C-N	-6.70	1.23	1.33
2	B	642	ASP	CA-C	-6.70	1.44	1.52
2	B	657	HIS	CA-C	-6.70	1.44	1.52
4	E	164	LEU	N-CA	-6.70	1.38	1.46
4	E	63	ASN	CA-CB	6.70	1.63	1.53
1	A	973	ILE	CB-CG2	6.70	1.74	1.52
5	F	87	LYS	CE-NZ	6.70	1.69	1.49
1	A	16	GLU	C-O	6.69	1.32	1.23
2	B	1064	TYR	CA-CB	-6.69	1.43	1.53
1	A	301	ALA	CA-C	6.69	1.61	1.52
3	C	88	CYS	C-O	-6.69	1.14	1.23
7	I	57	GLY	C-O	-6.69	1.15	1.24
2	B	509	ALA	CA-C	6.69	1.67	1.52
2	B	53	GLN	C-O	6.69	1.32	1.24
2	B	176	SER	CA-CB	6.69	1.63	1.53
1	A	591	PHE	CA-CB	6.69	1.63	1.53
1	A	805	LEU	CA-C	-6.69	1.44	1.52
1	A	1145	SER	N-CA	6.69	1.54	1.46
2	B	567	GLU	CD-OE2	6.69	1.38	1.25
3	C	87	PHE	CD2-CE2	6.69	1.58	1.38
1	A	187	LYS	C-N	6.69	1.43	1.33
1	A	1013	ASP	CA-C	6.69	1.61	1.52
3	C	23	SER	N-CA	6.69	1.53	1.46
1	A	193	ASP	CB-CG	6.68	1.68	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1445	ILE	CB-CG2	6.68	1.74	1.52
1	A	162	VAL	C-N	6.68	1.43	1.33
10	L	68	GLU	CD-OE2	6.68	1.38	1.25
2	B	191	LYS	CG-CD	6.68	1.72	1.52
1	A	48	ALA	CA-C	6.68	1.61	1.52
1	A	1105	LEU	C-O	-6.68	1.15	1.24
1	A	1316	VAL	N-CA	6.68	1.54	1.46
2	B	547	VAL	N-CA	6.68	1.53	1.46
1	A	482	PHE	CE1-CZ	-6.68	1.18	1.38
1	A	1009	ASN	N-CA	6.68	1.54	1.46
6	H	121	LEU	CG-CD1	-6.68	1.30	1.52
1	A	594	GLY	C-O	-6.67	1.15	1.23
1	A	674	PRO	C-O	6.67	1.32	1.24
7	I	20	LYS	CA-C	6.67	1.61	1.52
1	A	37	PHE	CD2-CE2	6.67	1.58	1.38
1	A	290	GLU	C-O	-6.67	1.16	1.24
1	A	275	SER	CA-C	6.67	1.61	1.52
1	A	185	TRP	N-CA	-6.67	1.37	1.46
1	A	683	ILE	CA-C	-6.67	1.44	1.52
1	A	865	GLN	CA-C	6.67	1.60	1.52
7	I	58	VAL	C-N	-6.67	1.23	1.33
2	B	659	ALA	C-O	-6.67	1.16	1.24
5	F	152	ILE	C-O	-6.67	1.17	1.24
1	A	616	VAL	CB-CG1	-6.67	1.30	1.52
2	B	462	ALA	CA-CB	-6.67	1.43	1.53
1	A	1003	LYS	CB-CG	6.66	1.72	1.52
2	B	358	LYS	C-O	-6.66	1.15	1.24
2	B	935	ARG	CD-NE	6.66	1.55	1.46
4	E	99	HIS	C-O	6.66	1.31	1.24
1	A	766	GLY	C-O	-6.66	1.14	1.24
2	B	821	GLN	CA-C	-6.66	1.44	1.52
2	B	1081	LEU	C-O	-6.66	1.16	1.24
7	I	40	SER	CA-C	-6.66	1.44	1.52
4	E	177	ARG	C-O	-6.65	1.15	1.23
1	A	174	ILE	N-CA	-6.65	1.38	1.46
2	B	647	GLY	C-O	-6.65	1.15	1.23
2	B	763	GLN	C-O	6.65	1.31	1.23
1	A	969	GLN	CA-CB	6.65	1.64	1.53
4	E	91	LYS	CB-CG	6.65	1.72	1.52
1	A	514	PRO	N-CA	-6.64	1.38	1.47
1	A	1382	THR	C-O	6.64	1.32	1.24
2	B	109	THR	C-O	-6.64	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	650	GLU	CA-C	6.64	1.60	1.52
3	C	52	GLU	CA-CB	6.64	1.64	1.53
3	C	67	LEU	C-N	6.64	1.42	1.33
3	C	220	ASP	C-O	6.64	1.32	1.23
7	I	8	ARG	CA-C	6.64	1.61	1.52
2	B	1157	ALA	CA-CB	6.64	1.61	1.52
1	A	720	ARG	CD-NE	6.64	1.55	1.46
2	B	466	TRP	C-N	6.64	1.42	1.33
2	B	651	LEU	CG-CD1	-6.64	1.30	1.52
1	A	993	LEU	C-O	-6.64	1.16	1.24
1	A	686	ALA	C-O	-6.64	1.16	1.24
2	B	710	LEU	CG-CD1	-6.64	1.30	1.52
7	I	8	ARG	C-O	-6.64	1.15	1.24
1	A	230	ARG	CA-C	6.63	1.61	1.52
1	A	1296	GLY	N-CA	6.63	1.52	1.45
1	A	175	ARG	CG-CD	6.63	1.72	1.52
1	A	473	SER	N-CA	6.63	1.54	1.46
1	A	999	VAL	N-CA	-6.63	1.40	1.46
7	I	54	GLU	CD-OE1	6.63	1.38	1.25
6	H	117	SER	C-O	6.63	1.31	1.23
2	B	1180	PHE	N-CA	-6.62	1.38	1.46
3	C	103	ALA	CA-C	-6.62	1.44	1.52
3	C	195	GLN	CG-CD	6.62	1.68	1.52
1	A	726	ARG	CA-C	-6.62	1.44	1.52
7	I	1	MET	CA-CB	6.62	1.66	1.53
1	A	5	GLN	N-CA	6.62	1.54	1.45
1	A	987	VAL	CB-CG1	-6.62	1.30	1.52
1	A	1286	LYS	CA-CB	6.62	1.62	1.53
2	B	211	VAL	CA-CB	6.62	1.63	1.54
2	B	1204	PHE	CE1-CZ	-6.62	1.18	1.38
1	A	900	ASP	CA-C	-6.62	1.44	1.53
4	E	172	GLU	CA-CB	6.62	1.63	1.53
1	A	992	ASP	C-O	-6.62	1.16	1.24
1	A	1025	ARG	N-CA	-6.62	1.37	1.46
2	B	342	GLY	CA-C	-6.62	1.43	1.52
2	B	578	THR	C-O	-6.62	1.16	1.24
1	A	175	ARG	C-O	6.62	1.32	1.23
1	A	1336	MET	CA-CB	-6.62	1.42	1.53
2	B	955	THR	C-O	-6.61	1.18	1.24
1	A	11	LEU	CA-C	-6.61	1.44	1.52
2	B	493	SER	N-CA	-6.61	1.38	1.46
2	B	912	ILE	CA-CB	-6.61	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	826	ASP	C-O	-6.61	1.16	1.24
2	B	594	ALA	CA-C	-6.61	1.43	1.52
2	B	823	ALA	CA-CB	-6.61	1.43	1.53
6	H	8	ASP	C-O	6.61	1.32	1.24
1	A	57	ARG	C-O	-6.60	1.15	1.24
1	A	644	LYS	CE-NZ	6.60	1.69	1.49
2	B	130	VAL	CB-CG2	-6.60	1.30	1.52
1	A	1074	GLU	CD-OE2	6.60	1.37	1.25
2	B	792	MET	CG-SD	6.60	1.97	1.80
9	K	101	LEU	CA-C	6.60	1.61	1.52
3	C	207	CYS	N-CA	6.60	1.54	1.46
1	A	1107	VAL	N-CA	-6.60	1.38	1.46
2	B	1163	CYS	CA-C	6.60	1.61	1.52
1	A	650	GLN	CD-NE2	-6.60	1.19	1.33
1	A	758	ILE	CG1-CD1	-6.60	1.26	1.51
6	H	52	GLN	CA-C	6.60	1.61	1.52
2	B	212	LEU	N-CA	-6.59	1.38	1.46
2	B	633	VAL	C-N	6.59	1.42	1.33
1	A	104	GLU	CA-C	6.59	1.61	1.52
1	A	607	ILE	CG1-CD1	-6.59	1.26	1.51
1	A	836	TYR	CG-CD2	6.59	1.53	1.39
1	A	372	LYS	C-O	-6.59	1.15	1.24
1	A	904	THR	CB-OG1	6.59	1.54	1.43
8	J	24	LEU	CA-CB	-6.59	1.42	1.53
8	J	53	HIS	C-O	-6.59	1.16	1.23
4	E	99	HIS	CA-CB	6.59	1.63	1.53
1	A	1221	LYS	N-CA	6.58	1.54	1.46
2	B	245	GLU	CA-CB	6.58	1.64	1.53
2	B	1184	GLY	CA-C	-6.58	1.45	1.52
3	C	205	LYS	CG-CD	6.58	1.72	1.52
1	A	80	HIS	CA-C	6.58	1.60	1.52
1	A	767	GLN	CA-CB	-6.58	1.42	1.53
1	A	392	VAL	N-CA	-6.58	1.38	1.46
1	A	1447	GLU	C-O	6.58	1.31	1.24
2	B	916	THR	CB-CG2	6.58	1.74	1.52
1	A	561	PRO	CA-CB	6.58	1.63	1.53
2	B	952	VAL	CA-C	-6.58	1.44	1.52
1	A	934	LYS	CG-CD	6.58	1.72	1.52
8	J	1	MET	CA-CB	-6.58	1.40	1.53
1	A	243	PRO	CA-CB	-6.57	1.45	1.54
7	I	78	CYS	CA-CB	6.57	1.64	1.53
8	J	37	SER	C-O	-6.57	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	905	ASP	CA-CB	-6.57	1.42	1.53
2	B	275	TYR	CA-C	-6.57	1.44	1.52
2	B	790	ASP	CA-C	-6.57	1.44	1.52
4	E	30	ILE	CA-CB	6.57	1.64	1.54
2	B	136	THR	C-N	6.57	1.42	1.33
2	B	337	ARG	CZ-NH1	-6.57	1.23	1.32
1	A	386	ASP	CG-OD1	6.57	1.37	1.25
1	A	589	GLN	CD-NE2	6.57	1.47	1.33
2	B	581	PHE	CE2-CZ	-6.57	1.19	1.38
5	F	77	ASP	CG-OD1	6.57	1.37	1.25
1	A	640	GLN	CD-OE1	6.56	1.36	1.23
2	B	347	LYS	CA-CB	-6.56	1.42	1.53
1	A	539	THR	CB-CG2	-6.56	1.30	1.52
2	B	843	GLN	CG-CD	-6.56	1.35	1.52
2	B	855	PHE	CG-CD2	-6.56	1.25	1.38
2	B	1035	ALA	C-O	6.56	1.31	1.24
2	B	1096	ARG	CA-CB	6.56	1.63	1.53
2	B	768	THR	CA-C	6.56	1.61	1.52
2	B	1069	PHE	CB-CG	-6.56	1.35	1.50
1	A	99	ILE	C-O	6.56	1.31	1.24
1	A	219	PHE	N-CA	6.56	1.54	1.46
1	A	1450	LEU	CA-C	6.56	1.66	1.52
2	B	349	ILE	CA-CB	-6.56	1.46	1.54
1	A	127	ALA	C-O	6.56	1.32	1.24
1	A	1080	THR	C-N	6.56	1.42	1.33
4	E	74	ASP	CG-OD1	-6.56	1.12	1.25
1	A	455	MET	CA-C	-6.55	1.45	1.53
1	A	1139	GLU	CA-CB	-6.55	1.42	1.53
1	A	1200	ALA	CA-CB	-6.55	1.42	1.53
2	B	582	VAL	CA-CB	6.55	1.62	1.54
2	B	665	GLU	CA-C	-6.55	1.44	1.52
2	B	684	LEU	CA-CB	-6.55	1.43	1.53
4	E	82	PHE	CA-CB	6.55	1.64	1.53
1	A	517	ASN	CG-OD1	-6.55	1.11	1.23
1	A	526	ASP	CA-C	-6.55	1.44	1.52
1	A	748	MET	C-N	-6.55	1.25	1.34
2	B	1095	LEU	CA-C	-6.55	1.44	1.52
2	B	840	ILE	C-O	-6.55	1.17	1.24
6	H	39	THR	CA-C	-6.55	1.44	1.52
9	K	114	LEU	CA-C	6.55	1.66	1.52
2	B	608	ASP	CG-OD2	6.54	1.37	1.25
1	A	686	ALA	CA-C	-6.54	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	420	LEU	N-CA	-6.54	1.37	1.46
2	B	624	LEU	C-O	-6.54	1.16	1.24
1	A	369	SER	CA-CB	-6.54	1.42	1.53
2	B	203	PHE	CA-CB	-6.54	1.42	1.53
3	C	7	GLN	CB-CG	6.54	1.72	1.52
7	I	72	ASP	CG-OD1	6.54	1.37	1.25
1	A	1029	ARG	N-CA	-6.54	1.38	1.46
2	B	192	LEU	CG-CD2	6.54	1.74	1.52
3	C	154	LYS	CA-C	-6.54	1.44	1.52
4	E	181	ALA	CA-CB	-6.54	1.43	1.53
1	A	529	CYS	C-N	-6.53	1.24	1.33
2	B	703	ILE	CA-CB	-6.53	1.46	1.54
2	B	654	ARG	CA-CB	-6.53	1.43	1.53
9	K	6	ARG	CB-CG	-6.53	1.32	1.52
1	A	516	SER	CA-C	-6.53	1.45	1.52
1	A	924	LYS	CA-CB	-6.53	1.42	1.53
1	A	1113	THR	C-O	-6.53	1.15	1.24
3	C	118	LEU	N-CA	6.53	1.54	1.46
1	A	1376	THR	C-O	-6.53	1.15	1.24
2	B	49	ASP	C-N	-6.53	1.24	1.33
1	A	202	LEU	N-CA	6.52	1.54	1.46
1	A	703	THR	CB-CG2	6.52	1.74	1.52
4	E	3	GLN	N-CA	6.52	1.54	1.46
6	H	99	GLY	C-O	6.52	1.32	1.23
2	B	779	GLY	C-O	-6.52	1.15	1.23
1	A	685	GLU	N-CA	-6.52	1.37	1.46
1	A	1225	PHE	CG-CD2	6.52	1.52	1.38
4	E	92	THR	CA-CB	6.52	1.63	1.53
2	B	875	GLU	C-O	-6.52	1.15	1.23
8	J	53	HIS	CG-CD2	-6.52	1.28	1.35
2	B	180	TYR	C-O	6.51	1.32	1.24
2	B	1033	LYS	CB-CG	-6.51	1.32	1.52
3	C	86	CYS	C-O	6.51	1.31	1.23
1	A	592	ASP	N-CA	6.51	1.54	1.46
2	B	661	LEU	C-N	-6.51	1.25	1.33
3	C	76	ASP	CA-CB	6.51	1.62	1.52
1	A	664	THR	C-O	-6.51	1.16	1.23
2	B	1032	SER	C-O	6.51	1.32	1.24
1	A	526	ASP	CA-CB	6.51	1.63	1.53
2	B	1077	THR	CA-CB	-6.51	1.45	1.54
8	J	25	LEU	CA-C	6.51	1.61	1.52
2	B	1085	ILE	CB-CG2	-6.50	1.31	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	993	THR	C-O	-6.50	1.16	1.23
2	B	1200	ALA	C-O	-6.50	1.16	1.24
1	A	482	PHE	C-O	-6.50	1.14	1.23
1	A	1132	LYS	CE-NZ	6.50	1.68	1.49
2	B	1069	PHE	CG-CD2	-6.50	1.25	1.38
1	A	123	ARG	CZ-NH2	6.50	1.42	1.33
1	A	593	GLU	CA-C	6.50	1.61	1.52
2	B	1224	PHE	CG-CD2	6.50	1.52	1.38
1	A	364	VAL	C-N	-6.50	1.26	1.33
1	A	440	ASP	C-N	-6.50	1.26	1.33
1	A	628	GLY	CA-C	-6.50	1.45	1.52
1	A	1269	GLU	N-CA	6.50	1.54	1.46
8	J	39	LEU	CA-C	-6.50	1.38	1.52
9	K	31	VAL	CA-CB	6.50	1.66	1.55
2	B	292	ILE	CA-CB	6.50	1.62	1.54
2	B	1041	GLU	C-N	-6.50	1.29	1.33
1	A	1192	LEU	CB-CG	6.50	1.66	1.53
2	B	68	THR	CA-C	6.49	1.60	1.52
2	B	1155	SER	C-O	6.49	1.32	1.24
3	C	33	LEU	CA-CB	6.49	1.63	1.53
4	E	160	GLU	C-N	-6.49	1.25	1.33
1	A	139	TRP	N-CA	6.49	1.54	1.46
1	A	676	MET	CA-C	-6.49	1.43	1.52
1	A	532	ARG	C-O	-6.49	1.16	1.24
1	A	555	ASP	CA-CB	6.49	1.61	1.53
2	B	19	GLU	CA-CB	6.49	1.64	1.53
8	J	2	ILE	C-N	6.49	1.40	1.33
1	A	511	ILE	CA-C	-6.49	1.44	1.52
2	B	397	ASP	CG-OD2	6.49	1.37	1.25
2	B	959	ASP	CA-C	6.49	1.61	1.52
3	C	209	TYR	CD2-CE2	6.49	1.58	1.38
1	A	972	HIS	C-O	-6.48	1.14	1.23
7	I	23	ASN	C-O	-6.48	1.14	1.23
1	A	891	ALA	CA-C	-6.48	1.44	1.52
2	B	65	GLU	CA-C	6.48	1.62	1.53
6	H	112	ILE	CA-C	6.48	1.60	1.52
2	B	635	ARG	C-O	-6.48	1.17	1.24
1	A	757	ASN	CA-CB	-6.47	1.43	1.53
3	C	98	VAL	C-O	-6.47	1.17	1.24
2	B	294	ASP	N-CA	6.47	1.54	1.46
6	H	34	ASP	CA-C	6.47	1.61	1.52
1	A	373	THR	CB-CG2	-6.47	1.31	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	499	ASN	C-O	-6.47	1.16	1.23
1	A	862	ASN	CA-C	-6.47	1.44	1.52
9	K	23	PRO	CA-C	-6.47	1.45	1.52
4	E	57	MET	C-O	6.46	1.32	1.24
3	C	26	ASP	CB-CG	6.46	1.68	1.52
6	H	119	GLY	C-O	6.46	1.32	1.23
2	B	563	MET	C-O	-6.46	1.16	1.23
4	E	154	ILE	CB-CG2	-6.46	1.31	1.52
7	I	66	PRO	CA-C	-6.46	1.41	1.52
4	E	170	LEU	CA-C	-6.46	1.45	1.52
1	A	1333	ILE	CB-CG2	-6.46	1.31	1.52
2	B	175	ARG	N-CA	6.46	1.53	1.46
2	B	999	MET	CA-C	-6.46	1.44	1.52
4	E	94	LYS	CG-CD	6.46	1.71	1.52
3	C	192	TRP	CB-CG	6.45	1.70	1.50
1	A	660	ASN	CG-ND2	-6.45	1.19	1.33
4	E	180	ARG	CD-NE	6.45	1.55	1.46
1	A	1142	THR	C-N	6.45	1.42	1.34
2	B	320	ASP	CG-OD1	6.45	1.37	1.25
2	B	637	LEU	CA-C	6.45	1.60	1.52
2	B	1224	PHE	N-CA	6.45	1.58	1.46
2	B	486	TYR	CA-C	-6.45	1.44	1.52
4	E	28	TYR	CE1-CZ	-6.44	1.22	1.38
2	B	513	GLN	C-O	-6.44	1.15	1.23
2	B	1079	LYS	C-O	-6.44	1.16	1.23
3	C	37	MET	CA-CB	-6.44	1.43	1.53
2	B	529	GLU	C-O	6.44	1.32	1.23
3	C	211	ASP	CG-OD2	6.44	1.37	1.25
4	E	108	GLY	C-N	-6.44	1.24	1.33
7	I	18	GLU	CA-CB	6.44	1.62	1.53
2	B	1151	LEU	N-CA	-6.44	1.37	1.46
2	B	65	GLU	CG-CD	6.43	1.68	1.52
2	B	235	SER	N-CA	-6.43	1.37	1.46
2	B	1109	GLY	C-O	6.43	1.32	1.24
2	B	1178	ASN	CB-CG	-6.43	1.35	1.52
3	C	218	PRO	CG-CD	6.43	1.72	1.50
1	A	1129	GLU	CA-CB	6.43	1.64	1.53
1	A	1221	LYS	CG-CD	6.43	1.71	1.52
2	B	953	LEU	N-CA	-6.43	1.38	1.46
3	C	27	LEU	CA-C	-6.43	1.43	1.52
4	E	20	LYS	CD-CE	6.43	1.71	1.52
1	A	446	ARG	CA-CB	-6.43	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	404	TYR	N-CA	-6.42	1.37	1.45
2	B	137	TYR	CA-CB	6.42	1.64	1.53
1	A	1221	LYS	CA-CB	6.42	1.64	1.53
1	A	1377	THR	CB-OG1	-6.42	1.33	1.43
10	L	49	LYS	CG-CD	6.42	1.71	1.52
1	A	787	PHE	CD1-CE1	6.42	1.57	1.38
1	A	1017	LEU	CG-CD1	-6.42	1.31	1.52
2	B	851	PHE	CB-CG	6.42	1.65	1.50
1	A	763	ALA	CA-C	-6.42	1.47	1.52
2	B	936	ASP	N-CA	6.42	1.54	1.46
8	J	42	LYS	C-O	6.42	1.33	1.23
1	A	347	PHE	CG-CD2	6.42	1.52	1.38
2	B	218	SER	CA-C	-6.42	1.44	1.52
1	A	1116	LEU	N-CA	-6.42	1.38	1.46
2	B	1067	ARG	C-N	-6.42	1.23	1.33
1	A	129	LYS	CA-C	6.41	1.60	1.52
2	B	866	TYR	CA-CB	6.41	1.62	1.53
3	C	123	ASN	C-O	-6.41	1.16	1.24
1	A	1272	THR	CB-CG2	6.41	1.73	1.52
2	B	328	GLU	C-O	-6.41	1.16	1.24
1	A	832	ALA	C-O	-6.41	1.16	1.24
1	A	4	GLN	C-N	6.41	1.41	1.33
1	A	1146	VAL	N-CA	-6.41	1.38	1.46
2	B	250	PHE	CG-CD2	6.41	1.52	1.38
2	B	398	ARG	NE-CZ	-6.41	1.26	1.33
6	H	28	ALA	C-O	6.41	1.31	1.23
8	J	37	SER	N-CA	6.41	1.54	1.46
1	A	487	MET	CG-SD	6.41	1.96	1.80
1	A	1130	GLN	N-CA	6.41	1.54	1.46
6	H	105	GLU	CA-CB	6.41	1.64	1.53
1	A	746	MET	CG-SD	-6.40	1.64	1.80
1	A	387	ARG	CA-C	6.40	1.61	1.52
1	A	411	ASP	C-O	-6.40	1.16	1.23
1	A	1340	GLY	C-O	-6.40	1.16	1.23
2	B	974	PRO	CA-C	-6.40	1.45	1.52
3	C	260	LEU	CA-CB	6.40	1.64	1.53
1	A	1450	LEU	CA-CB	6.40	1.66	1.53
2	B	466	TRP	C-O	6.40	1.32	1.24
2	B	819	ALA	C-O	-6.40	1.16	1.23
9	K	60	ALA	N-CA	6.40	1.54	1.46
1	A	274	ILE	N-CA	6.40	1.54	1.46
1	A	391	LEU	CA-C	6.40	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	815	PHE	CG-CD2	-6.40	1.25	1.38
1	A	1284	MET	N-CA	6.40	1.54	1.46
2	B	541	LEU	CA-CB	-6.40	1.42	1.53
2	B	566	LEU	C-O	-6.40	1.16	1.24
1	A	143	LYS	CG-CD	6.40	1.71	1.52
1	A	1448	GLU	CA-CB	6.40	1.64	1.53
6	H	30	SER	N-CA	6.40	1.54	1.46
1	A	389	THR	C-O	6.39	1.31	1.24
2	B	1142	GLY	CA-C	-6.39	1.42	1.51
10	L	62	LYS	CE-NZ	6.39	1.68	1.49
2	B	24	PRO	N-CA	-6.39	1.39	1.46
2	B	567	GLU	C-O	-6.39	1.16	1.24
4	E	148	GLU	CA-C	-6.39	1.43	1.52
2	B	229	ALA	CA-C	-6.39	1.44	1.52
8	J	41	LEU	CA-C	-6.39	1.44	1.52
1	A	804	TYR	CA-C	-6.39	1.44	1.52
3	C	29	MET	CA-C	6.39	1.61	1.52
9	K	26	LYS	CD-CE	6.39	1.71	1.52
8	J	61	LEU	CA-CB	-6.38	1.42	1.53
1	A	80	HIS	C-O	6.38	1.32	1.23
1	A	868	TYR	C-O	6.38	1.31	1.23
1	A	1222	ASN	C-N	6.38	1.42	1.33
1	A	1365	TYR	CA-C	-6.38	1.43	1.52
2	B	323	VAL	C-N	-6.38	1.25	1.33
2	B	991	GLY	C-O	-6.38	1.15	1.23
1	A	130	ASP	CG-OD1	6.38	1.37	1.25
2	B	981	ALA	C-O	-6.38	1.16	1.23
1	A	441	PRO	C-O	-6.38	1.16	1.23
1	A	1298	TYR	CG-CD2	-6.38	1.25	1.39
2	B	353	LYS	CD-CE	6.38	1.71	1.52
2	B	483	LEU	CB-CG	-6.38	1.40	1.53
1	A	581	ALA	CA-CB	-6.38	1.43	1.53
1	A	1414	ALA	CA-C	-6.38	1.43	1.52
2	B	598	GLU	C-O	-6.38	1.16	1.24
1	A	995	GLU	CA-C	-6.37	1.43	1.52
2	B	899	ILE	C-O	-6.37	1.15	1.24
1	A	833	GLU	CA-C	6.37	1.61	1.52
2	B	834	ASN	CA-CB	6.37	1.61	1.53
1	A	1363	VAL	C-O	6.37	1.30	1.24
2	B	795	ILE	CA-C	-6.37	1.44	1.52
2	B	406	LEU	CA-C	6.37	1.60	1.52
4	E	12	LEU	CA-CB	6.37	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	277	GLU	CA-C	6.37	1.61	1.52
1	A	820	GLY	C-N	-6.37	1.25	1.33
2	B	1194	ILE	N-CA	-6.37	1.39	1.46
1	A	968	GLN	CA-C	-6.36	1.43	1.52
3	C	136	ASP	CG-OD1	-6.36	1.13	1.25
9	K	1	MET	N-CA	6.36	1.58	1.46
1	A	28	ARG	C-O	6.36	1.31	1.24
1	A	1151	GLU	C-O	6.36	1.31	1.23
1	A	569	LYS	C-O	-6.36	1.17	1.24
1	A	920	LEU	CA-C	-6.36	1.44	1.52
3	C	231	ASN	CA-C	-6.36	1.44	1.52
4	E	60	PHE	C-O	-6.36	1.16	1.23
2	B	615	MET	C-O	6.36	1.30	1.23
1	A	131	SER	CA-C	6.36	1.61	1.52
1	A	169	ASN	C-O	-6.36	1.15	1.23
1	A	452	LYS	CA-C	-6.36	1.43	1.52
2	B	1064	TYR	CZ-OH	6.36	1.51	1.38
1	A	1176	LEU	CB-CG	6.36	1.66	1.53
2	B	785	TYR	CG-CD1	-6.36	1.26	1.39
2	B	1220	ARG	NE-CZ	6.36	1.40	1.33
1	A	135	PHE	CE2-CZ	-6.35	1.19	1.38
1	A	1079	MET	CA-C	6.35	1.63	1.52
1	A	1119	TYR	CG-CD1	-6.35	1.26	1.39
5	F	103	MET	CA-CB	-6.35	1.44	1.52
1	A	204	THR	C-N	6.35	1.42	1.33
1	A	975	HIS	CB-CG	6.35	1.59	1.50
2	B	497	ARG	C-O	-6.35	1.15	1.23
6	H	129	TYR	CE1-CZ	6.35	1.53	1.38
8	J	49	MET	C-O	-6.35	1.16	1.24
1	A	589	GLN	CG-CD	6.34	1.68	1.52
1	A	1325	THR	CB-CG2	-6.34	1.31	1.52
1	A	1336	MET	CB-CG	-6.34	1.33	1.52
2	B	311	LEU	N-CA	-6.34	1.38	1.46
1	A	210	ILE	CA-C	6.34	1.60	1.52
1	A	977	LYS	CB-CG	6.34	1.71	1.52
4	E	57	MET	CG-SD	6.34	1.96	1.80
2	B	710	LEU	CA-CB	-6.34	1.43	1.53
1	A	711	ARG	C-O	-6.34	1.16	1.24
5	F	149	GLU	C-O	6.34	1.31	1.24
1	A	507	VAL	CB-CG2	-6.34	1.31	1.52
1	A	1211	GLN	CB-CG	6.34	1.71	1.52
2	B	1000	PRO	N-CA	-6.34	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	810	PRO	CG-CD	6.34	1.72	1.50
4	E	192	ARG	CA-C	-6.34	1.45	1.52
2	B	889	THR	CA-CB	6.33	1.62	1.53
4	E	44	ALA	C-O	6.33	1.31	1.24
6	H	87	ARG	CD-NE	6.33	1.55	1.46
1	A	1301	GLU	CD-OE1	6.33	1.37	1.25
2	B	106	ASP	CA-CB	6.33	1.64	1.53
2	B	812	LEU	CA-C	-6.33	1.43	1.52
2	B	865	LYS	N-CA	6.33	1.54	1.46
2	B	1052	VAL	CA-CB	6.33	1.63	1.54
3	C	256	ALA	C-O	6.33	1.32	1.24
1	A	1283	VAL	CB-CG2	-6.32	1.31	1.52
1	A	1304	TRP	CA-C	-6.32	1.44	1.52
9	K	62	LYS	C-O	6.32	1.31	1.23
1	A	696	GLU	CA-C	6.32	1.60	1.52
2	B	204	ILE	C-O	-6.32	1.17	1.24
2	B	366	GLN	N-CA	6.32	1.53	1.46
2	B	1109	GLY	CA-C	6.32	1.60	1.51
2	B	1198	TYR	C-O	6.32	1.31	1.24
1	A	546	VAL	CA-C	-6.32	1.44	1.52
1	A	880	LYS	N-CA	-6.32	1.38	1.46
1	A	623	GLY	CA-C	-6.32	1.43	1.52
2	B	822	ASN	CA-CB	-6.32	1.45	1.53
4	E	187	TYR	CG-CD1	-6.32	1.26	1.39
3	C	56	THR	CA-CB	-6.31	1.42	1.53
2	B	312	GLU	N-CA	-6.31	1.38	1.46
2	B	385	LEU	C-O	-6.31	1.16	1.24
2	B	510	LYS	CB-CG	-6.31	1.33	1.52
3	C	146	LYS	CB-CG	6.31	1.71	1.52
9	K	83	PRO	C-O	-6.31	1.16	1.24
1	A	411	ASP	CG-OD1	6.31	1.37	1.25
2	B	764	SER	C-O	-6.31	1.18	1.24
1	A	1159	ARG	CD-NE	6.31	1.55	1.46
1	A	845	LEU	N-CA	6.30	1.54	1.46
1	A	1109	LYS	CA-CB	6.30	1.64	1.53
2	B	733	HIS	CA-CB	6.30	1.64	1.53
9	K	61	TYR	CZ-OH	-6.30	1.24	1.38
8	J	2	ILE	CA-C	-6.30	1.45	1.52
8	J	54	VAL	C-O	6.30	1.31	1.24
2	B	48	LEU	N-CA	-6.30	1.38	1.46
2	B	343	ILE	CA-CB	-6.30	1.44	1.53
2	B	344	LYS	CG-CD	6.30	1.71	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	61	ILE	CB-CG2	6.30	1.73	1.52
1	A	669	THR	N-CA	-6.30	1.37	1.46
6	H	95	TYR	C-N	-6.30	1.25	1.33
1	A	531	ILE	N-CA	6.29	1.54	1.46
1	A	326	ARG	CG-CD	6.29	1.71	1.52
1	A	1371	LEU	N-CA	-6.29	1.38	1.46
3	C	137	LYS	CD-CE	6.29	1.71	1.52
5	F	136	ARG	NE-CZ	-6.29	1.26	1.33
1	A	1234	GLU	C-O	-6.29	1.16	1.24
2	B	394	ASP	CB-CG	6.29	1.67	1.52
2	B	434	ARG	CD-NE	6.29	1.55	1.46
2	B	857	ARG	CA-CB	-6.29	1.42	1.53
4	E	214	CYS	CA-C	-6.29	1.44	1.52
3	C	233	GLU	C-O	-6.29	1.16	1.23
5	F	116	ASP	CA-C	-6.29	1.45	1.52
1	A	1227	ILE	CA-C	-6.29	1.46	1.52
1	A	1278	ASN	C-O	-6.29	1.16	1.24
10	L	57	LEU	CA-C	6.29	1.60	1.52
1	A	646	PHE	C-O	-6.29	1.16	1.24
1	A	708	MET	CB-CG	-6.29	1.33	1.52
2	B	794	ASN	N-CA	-6.29	1.38	1.46
4	E	67	GLU	C-O	6.29	1.31	1.24
1	A	605	MET	C-O	6.28	1.31	1.23
2	B	795	ILE	CA-CB	-6.28	1.46	1.54
2	B	292	ILE	CG1-CD1	-6.28	1.27	1.51
2	B	1024	ALA	CA-CB	-6.28	1.43	1.53
6	H	116	TYR	C-O	6.28	1.31	1.24
1	A	494	SER	CA-C	-6.28	1.44	1.52
2	B	640	VAL	CB-CG1	-6.28	1.31	1.52
2	B	983	ARG	CZ-NH2	-6.28	1.25	1.33
4	E	75	MET	SD-CE	6.28	1.95	1.79
1	A	711	ARG	CA-C	-6.28	1.44	1.52
2	B	1153	GLU	CA-C	6.28	1.61	1.52
4	E	149	LEU	CA-CB	-6.28	1.42	1.53
6	H	139	ASN	CA-C	6.28	1.61	1.52
2	B	1095	LEU	CA-CB	-6.27	1.43	1.53
6	H	97	MET	CA-CB	-6.27	1.44	1.53
2	B	778	MET	CB-CG	-6.27	1.33	1.52
3	C	164	ALA	N-CA	6.27	1.54	1.46
1	A	461	LYS	CA-CB	-6.27	1.43	1.53
1	A	596	THR	C-O	-6.27	1.16	1.24
1	A	903	ASN	CB-CG	-6.27	1.36	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	221	ASN	CA-C	6.26	1.61	1.52
1	A	192	GLY	CA-C	6.26	1.59	1.52
2	B	303	TYR	C-O	6.26	1.33	1.23
2	B	344	LYS	CA-C	6.26	1.60	1.52
2	B	303	TYR	CG-CD2	-6.26	1.26	1.39
1	A	777	PHE	C-N	-6.26	1.25	1.34
2	B	36	ALA	C-O	6.26	1.31	1.24
8	J	54	VAL	C-N	6.26	1.42	1.33
1	A	264	PHE	CG-CD2	6.26	1.51	1.38
2	B	1150	ARG	C-O	-6.26	1.16	1.24
1	A	525	GLN	C-O	-6.26	1.16	1.24
1	A	594	GLY	C-N	-6.26	1.25	1.33
2	B	96	TYR	CE2-CZ	6.26	1.53	1.38
2	B	250	PHE	CB-CG	6.26	1.65	1.50
2	B	875	GLU	CG-CD	6.26	1.67	1.52
1	A	295	LEU	C-N	6.25	1.41	1.33
2	B	249	ARG	C-O	6.25	1.31	1.24
2	B	964	VAL	CA-CB	-6.25	1.44	1.55
2	B	1008	PRO	N-CA	-6.25	1.39	1.47
5	F	141	GLY	C-O	-6.25	1.15	1.24
6	H	17	PRO	C-O	-6.25	1.15	1.24
9	K	108	GLU	CD-OE2	6.25	1.37	1.25
1	A	688	LYS	CG-CD	6.25	1.71	1.52
1	A	807	GLY	CA-C	6.25	1.60	1.52
3	C	35	ARG	CG-CD	6.25	1.71	1.52
8	J	48	ARG	CZ-NH1	-6.25	1.24	1.32
2	B	579	ARG	C-O	-6.25	1.16	1.23
3	C	228	PHE	C-O	-6.25	1.17	1.24
1	A	1155	ASP	CB-CG	-6.25	1.36	1.52
1	A	1325	THR	CA-CB	-6.25	1.43	1.53
1	A	1347	ALA	CA-C	-6.25	1.44	1.52
2	B	404	LYS	N-CA	-6.25	1.38	1.45
3	C	218	PRO	CA-CB	6.25	1.62	1.53
3	C	220	ASP	CB-CG	6.25	1.67	1.52
5	F	132	LEU	C-O	-6.25	1.16	1.23
1	A	639	PRO	CG-CD	-6.24	1.29	1.50
2	B	1195	HIS	N-CA	-6.24	1.38	1.46
1	A	904	THR	N-CA	-6.24	1.38	1.46
4	E	61	GLN	CB-CG	6.24	1.71	1.52
1	A	91	PHE	CG-CD1	-6.24	1.25	1.38
1	A	885	THR	CA-CB	6.24	1.64	1.53
1	A	931	GLU	N-CA	-6.24	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1039	LYS	CE-NZ	6.24	1.68	1.49
6	H	104	PHE	CG-CD1	6.24	1.51	1.38
7	I	79	HIS	CA-CB	6.24	1.64	1.53
8	J	47	ARG	C-O	6.24	1.31	1.24
2	B	337	ARG	CZ-NH2	-6.24	1.25	1.33
1	A	744	LYS	CG-CD	6.24	1.71	1.52
1	A	806	ARG	CB-CG	6.24	1.71	1.52
4	E	111	VAL	CA-C	-6.24	1.45	1.52
5	F	115	THR	C-O	-6.23	1.15	1.24
1	A	11	LEU	N-CA	6.23	1.53	1.46
1	A	813	PHE	C-N	-6.23	1.25	1.33
2	B	304	ASP	CG-OD1	6.23	1.37	1.25
3	C	139	GLY	N-CA	6.23	1.54	1.45
4	E	33	GLU	CD-OE1	6.23	1.37	1.25
1	A	276	LEU	C-O	-6.23	1.16	1.24
1	A	924	LYS	CG-CD	6.23	1.71	1.52
2	B	459	TYR	CE2-CZ	6.23	1.53	1.38
5	F	120	ILE	CA-CB	6.23	1.62	1.54
2	B	237	VAL	N-CA	-6.22	1.39	1.46
1	A	516	SER	CA-CB	-6.22	1.44	1.53
9	K	56	VAL	N-CA	6.22	1.53	1.46
1	A	205	GLU	CG-CD	6.22	1.67	1.52
7	I	14	LEU	CA-C	-6.22	1.45	1.52
1	A	173	THR	CA-CB	6.22	1.62	1.53
2	B	565	PRO	CA-CB	-6.22	1.45	1.53
2	B	680	THR	C-O	6.22	1.31	1.23
2	B	1189	ILE	CB-CG2	6.22	1.73	1.52
7	I	17	ARG	C-O	-6.22	1.16	1.23
8	J	42	LYS	CD-CE	6.22	1.71	1.52
1	A	396	PRO	CA-CB	-6.21	1.44	1.53
4	E	58	MET	CB-CG	-6.21	1.33	1.52
1	A	1267	MET	C-N	-6.21	1.25	1.33
1	A	1419	ASP	CG-OD2	6.21	1.37	1.25
7	I	46	HIS	C-O	6.21	1.31	1.24
1	A	236	LEU	N-CA	-6.21	1.38	1.45
1	A	604	GLY	CA-C	-6.21	1.43	1.52
2	B	733	HIS	CB-CG	6.21	1.58	1.50
2	B	1052	VAL	CB-CG2	-6.21	1.32	1.52
2	B	1127	GLY	CA-C	6.21	1.63	1.52
2	B	228	LYS	CB-CG	6.21	1.71	1.52
4	E	129	PRO	CB-CG	6.21	1.75	1.51
2	B	699	GLU	CA-C	-6.21	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	469	ARG	CB-CG	6.21	1.71	1.52
1	A	1238	ILE	CA-C	6.21	1.60	1.52
8	J	18	TRP	CA-CB	-6.21	1.43	1.53
2	B	328	GLU	CD-OE1	6.21	1.37	1.25
2	B	829	CYS	CA-C	-6.20	1.44	1.52
7	I	51	ASN	CG-OD1	6.20	1.35	1.23
2	B	649	LYS	CB-CG	-6.20	1.33	1.52
10	L	68	GLU	N-CA	-6.20	1.37	1.46
1	A	665	GLY	CA-C	-6.20	1.44	1.51
1	A	932	GLU	CD-OE2	6.20	1.37	1.25
1	A	1176	LEU	CA-CB	6.20	1.65	1.53
2	B	431	TYR	N-CA	6.20	1.52	1.46
2	B	704	ALA	CA-CB	-6.20	1.43	1.53
4	E	69	ILE	N-CA	6.20	1.54	1.46
1	A	467	THR	N-CA	-6.20	1.38	1.45
2	B	883	LEU	CA-C	6.20	1.61	1.53
3	C	41	ILE	N-CA	-6.20	1.41	1.46
1	A	837	ILE	C-N	-6.20	1.26	1.33
2	B	1215	ARG	CZ-NH2	-6.20	1.25	1.33
2	B	39	ARG	CZ-NH1	6.19	1.41	1.32
2	B	303	TYR	N-CA	6.19	1.54	1.46
2	B	519	TRP	N-CA	-6.19	1.38	1.46
2	B	916	THR	N-CA	6.19	1.58	1.46
8	J	29	GLU	C-O	6.19	1.32	1.23
1	A	648	ASN	CA-C	6.19	1.61	1.52
1	A	1147	THR	CB-OG1	6.19	1.53	1.43
2	B	411	PRO	CA-C	6.19	1.61	1.52
2	B	599	THR	C-O	6.19	1.31	1.24
9	K	40	HIS	CA-CB	6.19	1.63	1.53
1	A	1048	ASN	CG-ND2	6.19	1.46	1.33
1	A	1239	ARG	CZ-NH2	-6.19	1.25	1.33
3	C	146	LYS	CG-CD	6.19	1.71	1.52
1	A	688	LYS	C-O	-6.19	1.16	1.24
9	K	61	TYR	CG-CD2	-6.19	1.26	1.39
1	A	441	PRO	CA-CB	-6.18	1.45	1.53
2	B	568	ASP	CA-CB	6.18	1.63	1.53
2	B	605	ARG	CZ-NH1	-6.18	1.24	1.32
7	I	60	GLN	C-N	-6.18	1.25	1.33
2	B	319	GLU	CG-CD	6.18	1.67	1.52
5	F	136	ARG	N-CA	-6.18	1.38	1.46
1	A	95	PHE	CD1-CE1	6.18	1.57	1.38
1	A	220	THR	CB-OG1	6.18	1.53	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	69	THR	N-CA	6.18	1.54	1.46
1	A	1013	ASP	CG-OD2	6.18	1.37	1.25
1	A	1072	ILE	CA-CB	6.18	1.63	1.54
1	A	1137	ALA	CA-CB	-6.18	1.42	1.53
2	B	747	MET	CG-SD	6.18	1.96	1.80
1	A	62	ASP	CA-CB	6.18	1.64	1.53
2	B	615	MET	N-CA	-6.18	1.38	1.46
4	E	110	PHE	CA-C	-6.18	1.45	1.52
2	B	986	GLN	CB-CG	6.17	1.71	1.52
4	E	192	ARG	C-O	6.17	1.31	1.23
2	B	1046	PRO	CA-C	6.17	1.60	1.52
1	A	907	THR	N-CA	6.17	1.53	1.45
1	A	763	ALA	N-CA	-6.17	1.38	1.46
2	B	253	THR	CA-CB	-6.17	1.45	1.53
1	A	805	LEU	CG-CD1	-6.17	1.32	1.52
1	A	1209	MET	CA-C	-6.17	1.44	1.52
8	J	55	ASP	N-CA	6.17	1.54	1.46
1	A	877	HIS	N-CA	-6.17	1.39	1.46
3	C	38	ILE	N-CA	6.17	1.53	1.46
1	A	900	ASP	N-CA	6.16	1.54	1.46
4	E	83	CYS	N-CA	-6.16	1.38	1.46
1	A	498	ARG	C-N	6.16	1.42	1.33
10	L	48	CYS	C-O	6.16	1.30	1.23
1	A	530	GLY	N-CA	-6.16	1.36	1.45
2	B	567	GLU	CB-CG	6.16	1.71	1.52
2	B	745	PRO	N-CD	-6.16	1.39	1.47
1	A	66	LYS	CA-CB	6.16	1.67	1.53
1	A	1198	ASP	CA-CB	6.16	1.61	1.53
4	E	139	ALA	CA-CB	6.16	1.64	1.53
9	K	79	GLU	CG-CD	6.16	1.67	1.52
1	A	352	VAL	CB-CG2	6.15	1.72	1.52
1	A	379	VAL	CB-CG1	-6.15	1.32	1.52
1	A	656	TRP	C-O	6.15	1.31	1.24
1	A	1206	ASP	CB-CG	6.15	1.67	1.52
2	B	554	ILE	CA-C	-6.15	1.45	1.52
2	B	1050	ILE	C-N	-6.15	1.24	1.33
2	B	491	THR	C-O	6.15	1.31	1.24
2	B	875	GLU	CA-C	-6.15	1.44	1.52
1	A	1102	LYS	CA-C	6.15	1.60	1.52
1	A	1193	LEU	CG-CD1	-6.15	1.32	1.52
2	B	251	ILE	CA-CB	6.15	1.62	1.54
1	A	915	SER	CA-CB	6.15	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	616	ILE	N-CA	6.15	1.54	1.46
9	K	5	ASP	CA-CB	-6.15	1.43	1.53
1	A	495	GLU	CA-C	6.14	1.60	1.52
3	C	199	LYS	CA-C	-6.14	1.44	1.52
9	K	78	THR	C-N	6.14	1.42	1.33
1	A	202	LEU	CA-C	-6.14	1.45	1.52
6	H	20	TYR	CD2-CE2	-6.14	1.20	1.38
1	A	670	ILE	CA-C	6.14	1.60	1.52
1	A	1369	ALA	N-CA	-6.14	1.38	1.46
2	B	320	ASP	CA-C	-6.14	1.44	1.52
9	K	65	HIS	C-N	-6.14	1.28	1.34
1	A	1337	GLU	CA-C	-6.14	1.44	1.52
1	A	1450	LEU	CG-CD2	6.14	1.72	1.52
2	B	1074	ASN	N-CA	-6.14	1.38	1.46
7	I	100	PHE	CE1-CZ	-6.14	1.20	1.38
10	L	47	ARG	CD-NE	6.14	1.54	1.46
2	B	229	ALA	N-CA	6.14	1.53	1.46
1	A	1092	LYS	CB-CG	6.14	1.70	1.52
5	F	76	LYS	CG-CD	6.14	1.70	1.52
1	A	1146	VAL	C-O	-6.13	1.17	1.24
1	A	1312	ASN	CG-OD1	6.13	1.35	1.23
1	A	806	ARG	CZ-NH1	6.13	1.41	1.32
1	A	827	THR	C-O	-6.13	1.17	1.24
1	A	1036	ARG	C-O	-6.13	1.15	1.23
2	B	527	THR	CA-C	-6.13	1.45	1.52
2	B	848	ARG	CA-CB	-6.13	1.43	1.53
2	B	1183	LYS	C-O	6.13	1.31	1.24
1	A	659	HIS	CG-CD2	6.13	1.42	1.35
1	A	919	ILE	CG1-CD1	6.13	1.75	1.51
1	A	881	GLN	CD-NE2	6.13	1.46	1.33
2	B	667	GLN	N-CA	6.13	1.54	1.46
1	A	172	PRO	CA-CB	6.12	1.61	1.53
1	A	428	TYR	C-O	6.12	1.31	1.23
1	A	1440	ALA	C-O	6.12	1.31	1.24
5	F	76	LYS	CE-NZ	6.12	1.67	1.49
7	I	89	GLN	C-O	-6.12	1.15	1.24
1	A	504	LEU	C-O	-6.12	1.16	1.24
1	A	768	GLN	CA-CB	-6.12	1.44	1.53
1	A	1002	GLY	C-O	6.12	1.32	1.23
3	C	135	GLN	CA-C	6.12	1.60	1.52
6	H	142	LEU	CA-CB	-6.12	1.41	1.53
2	B	327	ARG	CA-C	-6.12	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	15	LYS	N-CA	6.12	1.54	1.46
1	A	180	LYS	CA-C	-6.12	1.45	1.52
1	A	919	ILE	C-O	-6.12	1.17	1.24
1	A	1346	ALA	C-O	-6.12	1.16	1.24
2	B	126	SER	CA-CB	-6.12	1.43	1.54
9	K	44	ASN	CA-C	6.12	1.61	1.52
2	B	243	ALA	CA-CB	6.11	1.64	1.53
2	B	447	ALA	CA-CB	-6.11	1.43	1.53
1	A	688	LYS	CD-CE	6.11	1.70	1.52
1	A	864	ILE	N-CA	-6.11	1.38	1.46
1	A	1162	VAL	CB-CG1	6.11	1.72	1.52
3	C	254	LYS	CD-CE	-6.11	1.34	1.52
1	A	74	MET	CA-CB	6.11	1.63	1.53
1	A	960	ILE	CG1-CD1	-6.11	1.27	1.51
2	B	239	GLU	CD-OE1	6.11	1.36	1.25
2	B	969	ARG	N-CA	-6.11	1.38	1.46
3	C	9	LYS	C-O	-6.11	1.16	1.24
3	C	50	GLU	N-CA	6.11	1.53	1.46
1	A	404	TYR	C-O	-6.11	1.16	1.23
1	A	517	ASN	CA-C	-6.11	1.44	1.53
2	B	667	GLN	CA-C	6.11	1.60	1.53
2	B	995	ARG	N-CA	6.11	1.53	1.45
3	C	40	GLU	C-O	-6.11	1.15	1.24
4	E	3	GLN	CA-CB	6.11	1.63	1.53
1	A	699	ALA	C-N	-6.11	1.25	1.33
2	B	983	ARG	CZ-NH1	-6.11	1.24	1.32
3	C	180	TYR	CD2-CE2	6.11	1.56	1.38
1	A	534	LEU	CB-CG	-6.11	1.41	1.53
3	C	132	PRO	N-CA	-6.11	1.39	1.47
1	A	219	PHE	CD2-CE2	-6.10	1.20	1.38
1	A	569	LYS	N-CA	6.10	1.55	1.46
1	A	835	GLY	CA-C	6.10	1.58	1.52
1	A	869	GLY	C-O	-6.10	1.15	1.23
4	E	72	PHE	CE2-CZ	6.10	1.56	1.38
6	H	12	VAL	N-CA	6.10	1.53	1.46
1	A	559	VAL	CA-C	-6.10	1.45	1.52
1	A	998	LEU	CA-CB	6.10	1.62	1.53
1	A	1066	VAL	C-O	6.10	1.31	1.24
2	B	359	GLU	CD-OE1	6.10	1.36	1.25
2	B	914	LYS	C-N	6.10	1.41	1.33
6	H	144	ILE	CG1-CD1	6.10	1.75	1.51
4	E	172	GLU	C-O	-6.10	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	J	60	PHE	CE1-CZ	-6.10	1.20	1.38
1	A	964	ILE	C-O	6.10	1.30	1.24
1	A	1068	ALA	C-N	-6.10	1.25	1.33
1	A	1093	LYS	CG-CD	6.09	1.70	1.52
2	B	635	ARG	CA-C	-6.09	1.45	1.52
2	B	707	PRO	C-N	-6.09	1.23	1.33
3	C	106	GLU	CD-OE1	6.09	1.36	1.25
1	A	218	ASP	CG-OD2	6.09	1.36	1.25
1	A	888	GLY	C-O	-6.09	1.16	1.23
2	B	1173	ALA	C-O	6.09	1.30	1.23
3	C	37	MET	N-CA	-6.09	1.39	1.46
1	A	1023	ARG	C-O	-6.09	1.16	1.24
2	B	335	GLY	C-O	-6.09	1.16	1.23
2	B	1209	ALA	CA-C	6.09	1.61	1.52
1	A	1191	TRP	CG-CD1	6.09	1.52	1.36
7	I	8	ARG	CZ-NH2	6.09	1.41	1.33
1	A	942	PHE	C-N	-6.09	1.25	1.33
1	A	986	ILE	CA-CB	-6.09	1.47	1.54
1	A	1417	GLU	N-CA	6.08	1.53	1.46
7	I	70	ARG	CA-C	-6.08	1.45	1.52
1	A	350	ARG	C-O	-6.08	1.17	1.23
1	A	1012	ARG	NE-CZ	6.08	1.39	1.33
1	A	1044	TRP	N-CA	6.08	1.53	1.46
3	C	220	ASP	N-CA	-6.08	1.38	1.46
1	A	1157	ASP	CB-CG	6.08	1.67	1.52
4	E	191	LYS	N-CA	-6.08	1.38	1.45
1	A	572	TRP	CG-CD1	-6.08	1.21	1.36
1	A	121	LEU	C-O	-6.08	1.16	1.24
1	A	960	ILE	CB-CG2	-6.08	1.32	1.52
1	A	1030	ARG	CB-CG	-6.08	1.34	1.52
2	B	327	ARG	C-O	-6.08	1.16	1.24
2	B	773	MET	C-O	-6.08	1.17	1.24
2	B	1193	GLN	C-N	-6.08	1.25	1.33
1	A	481	ASP	C-N	6.08	1.43	1.33
1	A	882	SER	CB-OG	-6.08	1.29	1.42
1	A	1126	ALA	CA-C	6.08	1.60	1.52
10	L	40	LEU	C-N	6.08	1.42	1.33
1	A	463	ILE	CB-CG2	-6.07	1.32	1.52
2	B	1222	ARG	CD-NE	-6.07	1.37	1.46
5	F	96	THR	CA-C	6.07	1.60	1.52
5	F	119	ARG	CZ-NH1	6.07	1.41	1.32
1	A	967	ALA	C-O	-6.07	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	238	ILE	CA-C	-6.07	1.46	1.52
1	A	780	VAL	C-O	6.07	1.29	1.23
1	A	1139	GLU	C-O	6.07	1.31	1.23
1	A	728	LYS	CE-NZ	6.07	1.67	1.49
1	A	899	VAL	CB-CG1	-6.07	1.32	1.52
1	A	66	LYS	N-CA	6.07	1.53	1.46
2	B	191	LYS	CB-CG	6.07	1.70	1.52
2	B	297	ILE	C-O	-6.07	1.17	1.24
2	B	343	ILE	CG1-CD1	6.07	1.75	1.51
2	B	332	ASP	C-O	-6.06	1.17	1.24
2	B	405	ARG	C-O	-6.06	1.16	1.23
2	B	1100	ASP	C-O	6.06	1.31	1.24
1	A	527	THR	C-O	-6.06	1.16	1.24
1	A	610	GLY	C-N	6.06	1.41	1.33
1	A	1078	GLN	CD-NE2	6.06	1.46	1.33
2	B	200	GLY	CA-C	-6.06	1.44	1.52
2	B	564	GLU	CD-OE2	6.06	1.36	1.25
3	C	15	LYS	CD-CE	6.06	1.70	1.52
3	C	119	VAL	CA-C	6.06	1.60	1.52
1	A	285	PRO	CA-C	-6.06	1.45	1.52
1	A	1234	GLU	CA-C	-6.06	1.44	1.52
1	A	612	ILE	CA-CB	-6.06	1.46	1.54
2	B	378	LEU	CG-CD2	-6.06	1.32	1.52
2	B	351	TYR	CA-CB	6.06	1.62	1.53
1	A	387	ARG	NE-CZ	6.06	1.39	1.33
9	K	33	ILE	C-O	-6.06	1.17	1.24
1	A	132	LYS	CG-CD	6.05	1.70	1.52
2	B	452	THR	CA-CB	6.05	1.63	1.53
2	B	699	GLU	CA-CB	-6.05	1.42	1.53
1	A	268	ASP	CA-CB	6.05	1.63	1.53
1	A	1377	THR	C-O	-6.05	1.16	1.24
1	A	925	LEU	CA-C	-6.05	1.45	1.52
1	A	298	PHE	C-O	-6.05	1.16	1.24
1	A	416	ARG	CA-C	-6.05	1.44	1.52
2	B	348	ARG	CZ-NH1	-6.05	1.24	1.32
2	B	1057	LYS	CA-CB	-6.05	1.44	1.53
1	A	940	ARG	CG-CD	6.05	1.70	1.52
1	A	1134	ILE	C-O	6.05	1.30	1.24
2	B	1021	MET	CB-CG	6.05	1.70	1.52
2	B	1071	VAL	CA-C	-6.05	1.45	1.52
2	B	667	GLN	CD-OE1	6.04	1.35	1.23
2	B	1150	ARG	C-N	-6.04	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	166	GLU	C-O	-6.04	1.16	1.24
1	A	724	GLU	CD-OE2	6.04	1.36	1.25
1	A	747	VAL	CA-C	-6.04	1.45	1.52
4	E	23	VAL	N-CA	-6.04	1.39	1.46
4	E	151	PRO	CA-C	-6.04	1.46	1.53
1	A	427	GLN	CG-CD	6.04	1.67	1.52
2	B	1060	ARG	CD-NE	6.04	1.54	1.46
3	C	259	LEU	CA-CB	-6.04	1.43	1.53
2	B	990	ILE	CG1-CD1	-6.04	1.28	1.51
1	A	632	VAL	CA-C	-6.04	1.45	1.52
1	A	1217	LYS	CA-C	6.04	1.60	1.52
1	A	1335	ILE	CB-CG2	-6.03	1.32	1.52
2	B	220	GLY	C-O	-6.03	1.14	1.23
7	I	32	CYS	C-O	6.03	1.32	1.23
2	B	47	GLN	CA-C	6.03	1.60	1.52
2	B	420	LEU	C-O	-6.03	1.16	1.24
2	B	486	TYR	CA-CB	-6.03	1.43	1.53
2	B	825	VAL	CA-C	-6.03	1.44	1.52
4	E	38	PRO	CA-C	-6.03	1.43	1.52
1	A	988	LEU	CG-CD2	-6.03	1.32	1.52
6	H	114	VAL	CA-CB	6.03	1.62	1.54
3	C	20	PHE	CB-CG	-6.03	1.36	1.50
1	A	80	HIS	CG-CD2	6.03	1.42	1.35
1	A	1021	LEU	CA-C	-6.03	1.44	1.52
2	B	96	TYR	CE1-CZ	6.03	1.52	1.38
2	B	308	TRP	N-CA	-6.03	1.38	1.46
7	I	99	LEU	CB-CG	-6.03	1.41	1.53
1	A	1374	VAL	N-CA	6.02	1.53	1.46
1	A	775	ILE	CA-C	-6.02	1.45	1.52
1	A	965	GLN	CD-NE2	6.02	1.45	1.33
1	A	1329	THR	CA-C	-6.02	1.45	1.52
1	A	1341	ILE	C-O	-6.02	1.17	1.24
1	A	1343	ALA	N-CA	6.02	1.53	1.46
7	I	60	GLN	CG-CD	6.02	1.67	1.52
1	A	53	LEU	CA-C	6.02	1.61	1.53
1	A	399	HIS	N-CA	6.02	1.53	1.45
1	A	888	GLY	N-CA	-6.02	1.38	1.45
2	B	320	ASP	C-N	-6.02	1.27	1.33
3	C	35	ARG	CB-CG	6.02	1.70	1.52
1	A	681	GLU	CA-C	-6.02	1.44	1.52
2	B	1019	SER	CA-CB	-6.02	1.43	1.53
5	F	127	GLU	C-O	-6.02	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1153	GLU	CD-OE2	6.02	1.36	1.25
1	A	596	THR	CB-CG2	6.01	1.72	1.52
1	A	1290	LYS	C-N	-6.01	1.28	1.33
2	B	96	TYR	CG-CD2	6.01	1.51	1.39
2	B	1130	PHE	C-O	-6.01	1.15	1.23
1	A	1441	PHE	CG-CD1	-6.01	1.26	1.38
2	B	50	SER	CB-OG	-6.01	1.30	1.42
5	F	133	VAL	CA-CB	-6.01	1.47	1.54
7	I	23	ASN	CA-C	-6.01	1.45	1.53
2	B	1102	LYS	CA-C	6.01	1.58	1.52
1	A	237	THR	CA-CB	-6.01	1.43	1.53
2	B	349	ILE	CB-CG2	-6.01	1.32	1.52
2	B	405	ARG	CZ-NH2	-6.01	1.25	1.33
1	A	264	PHE	CG-CD1	6.01	1.51	1.38
2	B	458	LYS	CG-CD	6.01	1.70	1.52
2	B	497	ARG	CA-C	-6.01	1.44	1.53
3	C	159	ALA	CA-CB	6.01	1.63	1.53
6	H	121	LEU	CA-CB	-6.01	1.44	1.53
1	A	1262	LYS	C-N	6.01	1.41	1.33
1	A	1303	GLU	CD-OE2	6.01	1.36	1.25
3	C	167	HIS	CA-CB	-6.01	1.43	1.53
5	F	108	PHE	N-CA	-6.01	1.38	1.46
7	I	93	LYS	C-N	6.01	1.41	1.33
10	L	66	GLN	CD-OE1	6.01	1.34	1.23
2	B	860	MET	SD-CE	6.00	1.94	1.79
6	H	102	TYR	CG-CD2	-6.00	1.26	1.39
2	B	723	VAL	CB-CG2	6.00	1.72	1.52
2	B	1179	GLN	CA-CB	6.00	1.62	1.53
1	A	139	TRP	CG-CD2	-6.00	1.32	1.43
1	A	285	PRO	CB-CG	-6.00	1.19	1.49
1	A	411	ASP	CA-CB	6.00	1.63	1.53
1	A	735	VAL	N-CA	-6.00	1.39	1.46
6	H	14	GLU	CA-C	-6.00	1.44	1.52
1	A	464	PRO	CA-CB	-6.00	1.45	1.53
2	B	456	GLY	N-CA	6.00	1.54	1.45
2	B	991	GLY	C-N	6.00	1.36	1.33
9	K	70	ARG	C-O	-6.00	1.16	1.23
1	A	21	LEU	CA-C	6.00	1.59	1.52
2	B	401	PHE	N-CA	6.00	1.54	1.46
2	B	1061	GLU	CB-CG	6.00	1.70	1.52
1	A	1188	GLN	CA-C	6.00	1.60	1.52
2	B	1087	PHE	CD2-CE2	-6.00	1.20	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	150	VAL	CB-CG1	6.00	1.72	1.52
1	A	99	ILE	N-CA	-5.99	1.39	1.46
1	A	367	PRO	C-O	-5.99	1.16	1.23
1	A	1331	SER	CA-C	5.99	1.60	1.52
2	B	288	ALA	CA-C	-5.99	1.44	1.52
2	B	550	ASP	C-O	5.99	1.32	1.23
2	B	1165	ILE	CG1-CD1	5.99	1.75	1.51
3	C	31	ASN	CG-ND2	5.99	1.45	1.33
9	K	63	VAL	CA-C	-5.99	1.45	1.52
1	A	939	ASP	CB-CG	5.99	1.67	1.52
3	C	209	TYR	CG-CD1	5.99	1.51	1.39
7	I	13	MET	N-CA	-5.99	1.38	1.45
1	A	84	ILE	CA-C	-5.99	1.45	1.52
4	E	93	MET	CG-SD	5.99	1.95	1.80
8	J	24	LEU	CB-CG	-5.99	1.41	1.53
1	A	1081	LEU	N-CA	5.98	1.57	1.46
2	B	287	ARG	CA-CB	-5.98	1.42	1.53
4	E	168	TYR	C-N	-5.98	1.25	1.33
9	K	24	ASP	CA-CB	-5.98	1.44	1.53
1	A	1127	ASP	CG-OD2	5.98	1.36	1.25
2	B	289	LEU	C-O	-5.98	1.16	1.24
3	C	122	SER	CB-OG	5.98	1.54	1.42
1	A	1234	GLU	N-CA	5.98	1.53	1.46
2	B	296	GLU	CD-OE2	5.98	1.36	1.25
1	A	855	THR	C-O	-5.98	1.16	1.23
1	A	623	GLY	C-O	-5.97	1.18	1.23
2	B	370	PHE	CD2-CE2	5.97	1.56	1.38
2	B	836	GLU	C-N	5.97	1.41	1.33
9	K	56	VAL	CA-CB	5.97	1.60	1.53
1	A	790	ASP	CA-CB	-5.97	1.43	1.53
2	B	115	GLN	C-O	-5.97	1.16	1.24
2	B	418	LYS	CA-C	-5.97	1.45	1.52
2	B	1181	GLU	CA-CB	5.97	1.65	1.53
1	A	716	ASP	CA-C	5.97	1.60	1.52
2	B	308	TRP	CE2-CZ2	-5.97	1.27	1.39
3	C	34	ARG	CA-CB	-5.97	1.43	1.53
1	A	1338	VAL	CA-C	5.97	1.59	1.52
1	A	1380	GLY	C-N	-5.97	1.25	1.33
10	L	42	ARG	CD-NE	5.97	1.54	1.46
1	A	474	VAL	C-O	-5.97	1.16	1.24
1	A	630	ILE	CG1-CD1	-5.97	1.28	1.51
1	A	834	THR	CA-C	-5.97	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1060	PRO	N-CA	-5.97	1.39	1.47
3	C	78	GLU	CD-OE2	5.97	1.36	1.25
4	E	8	ASN	CG-OD1	5.97	1.34	1.23
2	B	1080	LYS	CA-CB	5.96	1.63	1.53
3	C	80	LEU	N-CA	5.96	1.53	1.46
6	H	106	GLU	CA-C	5.96	1.62	1.52
1	A	1059	HIS	CD2-NE2	-5.96	1.31	1.37
2	B	1087	PHE	CA-CB	-5.96	1.43	1.53
1	A	162	VAL	CB-CG2	5.96	1.72	1.52
2	B	195	CYS	CA-CB	-5.96	1.44	1.53
1	A	209	ASN	CA-CB	5.96	1.63	1.53
1	A	626	ASN	CA-CB	5.96	1.63	1.53
1	A	1060	PRO	CA-C	-5.96	1.45	1.52
2	B	944	THR	N-CA	5.96	1.53	1.46
2	B	1100	ASP	CB-CG	5.96	1.67	1.52
7	I	27	PHE	CE1-CZ	-5.96	1.20	1.38
1	A	72	GLU	CA-C	5.96	1.60	1.52
1	A	521	MET	N-CA	5.96	1.53	1.46
2	B	287	ARG	N-CA	5.96	1.53	1.46
2	B	655	LYS	CG-CD	5.96	1.70	1.52
1	A	772	GLY	CA-C	-5.96	1.43	1.51
2	B	1034	VAL	N-CA	-5.96	1.39	1.46
7	I	114	GLN	N-CA	-5.96	1.38	1.46
1	A	53	LEU	CB-CG	5.95	1.65	1.53
1	A	1262	LYS	CB-CG	5.95	1.70	1.52
2	B	196	PRO	C-O	5.95	1.31	1.24
2	B	350	GLN	CA-CB	-5.95	1.43	1.53
3	C	134	ILE	CA-C	-5.95	1.45	1.52
2	B	20	ASP	C-O	-5.95	1.16	1.23
2	B	387	LEU	CG-CD1	-5.95	1.32	1.52
4	E	64	PRO	CA-CB	5.95	1.62	1.53
10	L	57	LEU	CG-CD1	5.95	1.72	1.52
2	B	318	VAL	C-O	5.95	1.30	1.24
2	B	347	LYS	C-O	-5.95	1.17	1.24
5	F	118	LEU	CG-CD1	-5.95	1.32	1.52
8	J	22	LEU	CG-CD2	-5.95	1.32	1.52
8	J	44	TYR	CA-CB	-5.95	1.42	1.53
2	B	108	VAL	N-CA	5.95	1.53	1.46
1	A	129	LYS	CB-CG	5.95	1.70	1.52
1	A	1285	MET	CG-SD	5.95	1.95	1.80
2	B	39	ARG	CD-NE	5.95	1.54	1.46
2	B	824	ILE	CA-CB	5.95	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	178	PHE	CA-C	-5.95	1.44	1.52
1	A	635	ARG	C-O	-5.94	1.16	1.24
1	A	979	SER	N-CA	-5.94	1.38	1.45
1	A	69	THR	C-N	5.94	1.42	1.33
2	B	214	ALA	N-CA	-5.94	1.38	1.46
6	H	126	GLU	CD-OE1	5.94	1.36	1.25
6	H	132	LEU	N-CA	5.94	1.53	1.46
1	A	382	PRO	CG-CD	-5.94	1.30	1.50
2	B	173	MET	SD-CE	-5.94	1.64	1.79
2	B	367	LEU	CG-CD2	5.94	1.72	1.52
3	C	175	ALA	N-CA	-5.94	1.37	1.45
6	H	33	GLN	C-O	-5.94	1.16	1.23
1	A	387	ARG	CZ-NH2	-5.94	1.25	1.33
1	A	997	LEU	C-O	-5.94	1.16	1.23
4	E	103	LYS	CE-NZ	5.94	1.67	1.49
6	H	45	GLU	CD-OE1	5.94	1.36	1.25
1	A	29	ALA	CA-CB	5.94	1.63	1.53
1	A	704	ALA	CA-C	-5.94	1.45	1.53
2	B	385	LEU	CG-CD2	5.94	1.72	1.52
2	B	707	PRO	CA-C	5.94	1.61	1.52
2	B	850	LEU	CG-CD2	-5.94	1.32	1.52
2	B	421	PHE	C-O	-5.94	1.16	1.24
2	B	327	ARG	NE-CZ	-5.93	1.26	1.33
2	B	529	GLU	CA-C	5.93	1.60	1.52
2	B	835	GLN	C-O	-5.93	1.16	1.23
3	C	26	ASP	CA-C	5.93	1.60	1.52
4	E	5	ASN	CA-CB	5.93	1.63	1.53
4	E	136	ASN	CG-ND2	5.93	1.45	1.33
3	C	164	ALA	C-N	5.93	1.42	1.33
2	B	835	GLN	N-CA	5.93	1.53	1.45
1	A	186	LYS	CD-CE	5.93	1.70	1.52
1	A	374	LEU	C-N	-5.93	1.25	1.33
2	B	853	SER	CB-OG	5.93	1.54	1.42
2	B	1174	LYS	CA-CB	5.93	1.60	1.52
6	H	2	SER	N-CA	5.93	1.57	1.46
9	K	71	PHE	C-O	5.93	1.31	1.23
1	A	917	SER	CA-CB	-5.93	1.44	1.53
2	B	625	LYS	C-N	-5.93	1.24	1.33
2	B	692	TYR	CA-CB	-5.93	1.45	1.53
2	B	888	GLY	N-CA	5.93	1.50	1.44
1	A	1191	TRP	CG-CD2	-5.92	1.33	1.43
2	B	847	ASP	CG-OD2	5.92	1.36	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	88	SER	C-O	-5.92	1.16	1.23
2	B	234	ILE	CA-CB	-5.92	1.47	1.54
2	B	633	VAL	C-O	5.92	1.32	1.24
2	B	1055	ILE	CA-C	-5.92	1.44	1.52
10	L	65	VAL	CA-CB	-5.92	1.47	1.54
1	A	325	ILE	C-O	-5.92	1.17	1.24
1	A	862	ASN	CG-OD1	5.92	1.34	1.23
10	L	38	LEU	N-CA	-5.92	1.37	1.45
1	A	436	ILE	CG1-CD1	-5.92	1.28	1.51
6	H	41	ASP	CA-CB	5.92	1.61	1.53
1	A	390	GLN	CD-OE1	5.92	1.34	1.23
1	A	1166	ASP	CG-OD2	5.92	1.36	1.25
2	B	948	ILE	CG1-CD1	-5.92	1.28	1.51
3	C	7	GLN	CA-CB	5.92	1.62	1.53
7	I	97	MET	N-CA	-5.92	1.39	1.46
4	E	115	ASN	C-O	5.91	1.30	1.23
1	A	220	THR	CA-C	-5.91	1.45	1.52
9	K	39	ASP	C-N	-5.91	1.25	1.34
1	A	793	SER	CA-CB	-5.91	1.45	1.53
2	B	595	ARG	C-N	-5.91	1.26	1.33
4	E	130	ALA	CA-CB	5.91	1.62	1.53
1	A	447	GLN	CA-C	-5.91	1.45	1.53
1	A	923	LEU	C-O	5.91	1.31	1.24
5	F	83	PRO	N-CA	-5.91	1.39	1.47
8	J	2	ILE	N-CA	-5.91	1.39	1.46
1	A	955	PRO	CA-C	-5.91	1.45	1.52
2	B	768	THR	N-CA	-5.91	1.39	1.46
1	A	426	LEU	CA-C	-5.91	1.45	1.52
1	A	1290	LYS	N-CA	5.91	1.53	1.46
2	B	138	GLU	CD-OE2	-5.91	1.14	1.25
3	C	50	GLU	CB-CG	5.91	1.70	1.52
9	K	67	PHE	CA-C	-5.90	1.44	1.52
1	A	1230	GLU	CD-OE2	5.90	1.36	1.25
2	B	119	LEU	CA-CB	-5.90	1.43	1.53
2	B	620	ARG	CD-NE	-5.90	1.38	1.46
9	K	55	LYS	CG-CD	5.90	1.70	1.52
1	A	130	ASP	CB-CG	5.90	1.66	1.52
2	B	128	LEU	N-CA	-5.90	1.39	1.46
1	A	829	VAL	CB-CG2	5.90	1.72	1.52
1	A	1261	LYS	CG-CD	5.90	1.70	1.52
2	B	1102	LYS	C-N	5.90	1.41	1.33
6	H	6	PHE	C-O	-5.90	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	468	PHE	CD2-CE2	-5.89	1.21	1.38
2	B	785	TYR	N-CA	5.89	1.53	1.46
2	B	804	GLY	C-O	-5.89	1.16	1.23
3	C	81	GLU	N-CA	-5.89	1.38	1.45
1	A	703	THR	C-O	-5.89	1.16	1.24
1	A	940	ARG	C-O	-5.89	1.17	1.24
2	B	404	LYS	C-O	-5.89	1.16	1.23
3	C	196	ASP	CG-OD1	5.89	1.36	1.25
4	E	59	SER	C-O	5.89	1.31	1.24
7	I	98	VAL	CA-C	5.89	1.62	1.53
1	A	951	GLU	CA-C	-5.89	1.44	1.52
2	B	319	GLU	CB-CG	5.89	1.70	1.52
2	B	306	ASN	CB-CG	5.89	1.66	1.52
1	A	303	TYR	C-O	-5.89	1.17	1.24
1	A	396	PRO	C-O	-5.89	1.16	1.24
1	A	458	HIS	C-N	5.89	1.41	1.33
2	B	610	ASN	CG-ND2	-5.89	1.20	1.33
2	B	1146	PHE	CA-C	-5.89	1.45	1.52
2	B	1208	MET	CA-C	5.89	1.60	1.52
7	I	12	ASN	CA-C	5.89	1.61	1.53
1	A	229	SER	CB-OG	5.88	1.53	1.42
1	A	645	LEU	C-N	-5.88	1.25	1.33
1	A	874	ASP	CA-C	-5.88	1.45	1.52
7	I	78	CYS	CB-SG	5.88	2.00	1.81
1	A	124	GLN	CD-NE2	5.88	1.45	1.33
1	A	626	ASN	CG-OD1	5.88	1.34	1.23
3	C	106	GLU	C-O	5.88	1.30	1.23
1	A	36	ARG	C-O	-5.88	1.16	1.24
1	A	502	SER	N-CA	5.88	1.53	1.46
1	A	575	LYS	N-CA	5.88	1.53	1.46
1	A	1449	SER	C-N	5.88	1.41	1.33
2	B	461	LEU	CA-CB	-5.88	1.43	1.53
2	B	1008	PRO	CG-CD	-5.88	1.30	1.50
4	E	65	THR	CB-OG1	5.88	1.53	1.43
9	K	10	PHE	CB-CG	5.88	1.64	1.50
1	A	442	VAL	C-O	-5.88	1.16	1.23
2	B	356	LEU	CA-C	5.88	1.60	1.52
2	B	1045	SER	N-CA	-5.88	1.36	1.45
3	C	138	GLU	C-O	5.88	1.31	1.24
1	A	756	ILE	C-O	5.88	1.31	1.24
1	A	1126	ALA	C-O	-5.88	1.16	1.24
2	B	249	ARG	CD-NE	5.88	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1160	SER	CB-OG	5.88	1.53	1.42
1	A	1314	SER	CA-C	-5.88	1.44	1.52
2	B	235	SER	CB-OG	-5.87	1.30	1.42
2	B	501	PRO	CA-C	-5.87	1.46	1.52
4	E	153	HIS	CG-ND1	-5.87	1.31	1.38
1	A	221	SER	CB-OG	-5.87	1.30	1.42
1	A	836	TYR	N-CA	-5.87	1.39	1.46
1	A	112	LYS	C-O	-5.87	1.17	1.24
1	A	404	TYR	CA-C	-5.87	1.45	1.52
2	B	303	TYR	C-N	5.87	1.42	1.33
2	B	585	VAL	CA-CB	5.87	1.61	1.54
5	F	87	LYS	CD-CE	5.87	1.70	1.52
1	A	148	CYS	CB-SG	-5.87	1.61	1.81
2	B	418	LYS	CG-CD	5.87	1.70	1.52
7	I	9	ASP	N-CA	-5.87	1.39	1.46
3	C	112	ASN	N-CA	-5.86	1.38	1.45
1	A	1291	VAL	CB-CG1	-5.86	1.33	1.52
3	C	54	ASN	CA-CB	-5.86	1.44	1.52
7	I	95	THR	CB-CG2	-5.86	1.33	1.52
9	K	6	ARG	CA-CB	-5.86	1.43	1.53
6	H	11	GLN	CB-CG	5.86	1.70	1.52
2	B	593	PRO	CG-CD	5.86	1.70	1.50
1	A	185	TRP	CG-CD2	-5.86	1.33	1.43
1	A	691	LEU	CA-CB	-5.86	1.43	1.53
2	B	112	LEU	CA-CB	-5.86	1.44	1.53
1	A	1211	GLN	CD-OE1	5.85	1.34	1.23
2	B	137	TYR	CA-C	5.85	1.60	1.52
1	A	943	LEU	N-CA	-5.85	1.38	1.46
2	B	1130	PHE	N-CA	-5.85	1.36	1.46
4	E	81	GLU	CA-C	-5.85	1.45	1.52
1	A	425	GLN	CD-NE2	5.85	1.45	1.33
2	B	826	ALA	CA-C	5.85	1.60	1.52
1	A	620	LYS	CA-C	5.85	1.60	1.52
3	C	67	LEU	CG-CD1	-5.85	1.33	1.52
1	A	83	HIS	C-O	5.85	1.30	1.23
1	A	1110	ASN	C-N	-5.85	1.24	1.33
2	B	825	VAL	C-O	-5.85	1.17	1.24
2	B	238	ALA	CA-C	-5.84	1.45	1.52
2	B	346	GLU	CD-OE1	5.84	1.36	1.25
1	A	1236	LEU	CB-CG	5.84	1.65	1.53
3	C	81	GLU	CA-C	5.84	1.60	1.52
4	E	58	MET	CA-C	5.84	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	186	LEU	C-O	-5.84	1.17	1.24
2	B	328	GLU	CA-CB	5.84	1.62	1.53
3	C	183	TRP	CA-CB	5.84	1.61	1.53
2	B	230	ALA	C-N	5.84	1.40	1.34
2	B	478	GLY	CA-C	5.84	1.59	1.51
1	A	350	ARG	CG-CD	-5.84	1.34	1.52
1	A	529	CYS	CA-C	-5.84	1.44	1.52
1	A	1164	PRO	CA-CB	5.84	1.62	1.53
7	I	91	ARG	N-CA	-5.84	1.38	1.47
1	A	1148	ILE	CA-CB	5.83	1.61	1.54
1	A	325	ILE	CA-CB	5.83	1.61	1.54
1	A	876	ALA	C-N	-5.83	1.26	1.33
1	A	514	PRO	CA-C	-5.83	1.42	1.52
2	B	185	THR	CA-C	-5.83	1.45	1.53
3	C	239	PRO	CA-C	-5.83	1.45	1.52
1	A	194	ALA	CA-CB	5.83	1.61	1.52
8	J	62	ARG	N-CA	-5.83	1.38	1.46
2	B	880	THR	CB-CG2	5.83	1.71	1.52
2	B	1007	VAL	CB-CG1	-5.83	1.33	1.52
1	A	728	LYS	C-N	-5.83	1.25	1.33
1	A	1049	ILE	C-O	-5.83	1.17	1.24
2	B	105	SER	C-O	5.83	1.31	1.24
2	B	1135	ARG	CD-NE	-5.83	1.38	1.46
3	C	75	MET	CB-CG	-5.83	1.34	1.52
9	K	7	PHE	CB-CG	-5.83	1.37	1.50
1	A	48	ALA	CA-CB	5.82	1.63	1.53
2	B	217	ARG	CA-C	-5.82	1.45	1.52
2	B	235	SER	CA-CB	-5.82	1.44	1.54
2	B	1039	GLY	CA-C	-5.82	1.43	1.51
1	A	161	LEU	CA-C	-5.82	1.45	1.52
2	B	370	PHE	CG-CD1	5.82	1.51	1.38
2	B	526	GLU	CA-CB	5.82	1.60	1.53
2	B	776	GLN	C-O	-5.82	1.16	1.24
5	F	97	ARG	CB-CG	-5.82	1.34	1.52
1	A	393	ARG	CG-CD	5.82	1.70	1.52
1	A	420	ARG	C-O	-5.82	1.16	1.24
1	A	1092	LYS	CA-C	5.82	1.65	1.52
1	A	592	ASP	C-O	-5.82	1.16	1.24
4	E	41	ASP	CG-OD2	5.82	1.36	1.25
6	H	19	ARG	CZ-NH2	5.82	1.41	1.33
1	A	210	ILE	CA-CB	-5.82	1.47	1.54
1	A	1408	ILE	CG1-CD1	5.82	1.74	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	220	GLY	N-CA	-5.82	1.38	1.45
2	B	457	LEU	CA-CB	5.82	1.61	1.53
2	B	770	GLN	N-CA	5.82	1.53	1.46
3	C	223	ALA	C-O	-5.82	1.16	1.23
1	A	846	GLU	CG-CD	5.82	1.66	1.52
2	B	666	TYR	CE1-CZ	5.82	1.52	1.38
2	B	691	GLU	CA-C	-5.82	1.45	1.52
2	B	1003	ALA	C-O	-5.82	1.16	1.24
3	C	188	HIS	CB-CG	-5.82	1.42	1.50
4	E	146	HIS	C-O	-5.82	1.16	1.24
1	A	1037	LEU	CA-C	-5.81	1.45	1.52
3	C	23	SER	CA-C	-5.81	1.45	1.52
2	B	399	ASP	C-O	-5.81	1.16	1.23
2	B	1154	ALA	C-O	5.81	1.31	1.24
1	A	627	GLY	C-O	-5.81	1.15	1.23
1	A	721	PHE	CA-CB	5.81	1.62	1.53
1	A	1420	ASP	N-CA	5.81	1.54	1.46
2	B	305	VAL	C-O	5.81	1.31	1.24
2	B	769	TYR	CB-CG	5.81	1.64	1.51
2	B	822	ASN	CG-ND2	5.81	1.45	1.33
2	B	67	SER	CA-C	5.81	1.60	1.52
2	B	612	GLU	C-O	-5.81	1.16	1.24
6	H	78	SER	CA-C	-5.81	1.45	1.52
9	K	87	LEU	C-N	5.81	1.41	1.33
1	A	932	GLU	CD-OE1	5.81	1.36	1.25
2	B	496	ARG	N-CA	-5.80	1.40	1.46
1	A	164	ARG	NE-CZ	5.80	1.39	1.33
1	A	459	ARG	CG-CD	5.80	1.69	1.52
9	K	91	CYS	C-O	5.80	1.30	1.24
1	A	489	LEU	CA-CB	-5.80	1.40	1.53
2	B	127	GLY	C-N	-5.80	1.25	1.33
2	B	396	ASP	C-N	5.80	1.41	1.33
3	C	252	GLN	CB-CG	5.80	1.69	1.52
1	A	165	GLY	N-CA	5.80	1.53	1.45
2	B	19	GLU	CA-C	5.80	1.60	1.52
1	A	821	ARG	N-CA	-5.80	1.39	1.46
8	J	31	ASP	C-N	5.80	1.41	1.33
1	A	1237	ILE	C-O	5.80	1.29	1.24
1	A	1267	MET	CA-C	-5.80	1.45	1.52
2	B	231	PRO	N-CA	5.80	1.55	1.47
2	B	279	ASP	N-CA	5.80	1.53	1.46
2	B	1133	MET	CA-CB	-5.80	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	148	ARG	CZ-NH1	5.80	1.40	1.32
9	K	41	THR	C-O	-5.80	1.17	1.24
2	B	403	LYS	N-CA	-5.79	1.38	1.46
2	B	988	GLY	C-O	-5.79	1.18	1.23
1	A	451	HIS	C-O	-5.79	1.16	1.23
2	B	1077	THR	C-N	-5.79	1.25	1.33
1	A	26	GLU	CA-C	-5.79	1.44	1.52
1	A	386	ASP	CA-CB	5.79	1.62	1.53
1	A	572	TRP	CD2-CE2	-5.79	1.31	1.41
1	A	710	LEU	CG-CD1	5.79	1.71	1.52
1	A	712	GLU	C-O	-5.79	1.16	1.24
5	F	82	THR	N-CA	5.79	1.53	1.45
10	L	58	LYS	N-CA	-5.79	1.38	1.46
3	C	202	PRO	C-O	-5.79	1.17	1.23
4	E	180	ARG	CG-CD	5.79	1.69	1.52
1	A	156	ASP	N-CA	5.79	1.53	1.46
1	A	469	ARG	CG-CD	5.79	1.69	1.52
1	A	1059	HIS	CG-ND1	-5.79	1.31	1.38
3	C	180	TYR	C-N	-5.79	1.25	1.33
3	C	256	ALA	N-CA	-5.79	1.38	1.46
4	E	175	LEU	C-N	-5.79	1.26	1.33
1	A	126	LEU	CA-C	5.79	1.60	1.52
1	A	1022	LEU	CA-CB	-5.79	1.44	1.53
1	A	1211	GLN	CG-CD	5.79	1.66	1.52
2	B	46	GLN	CG-CD	-5.79	1.37	1.52
3	C	260	LEU	C-O	5.79	1.31	1.24
4	E	98	ILE	C-N	5.78	1.41	1.33
7	I	38	ALA	N-CA	5.78	1.53	1.46
9	K	28	PRO	CA-C	5.78	1.58	1.52
9	K	70	ARG	CA-C	-5.78	1.45	1.52
1	A	1078	GLN	CA-CB	5.78	1.61	1.53
2	B	1217	TYR	N-CA	-5.78	1.39	1.46
1	A	779	PHE	C-O	-5.78	1.16	1.23
1	A	1289	ARG	N-CA	5.78	1.53	1.46
2	B	722	ASP	CB-CG	5.78	1.66	1.52
1	A	842	VAL	C-N	-5.78	1.26	1.33
1	A	1238	ILE	CA-CB	-5.78	1.47	1.54
2	B	1074	ASN	C-N	-5.78	1.25	1.33
3	C	248	ILE	CG1-CD1	-5.78	1.29	1.51
1	A	8	SER	CA-C	5.77	1.60	1.52
1	A	511	ILE	C-N	-5.77	1.26	1.33
1	A	668	ASP	CA-CB	-5.77	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1007	VAL	CA-CB	-5.77	1.46	1.54
9	K	40	HIS	CD2-NE2	-5.77	1.31	1.37
3	C	118	LEU	CA-CB	5.77	1.61	1.53
1	A	1130	GLN	CA-CB	5.77	1.63	1.53
2	B	31	TRP	C-N	-5.77	1.26	1.33
2	B	908	GLU	CB-CG	5.77	1.69	1.52
4	E	172	GLU	CA-C	-5.77	1.45	1.52
1	A	400	PRO	N-CA	-5.77	1.40	1.47
1	A	826	ASP	C-N	-5.77	1.26	1.33
2	B	107	GLY	CA-C	5.77	1.60	1.51
2	B	210	LYS	C-N	-5.77	1.25	1.33
2	B	555	ILE	CG1-CD1	-5.77	1.29	1.51
3	C	3	GLU	CD-OE1	5.77	1.36	1.25
5	F	145	ASP	CA-CB	-5.77	1.44	1.53
1	A	1157	ASP	N-CA	-5.77	1.40	1.46
6	H	103	LYS	N-CA	-5.77	1.38	1.46
1	A	1019	CYS	CA-C	-5.76	1.44	1.52
2	B	401	PHE	CG-CD2	-5.76	1.26	1.38
2	B	415	GLN	CA-CB	5.76	1.62	1.53
2	B	780	VAL	CA-CB	-5.76	1.47	1.53
3	C	110	THR	N-CA	5.76	1.53	1.46
2	B	273	LEU	C-O	5.76	1.31	1.24
6	H	63	LEU	C-O	5.76	1.35	1.23
1	A	572	TRP	N-CA	5.76	1.53	1.45
1	A	1339	LEU	N-CA	-5.76	1.38	1.45
2	B	205	ILE	CG1-CD1	-5.76	1.29	1.51
2	B	537	LYS	C-O	-5.76	1.16	1.23
1	A	1274	ARG	CZ-NH2	5.76	1.41	1.33
2	B	40	GLU	N-CA	-5.76	1.39	1.46
9	K	66	PRO	CB-CG	-5.76	1.20	1.49
1	A	754	SER	C-O	-5.76	1.16	1.23
6	H	141	TYR	CA-C	-5.76	1.45	1.53
8	J	42	LYS	CG-CD	5.76	1.69	1.52
1	A	170	THR	CA-CB	5.76	1.62	1.53
1	A	201	VAL	C-O	5.76	1.31	1.24
2	B	978	ASP	C-O	-5.76	1.16	1.23
3	C	34	ARG	CG-CD	5.76	1.69	1.52
10	L	60	ARG	CD-NE	5.76	1.54	1.46
1	A	1044	TRP	CB-CG	-5.75	1.32	1.50
4	E	11	ARG	N-CA	5.75	1.53	1.46
1	A	511	ILE	N-CA	5.75	1.53	1.46
1	A	861	GLY	CA-C	-5.75	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	128	LYS	CA-C	-5.75	1.45	1.53
1	A	400	PRO	CB-CG	-5.75	1.21	1.49
1	A	973	ILE	CA-CB	5.75	1.61	1.54
2	B	641	GLU	CD-OE2	5.75	1.36	1.25
7	I	120	GLN	CA-CB	5.75	1.63	1.53
1	A	659	HIS	C-N	-5.75	1.25	1.33
1	A	717	ASN	CG-ND2	-5.75	1.21	1.33
1	A	995	GLU	CD-OE1	5.75	1.36	1.25
1	A	1049	ILE	C-N	-5.75	1.26	1.33
1	A	1442	ASP	CA-CB	-5.75	1.44	1.53
1	A	433	GLU	CD-OE1	5.75	1.36	1.25
1	A	722	LEU	CA-C	-5.75	1.44	1.52
2	B	92	PHE	CA-C	5.75	1.60	1.52
2	B	194	GLU	CD-OE2	5.74	1.36	1.25
1	A	274	ILE	CG1-CD1	5.74	1.74	1.51
1	A	1206	ASP	CA-CB	5.74	1.62	1.53
4	E	15	ALA	CA-C	-5.74	1.45	1.52
5	F	97	ARG	CA-CB	-5.74	1.44	1.53
1	A	460	VAL	CB-CG2	-5.74	1.33	1.52
1	A	567	LYS	CA-C	-5.74	1.45	1.52
1	A	1052	GLN	N-CA	-5.74	1.39	1.46
2	B	54	PHE	C-O	-5.74	1.17	1.24
2	B	685	LEU	CG-CD1	-5.74	1.33	1.52
2	B	1093	GLN	C-O	-5.74	1.17	1.24
3	C	173	ALA	N-CA	5.74	1.52	1.45
8	J	9	SER	N-CA	-5.74	1.38	1.46
3	C	178	PHE	C-O	-5.74	1.16	1.24
1	A	1196	GLU	C-O	-5.74	1.17	1.24
7	I	36	GLU	CA-C	-5.74	1.45	1.52
1	A	1150	SER	CA-C	5.73	1.59	1.52
1	A	611	GLN	C-O	5.73	1.30	1.23
1	A	62	ASP	CA-C	5.73	1.60	1.52
1	A	841	LEU	CB-CG	-5.73	1.42	1.53
2	B	18	PHE	CG-CD2	5.73	1.50	1.38
2	B	538	ASN	N-CA	-5.73	1.38	1.46
2	B	903	VAL	CA-C	-5.73	1.46	1.52
2	B	485	ARG	N-CA	-5.73	1.37	1.46
2	B	950	ASP	C-N	-5.73	1.26	1.33
1	A	135	PHE	CG-CD1	-5.73	1.26	1.38
1	A	1074	GLU	CA-CB	5.73	1.62	1.53
2	B	336	ARG	CZ-NH1	5.73	1.40	1.32
2	B	547	VAL	CB-CG1	-5.73	1.33	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	72	ASP	CA-CB	5.73	1.61	1.53
1	A	459	ARG	CA-CB	-5.72	1.44	1.53
1	A	836	TYR	CE1-CZ	5.72	1.51	1.38
1	A	1017	LEU	CA-C	-5.72	1.45	1.52
1	A	1355	VAL	C-N	-5.72	1.26	1.33
2	B	254	LEU	N-CA	-5.72	1.38	1.46
3	C	160	LYS	C-O	5.72	1.30	1.23
1	A	193	ASP	CA-C	5.72	1.60	1.52
1	A	1423	GLY	C-N	-5.72	1.26	1.33
2	B	563	MET	CA-CB	-5.72	1.44	1.53
6	H	134	ASN	CA-C	-5.72	1.45	1.53
7	I	27	PHE	CA-CB	-5.72	1.45	1.53
7	I	73	ARG	CB-CG	-5.72	1.35	1.52
2	B	216	GLU	N-CA	5.72	1.53	1.46
5	F	91	ALA	CA-C	-5.72	1.45	1.52
1	A	190	ALA	N-CA	5.72	1.53	1.46
2	B	1192	TYR	CA-CB	-5.72	1.43	1.54
9	K	32	VAL	CA-CB	-5.72	1.46	1.54
1	A	286	HIS	C-O	-5.72	1.16	1.24
1	A	672	ASP	CB-CG	-5.72	1.37	1.52
1	A	110	CYS	N-CA	5.72	1.53	1.46
1	A	220	THR	C-N	-5.72	1.25	1.33
1	A	1262	LYS	CA-C	5.72	1.59	1.52
2	B	347	LYS	CA-C	5.72	1.60	1.52
2	B	449	ASN	N-CA	5.72	1.53	1.46
3	C	106	GLU	CD-OE2	5.72	1.36	1.25
1	A	451	HIS	N-CA	-5.71	1.38	1.45
1	A	887	GLY	C-O	-5.71	1.16	1.23
1	A	1194	ARG	CA-C	-5.71	1.45	1.52
2	B	60	GLN	CB-CG	-5.71	1.35	1.52
2	B	94	LYS	C-N	5.71	1.41	1.33
2	B	734	HIS	CB-CG	5.71	1.58	1.50
9	K	69	ALA	CA-C	-5.71	1.45	1.52
1	A	888	GLY	CA-C	-5.71	1.46	1.52
1	A	948	VAL	CB-CG1	-5.71	1.33	1.52
2	B	1041	GLU	C-O	-5.71	1.16	1.24
1	A	464	PRO	N-CA	-5.71	1.40	1.47
1	A	1103	GLU	N-CA	-5.71	1.39	1.46
2	B	794	ASN	C-O	-5.71	1.17	1.24
7	I	70	ARG	C-O	-5.71	1.16	1.23
10	L	35	SER	N-CA	5.71	1.53	1.46
6	H	109	LYS	N-CA	5.71	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	77	LYS	CG-CD	5.71	1.69	1.52
1	A	386	ASP	N-CA	-5.71	1.39	1.46
1	A	906	HIS	CA-C	-5.71	1.45	1.52
2	B	800	GLN	CG-CD	5.71	1.66	1.52
2	B	899	ILE	CA-C	-5.71	1.46	1.53
3	C	227	THR	CA-C	5.71	1.58	1.52
7	I	49	ILE	CB-CG2	5.71	1.71	1.52
1	A	211	PHE	CB-CG	5.71	1.63	1.50
1	A	248	PRO	N-CD	5.71	1.55	1.47
1	A	436	ILE	N-CA	-5.71	1.36	1.46
1	A	1421	CYS	N-CA	-5.71	1.38	1.46
9	K	34	THR	C-O	5.71	1.30	1.24
2	B	869	SER	N-CA	5.71	1.53	1.46
6	H	50	ALA	CA-CB	5.71	1.62	1.53
1	A	473	SER	C-O	-5.70	1.16	1.24
2	B	133	LYS	CA-C	5.70	1.59	1.52
7	I	41	PRO	CA-CB	-5.70	1.45	1.53
1	A	1441	PHE	C-O	-5.70	1.17	1.23
1	A	933	TYR	CG-CD1	-5.70	1.27	1.39
1	A	1337	GLU	CD-OE1	5.70	1.36	1.25
2	B	654	ARG	NE-CZ	-5.70	1.26	1.33
1	A	402	ALA	C-O	-5.70	1.16	1.23
1	A	555	ASP	CA-C	-5.70	1.46	1.53
1	A	976	THR	CB-CG2	5.70	1.71	1.52
1	A	1281	ARG	CG-CD	5.70	1.69	1.52
2	B	1177	HIS	C-O	-5.70	1.15	1.24
4	E	40	GLU	CD-OE1	5.70	1.36	1.25
9	K	6	ARG	C-O	5.70	1.31	1.24
1	A	427	GLN	CB-CG	5.70	1.69	1.52
3	C	75	MET	C-O	-5.70	1.17	1.24
4	E	13	TRP	C-O	5.70	1.31	1.24
4	E	144	ILE	C-O	-5.70	1.16	1.24
4	E	206	GLY	C-O	-5.69	1.17	1.23
8	J	32	GLU	CD-OE1	5.69	1.36	1.25
1	A	806	ARG	CA-CB	-5.69	1.43	1.53
3	C	111	THR	CB-CG2	5.69	1.71	1.52
5	F	104	ASN	CG-ND2	5.69	1.45	1.33
9	K	113	THR	CA-CB	5.69	1.67	1.53
1	A	420	ARG	CZ-NH1	-5.69	1.24	1.32
1	A	1108	ALA	CA-CB	-5.69	1.44	1.53
1	A	1347	ALA	N-CA	-5.69	1.39	1.46
2	B	732	SER	C-N	5.69	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	140	ASN	CG-OD1	5.69	1.34	1.23
3	C	240	VAL	C-O	-5.69	1.17	1.24
7	I	12	ASN	N-CA	-5.69	1.39	1.45
8	J	21	TYR	CB-CG	5.69	1.64	1.51
10	L	47	ARG	CZ-NH2	5.69	1.40	1.33
1	A	155	GLU	CG-CD	5.69	1.66	1.52
2	B	279	ASP	CG-OD2	5.69	1.36	1.25
2	B	1023	VAL	N-CA	-5.69	1.39	1.46
4	E	131	THR	CA-C	-5.69	1.46	1.52
1	A	633	VAL	CA-CB	-5.69	1.47	1.54
1	A	474	VAL	CB-CG2	-5.69	1.33	1.52
1	A	1316	VAL	CA-CB	5.69	1.62	1.54
1	A	621	THR	C-N	-5.68	1.27	1.33
1	A	1155	ASP	C-O	-5.68	1.17	1.24
1	A	401	GLY	N-CA	-5.68	1.37	1.45
1	A	552	TRP	CG-CD1	-5.68	1.22	1.36
1	A	607	ILE	CA-CB	5.68	1.62	1.54
1	A	1301	GLU	CD-OE2	5.68	1.36	1.25
6	H	13	SER	CA-C	-5.68	1.45	1.52
2	B	802	PRO	N-CA	-5.68	1.40	1.47
1	A	589	GLN	N-CA	-5.68	1.38	1.45
1	A	1005	GLU	CD-OE2	5.68	1.36	1.25
3	C	128	ASN	CG-OD1	5.68	1.34	1.23
4	E	148	GLU	CD-OE2	5.68	1.36	1.25
1	A	1223	ASP	C-O	-5.68	1.16	1.24
5	F	88	TYR	C-N	-5.68	1.26	1.33
7	I	34	TYR	CE1-CZ	-5.68	1.24	1.38
1	A	720	ARG	NE-CZ	5.68	1.39	1.33
1	A	1359	ASP	C-O	-5.68	1.16	1.24
2	B	1004	GLU	C-O	5.68	1.38	1.24
7	I	49	ILE	CA-CB	5.68	1.60	1.53
2	B	632	ARG	C-N	-5.67	1.20	1.33
5	F	136	ARG	CZ-NH1	-5.67	1.24	1.32
6	H	117	SER	N-CA	5.67	1.53	1.46
7	I	24	ARG	CD-NE	5.67	1.54	1.46
1	A	398	GLU	CD-OE2	5.67	1.36	1.25
1	A	653	VAL	CB-CG2	-5.67	1.33	1.52
1	A	836	TYR	CE2-CZ	5.67	1.51	1.38
1	A	872	GLY	CA-C	-5.67	1.43	1.51
1	A	1008	GLN	CA-C	-5.67	1.45	1.52
1	A	1218	GLN	CA-C	-5.67	1.45	1.52
2	B	307	ASP	CB-CG	-5.67	1.37	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	730	ARG	CZ-NH1	-5.67	1.24	1.32
4	E	32	GLN	C-O	-5.67	1.17	1.24
1	A	1381	LEU	CG-CD1	-5.67	1.33	1.52
1	A	1012	ARG	C-N	5.67	1.41	1.33
1	A	1138	ILE	CA-CB	-5.67	1.47	1.54
2	B	388	CYS	CA-C	-5.67	1.45	1.52
2	B	510	LYS	C-N	-5.67	1.26	1.34
1	A	292	ALA	CA-CB	5.67	1.62	1.53
1	A	957	PRO	N-CA	-5.67	1.40	1.46
1	A	1197	LEU	C-N	-5.67	1.25	1.33
9	K	96	ASN	C-O	5.67	1.30	1.24
1	A	1050	GLU	CD-OE1	5.67	1.36	1.25
2	B	451	LYS	N-CA	-5.67	1.38	1.46
3	C	137	LYS	CA-CB	5.67	1.62	1.53
1	A	634	THR	CA-C	-5.66	1.45	1.52
1	A	1350	LYS	CE-NZ	5.66	1.66	1.49
2	B	373	ARG	CD-NE	5.66	1.54	1.46
3	C	50	GLU	CD-OE2	5.66	1.36	1.25
1	A	1124	HIS	CA-CB	5.66	1.60	1.53
10	L	63	ARG	N-CA	5.66	1.53	1.46
2	B	384	ARG	CG-CD	5.66	1.69	1.52
2	B	1155	SER	CB-OG	5.66	1.53	1.42
8	J	45	CYS	N-CA	-5.66	1.39	1.46
1	A	188	ASP	C-O	5.66	1.31	1.24
1	A	196	GLU	N-CA	5.66	1.54	1.46
2	B	1034	VAL	CA-CB	-5.66	1.47	1.54
2	B	1086	PHE	CA-C	-5.66	1.45	1.52
2	B	1168	LEU	N-CA	5.66	1.53	1.45
2	B	1217	TYR	CG-CD1	-5.66	1.27	1.39
4	E	95	THR	CA-C	-5.66	1.45	1.52
8	J	46	CYS	N-CA	5.66	1.53	1.46
2	B	846	ILE	CB-CG2	5.66	1.71	1.52
2	B	1039	GLY	C-O	-5.66	1.16	1.23
8	J	15	GLY	C-O	5.66	1.30	1.23
1	A	62	ASP	N-CA	5.65	1.53	1.46
1	A	1325	THR	CA-C	5.65	1.60	1.52
1	A	1404	GLU	N-CA	5.65	1.52	1.45
3	C	138	GLU	CA-C	-5.65	1.45	1.52
1	A	359	LEU	CG-CD2	-5.65	1.33	1.52
2	B	174	LEU	C-N	-5.65	1.25	1.33
2	B	522	VAL	N-CA	5.65	1.52	1.46
1	A	1212	VAL	CB-CG1	-5.65	1.33	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	43	ASN	CB-CG	5.65	1.66	1.52
7	I	5	ARG	CA-C	-5.65	1.45	1.52
4	E	40	GLU	N-CA	5.65	1.53	1.46
1	A	542	GLU	CD-OE1	5.64	1.36	1.25
1	A	620	LYS	C-O	-5.64	1.17	1.24
9	K	54	ARG	CZ-NH1	5.64	1.40	1.32
1	A	825	ILE	CA-CB	-5.64	1.47	1.54
2	B	832	GLY	CA-C	-5.64	1.43	1.51
6	H	92	ASP	CA-CB	5.64	1.61	1.53
1	A	983	ILE	CB-CG2	-5.64	1.33	1.52
2	B	874	PHE	CD2-CE2	-5.64	1.21	1.38
8	J	62	ARG	C-N	-5.64	1.25	1.33
1	A	188	ASP	C-N	5.64	1.41	1.33
1	A	936	LEU	C-O	-5.64	1.17	1.24
2	B	248	SER	N-CA	5.64	1.53	1.46
2	B	900	ALA	CA-CB	-5.64	1.42	1.54
2	B	325	GLN	CB-CG	-5.64	1.35	1.52
1	A	123	ARG	CA-C	-5.64	1.45	1.52
1	A	125	ALA	C-O	-5.64	1.16	1.24
1	A	218	ASP	C-N	5.64	1.42	1.33
1	A	994	GLN	CD-OE1	-5.64	1.12	1.23
6	H	135	LEU	CA-CB	5.64	1.62	1.53
1	A	353	ILE	CA-C	-5.63	1.45	1.52
1	A	674	PRO	N-CA	-5.63	1.40	1.47
2	B	115	GLN	N-CA	5.63	1.53	1.46
2	B	869	SER	C-N	5.63	1.41	1.33
1	A	46	THR	CA-CB	5.63	1.77	1.54
1	A	945	GLU	CD-OE1	5.63	1.36	1.25
1	A	1366	ARG	C-O	-5.63	1.16	1.24
2	B	710	LEU	C-O	-5.63	1.17	1.24
2	B	1129	ARG	CZ-NH1	5.63	1.40	1.32
5	F	93	ILE	CA-C	5.63	1.59	1.52
6	H	86	ASP	N-CA	5.63	1.53	1.46
9	K	64	GLU	C-N	-5.63	1.25	1.33
4	E	162	ARG	C-N	-5.63	1.26	1.33
1	A	440	ASP	CB-CG	-5.63	1.38	1.52
2	B	380	TYR	CA-C	-5.63	1.45	1.52
2	B	709	ASP	C-N	-5.63	1.25	1.33
2	B	844	SER	CA-CB	-5.63	1.44	1.53
2	B	979	LYS	CB-CG	-5.63	1.35	1.52
1	A	1315	GLU	C-N	-5.63	1.27	1.34
1	A	1317	MET	SD-CE	-5.63	1.65	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	715	GLU	CA-C	-5.62	1.45	1.52
3	C	91	HIS	C-O	-5.62	1.16	1.23
4	E	84	ASP	CA-C	5.62	1.60	1.52
7	I	109	ILE	N-CA	-5.62	1.39	1.46
2	B	56	ASP	C-O	-5.62	1.16	1.24
2	B	499	ASN	CG-ND2	5.62	1.45	1.33
8	J	56	LEU	C-N	-5.62	1.27	1.34
1	A	808	LEU	CG-CD1	-5.62	1.34	1.52
1	A	295	LEU	CG-CD1	5.62	1.71	1.52
2	B	761	HIS	CE1-NE2	5.62	1.38	1.32
1	A	655	PHE	C-N	-5.62	1.26	1.34
2	B	618	ASP	CB-CG	-5.62	1.38	1.52
3	C	13	ALA	C-O	-5.62	1.17	1.23
6	H	9	ILE	CB-CG1	5.62	1.64	1.53
10	L	64	LEU	CA-CB	5.62	1.62	1.53
1	A	809	THR	C-N	-5.62	1.26	1.34
2	B	204	ILE	CA-C	5.62	1.59	1.52
1	A	527	THR	CA-CB	-5.62	1.43	1.53
2	B	278	GLN	N-CA	-5.62	1.38	1.45
2	B	958	GLN	CD-NE2	5.62	1.45	1.33
3	C	179	GLU	CD-OE1	-5.62	1.14	1.25
6	H	80	ARG	CZ-NH2	5.62	1.40	1.33
3	C	77	ILE	N-CA	5.61	1.53	1.46
3	C	210	GLU	C-O	-5.61	1.17	1.23
4	E	66	GLU	CG-CD	5.61	1.66	1.52
1	A	645	LEU	CA-C	5.61	1.60	1.52
2	B	1060	ARG	CB-CG	-5.61	1.35	1.52
4	E	210	SER	CB-OG	5.61	1.53	1.42
1	A	1078	GLN	CG-CD	5.61	1.66	1.52
2	B	229	ALA	CA-CB	-5.61	1.45	1.53
10	L	33	GLU	C-O	5.61	1.31	1.24
1	A	693	VAL	CA-CB	-5.60	1.46	1.54
2	B	291	ILE	CG1-CD1	-5.60	1.29	1.51
2	B	1026	LEU	C-O	-5.60	1.17	1.24
2	B	1196	ILE	CA-C	5.60	1.58	1.52
2	B	1224	PHE	CG-CD1	5.60	1.50	1.38
8	J	49	MET	CB-CG	-5.60	1.35	1.52
1	A	268	ASP	CB-CG	5.60	1.66	1.52
1	A	949	ASP	CA-C	-5.60	1.44	1.52
1	A	1306	LEU	CA-C	5.60	1.60	1.52
1	A	56	PRO	C-N	5.60	1.41	1.33
2	B	1043	ASP	CG-OD2	5.60	1.35	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	3	THR	CB-CG2	5.60	1.71	1.52
1	A	248	PRO	CB-CG	5.60	1.77	1.49
1	A	286	HIS	CA-C	-5.60	1.45	1.52
7	I	30	ARG	C-N	-5.60	1.25	1.33
7	I	59	VAL	CB-CG1	-5.60	1.34	1.52
8	J	27	GLU	CA-C	5.60	1.60	1.52
1	A	277	GLU	CA-CB	5.60	1.62	1.53
2	B	855	PHE	CG-CD1	-5.60	1.27	1.38
2	B	90	ILE	C-N	5.59	1.40	1.33
1	A	719	VAL	CB-CG1	-5.59	1.34	1.52
2	B	935	ARG	C-O	5.59	1.30	1.23
2	B	1020	ARG	CA-C	5.59	1.60	1.52
7	I	24	ARG	N-CA	5.59	1.53	1.45
1	A	1286	LYS	CB-CG	5.59	1.69	1.52
2	B	1056	SER	C-O	-5.59	1.17	1.24
3	C	134	ILE	CB-CG2	-5.59	1.34	1.52
5	F	134	ILE	CB-CG2	-5.59	1.34	1.52
9	K	26	LYS	C-N	-5.59	1.26	1.33
1	A	303	TYR	CA-CB	5.59	1.62	1.53
2	B	1101	ASP	N-CA	5.59	1.53	1.46
1	A	1384	VAL	CB-CG2	5.59	1.71	1.52
1	A	225	ASN	CG-ND2	-5.59	1.21	1.33
3	C	132	PRO	N-CD	-5.59	1.40	1.47
1	A	228	PHE	N-CA	5.58	1.53	1.46
5	F	105	ALA	N-CA	-5.58	1.37	1.45
1	A	80	HIS	CA-CB	5.58	1.62	1.53
1	A	470	LEU	N-CA	-5.58	1.39	1.45
2	B	276	ILE	N-CA	-5.58	1.39	1.46
7	I	93	LYS	N-CA	-5.58	1.39	1.46
9	K	18	LYS	N-CA	5.58	1.53	1.46
2	B	644	GLU	CD-OE1	5.58	1.35	1.25
2	B	1028	GLU	C-N	-5.58	1.26	1.33
1	A	956	LEU	C-N	-5.58	1.26	1.33
2	B	265	SER	C-O	5.58	1.30	1.24
2	B	638	PHE	N-CA	-5.58	1.38	1.45
1	A	782	ARG	NE-CZ	5.58	1.39	1.33
2	B	206	ASN	C-O	-5.58	1.16	1.23
2	B	984	HIS	CG-ND1	-5.58	1.32	1.38
7	I	8	ARG	CB-CG	5.58	1.69	1.52
1	A	736	ASN	CA-C	-5.58	1.43	1.52
1	A	865	GLN	C-O	-5.58	1.17	1.23
2	B	698	GLU	CA-C	5.58	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	20	TYR	CE2-CZ	-5.58	1.24	1.38
1	A	398	GLU	C-O	-5.57	1.17	1.24
9	K	105	PHE	CE2-CZ	5.57	1.55	1.38
1	A	541	ILE	N-CA	-5.57	1.39	1.46
1	A	1450	LEU	CB-CG	5.57	1.64	1.53
2	B	645	SER	C-O	-5.57	1.17	1.24
1	A	785	PRO	CA-CB	5.57	1.63	1.53
3	C	118	LEU	CA-C	5.57	1.59	1.52
2	B	787	VAL	CA-C	-5.57	1.44	1.52
6	H	21	ASN	CA-CB	-5.57	1.45	1.53
6	H	39	THR	N-CA	5.57	1.53	1.46
3	C	32	SER	C-O	5.57	1.31	1.24
9	K	2	ASN	C-N	5.57	1.43	1.33
1	A	763	ALA	CA-CB	-5.56	1.44	1.53
2	B	587	HIS	C-N	5.56	1.41	1.33
9	K	94	ILE	CA-C	-5.56	1.46	1.52
2	B	255	GLN	C-O	-5.56	1.16	1.24
2	B	346	GLU	CD-OE2	5.56	1.35	1.25
2	B	845	SER	C-O	5.56	1.31	1.24
1	A	109	HIS	N-CA	-5.56	1.40	1.47
1	A	835	GLY	N-CA	5.56	1.52	1.45
2	B	969	ARG	NE-CZ	-5.56	1.26	1.33
1	A	868	TYR	CA-C	-5.56	1.45	1.52
1	A	1413	GLY	C-N	-5.56	1.25	1.33
2	B	852	ARG	N-CA	-5.56	1.39	1.46
2	B	1055	ILE	C-N	-5.56	1.26	1.33
3	C	100	THR	CA-CB	-5.56	1.41	1.53
1	A	983	ILE	C-O	-5.55	1.17	1.24
1	A	1006	ILE	C-O	-5.55	1.18	1.24
2	B	215	GLN	CA-C	-5.55	1.46	1.52
2	B	1211	ASN	N-CA	5.55	1.53	1.46
3	C	249	ASP	CG-OD1	5.55	1.35	1.25
4	E	100	ILE	CG1-CD1	-5.55	1.30	1.51
2	B	808	ALA	N-CA	5.55	1.53	1.46
9	K	63	VAL	C-N	-5.55	1.26	1.34
1	A	546	VAL	CB-CG2	-5.55	1.34	1.52
1	A	451	HIS	CA-CB	-5.55	1.43	1.53
1	A	862	ASN	CA-CB	-5.55	1.44	1.53
1	A	900	ASP	C-O	5.55	1.30	1.24
1	A	1191	TRP	CZ3-CH2	-5.55	1.26	1.40
4	E	75	MET	N-CA	-5.55	1.39	1.46
7	I	31	THR	C-O	-5.55	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	37	PHE	CE1-CZ	5.55	1.55	1.38
1	A	549	MET	C-O	-5.55	1.17	1.24
2	B	525	ALA	N-CA	-5.55	1.39	1.46
6	H	142	LEU	CA-C	5.55	1.59	1.52
10	L	32	ALA	CA-C	5.55	1.60	1.52
1	A	652	VAL	N-CA	-5.55	1.39	1.46
8	J	43	ARG	CZ-NH1	-5.55	1.25	1.32
1	A	152	VAL	C-O	5.54	1.31	1.24
1	A	759	ALA	CA-C	-5.54	1.45	1.52
1	A	1196	GLU	CD-OE2	5.54	1.35	1.25
2	B	166	PHE	CA-C	-5.54	1.45	1.52
6	H	93	TYR	CG-CD1	5.54	1.50	1.39
1	A	1284	MET	CG-SD	-5.54	1.66	1.80
2	B	905	VAL	CA-CB	-5.54	1.46	1.54
2	B	1072	MET	C-O	5.54	1.31	1.23
4	E	196	VAL	CA-C	5.54	1.59	1.52
1	A	194	ALA	CA-C	5.54	1.59	1.53
2	B	515	HIS	CG-CD2	-5.54	1.29	1.35
2	B	564	GLU	N-CA	-5.54	1.37	1.46
2	B	770	GLN	CG-CD	-5.54	1.38	1.52
2	B	1143	ALA	CA-C	-5.54	1.47	1.53
4	E	15	ALA	C-O	5.54	1.31	1.24
7	I	72	ASP	N-CA	5.54	1.52	1.46
2	B	193	LYS	CG-CD	5.54	1.69	1.52
2	B	592	ASN	CG-ND2	5.54	1.44	1.33
1	A	749	ALA	CA-CB	5.54	1.62	1.53
1	A	1262	LYS	CG-CD	5.54	1.69	1.52
1	A	1311	VAL	C-N	5.54	1.41	1.33
2	B	685	LEU	C-N	-5.54	1.26	1.33
6	H	107	VAL	CB-CG1	5.54	1.70	1.52
1	A	992	ASP	CB-CG	5.53	1.65	1.52
9	K	75	ILE	CG1-CD1	-5.53	1.30	1.51
4	E	155	ARG	CZ-NH1	5.53	1.40	1.32
7	I	15	TYR	N-CA	-5.53	1.37	1.45
1	A	513	SER	C-O	-5.53	1.18	1.24
1	A	810	PRO	C-O	-5.53	1.16	1.24
2	B	370	PHE	C-N	5.53	1.41	1.33
2	B	509	ALA	N-CA	-5.53	1.35	1.46
5	F	96	THR	CB-OG1	-5.53	1.34	1.43
1	A	1314	SER	N-CA	-5.53	1.39	1.46
2	B	224	GLN	CB-CG	5.53	1.69	1.52
2	B	585	VAL	C-O	-5.53	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1224	PHE	CD2-CE2	5.53	1.55	1.38
1	A	704	ALA	CA-CB	-5.53	1.44	1.53
2	B	615	MET	CA-CB	-5.53	1.44	1.53
2	B	862	GLN	CD-OE1	5.53	1.34	1.23
2	B	979	LYS	CA-CB	-5.53	1.44	1.53
3	C	194	GLU	CA-CB	5.53	1.62	1.53
1	A	445	ASN	CA-C	5.52	1.59	1.52
1	A	597	LEU	C-N	-5.52	1.25	1.33
1	A	1015	VAL	C-O	-5.52	1.15	1.24
2	B	595	ARG	CZ-NH2	-5.52	1.26	1.33
1	A	278	THR	CA-CB	5.52	1.62	1.53
2	B	616	ILE	C-O	5.52	1.30	1.24
2	B	973	ILE	CG1-CD1	-5.52	1.30	1.51
1	A	382	PRO	CA-CB	-5.52	1.44	1.53
1	A	920	LEU	CB-CG	-5.52	1.42	1.53
1	A	1283	VAL	N-CA	-5.52	1.39	1.46
2	B	935	ARG	CA-CB	5.52	1.59	1.52
3	C	222	LYS	C-O	5.52	1.31	1.24
2	B	1053	GLU	CA-C	-5.52	1.45	1.52
1	A	675	THR	CA-C	5.51	1.60	1.52
1	A	1352	VAL	N-CA	5.51	1.53	1.46
2	B	841	MET	CG-SD	-5.51	1.67	1.80
5	F	115	THR	N-CA	5.51	1.53	1.45
9	K	40	HIS	C-O	5.51	1.31	1.24
1	A	590	ARG	NE-CZ	-5.51	1.26	1.33
1	A	710	LEU	CA-CB	-5.51	1.44	1.53
2	B	41	LYS	CE-NZ	5.51	1.65	1.49
2	B	767	ASN	N-CA	-5.51	1.39	1.46
3	C	94	LYS	CA-CB	5.51	1.63	1.53
1	A	1136	SER	C-N	5.51	1.41	1.33
2	B	1151	LEU	CG-CD2	-5.51	1.34	1.52
4	E	20	LYS	C-O	5.51	1.30	1.24
1	A	830	LYS	N-CA	5.51	1.52	1.46
3	C	124	LEU	C-O	5.51	1.31	1.24
4	E	176	PRO	C-O	5.51	1.30	1.23
1	A	461	LYS	C-N	5.51	1.39	1.33
1	A	655	PHE	CG-CD2	-5.51	1.27	1.38
1	A	773	LYS	CA-C	-5.51	1.45	1.52
1	A	1416	ALA	CA-CB	-5.51	1.45	1.53
2	B	285	ILE	CA-C	5.51	1.59	1.52
3	C	211	ASP	CG-OD1	5.51	1.35	1.25
2	B	354	ASP	C-O	5.50	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1222	ASN	CG-OD1	5.50	1.34	1.23
1	A	1307	GLU	CA-CB	-5.50	1.43	1.53
1	A	1345	ARG	CZ-NH2	-5.50	1.26	1.33
2	B	971	THR	CA-CB	-5.50	1.45	1.53
4	E	100	ILE	CA-CB	-5.50	1.48	1.54
5	F	80	ALA	N-CA	-5.50	1.38	1.45
1	A	1031	VAL	N-CA	-5.50	1.40	1.46
2	B	859	TYR	C-O	-5.50	1.17	1.23
5	F	152	ILE	CG1-CD1	-5.50	1.30	1.51
6	H	98	TYR	CE1-CZ	-5.50	1.25	1.38
6	H	104	PHE	CE2-CZ	5.50	1.55	1.38
7	I	32	CYS	N-CA	5.50	1.54	1.46
1	A	8	SER	CA-CB	5.50	1.63	1.53
2	B	462	ALA	CA-C	-5.50	1.45	1.52
6	H	145	ARG	N-CA	5.50	1.52	1.45
1	A	394	ASN	CA-CB	-5.50	1.44	1.53
1	A	931	GLU	CD-OE1	5.50	1.35	1.25
1	A	1190	PRO	N-CD	5.50	1.55	1.47
2	B	451	LYS	CG-CD	5.50	1.69	1.52
2	B	1093	GLN	CD-OE1	5.50	1.33	1.23
9	K	61	TYR	CA-C	-5.50	1.46	1.52
1	A	73	GLY	CA-C	-5.50	1.45	1.52
1	A	1114	PRO	C-O	-5.50	1.17	1.23
2	B	64	CYS	CA-C	-5.50	1.45	1.52
2	B	788	ARG	CZ-NH1	-5.50	1.25	1.32
2	B	871	THR	N-CA	5.50	1.52	1.45
2	B	1014	PRO	CA-C	-5.49	1.44	1.52
2	B	666	TYR	C-O	-5.49	1.17	1.24
3	C	179	GLU	CD-OE2	-5.49	1.15	1.25
1	A	24	PRO	CG-CD	-5.49	1.32	1.50
1	A	568	PRO	CA-C	-5.49	1.43	1.52
1	A	899	VAL	CA-CB	-5.49	1.47	1.53
2	B	281	PRO	C-O	-5.49	1.16	1.24
8	J	30	LEU	CA-CB	-5.49	1.44	1.53
1	A	191	THR	CB-CG2	5.49	1.70	1.52
1	A	203	SER	C-O	-5.49	1.16	1.23
2	B	105	SER	CA-CB	5.49	1.62	1.53
2	B	355	ILE	C-N	-5.49	1.26	1.33
6	H	87	ARG	CB-CG	5.49	1.69	1.52
2	B	418	LYS	C-O	-5.49	1.17	1.24
3	C	191	TYR	CG-CD2	-5.49	1.27	1.39
1	A	454	SER	CA-C	-5.48	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	629	LEU	CA-CB	-5.48	1.44	1.53
1	A	500	GLU	CA-CB	-5.48	1.44	1.53
1	A	601	LYS	CA-C	5.48	1.60	1.52
1	A	1079	MET	C-O	5.48	1.31	1.24
1	A	1380	GLY	N-CA	5.48	1.53	1.45
3	C	171	GLY	C-O	5.48	1.31	1.24
1	A	748	MET	N-CA	5.48	1.53	1.46
1	A	877	HIS	CG-CD2	-5.48	1.29	1.35
1	A	1201	ALA	CA-C	5.48	1.60	1.52
2	B	213	ILE	C-O	5.48	1.30	1.24
2	B	690	VAL	CB-CG1	-5.48	1.34	1.52
3	C	169	LYS	C-N	-5.48	1.25	1.33
1	A	752	LYS	N-CA	-5.48	1.39	1.46
1	A	801	GLU	CA-C	-5.48	1.45	1.52
6	H	93	TYR	N-CA	5.48	1.52	1.45
6	H	97	MET	SD-CE	5.48	1.93	1.79
2	B	365	THR	CA-CB	5.48	1.63	1.53
2	B	493	SER	CA-C	5.48	1.60	1.52
7	I	31	THR	N-CA	-5.48	1.39	1.46
7	I	105	SER	C-O	-5.48	1.17	1.24
7	I	119	THR	CA-CB	5.48	1.62	1.53
9	K	55	LYS	CD-CE	5.48	1.68	1.52
2	B	392	ARG	C-O	-5.48	1.16	1.24
2	B	591	ARG	CA-CB	-5.48	1.46	1.54
2	B	401	PHE	CB-CG	-5.47	1.38	1.50
2	B	601	ARG	CD-NE	5.47	1.53	1.46
2	B	842	ASN	N-CA	5.47	1.52	1.46
7	I	73	ARG	NE-CZ	5.47	1.39	1.33
1	A	351	THR	CB-CG2	-5.47	1.34	1.52
2	B	551	PRO	N-CD	-5.47	1.40	1.47
4	E	103	LYS	C-O	5.47	1.31	1.24
1	A	177	ASP	CB-CG	5.47	1.65	1.52
1	A	655	PHE	N-CA	5.47	1.52	1.46
1	A	669	THR	CA-CB	5.47	1.62	1.53
1	A	1342	GLU	CD-OE1	5.47	1.35	1.25
2	B	1091	TYR	CB-CG	-5.47	1.39	1.51
1	A	551	TYR	C-N	5.47	1.41	1.34
1	A	619	LYS	C-N	-5.47	1.26	1.33
2	B	372	SER	C-N	-5.47	1.26	1.33
2	B	662	MET	C-O	-5.47	1.17	1.24
2	B	969	ARG	CZ-NH1	5.47	1.40	1.32
1	A	434	ARG	CA-CB	-5.47	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1100	ARG	NE-CZ	5.47	1.39	1.33
2	B	970	THR	CA-C	-5.47	1.46	1.52
1	A	533	LYS	C-N	-5.47	1.26	1.33
9	K	72	LYS	N-CA	-5.47	1.39	1.46
1	A	829	VAL	C-O	-5.46	1.18	1.24
2	B	100	PRO	CB-CG	-5.46	1.22	1.49
7	I	34	TYR	CA-C	-5.46	1.45	1.52
1	A	1265	ASN	CA-CB	5.46	1.61	1.53
3	C	28	ALA	N-CA	5.46	1.52	1.46
3	C	116	LYS	N-CA	5.46	1.53	1.46
7	I	26	LEU	N-CA	-5.46	1.39	1.45
8	J	2	ILE	CA-CB	5.46	1.63	1.55
2	B	350	GLN	N-CA	-5.46	1.39	1.46
1	A	19	PHE	CD1-CE1	-5.46	1.22	1.38
1	A	106	VAL	CA-C	5.46	1.59	1.52
2	B	512	ARG	CD-NE	-5.46	1.38	1.46
3	C	17	ASN	C-O	-5.46	1.17	1.23
4	E	137	GLU	CA-C	-5.46	1.46	1.52
9	K	16	GLU	CG-CD	5.46	1.65	1.52
2	B	515	HIS	C-O	-5.46	1.17	1.23
3	C	77	ILE	CB-CG1	-5.46	1.42	1.53
3	C	191	TYR	CB-CG	5.46	1.63	1.51
1	A	187	LYS	CA-CB	5.45	1.61	1.54
1	A	1077	THR	CB-CG2	5.45	1.70	1.52
2	B	957	ASN	N-CA	5.45	1.53	1.46
4	E	64	PRO	CG-CD	5.45	1.69	1.50
6	H	146	ARG	NE-CZ	5.45	1.39	1.33
9	K	64	GLU	CD-OE2	-5.45	1.15	1.25
2	B	1098	MET	SD-CE	5.45	1.93	1.79
3	C	97	VAL	N-CA	-5.45	1.39	1.46
9	K	101	LEU	C-O	-5.45	1.17	1.24
1	A	389	THR	CB-CG2	5.45	1.70	1.52
1	A	1032	LEU	C-O	-5.45	1.16	1.23
1	A	1053	PHE	C-N	-5.45	1.26	1.34
2	B	356	LEU	CA-CB	5.45	1.61	1.53
2	B	845	SER	C-N	-5.45	1.27	1.33
6	H	20	TYR	CD1-CE1	-5.45	1.22	1.38
9	K	2	ASN	CB-CG	5.45	1.65	1.52
2	B	174	LEU	CG-CD1	5.45	1.70	1.52
1	A	53	LEU	C-O	5.45	1.31	1.23
2	B	257	LYS	CA-C	-5.45	1.46	1.52
2	B	996	ARG	NE-CZ	-5.45	1.27	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	217	ASP	CA-C	5.45	1.59	1.52
6	H	132	LEU	CB-CG	5.45	1.64	1.53
1	A	268	ASP	CG-OD1	5.44	1.35	1.25
1	A	288	ALA	C-O	-5.44	1.17	1.24
2	B	329	THR	C-O	-5.44	1.17	1.24
2	B	502	ILE	CB-CG2	5.44	1.70	1.52
2	B	758	PHE	CG-CD2	-5.44	1.27	1.38
2	B	1034	VAL	CA-C	-5.44	1.45	1.52
2	B	1188	LYS	C-N	5.44	1.41	1.33
10	L	62	LYS	CA-C	5.44	1.60	1.52
1	A	26	GLU	CA-CB	-5.44	1.45	1.53
1	A	458	HIS	CG-CD2	-5.44	1.29	1.35
1	A	593	GLU	C-N	5.44	1.41	1.33
2	B	679	TYR	CA-CB	-5.44	1.45	1.53
2	B	797	TYR	CE1-CZ	-5.44	1.25	1.38
6	H	81	PRO	CG-CD	5.44	1.69	1.50
1	A	372	LYS	N-CA	5.44	1.53	1.46
1	A	613	ILE	CB-CG1	-5.44	1.42	1.53
1	A	782	ARG	CB-CG	-5.44	1.36	1.52
1	A	847	ASP	CA-CB	5.44	1.63	1.53
1	A	956	LEU	CG-CD2	-5.44	1.34	1.52
1	A	1141	THR	CA-CB	-5.44	1.44	1.53
1	A	298	PHE	CG-CD2	5.44	1.50	1.38
2	B	488	TYR	CA-C	5.44	1.60	1.52
2	B	1206	GLU	CD-OE1	5.44	1.35	1.25
6	H	118	PHE	CA-C	5.44	1.60	1.53
1	A	893	PHE	N-CA	-5.44	1.39	1.46
3	C	157	CYS	CB-SG	-5.44	1.63	1.81
9	K	58	PHE	CB-CG	5.44	1.63	1.50
1	A	391	LEU	CG-CD2	-5.43	1.34	1.52
2	B	266	ALA	CA-CB	5.43	1.62	1.53
2	B	1196	ILE	CA-CB	-5.43	1.45	1.54
7	I	47	GLU	CG-CD	5.43	1.65	1.52
1	A	70	CYS	CA-CB	5.43	1.62	1.53
2	B	381	MET	CG-SD	5.43	1.94	1.80
1	A	528	LEU	C-O	5.43	1.30	1.24
2	B	452	THR	CA-C	5.43	1.60	1.52
3	C	173	ALA	CA-CB	-5.43	1.44	1.53
3	C	253	LYS	N-CA	5.43	1.53	1.46
6	H	2	SER	CA-CB	5.43	1.64	1.53
1	A	782	ARG	CA-C	-5.43	1.45	1.52
3	C	60	ASP	CG-OD2	5.43	1.35	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	79	TRP	N-CA	-5.43	1.39	1.46
9	K	107	THR	CA-C	-5.43	1.46	1.52
1	A	591	PHE	CA-C	-5.42	1.46	1.52
1	A	1114	PRO	N-CA	-5.42	1.40	1.47
2	B	1027	ILE	C-N	-5.42	1.26	1.33
2	B	1211	ASN	CB-CG	-5.42	1.38	1.52
1	A	264	PHE	CE2-CZ	5.42	1.54	1.38
1	A	1064	VAL	C-O	-5.42	1.17	1.24
7	I	6	PHE	CD1-CE1	5.42	1.54	1.38
1	A	794	PRO	C-N	-5.42	1.26	1.33
7	I	73	ARG	C-O	-5.42	1.16	1.23
9	K	109	TRP	C-O	5.42	1.31	1.24
2	B	356	LEU	N-CA	-5.42	1.39	1.46
2	B	953	LEU	CA-C	-5.42	1.46	1.52
2	B	965	LYS	CD-CE	5.42	1.68	1.52
5	F	128	LYS	CG-CD	5.42	1.68	1.52
1	A	65	LEU	N-CA	5.42	1.53	1.46
2	B	288	ALA	CA-CB	5.42	1.62	1.53
2	B	301	ILE	CA-CB	-5.42	1.49	1.55
2	B	348	ARG	CD-NE	-5.42	1.38	1.46
2	B	754	SER	CA-CB	-5.42	1.44	1.53
8	J	63	TYR	CA-CB	5.42	1.62	1.53
1	A	1140	HIS	CB-CG	-5.42	1.42	1.50
2	B	741	CYS	CA-C	5.42	1.59	1.52
3	C	71	PRO	N-CA	-5.42	1.40	1.47
1	A	109	HIS	CA-CB	5.41	1.60	1.53
1	A	422	GLY	C-N	-5.41	1.26	1.33
3	C	96	SER	N-CA	-5.41	1.39	1.46
5	F	122	MET	C-O	-5.41	1.17	1.24
1	A	55	ASP	N-CA	5.41	1.53	1.46
1	A	1267	MET	N-CA	5.41	1.52	1.46
1	A	1136	SER	CB-OG	5.41	1.52	1.42
2	B	61	ASP	CG-OD1	5.41	1.35	1.25
6	H	23	VAL	N-CA	-5.41	1.39	1.46
3	C	199	LYS	C-O	-5.41	1.17	1.24
1	A	137	ALA	CA-CB	-5.41	1.45	1.53
1	A	203	SER	CA-CB	5.41	1.62	1.53
1	A	387	ARG	CD-NE	5.41	1.53	1.46
1	A	1365	TYR	CD2-CE2	5.41	1.54	1.38
2	B	363	HIS	C-O	-5.41	1.17	1.24
2	B	368	GLU	C-O	5.41	1.30	1.24
2	B	1220	ARG	N-CA	5.41	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	711	ARG	N-CA	-5.40	1.39	1.46
1	A	933	TYR	CE2-CZ	-5.40	1.25	1.38
2	B	597	MET	C-N	5.40	1.41	1.33
4	E	85	GLU	CA-CB	5.40	1.62	1.52
2	B	198	ASP	CA-C	-5.40	1.46	1.52
2	B	422	LYS	C-O	-5.40	1.17	1.24
1	A	1002	GLY	CA-C	5.40	1.59	1.51
2	B	598	GLU	CA-C	5.40	1.59	1.52
2	B	1193	GLN	CD-OE1	5.40	1.33	1.23
4	E	42	PHE	CE1-CZ	-5.40	1.22	1.38
5	F	123	LYS	CG-CD	5.40	1.68	1.52
4	E	67	GLU	C-N	5.40	1.40	1.33
9	K	51	LEU	CA-C	5.40	1.60	1.52
1	A	1063	MET	C-O	-5.39	1.16	1.23
2	B	365	THR	CB-CG2	-5.39	1.34	1.52
2	B	625	LYS	CD-CE	5.39	1.68	1.52
2	B	665	GLU	C-O	-5.39	1.17	1.24
4	E	88	VAL	N-CA	-5.39	1.39	1.46
1	A	451	HIS	CB-CG	-5.39	1.42	1.50
7	I	63	GLY	C-N	-5.39	1.25	1.33
1	A	129	LYS	CG-CD	5.39	1.68	1.52
1	A	1070	GLN	N-CA	-5.39	1.39	1.46
2	B	214	ALA	CA-CB	-5.39	1.44	1.53
9	K	75	ILE	CB-CG1	5.39	1.64	1.53
1	A	832	ALA	CA-C	5.39	1.59	1.52
1	A	969	GLN	C-N	-5.39	1.26	1.34
2	B	232	SER	CA-C	-5.39	1.46	1.53
2	B	273	LEU	C-N	5.39	1.40	1.33
2	B	345	LYS	CA-CB	-5.39	1.45	1.53
7	I	87	GLN	CB-CG	5.39	1.68	1.52
1	A	385	ILE	C-O	-5.39	1.17	1.24
1	A	1064	VAL	CA-CB	5.39	1.60	1.54
1	A	1072	ILE	C-O	-5.39	1.18	1.23
1	A	1129	GLU	CA-C	5.39	1.60	1.52
2	B	756	ILE	N-CA	5.39	1.52	1.46
2	B	934	LYS	CA-C	5.39	1.59	1.53
1	A	656	TRP	CE3-CZ3	5.38	1.54	1.38
1	A	840	ARG	N-CA	-5.38	1.39	1.46
1	A	1385	THR	C-O	5.38	1.34	1.23
2	B	50	SER	C-O	5.38	1.31	1.24
2	B	1189	ILE	N-CA	5.38	1.53	1.46
3	C	108	GLU	CA-C	5.38	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	209	TYR	CD1-CE1	5.38	1.54	1.38
7	I	34	TYR	CE2-CZ	-5.38	1.25	1.38
1	A	497	THR	CA-CB	-5.38	1.45	1.53
2	B	488	TYR	CG-CD2	-5.38	1.28	1.39
6	H	102	TYR	C-N	-5.38	1.26	1.33
1	A	143	LYS	CE-NZ	5.38	1.65	1.49
1	A	1133	LEU	N-CA	-5.38	1.39	1.46
1	A	556	TRP	C-O	5.38	1.30	1.23
3	C	219	PHE	CE1-CZ	-5.38	1.22	1.38
2	B	91	SER	CA-C	-5.38	1.46	1.52
2	B	250	PHE	CG-CD1	5.38	1.50	1.38
2	B	315	LYS	CA-C	5.38	1.59	1.52
2	B	730	ARG	CA-C	5.38	1.59	1.52
2	B	782	LEU	CB-CG	-5.38	1.42	1.53
1	A	416	ARG	C-N	-5.38	1.26	1.33
1	A	868	TYR	CE2-CZ	-5.38	1.25	1.38
8	J	57	ILE	CA-CB	-5.38	1.46	1.54
1	A	1242	VAL	CA-C	5.38	1.59	1.52
7	I	85	PHE	N-CA	5.38	1.52	1.45
9	K	50	LEU	CG-CD2	-5.38	1.34	1.52
1	A	17	VAL	C-O	-5.37	1.18	1.24
2	B	542	MET	C-O	5.37	1.31	1.24
3	C	11	ARG	NE-CZ	5.37	1.39	1.33
1	A	273	ASN	CB-CG	5.37	1.65	1.52
1	A	1234	GLU	CG-CD	5.37	1.65	1.52
2	B	249	ARG	CG-CD	5.37	1.68	1.52
2	B	311	LEU	CG-CD1	-5.37	1.34	1.52
2	B	1183	LYS	CG-CD	5.37	1.68	1.52
3	C	64	ALA	C-O	-5.37	1.17	1.24
1	A	1426	GLU	N-CA	-5.37	1.40	1.46
9	K	21	ILE	C-N	-5.37	1.26	1.33
9	K	90	ALA	CA-CB	-5.37	1.44	1.53
1	A	120	GLU	CD-OE1	5.37	1.35	1.25
2	B	798	TYR	N-CA	5.37	1.52	1.46
2	B	573	GLN	CD-OE1	5.36	1.33	1.23
1	A	859	SER	N-CA	-5.36	1.39	1.46
2	B	841	MET	SD-CE	-5.36	1.66	1.79
6	H	61	SER	CA-C	-5.36	1.45	1.52
1	A	1010	ALA	CA-CB	-5.36	1.44	1.53
2	B	465	ASN	CG-ND2	5.36	1.44	1.33
9	K	109	TRP	CA-C	5.36	1.59	1.52
2	B	1073	TYR	CA-C	-5.36	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	196	ASP	CG-OD2	5.36	1.35	1.25
1	A	527	THR	N-CA	-5.36	1.39	1.46
1	A	1134	ILE	C-N	-5.36	1.26	1.33
1	A	1140	HIS	CA-C	-5.36	1.45	1.52
2	B	626	ILE	N-CA	-5.36	1.40	1.46
1	A	144	THR	CB-OG1	-5.36	1.35	1.43
1	A	734	GLU	CG-CD	5.36	1.65	1.52
1	A	796	SER	C-O	-5.36	1.17	1.24
1	A	931	GLU	CG-CD	5.36	1.65	1.52
3	C	183	TRP	NE1-CE2	-5.36	1.31	1.37
4	E	25	ASP	N-CA	5.36	1.53	1.46
10	L	34	CYS	C-O	-5.35	1.16	1.24
1	A	43	GLU	C-N	5.35	1.41	1.33
2	B	186	GLU	C-O	5.35	1.30	1.24
9	K	58	PHE	C-O	5.35	1.29	1.23
1	A	659	HIS	CA-C	-5.35	1.45	1.52
2	B	200	GLY	C-N	-5.35	1.25	1.33
2	B	387	LEU	CA-C	5.35	1.59	1.52
2	B	957	ASN	C-O	5.35	1.30	1.24
1	A	941	LYS	C-N	-5.35	1.27	1.33
1	A	1210	GLY	C-N	5.35	1.41	1.33
2	B	279	ASP	CA-C	5.35	1.59	1.52
2	B	746	SER	CB-OG	-5.35	1.31	1.42
2	B	797	TYR	CG-CD2	-5.35	1.28	1.39
2	B	1055	ILE	C-O	-5.35	1.17	1.24
2	B	1103	ILE	CA-CB	5.35	1.61	1.54
1	A	346	ASP	CG-OD2	5.35	1.35	1.25
3	C	211	ASP	C-O	5.34	1.31	1.24
7	I	69	PRO	N-CA	-5.34	1.40	1.47
1	A	179	LEU	CG-CD2	-5.34	1.34	1.52
1	A	208	LEU	CG-CD1	-5.34	1.34	1.52
1	A	544	ASP	CG-OD1	5.34	1.35	1.25
1	A	719	VAL	C-O	-5.34	1.16	1.24
1	A	1187	GLN	CA-CB	5.34	1.64	1.53
2	B	762	ASN	CG-OD1	-5.34	1.13	1.23
1	A	1446	ASP	CG-OD2	5.34	1.35	1.25
4	E	121	MET	CA-C	5.34	1.60	1.52
7	I	79	HIS	N-CA	5.34	1.53	1.46
1	A	468	PHE	CE2-CZ	-5.34	1.22	1.38
2	B	1152	MET	C-O	-5.34	1.15	1.23
1	A	1324	PRO	N-CD	-5.34	1.40	1.47
2	B	490	SER	CA-CB	5.34	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1109	GLY	C-N	5.34	1.43	1.34
5	F	79	ARG	CD-NE	-5.34	1.38	1.46
1	A	324	SER	CA-C	5.33	1.64	1.52
1	A	945	GLU	CD-OE2	5.33	1.35	1.25
2	B	552	MET	N-CA	-5.33	1.41	1.46
1	A	198	GLU	CD-OE2	5.33	1.35	1.25
1	A	217	LYS	N-CA	5.33	1.52	1.46
2	B	278	GLN	CB-CG	-5.33	1.36	1.52
2	B	451	LYS	CD-CE	5.33	1.68	1.52
2	B	552	MET	CA-C	5.33	1.59	1.52
9	K	66	PRO	N-CD	-5.33	1.40	1.47
1	A	376	TYR	CG-CD1	-5.33	1.28	1.39
2	B	309	GLN	N-CA	5.33	1.53	1.46
2	B	864	LYS	C-O	5.33	1.30	1.24
2	B	1224	PHE	CB-CG	5.33	1.62	1.50
3	C	203	GLN	CB-CG	5.33	1.68	1.52
1	A	626	ASN	N-CA	5.33	1.53	1.46
2	B	911	ILE	CA-C	-5.33	1.46	1.52
2	B	1084	GLN	CD-OE1	5.33	1.33	1.23
1	A	490	HIS	CG-ND1	-5.33	1.32	1.38
2	B	31	TRP	CG-CD1	-5.33	1.23	1.36
2	B	459	TYR	CD2-CE2	5.33	1.54	1.38
3	C	126	GLY	CA-C	5.33	1.59	1.51
1	A	578	LEU	CG-CD1	-5.33	1.34	1.52
1	A	952	ALA	N-CA	-5.33	1.39	1.46
3	C	214	ASN	C-O	5.33	1.30	1.24
1	A	503	GLN	CD-OE1	5.32	1.33	1.23
2	B	638	PHE	CG-CD2	-5.32	1.27	1.38
3	C	149	LYS	C-N	5.32	1.41	1.33
10	L	27	LEU	CG-CD2	5.32	1.70	1.52
1	A	533	LYS	CA-C	-5.32	1.45	1.52
2	B	181	LEU	CA-CB	-5.32	1.44	1.53
4	E	116	ILE	CA-CB	5.32	1.62	1.54
7	I	23	ASN	CG-ND2	5.32	1.44	1.33
1	A	51	GLY	C-O	-5.32	1.16	1.23
1	A	376	TYR	C-O	-5.32	1.18	1.24
2	B	752	ALA	C-O	-5.32	1.17	1.24
2	B	968	VAL	CB-CG2	-5.32	1.34	1.52
3	C	267	GLN	CA-CB	5.32	1.62	1.53
7	I	21	GLU	C-N	-5.32	1.26	1.33
8	J	39	LEU	CA-CB	-5.32	1.45	1.53
2	B	203	PHE	CG-CD2	-5.32	1.27	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	76	ASP	CA-C	5.32	1.60	1.52
3	C	131	HIS	CA-CB	5.32	1.63	1.53
1	A	385	ILE	C-N	-5.32	1.27	1.33
2	B	178	ASN	C-O	-5.32	1.17	1.24
2	B	535	LEU	CG-CD1	-5.32	1.35	1.52
1	A	18	GLN	C-O	5.32	1.30	1.24
1	A	118	HIS	CA-CB	5.32	1.62	1.53
2	B	189	LEU	CA-C	5.32	1.59	1.52
2	B	946	ASN	N-CA	-5.32	1.39	1.46
5	F	123	LYS	CB-CG	5.32	1.68	1.52
9	K	91	CYS	CB-SG	-5.32	1.63	1.81
1	A	30	ILE	CB-CG2	5.31	1.70	1.52
1	A	1135	ARG	CA-C	5.31	1.59	1.52
2	B	875	GLU	CD-OE2	5.31	1.35	1.25
1	A	80	HIS	CB-CG	5.31	1.57	1.50
1	A	141	LEU	C-O	5.31	1.31	1.24
2	B	529	GLU	N-CA	5.31	1.52	1.45
5	F	123	LYS	C-O	5.31	1.30	1.24
6	H	105	GLU	CG-CD	5.31	1.65	1.52
10	L	59	ALA	C-O	-5.31	1.17	1.24
1	A	20	GLY	CA-C	-5.31	1.44	1.51
2	B	218	SER	C-N	-5.31	1.26	1.33
3	C	123	ASN	CB-CG	5.31	1.65	1.52
7	I	89	GLN	CG-CD	-5.31	1.38	1.52
1	A	218	ASP	CG-OD1	5.31	1.35	1.25
3	C	135	GLN	CA-CB	-5.31	1.45	1.54
4	E	11	ARG	C-N	5.31	1.40	1.33
1	A	374	LEU	CA-C	-5.31	1.46	1.52
1	A	423	ASP	CG-OD2	5.31	1.35	1.25
1	A	620	LYS	CA-CB	5.31	1.61	1.53
4	E	2	ASP	C-O	5.31	1.30	1.24
4	E	88	VAL	CA-C	5.31	1.59	1.52
1	A	390	GLN	CB-CG	5.31	1.68	1.52
1	A	555	ASP	CG-OD1	5.31	1.35	1.25
1	A	1422	ARG	CZ-NH1	5.31	1.40	1.32
2	B	650	GLU	CD-OE1	5.31	1.35	1.25
2	B	697	GLU	CD-OE2	5.31	1.35	1.25
2	B	899	ILE	CB-CG1	-5.31	1.42	1.53
2	B	941	LEU	N-CA	-5.31	1.39	1.46
1	A	863	VAL	CB-CG2	5.30	1.70	1.52
2	B	350	GLN	CD-OE1	5.30	1.33	1.23
2	B	806	THR	N-CA	5.30	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	87	LYS	CG-CD	5.30	1.68	1.52
1	A	223	GLY	C-O	5.30	1.31	1.24
5	F	84	TYR	CA-CB	-5.30	1.44	1.53
8	J	18	TRP	NE1-CE2	-5.30	1.31	1.37
2	B	194	GLU	C-O	-5.30	1.17	1.24
4	E	137	GLU	CA-CB	5.30	1.61	1.53
2	B	993	THR	CB-OG1	-5.30	1.35	1.43
1	A	69	THR	C-O	5.30	1.30	1.24
10	L	47	ARG	CB-CG	5.30	1.68	1.52
1	A	745	GLN	CA-C	5.29	1.59	1.52
2	B	1207	LEU	CA-C	5.29	1.59	1.52
4	E	33	GLU	CA-CB	5.29	1.63	1.53
7	I	99	LEU	CG-CD1	-5.29	1.35	1.52
2	B	249	ARG	N-CA	5.29	1.53	1.46
2	B	912	ILE	C-N	5.29	1.38	1.33
1	A	28	ARG	CZ-NH1	5.29	1.40	1.32
2	B	452	THR	N-CA	5.29	1.53	1.46
2	B	851	PHE	C-O	-5.29	1.15	1.24
3	C	211	ASP	CA-CB	5.29	1.61	1.52
9	K	61	TYR	CE2-CZ	-5.29	1.25	1.38
1	A	201	VAL	C-N	5.29	1.41	1.33
1	A	483	ASP	N-CA	5.29	1.51	1.46
1	A	1009	ASN	CA-CB	5.29	1.61	1.53
2	B	1048	THR	C-O	-5.29	1.17	1.24
1	A	98	LYS	C-O	5.29	1.30	1.24
1	A	117	GLU	N-CA	5.29	1.52	1.46
1	A	145	LYS	CA-C	-5.29	1.46	1.52
1	A	459	ARG	CA-C	5.29	1.59	1.52
3	C	50	GLU	CD-OE1	5.29	1.35	1.25
4	E	46	TYR	CD2-CE2	5.29	1.54	1.38
1	A	897	TYR	N-CA	5.29	1.52	1.46
3	C	63	ILE	C-N	5.29	1.41	1.34
4	E	109	ILE	CB-CG2	-5.28	1.35	1.52
8	J	63	TYR	N-CA	5.28	1.51	1.45
3	C	24	ASN	C-O	5.28	1.30	1.23
3	C	250	THR	CA-C	5.28	1.59	1.52
3	C	185	LYS	CB-CG	5.28	1.68	1.52
4	E	131	THR	C-O	-5.28	1.17	1.23
7	I	29	CYS	C-N	5.28	1.40	1.33
10	L	54	ARG	CB-CG	5.28	1.68	1.52
2	B	198	ASP	C-N	-5.28	1.25	1.33
2	B	1069	PHE	CE2-CZ	-5.28	1.22	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	207	ARG	CG-CD	5.28	1.68	1.52
1	A	754	SER	CA-C	5.28	1.59	1.52
2	B	620	ARG	C-O	5.28	1.30	1.24
1	A	702	LEU	CG-CD1	5.28	1.70	1.52
1	A	982	THR	N-CA	-5.28	1.38	1.45
6	H	16	ASP	N-CA	5.28	1.54	1.46
1	A	728	LYS	CA-CB	5.27	1.61	1.53
1	A	786	HIS	CA-CB	-5.27	1.44	1.53
1	A	866	PHE	N-CA	5.27	1.53	1.46
1	A	909	ASP	CA-C	5.27	1.59	1.52
2	B	167	ILE	C-O	5.27	1.30	1.24
2	B	975	GLN	C-N	-5.27	1.27	1.33
4	E	6	GLU	C-O	-5.27	1.17	1.24
4	E	114	ASN	CB-CG	-5.27	1.38	1.52
2	B	595	ARG	CA-C	-5.27	1.46	1.52
2	B	1224	PHE	CA-C	5.27	1.64	1.52
4	E	3	GLN	CB-CG	5.27	1.68	1.52
1	A	571	LEU	CG-CD1	-5.27	1.35	1.52
1	A	793	SER	C-O	-5.27	1.17	1.23
1	A	979	SER	CB-OG	5.27	1.52	1.42
2	B	389	ALA	C-O	-5.27	1.17	1.24
2	B	1014	PRO	N-CA	-5.27	1.40	1.47
6	H	19	ARG	CA-CB	5.27	1.62	1.53
1	A	144	THR	N-CA	5.27	1.52	1.46
1	A	1292	PRO	CA-C	5.27	1.58	1.52
7	I	113	ASP	C-O	-5.27	1.17	1.23
5	F	123	LYS	CE-NZ	5.26	1.65	1.49
6	H	89	LEU	CA-C	5.26	1.59	1.52
7	I	7	CYS	N-CA	5.26	1.53	1.46
7	I	51	ASN	CB-CG	5.26	1.65	1.52
10	L	67	PHE	CA-C	-5.26	1.46	1.52
1	A	16	GLU	N-CA	5.26	1.52	1.46
1	A	138	ILE	CA-C	5.26	1.59	1.52
1	A	777	PHE	CD2-CE2	5.26	1.54	1.38
2	B	766	ARG	CA-C	-5.26	1.45	1.52
7	I	74	GLU	CG-CD	5.26	1.65	1.52
1	A	1062	GLU	CD-OE1	-5.26	1.15	1.25
1	A	1426	GLU	CA-C	5.26	1.59	1.52
2	B	935	ARG	CG-CD	5.26	1.68	1.52
2	B	807	ARG	CG-CD	5.26	1.68	1.52
4	E	198	ILE	C-O	-5.26	1.18	1.24
4	E	204	THR	C-N	5.26	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1242	VAL	CA-CB	-5.26	1.47	1.54
1	A	1446	ASP	N-CA	5.26	1.53	1.46
2	B	617	ARG	CA-CB	-5.26	1.46	1.53
2	B	895	ASP	CG-OD2	5.26	1.35	1.25
6	H	141	TYR	CA-CB	-5.26	1.44	1.53
1	A	660	ASN	N-CA	-5.25	1.39	1.46
1	A	1033	GLN	C-O	-5.25	1.17	1.24
2	B	1026	LEU	CA-C	5.25	1.59	1.52
1	A	214	ILE	C-N	5.25	1.40	1.33
3	C	82	TYR	CZ-OH	5.25	1.49	1.38
3	C	167	HIS	C-N	-5.25	1.26	1.33
3	C	191	TYR	N-CA	-5.25	1.39	1.46
9	K	94	ILE	C-O	-5.25	1.18	1.24
1	A	105	CYS	C-O	-5.25	1.17	1.23
2	B	884	ARG	N-CA	5.25	1.52	1.46
4	E	98	ILE	CB-CG1	5.25	1.64	1.53
1	A	237	THR	CA-C	-5.25	1.45	1.52
2	B	1043	ASP	CA-CB	5.25	1.59	1.52
1	A	205	GLU	CA-CB	5.25	1.61	1.53
1	A	947	PHE	C-O	-5.25	1.16	1.23
1	A	1334	ASP	C-N	-5.25	1.27	1.33
2	B	597	MET	C-O	-5.25	1.18	1.24
6	H	120	GLY	N-CA	5.25	1.53	1.45
7	I	79	HIS	CA-C	5.25	1.59	1.52
1	A	991	LYS	N-CA	5.25	1.52	1.46
1	A	999	VAL	CB-CG1	-5.25	1.35	1.52
6	H	53	ASP	N-CA	5.25	1.52	1.46
1	A	1176	LEU	CG-CD1	5.25	1.69	1.52
2	B	70	ILE	CB-CG2	5.25	1.69	1.52
2	B	312	GLU	CD-OE2	5.25	1.35	1.25
2	B	577	ALA	N-CA	5.25	1.52	1.46
2	B	1013	ASN	CG-ND2	-5.25	1.22	1.33
2	B	104	GLU	C-O	5.24	1.30	1.23
8	J	22	LEU	CG-CD1	-5.24	1.35	1.52
3	C	249	ASP	C-O	5.24	1.30	1.24
1	A	734	GLU	C-N	-5.24	1.27	1.33
1	A	1162	VAL	N-CA	-5.24	1.39	1.46
2	B	616	ILE	CB-CG1	-5.24	1.43	1.53
2	B	1215	ARG	CG-CD	5.24	1.68	1.52
3	C	185	LYS	CG-CD	5.24	1.68	1.52
3	C	215	GLU	N-CA	5.24	1.52	1.46
3	C	257	SER	C-O	-5.24	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	922	ASP	C-N	-5.24	1.26	1.33
1	A	1422	ARG	CA-C	-5.24	1.45	1.52
2	B	538	ASN	CB-CG	-5.24	1.39	1.52
3	C	207	CYS	CA-CB	5.24	1.61	1.53
3	C	220	ASP	CG-OD1	5.24	1.35	1.25
9	K	100	ALA	CA-CB	-5.24	1.45	1.53
1	A	935	GLN	CD-OE1	-5.24	1.13	1.23
2	B	124	TYR	C-N	5.24	1.40	1.33
2	B	274	PRO	CA-CB	5.24	1.60	1.53
2	B	781	PHE	N-CA	-5.24	1.39	1.46
4	E	146	HIS	C-N	-5.24	1.25	1.33
4	E	165	LEU	C-O	5.24	1.30	1.24
2	B	862	GLN	CG-CD	5.23	1.65	1.52
3	C	65	HIS	CB-CG	5.23	1.57	1.50
3	C	123	ASN	N-CA	-5.23	1.40	1.46
3	C	149	LYS	N-CA	-5.23	1.39	1.46
1	A	519	PRO	N-CA	-5.23	1.40	1.47
3	C	29	MET	CA-CB	-5.23	1.45	1.53
3	C	58	LEU	C-O	-5.23	1.17	1.24
1	A	864	ILE	CA-C	-5.23	1.47	1.52
1	A	1242	VAL	C-O	5.23	1.30	1.24
1	A	1298	TYR	CG-CD1	-5.23	1.28	1.39
3	C	133	ILE	CA-CB	5.23	1.61	1.54
2	B	875	GLU	CB-CG	5.23	1.68	1.52
2	B	1031	LEU	CA-CB	-5.22	1.45	1.53
9	K	20	LYS	N-CA	5.22	1.52	1.46
1	A	572	TRP	CE2-CZ2	-5.22	1.28	1.39
1	A	1214	GLU	CB-CG	5.22	1.68	1.52
2	B	37	PHE	CE2-CZ	-5.22	1.23	1.38
2	B	131	ASP	CA-CB	5.22	1.60	1.52
2	B	279	ASP	CB-CG	5.22	1.65	1.52
4	E	29	PHE	CA-CB	5.22	1.59	1.53
5	F	108	PHE	C-N	-5.22	1.26	1.33
1	A	1335	ILE	CG1-CD1	-5.22	1.31	1.51
2	B	951	GLN	CB-CG	5.22	1.68	1.52
1	A	230	ARG	CZ-NH1	5.22	1.40	1.32
2	B	913	GLY	C-O	-5.22	1.18	1.24
2	B	1040	ASN	C-O	-5.22	1.17	1.23
1	A	1119	TYR	CG-CD2	-5.22	1.28	1.39
7	I	11	ASN	CG-ND2	-5.22	1.22	1.33
8	J	24	LEU	C-N	-5.22	1.26	1.33
8	J	37	SER	CA-CB	-5.22	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1374	VAL	CA-CB	-5.21	1.48	1.54
2	B	373	ARG	CZ-NH1	5.21	1.40	1.32
2	B	1005	GLY	C-O	5.21	1.30	1.23
1	A	1012	ARG	CG-CD	5.21	1.68	1.52
2	B	1061	GLU	CD-OE1	5.21	1.35	1.25
7	I	69	PRO	N-CD	-5.21	1.40	1.47
1	A	705	LYS	CE-NZ	5.21	1.65	1.49
1	A	1372	VAL	CA-CB	-5.21	1.47	1.54
2	B	1091	TYR	CD2-CE2	5.21	1.54	1.38
3	C	114	TYR	CE2-CZ	-5.21	1.25	1.38
1	A	149	GLU	N-CA	-5.21	1.39	1.46
9	K	35	PHE	CA-C	-5.21	1.46	1.52
1	A	982	THR	C-N	5.21	1.40	1.33
4	E	19	VAL	CA-C	5.21	1.59	1.52
4	E	158	SER	CA-C	5.21	1.59	1.52
1	A	926	GLN	CA-C	-5.21	1.45	1.52
1	A	1189	SER	N-CA	5.21	1.53	1.46
6	H	123	MET	SD-CE	-5.21	1.66	1.79
8	J	6	ARG	N-CA	5.21	1.52	1.45
1	A	126	LEU	C-O	5.21	1.30	1.24
2	B	1094	ARG	CZ-NH1	-5.21	1.25	1.32
1	A	128	ILE	CA-C	-5.20	1.46	1.52
1	A	487	MET	N-CA	-5.20	1.39	1.45
1	A	739	ASP	CB-CG	5.20	1.65	1.52
1	A	1056	SER	N-CA	5.20	1.52	1.46
2	B	282	ILE	N-CA	-5.20	1.39	1.46
4	E	23	VAL	CA-CB	-5.20	1.48	1.54
4	E	35	VAL	CA-CB	-5.20	1.48	1.54
8	J	43	ARG	NE-CZ	-5.20	1.27	1.33
2	B	880	THR	CA-C	5.20	1.61	1.53
2	B	344	LYS	C-O	5.20	1.30	1.23
3	C	16	ASP	CG-OD1	-5.20	1.15	1.25
4	E	162	ARG	CZ-NH2	5.20	1.40	1.33
8	J	9	SER	C-O	-5.20	1.17	1.24
1	A	848	ILE	CG1-CD1	-5.20	1.31	1.51
2	B	94	LYS	CA-C	5.20	1.59	1.52
2	B	289	LEU	CA-CB	-5.20	1.44	1.53
2	B	1062	HIS	CB-CG	-5.20	1.42	1.50
1	A	1050	GLU	N-CA	-5.20	1.40	1.46
1	A	1117	THR	CA-CB	-5.20	1.46	1.53
2	B	295	GLY	C-O	5.20	1.30	1.23
9	K	46	ILE	C-O	-5.20	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	370	PHE	CE2-CZ	5.20	1.54	1.38
2	B	657	HIS	CA-CB	-5.20	1.45	1.53
2	B	700	SER	CA-CB	-5.20	1.45	1.53
2	B	821	GLN	N-CA	-5.20	1.39	1.45
9	K	40	HIS	CG-ND1	-5.20	1.32	1.38
1	A	1269	GLU	C-N	-5.19	1.27	1.33
3	C	192	TRP	N-CA	-5.19	1.39	1.46
5	F	84	TYR	CE2-CZ	5.19	1.50	1.38
8	J	6	ARG	CZ-NH1	-5.19	1.25	1.32
1	A	504	LEU	CG-CD1	-5.19	1.35	1.52
8	J	59	LYS	CE-NZ	-5.19	1.33	1.49
2	B	277	LYS	N-CA	-5.19	1.39	1.46
2	B	586	TRP	C-N	-5.19	1.25	1.33
3	C	78	GLU	C-N	-5.19	1.26	1.33
3	C	141	GLY	N-CA	5.19	1.52	1.45
5	F	75	PRO	CA-C	-5.19	1.46	1.52
1	A	493	GLN	C-O	-5.19	1.16	1.24
7	I	120	GLN	CG-CD	5.19	1.65	1.52
1	A	17	VAL	CA-C	-5.19	1.45	1.52
1	A	172	PRO	CG-CD	5.19	1.68	1.50
1	A	325	ILE	N-CA	5.19	1.53	1.46
1	A	352	VAL	C-O	5.19	1.29	1.24
1	A	615	GLY	CA-C	5.19	1.58	1.52
1	A	716	ASP	CG-OD1	5.19	1.35	1.25
3	C	3	GLU	CA-CB	-5.19	1.43	1.53
4	E	148	GLU	C-O	-5.19	1.17	1.24
7	I	28	GLU	N-CA	-5.19	1.40	1.45
1	A	221	SER	C-N	5.19	1.41	1.33
2	B	513	GLN	CD-NE2	5.19	1.44	1.33
8	J	58	GLU	N-CA	5.19	1.52	1.46
1	A	755	PHE	N-CA	-5.18	1.40	1.46
2	B	61	ASP	CA-C	-5.18	1.45	1.52
2	B	198	ASP	CG-OD2	-5.18	1.15	1.25
9	K	95	ILE	C-N	5.18	1.41	1.33
1	A	145	LYS	CA-CB	5.18	1.59	1.53
2	B	30	SER	CA-C	-5.18	1.46	1.52
2	B	57	TYR	CE1-CZ	-5.18	1.25	1.38
2	B	409	ALA	CA-C	-5.18	1.45	1.52
1	A	351	THR	CA-CB	5.18	1.61	1.53
2	B	414	ALA	C-O	-5.18	1.16	1.23
1	A	383	TYR	CA-C	5.18	1.59	1.52
1	A	743	VAL	CA-CB	-5.18	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1332	PHE	CB-CG	-5.18	1.38	1.50
2	B	952	VAL	CA-CB	-5.18	1.47	1.54
1	A	767	GLN	CB-CG	-5.18	1.36	1.52
2	B	269	ILE	CB-CG2	-5.18	1.35	1.52
1	A	698	GLN	CA-C	-5.18	1.45	1.52
1	A	732	LEU	CG-CD1	5.18	1.69	1.52
1	A	773	LYS	CB-CG	-5.18	1.36	1.52
1	A	1051	ALA	C-O	-5.18	1.18	1.24
8	J	14	VAL	CA-C	5.18	1.59	1.52
1	A	863	VAL	CA-CB	-5.17	1.47	1.54
1	A	906	HIS	C-O	-5.17	1.16	1.24
1	A	1265	ASN	C-O	-5.17	1.18	1.24
2	B	968	VAL	CB-CG1	5.17	1.69	1.52
2	B	1180	PHE	CA-CB	5.17	1.61	1.53
4	E	31	THR	CB-CG2	5.17	1.69	1.52
2	B	338	GLY	C-O	-5.17	1.17	1.23
7	I	11	ASN	CG-OD1	-5.17	1.13	1.23
1	A	445	ASN	N-CA	-5.17	1.40	1.46
5	F	154	ASP	CA-C	5.17	1.63	1.52
3	C	95	CYS	N-CA	5.17	1.52	1.46
4	E	18	THR	CA-C	-5.17	1.46	1.52
4	E	21	GLU	N-CA	5.17	1.52	1.46
1	A	536	LEU	CA-CB	-5.17	1.45	1.53
1	A	1225	PHE	CE1-CZ	5.17	1.54	1.38
6	H	19	ARG	CD-NE	5.17	1.53	1.46
7	I	15	TYR	CA-C	5.17	1.57	1.52
7	I	78	CYS	C-O	-5.17	1.17	1.24
9	K	54	ARG	C-O	-5.17	1.17	1.24
2	B	624	LEU	CG-CD1	-5.17	1.35	1.52
2	B	1129	ARG	CZ-NH2	5.17	1.40	1.33
10	L	63	ARG	CA-CB	5.17	1.61	1.53
1	A	912	LEU	CA-CB	-5.17	1.44	1.53
7	I	43	VAL	CA-C	-5.17	1.45	1.52
1	A	519	PRO	C-O	-5.16	1.17	1.23
1	A	546	VAL	C-O	-5.16	1.18	1.24
1	A	848	ILE	N-CA	-5.16	1.40	1.46
1	A	910	PRO	CA-CB	-5.16	1.46	1.53
6	H	84	ALA	C-O	5.16	1.30	1.24
4	E	99	HIS	CB-CG	5.16	1.57	1.50
2	B	255	GLN	CA-CB	-5.16	1.42	1.53
2	B	429	PHE	CA-C	5.16	1.64	1.52
2	B	905	VAL	CA-C	-5.16	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	67	THR	N-CA	5.16	1.52	1.46
2	B	411	PRO	N-CA	-5.16	1.40	1.47
3	C	197	SER	CB-OG	5.16	1.52	1.42
7	I	48	LEU	CA-CB	-5.16	1.45	1.53
1	A	1355	VAL	N-CA	-5.16	1.40	1.46
2	B	250	PHE	CE1-CZ	5.16	1.54	1.38
4	E	7	ARG	CG-CD	5.16	1.68	1.52
2	B	99	LYS	CD-CE	5.16	1.68	1.52
8	J	4	PRO	C-N	-5.16	1.27	1.33
9	K	12	LEU	CG-CD1	5.16	1.69	1.52
9	K	39	ASP	CB-CG	5.16	1.65	1.52
1	A	1200	ALA	CA-C	5.15	1.59	1.52
1	A	147	VAL	N-CA	-5.15	1.40	1.46
1	A	482	PHE	CG-CD2	-5.15	1.28	1.38
1	A	607	ILE	C-O	5.15	1.29	1.23
1	A	1293	SER	CB-OG	-5.15	1.31	1.42
2	B	1218	THR	CA-C	-5.15	1.45	1.52
1	A	538	ASP	CA-C	-5.15	1.45	1.52
2	B	408	LEU	C-O	-5.15	1.16	1.24
2	B	611	PRO	N-CA	-5.15	1.40	1.47
1	A	77	CYS	C-O	5.15	1.30	1.24
1	A	97	ALA	CA-C	-5.15	1.45	1.52
2	B	1176	ASN	CG-OD1	5.15	1.33	1.23
10	L	33	GLU	C-N	5.15	1.41	1.33
2	B	814	PHE	C-O	5.15	1.30	1.24
2	B	875	GLU	CD-OE1	5.15	1.35	1.25
3	C	123	ASN	C-N	-5.15	1.27	1.33
1	A	923	LEU	CG-CD1	-5.14	1.35	1.52
1	A	1112	LYS	CG-CD	5.14	1.67	1.52
1	A	1327	ILE	N-CA	-5.14	1.40	1.46
2	B	368	GLU	CA-C	5.14	1.59	1.52
2	B	711	GLU	CG-CD	5.14	1.65	1.52
2	B	1151	LEU	C-O	-5.14	1.17	1.24
6	H	123	MET	CA-C	-5.14	1.46	1.52
1	A	1133	LEU	CG-CD2	5.14	1.69	1.52
2	B	233	PRO	CB-CG	5.14	1.75	1.49
2	B	984	HIS	CA-CB	5.14	1.60	1.53
4	E	153	HIS	N-CA	-5.14	1.39	1.46
6	H	46	LEU	CA-C	5.14	1.59	1.52
10	L	27	LEU	N-CA	5.14	1.52	1.46
1	A	180	LYS	CA-CB	5.14	1.61	1.53
2	B	109	THR	CB-OG1	5.14	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	382	ILE	N-CA	-5.14	1.39	1.46
2	B	686	ASN	CG-OD1	5.14	1.33	1.23
2	B	797	TYR	CD2-CE2	5.14	1.54	1.38
2	B	522	VAL	CA-CB	-5.14	1.48	1.54
2	B	1084	GLN	CA-C	-5.14	1.46	1.53
7	I	86	PHE	N-CA	-5.14	1.39	1.45
1	A	824	LEU	C-O	-5.14	1.18	1.24
1	A	1361	SER	N-CA	5.14	1.52	1.45
2	B	291	ILE	CA-CB	-5.14	1.47	1.53
2	B	328	GLU	N-CA	5.14	1.52	1.46
2	B	393	LYS	CD-CE	5.14	1.67	1.52
3	C	138	GLU	CD-OE2	5.14	1.35	1.25
3	C	163	ILE	N-CA	5.14	1.51	1.46
1	A	1265	ASN	C-N	-5.13	1.27	1.33
2	B	892	LYS	CA-C	-5.13	1.46	1.52
8	J	49	MET	N-CA	5.13	1.52	1.46
2	B	680	THR	CB-CG2	-5.13	1.35	1.52
6	H	129	TYR	CG-CD2	5.13	1.50	1.39
1	A	682	THR	CA-C	-5.13	1.45	1.52
8	J	48	ARG	CG-CD	-5.13	1.37	1.52
1	A	137	ALA	CA-C	5.13	1.59	1.52
1	A	744	LYS	CD-CE	5.13	1.67	1.52
2	B	280	ILE	CA-CB	-5.13	1.48	1.54
5	F	81	THR	C-O	-5.13	1.16	1.23
1	A	799	PHE	C-O	-5.13	1.17	1.24
1	A	885	THR	CA-C	5.13	1.59	1.52
1	A	1338	VAL	N-CA	-5.13	1.39	1.46
2	B	217	ARG	CZ-NH2	5.13	1.40	1.33
2	B	1020	ARG	CG-CD	-5.13	1.37	1.52
7	I	86	PHE	C-O	-5.13	1.17	1.23
1	A	1206	ASP	C-O	5.12	1.30	1.23
1	A	1290	LYS	C-O	5.12	1.30	1.24
5	F	80	ALA	C-N	-5.12	1.26	1.33
1	A	33	ALA	CA-C	5.12	1.59	1.52
1	A	297	GLN	CA-C	-5.12	1.45	1.52
2	B	323	VAL	CB-CG1	5.12	1.69	1.52
6	H	45	GLU	CD-OE2	5.12	1.35	1.25
1	A	1379	GLY	N-CA	-5.12	1.36	1.44
2	B	870	ILE	CB-CG2	5.12	1.69	1.52
5	F	73	ALA	CA-C	-5.12	1.46	1.52
6	H	52	GLN	C-O	-5.12	1.17	1.24
1	A	575	LYS	CG-CD	-5.12	1.37	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	K	106	GLU	CA-C	5.12	1.59	1.52
1	A	710	LEU	C-N	-5.12	1.26	1.34
3	C	105	GLY	C-O	5.12	1.30	1.23
4	E	184	VAL	CB-CG1	-5.12	1.35	1.52
6	H	140	ALA	C-N	5.12	1.40	1.33
7	I	104	LEU	CA-C	-5.12	1.45	1.52
2	B	326	ASP	CG-OD2	5.12	1.35	1.25
2	B	915	THR	N-CA	5.12	1.52	1.45
1	A	724	GLU	N-CA	-5.12	1.39	1.46
4	E	196	VAL	CB-CG1	-5.12	1.35	1.52
7	I	11	ASN	CB-CG	-5.12	1.39	1.52
1	A	779	PHE	CA-CB	-5.11	1.45	1.53
1	A	1228	TRP	C-O	5.11	1.29	1.23
2	B	604	ARG	CB-CG	5.11	1.67	1.52
3	C	84	ARG	CD-NE	5.11	1.53	1.46
3	C	191	TYR	CA-CB	5.11	1.60	1.53
7	I	42	LEU	CA-C	-5.11	1.46	1.52
1	A	1263	ILE	N-CA	5.11	1.52	1.46
2	B	172	ILE	CA-CB	-5.11	1.48	1.54
4	E	49	SER	N-CA	5.11	1.53	1.46
5	F	131	PRO	CA-C	-5.11	1.48	1.52
9	K	81	TYR	CA-CB	5.11	1.61	1.53
1	A	280	GLU	C-O	-5.11	1.17	1.24
2	B	236	HIS	CA-C	-5.11	1.46	1.52
1	A	303	TYR	CG-CD2	-5.11	1.28	1.39
2	B	18	PHE	C-O	5.11	1.33	1.23
3	C	252	GLN	CA-CB	5.11	1.61	1.53
1	A	825	ILE	C-O	-5.11	1.18	1.24
1	A	1145	SER	C-N	-5.11	1.27	1.34
2	B	1172	ILE	CA-C	5.11	1.58	1.53
2	B	1179	GLN	N-CA	5.11	1.52	1.46
9	K	26	LYS	CE-NZ	5.11	1.64	1.49
9	K	67	PHE	N-CA	-5.11	1.39	1.46
1	A	84	ILE	CG1-CD1	-5.10	1.31	1.51
1	A	1161	THR	CB-OG1	-5.10	1.35	1.43
2	B	682	SER	CA-CB	-5.10	1.45	1.53
2	B	60	GLN	N-CA	-5.10	1.40	1.46
1	A	227	VAL	CA-CB	5.10	1.60	1.54
2	B	595	ARG	N-CA	5.10	1.52	1.46
4	E	8	ASN	CG-ND2	5.10	1.44	1.33
4	E	102	GLU	CD-OE1	5.10	1.35	1.25
6	H	40	LEU	N-CA	-5.10	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	110	ASP	CB-CG	5.10	1.64	1.52
1	A	208	LEU	CA-CB	-5.10	1.44	1.53
1	A	679	ILE	CB-CG1	-5.10	1.43	1.53
2	B	401	PHE	CA-C	-5.10	1.45	1.52
5	F	148	VAL	CA-CB	-5.10	1.48	1.54
1	A	907	THR	C-O	-5.10	1.18	1.23
3	C	17	ASN	CG-ND2	5.10	1.44	1.33
1	A	1425	SER	N-CA	5.09	1.52	1.46
2	B	1102	LYS	CG-CD	5.09	1.67	1.52
2	B	1224	PHE	CE1-CZ	5.09	1.53	1.38
4	E	194	GLU	C-O	-5.09	1.17	1.23
6	H	143	LEU	C-O	5.09	1.30	1.23
1	A	133	LYS	CG-CD	5.09	1.67	1.52
1	A	467	THR	C-O	-5.09	1.17	1.23
1	A	478	TYR	CG-CD1	-5.09	1.28	1.39
1	A	962	ARG	CD-NE	-5.09	1.39	1.46
1	A	1447	GLU	C-N	5.09	1.40	1.33
4	E	107	THR	CA-C	5.09	1.58	1.52
6	H	112	ILE	CA-CB	5.09	1.61	1.54
1	A	829	VAL	CA-C	5.09	1.59	1.52
1	A	1351	GLU	C-O	-5.09	1.18	1.24
2	B	108	VAL	CB-CG2	5.09	1.69	1.52
4	E	61	GLN	CA-C	-5.09	1.46	1.52
1	A	747	VAL	C-O	-5.09	1.18	1.24
1	A	1303	GLU	CG-CD	5.09	1.64	1.52
1	A	1362	TYR	CE1-CZ	-5.09	1.26	1.38
5	F	140	ASP	CA-CB	5.09	1.62	1.53
1	A	1376	THR	N-CA	5.09	1.52	1.45
7	I	20	LYS	CE-NZ	5.09	1.64	1.49
2	B	406	LEU	C-O	5.09	1.30	1.24
2	B	868	MET	CB-CG	5.09	1.67	1.52
2	B	883	LEU	CG-CD1	5.09	1.69	1.52
2	B	1044	ALA	CA-C	5.09	1.59	1.52
10	L	50	ASP	C-N	5.09	1.40	1.33
1	A	155	GLU	CD-OE2	5.08	1.35	1.25
6	H	140	ALA	CA-CB	-5.08	1.45	1.53
10	L	38	LEU	CG-CD2	5.08	1.69	1.52
3	C	54	ASN	C-N	-5.08	1.26	1.33
4	E	212	ARG	CG-CD	5.08	1.67	1.52
5	F	111	LEU	C-O	5.08	1.29	1.23
2	B	1026	LEU	CB-CG	-5.08	1.43	1.53
1	A	1419	ASP	CA-CB	5.08	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	761	HIS	N-CA	-5.08	1.40	1.46
3	C	180	TYR	CD1-CE1	5.08	1.53	1.38
4	E	96	PHE	CA-CB	5.08	1.61	1.53
1	A	188	ASP	CB-CG	5.08	1.64	1.52
2	B	513	GLN	CG-CD	-5.08	1.39	1.52
2	B	862	GLN	CA-C	-5.08	1.46	1.53
2	B	865	LYS	C-O	5.08	1.30	1.24
1	A	244	PRO	C-N	5.08	1.41	1.33
1	A	393	ARG	CD-NE	5.08	1.53	1.46
1	A	1272	THR	CA-CB	5.08	1.60	1.53
1	A	1375	MET	CA-CB	5.08	1.62	1.53
5	F	136	ARG	C-N	5.08	1.40	1.33
10	L	29	TYR	CG-CD2	-5.08	1.28	1.39
1	A	536	LEU	C-O	5.08	1.31	1.23
1	A	880	LYS	CG-CD	5.08	1.67	1.52
3	C	86	CYS	CB-SG	5.08	1.98	1.81
1	A	268	ASP	CA-C	5.07	1.59	1.52
2	B	939	THR	CA-CB	-5.07	1.46	1.53
2	B	1009	ASP	C-N	-5.07	1.27	1.33
4	E	157	SER	CA-CB	5.07	1.62	1.53
8	J	63	TYR	C-O	-5.07	1.17	1.23
2	B	104	GLU	N-CA	5.07	1.52	1.45
1	A	1166	ASP	C-O	5.07	1.30	1.24
1	A	1337	GLU	CD-OE2	5.07	1.34	1.25
2	B	250	PHE	CD2-CE2	5.07	1.53	1.38
2	B	562	GLY	CA-C	-5.07	1.44	1.51
1	A	153	PRO	C-O	5.07	1.29	1.23
1	A	184	SER	C-O	-5.07	1.17	1.23
1	A	958	VAL	CB-CG1	-5.07	1.35	1.52
1	A	1032	LEU	CG-CD1	-5.07	1.35	1.52
1	A	1362	TYR	N-CA	5.07	1.52	1.46
2	B	455	SER	CA-CB	5.07	1.61	1.53
3	C	133	ILE	C-N	5.07	1.39	1.33
3	C	170	TRP	CZ3-CH2	-5.07	1.27	1.40
9	K	20	LYS	CD-CE	5.07	1.67	1.52
1	A	279	LEU	C-N	-5.07	1.27	1.34
1	A	552	TRP	N-CA	5.07	1.52	1.46
2	B	794	ASN	CG-OD1	5.07	1.33	1.23
2	B	909	ASP	CG-OD1	-5.07	1.15	1.25
2	B	1224	PHE	CD1-CE1	5.07	1.53	1.38
2	B	616	ILE	CA-C	-5.07	1.46	1.52
2	B	833	TYR	CG-CD2	-5.07	1.28	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	14	ARG	CA-CB	-5.07	1.45	1.53
2	B	287	ARG	NE-CZ	-5.06	1.27	1.33
2	B	1141	HIS	CA-C	5.06	1.59	1.52
4	E	119	SER	C-O	5.06	1.30	1.24
1	A	419	LYS	CE-NZ	-5.06	1.34	1.49
2	B	202	TYR	C-O	-5.06	1.17	1.23
2	B	1090	THR	N-CA	-5.06	1.39	1.45
2	B	1156	ASP	CG-OD1	5.06	1.34	1.25
1	A	1147	THR	C-N	-5.06	1.27	1.33
2	B	483	LEU	C-O	-5.06	1.18	1.24
3	C	73	GLN	C-O	-5.06	1.18	1.23
3	C	134	ILE	N-CA	5.06	1.52	1.46
4	E	26	ARG	CB-CG	-5.06	1.37	1.52
2	B	434	ARG	C-N	5.06	1.40	1.33
2	B	995	ARG	CA-CB	-5.06	1.45	1.53
3	C	66	ARG	CZ-NH1	-5.06	1.25	1.32
10	L	59	ALA	CA-CB	5.06	1.62	1.53
2	B	1034	VAL	C-N	-5.06	1.27	1.33
2	B	1220	ARG	C-O	5.06	1.30	1.24
6	H	13	SER	C-O	-5.06	1.17	1.24
1	A	746	MET	C-O	-5.05	1.18	1.24
2	B	485	ARG	CZ-NH1	-5.05	1.25	1.32
1	A	213	HIS	CA-C	-5.05	1.45	1.52
1	A	469	ARG	CA-C	5.05	1.58	1.52
2	B	936	ASP	C-O	-5.05	1.17	1.24
7	I	41	PRO	C-N	-5.05	1.26	1.33
1	A	902	LEU	CG-CD1	5.05	1.69	1.52
2	B	56	ASP	CA-CB	-5.05	1.44	1.53
2	B	95	ILE	CA-CB	-5.05	1.48	1.54
2	B	1217	TYR	CA-CB	5.05	1.61	1.53
3	C	173	ALA	C-N	-5.05	1.27	1.32
6	H	80	ARG	C-O	-5.05	1.19	1.24
7	I	2	THR	CA-CB	-5.05	1.45	1.53
1	A	132	LYS	CA-C	5.05	1.59	1.52
1	A	567	LYS	CA-CB	-5.05	1.45	1.53
2	B	933	SER	C-O	5.05	1.33	1.23
1	A	1306	LEU	N-CA	-5.05	1.39	1.45
1	A	209	ASN	N-CA	-5.05	1.39	1.46
1	A	967	ALA	N-CA	5.05	1.52	1.46
1	A	1375	MET	SD-CE	-5.05	1.67	1.79
2	B	610	ASN	CA-C	5.05	1.58	1.53
2	B	892	LYS	CG-CD	5.05	1.67	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	349	ILE	CA-C	5.04	1.59	1.52
2	B	987	LYS	CA-C	-5.04	1.46	1.53
2	B	1107	ALA	CA-CB	-5.04	1.46	1.53
2	B	1150	ARG	CG-CD	-5.04	1.37	1.52
3	C	10	ILE	N-CA	-5.04	1.40	1.46
4	E	54	GLN	CG-CD	5.04	1.64	1.52
1	A	111	GLY	N-CA	5.04	1.52	1.45
1	A	657	LEU	C-O	-5.04	1.17	1.24
1	A	1042	PHE	CG-CD2	-5.04	1.28	1.38
2	B	313	MET	C-O	5.04	1.30	1.24
2	B	1190	ASP	CG-OD1	5.04	1.34	1.25
3	C	60	ASP	CA-C	-5.04	1.46	1.52
7	I	101	PHE	CD1-CE1	5.04	1.53	1.38
9	K	99	GLY	CA-C	5.04	1.58	1.51
1	A	115	LEU	N-CA	5.04	1.52	1.45
1	A	863	VAL	CA-C	-5.04	1.47	1.52
2	B	388	CYS	N-CA	-5.04	1.40	1.46
2	B	512	ARG	CZ-NH1	5.04	1.39	1.32
7	I	4	PHE	CA-C	-5.04	1.46	1.52
1	A	588	LEU	CA-C	5.04	1.58	1.52
2	B	733	HIS	C-O	5.04	1.30	1.24
7	I	69	PRO	CA-C	-5.04	1.46	1.52
8	J	58	GLU	CD-OE1	-5.04	1.15	1.25
1	A	243	PRO	C-O	-5.03	1.18	1.24
1	A	896	ARG	CA-C	-5.03	1.46	1.52
1	A	900	ASP	C-N	-5.03	1.26	1.33
1	A	1130	GLN	CD-OE1	5.03	1.33	1.23
1	A	1156	PRO	CA-C	5.03	1.60	1.52
2	B	1184	GLY	C-O	-5.03	1.18	1.24
2	B	1100	ASP	N-CA	5.03	1.52	1.46
1	A	273	ASN	CG-ND2	5.03	1.43	1.33
1	A	505	CYS	CA-C	-5.03	1.45	1.52
1	A	884	ASP	N-CA	5.03	1.52	1.46
1	A	885	THR	CB-OG1	-5.03	1.35	1.43
2	B	120	ARG	NE-CZ	5.03	1.38	1.33
2	B	209	GLU	N-CA	5.03	1.52	1.46
2	B	742	GLU	C-O	-5.03	1.17	1.23
2	B	842	ASN	C-O	-5.03	1.18	1.24
10	L	25	ALA	CA-CB	5.03	1.69	1.52
1	A	659	HIS	CD2-NE2	-5.03	1.32	1.37
2	B	589	VAL	N-CA	-5.03	1.40	1.46
2	B	887	HIS	CB-CG	5.03	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	453	MET	SD-CE	5.03	1.92	1.79
1	A	1040	GLN	N-CA	-5.03	1.40	1.46
1	A	1431	GLY	C-N	-5.03	1.27	1.33
2	B	916	THR	CA-CB	5.03	1.68	1.54
2	B	579	ARG	CG-CD	5.03	1.67	1.52
2	B	848	ARG	CD-NE	-5.03	1.39	1.46
3	C	99	LEU	CB-CG	-5.03	1.43	1.53
4	E	158	SER	N-CA	-5.03	1.39	1.46
5	F	104	ASN	N-CA	5.03	1.54	1.46
2	B	245	GLU	C-N	5.02	1.40	1.33
5	F	94	LEU	N-CA	-5.02	1.40	1.46
6	H	111	LEU	CG-CD1	5.02	1.69	1.52
1	A	1129	GLU	C-O	5.02	1.30	1.24
1	A	1321	GLY	N-CA	5.02	1.52	1.45
3	C	34	ARG	CA-C	-5.02	1.46	1.52
3	C	152	GLU	CA-C	-5.02	1.46	1.52
8	J	53	HIS	C-N	-5.02	1.27	1.33
9	K	2	ASN	CA-CB	5.02	1.61	1.53
4	E	214	CYS	C-O	-5.02	1.18	1.23
1	A	119	ASN	CG-ND2	-5.02	1.22	1.33
1	A	1200	ALA	N-CA	5.02	1.52	1.46
2	B	256	VAL	CA-C	5.02	1.59	1.52
2	B	797	TYR	CD1-CE1	5.02	1.53	1.38
3	C	44	LEU	C-N	5.02	1.39	1.33
3	C	137	LYS	CG-CD	5.02	1.67	1.52
6	H	46	LEU	N-CA	-5.02	1.39	1.46
1	A	553	VAL	C-O	-5.02	1.18	1.24
1	A	1024	SER	N-CA	-5.02	1.39	1.46
1	A	1078	GLN	CA-C	5.02	1.59	1.52
1	A	1130	GLN	C-O	-5.02	1.17	1.24
2	B	663	ALA	CA-C	-5.02	1.46	1.52
2	B	1069	PHE	CE1-CZ	-5.02	1.23	1.38
5	F	123	LYS	CA-C	5.02	1.59	1.52
9	K	5	ASP	CA-C	-5.02	1.46	1.52
2	B	38	PHE	CE1-CZ	-5.02	1.23	1.38
1	A	96	ILE	CA-C	5.01	1.59	1.52
1	A	444	PHE	CA-C	-5.01	1.46	1.52
2	B	246	LYS	C-O	5.01	1.30	1.23
2	B	769	TYR	CA-CB	-5.01	1.45	1.53
2	B	1161	HIS	CG-CD2	5.01	1.41	1.35
3	C	90	ASP	CA-CB	5.01	1.61	1.53
4	E	142	VAL	CA-C	5.01	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	449	SER	CA-C	5.01	1.59	1.52
1	A	1366	ARG	CG-CD	-5.01	1.37	1.52
1	A	132	LYS	C-O	5.01	1.30	1.23
1	A	815	PHE	CE2-CZ	-5.01	1.23	1.38
2	B	622	LYS	CE-NZ	5.01	1.64	1.49
2	B	698	GLU	C-N	-5.01	1.27	1.33
2	B	1150	ARG	CD-NE	-5.01	1.39	1.46
3	C	38	ILE	CA-CB	-5.01	1.48	1.54
1	A	507	VAL	CA-CB	5.01	1.57	1.53
2	B	597	MET	CG-SD	5.01	1.93	1.80
4	E	196	VAL	N-CA	5.01	1.52	1.46
7	I	6	PHE	CD2-CE2	5.01	1.53	1.38
9	K	25	THR	CA-C	-5.01	1.45	1.52
9	K	113	THR	CB-OG1	5.01	1.51	1.43
2	B	60	GLN	C-N	-5.00	1.26	1.33
2	B	817	LEU	CA-C	5.00	1.58	1.52
3	C	199	LYS	N-CA	5.00	1.52	1.46
1	A	65	LEU	C-N	5.00	1.39	1.33
1	A	974	ASP	C-O	-5.00	1.17	1.24
2	B	589	VAL	C-O	-5.00	1.19	1.24
3	C	36	VAL	CA-CB	-5.00	1.48	1.54
3	C	89	GLU	N-CA	5.00	1.52	1.46
3	C	143	LEU	CA-CB	-5.00	1.46	1.53
3	C	202	PRO	N-CD	-5.00	1.40	1.47
1	A	748	MET	CA-C	-5.00	1.46	1.52
1	A	1103	GLU	CB-CG	-5.00	1.37	1.52
2	B	105	SER	CB-OG	5.00	1.52	1.42
2	B	135	ARG	C-N	5.00	1.40	1.33
2	B	907	GLY	C-O	5.00	1.31	1.24
5	F	135	ARG	CA-CB	5.00	1.59	1.53

All (2921) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	399	HIS	CA-C-N	18.75	143.28	119.84
1	A	399	HIS	C-N-CA	18.75	143.28	119.84
2	B	1097	HIS	CB-CG-ND1	-18.22	95.37	122.70
3	C	240	VAL	N-CA-C	17.00	127.91	110.23
1	A	469	ARG	NE-CZ-NH2	-16.76	104.12	119.20
5	F	81	THR	N-CA-CB	-16.10	88.32	110.38
1	A	774	ARG	NE-CZ-NH1	15.94	137.44	121.50
1	A	1259	MET	N-CA-C	-15.52	94.36	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	183	TRP	CA-C-N	-15.43	98.07	123.37
3	C	183	TRP	C-N-CA	-15.43	98.07	123.37
7	I	43	VAL	N-CA-CB	-15.41	88.65	112.07
1	A	93	VAL	CB-CA-C	-15.19	91.26	112.22
1	A	1366	ARG	NE-CZ-NH1	14.54	136.04	121.50
3	C	35	ARG	NE-CZ-NH2	-14.34	106.29	119.20
3	C	34	ARG	NE-CZ-NH2	-14.32	106.32	119.20
1	A	1366	ARG	NE-CZ-NH2	-14.26	106.37	119.20
2	B	995	ARG	NE-CZ-NH2	-14.22	106.40	119.20
3	C	66	ARG	NE-CZ-NH2	13.81	131.63	119.20
2	B	620	ARG	NH1-CZ-NH2	13.37	136.68	119.30
1	A	538	ASP	CB-CA-C	-13.26	86.15	110.01
2	B	839	MET	CG-SD-CE	-13.23	71.80	100.90
2	B	802	PRO	CA-C-O	-13.21	105.51	120.97
6	H	57	VAL	N-CA-C	13.13	125.49	106.85
2	B	1150	ARG	NE-CZ-NH1	-13.09	108.41	121.50
3	C	124	LEU	N-CA-C	13.06	128.54	112.87
1	A	659	HIS	CB-CG-ND1	-12.88	103.38	122.70
1	A	896	ARG	NE-CZ-NH2	-12.78	107.70	119.20
1	A	949	ASP	N-CA-CB	-12.73	89.64	110.40
1	A	1062	GLU	CB-CA-C	-12.71	87.92	109.65
4	E	212	ARG	CD-NE-CZ	12.58	142.01	124.40
3	C	20	PHE	N-CA-C	12.56	126.57	108.86
1	A	1004	ASN	N-CA-C	12.55	126.53	110.33
2	B	620	ARG	NE-CZ-NH1	-12.54	108.96	121.50
2	B	1077	THR	N-CA-CB	-12.53	94.23	110.90
10	L	57	LEU	N-CA-C	12.47	129.53	108.20
2	B	1185	CYS	N-CA-C	-12.47	97.76	113.23
8	J	2	ILE	CG1-CB-CG2	-12.45	73.36	110.70
1	A	964	ILE	N-CA-C	-12.45	98.75	110.82
3	C	181	ASP	CA-C-O	-12.41	111.91	120.47
7	I	31	THR	N-CA-CB	-12.41	94.09	110.59
1	A	1336	MET	CG-SD-CE	12.29	127.95	100.90
3	C	163	ILE	CA-CB-CG2	12.29	131.39	110.50
7	I	33	SER	N-CA-C	-12.21	96.53	112.41
2	B	608	ASP	N-CA-C	-12.20	98.06	111.36
2	B	642	ASP	N-CA-C	-12.20	86.52	107.99
1	A	182	VAL	N-CA-C	12.13	125.09	108.11
6	H	106	GLU	N-CA-C	-12.09	98.81	113.19
4	E	77	SER	N-CA-C	-12.00	92.14	109.18
2	B	416	LEU	CB-CA-C	-11.89	92.53	110.95
8	J	38	ARG	N-CA-C	-11.85	97.38	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1019	SER	CB-CA-C	-11.79	86.34	110.38
3	C	81	GLU	N-CA-C	-11.70	91.72	110.32
1	A	137	ALA	N-CA-C	11.67	123.55	111.07
1	A	962	ARG	NE-CZ-NH2	-11.61	108.75	119.20
1	A	1100	ARG	NE-CZ-NH2	-11.56	108.80	119.20
1	A	982	THR	N-CA-CB	-11.52	92.94	110.45
8	J	43	ARG	NE-CZ-NH2	11.50	129.55	119.20
2	B	46	GLN	CA-CB-CG	-11.44	91.21	114.10
4	E	5	ASN	N-CA-C	-11.44	99.05	113.23
4	E	204	THR	CA-CB-CG2	11.44	129.94	110.50
1	A	1376	THR	N-CA-CB	-11.34	94.62	110.95
3	C	40	GLU	N-CA-C	11.28	127.07	112.41
1	A	446	ARG	NH1-CZ-NH2	11.23	133.90	119.30
3	C	18	VAL	CB-CA-C	-11.22	92.89	111.29
1	A	821	ARG	NE-CZ-NH2	-11.20	109.12	119.20
1	A	774	ARG	NE-CZ-NH2	-11.19	109.13	119.20
3	C	256	ALA	N-CA-C	-11.12	98.33	112.90
4	E	24	LYS	CD-CE-NZ	-11.06	76.50	111.90
2	B	1150	ARG	NH1-CZ-NH2	11.06	133.68	119.30
2	B	807	ARG	NE-CZ-NH2	-11.05	109.25	119.20
2	B	399	ASP	N-CA-C	11.03	127.07	113.17
1	A	474	VAL	N-CA-C	-11.02	101.92	112.83
10	L	40	LEU	CA-C-O	-11.01	109.88	120.56
1	A	434	ARG	NE-CZ-NH1	10.99	132.49	121.50
8	J	43	ARG	NE-CZ-NH1	-10.97	110.53	121.50
2	B	455	SER	N-CA-C	-10.94	100.04	113.50
1	A	883	LEU	N-CA-C	-10.92	90.72	108.52
2	B	680	THR	N-CA-CB	-10.91	93.94	111.62
7	I	10	CYS	N-CA-C	10.89	126.39	112.89
1	A	974	ASP	N-CA-CB	10.88	128.45	110.17
1	A	1358	SER	N-CA-C	-10.87	99.40	111.14
1	A	724	GLU	N-CA-C	-10.87	99.21	111.82
1	A	1318	THR	N-CA-CB	-10.87	94.34	110.53
1	A	1172	LEU	CB-CA-C	-10.85	97.77	111.22
3	C	160	LYS	CD-CE-NZ	10.82	146.52	111.90
3	C	35	ARG	NE-CZ-NH1	10.80	132.31	121.50
5	F	82	THR	CB-CA-C	-10.80	91.89	109.27
3	C	28	ALA	N-CA-C	10.78	122.61	111.07
1	A	466	SER	CB-CA-C	-10.78	92.51	110.72
2	B	559	SER	CA-CB-OG	-10.77	89.57	111.10
2	B	1042	GLY	CA-C-O	-10.76	111.55	120.91
9	K	47	ARG	NE-CZ-NH2	-10.75	109.52	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	102	TYR	CA-C-O	10.72	131.15	119.03
2	B	496	ARG	NE-CZ-NH1	10.71	132.22	121.50
2	B	791	THR	OG1-CB-CG2	-10.70	87.89	109.30
1	A	109	HIS	CA-C-N	10.70	135.48	120.29
1	A	109	HIS	C-N-CA	10.70	135.48	120.29
1	A	802	ASN	N-CA-C	10.68	125.56	110.50
1	A	1404	GLU	CA-C-N	-10.66	101.17	121.54
1	A	1404	GLU	C-N-CA	-10.66	101.17	121.54
1	A	789	LYS	N-CA-C	10.66	124.39	110.43
2	B	772	ALA	N-CA-C	10.66	122.47	111.07
1	A	394	ASN	N-CA-C	10.65	123.96	111.71
4	E	176	PRO	CB-CA-C	-10.65	97.00	110.95
1	A	419	LYS	N-CA-C	-10.62	99.42	112.38
8	J	22	LEU	N-CA-CB	-10.62	94.68	110.07
1	A	1338	VAL	N-CA-C	10.61	120.94	111.81
6	H	91	ASP	CA-C-O	10.61	131.65	120.30
1	A	725	ALA	N-CA-C	10.56	122.87	111.36
4	E	93	MET	N-CA-C	10.54	122.34	111.07
1	A	50	ILE	CB-CA-C	-10.54	96.51	110.84
1	A	613	ILE	N-CA-C	-10.53	101.58	111.48
3	C	89	GLU	N-CA-C	-10.52	92.24	108.96
1	A	1016	THR	N-CA-C	10.48	122.29	111.07
6	H	81	PRO	CB-CA-C	10.47	123.69	110.92
2	B	46	GLN	N-CA-C	-10.46	99.88	111.28
1	A	244	PRO	CA-C-O	-10.43	105.43	120.56
2	B	24	PRO	N-CD-CG	-10.43	87.56	103.20
1	A	469	ARG	NE-CZ-NH1	10.42	131.92	121.50
1	A	748	MET	CG-SD-CE	10.41	123.80	100.90
2	B	501	PRO	CA-C-O	-10.41	108.75	120.92
1	A	566	ILE	CB-CA-C	-10.40	98.83	111.94
8	J	1	MET	N-CA-CB	-10.38	92.84	110.50
8	J	7	CYS	CA-CB-SG	10.38	138.26	114.40
6	H	17	PRO	CA-C-O	-10.36	108.34	118.29
2	B	90	ILE	CB-CA-C	-10.34	94.33	111.29
2	B	895	ASP	N-CA-C	-10.34	100.06	112.89
3	C	229	TYR	N-CA-C	10.33	127.38	108.58
1	A	1228	TRP	CB-CA-C	-10.30	91.19	110.56
2	B	268	THR	N-CA-CB	-10.30	95.60	111.05
3	C	77	ILE	N-CA-C	-10.29	98.26	113.39
2	B	604	ARG	NE-CZ-NH2	-10.28	109.95	119.20
2	B	547	VAL	N-CA-CB	-10.26	100.93	112.21
2	B	414	ALA	N-CA-C	-10.25	99.54	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	996	ARG	NH1-CZ-NH2	10.23	132.60	119.30
1	A	1136	SER	N-CA-C	-10.22	100.55	113.23
1	A	752	LYS	CD-CE-NZ	10.21	144.58	111.90
4	E	197	LYS	N-CA-C	-10.20	92.65	109.07
1	A	709	THR	N-CA-CB	-10.20	95.05	110.04
2	B	598	GLU	N-CA-CB	10.18	125.08	110.12
1	A	1366	ARG	CD-NE-CZ	10.18	138.65	124.40
1	A	687	LYS	N-CA-C	10.15	124.74	111.75
2	B	974	PRO	CA-C-O	-10.15	110.06	121.43
8	J	49	MET	CG-SD-CE	-10.14	78.58	100.90
1	A	464	PRO	O-C-N	-10.14	108.95	122.64
1	A	610	GLY	O-C-N	10.12	134.17	122.33
2	B	648	HIS	N-CA-C	10.11	125.06	109.60
2	B	620	ARG	CG-CD-NE	-10.08	89.83	112.00
7	I	84	VAL	N-CA-CB	-10.06	95.58	112.47
1	A	459	ARG	NE-CZ-NH2	-10.05	110.15	119.20
2	B	498	THR	N-CA-CB	-10.05	94.06	111.55
4	E	66	GLU	N-CA-C	-10.04	100.42	111.36
2	B	1160	VAL	CB-CA-C	-10.03	94.84	111.29
1	A	728	LYS	N-CA-CB	10.02	124.85	110.12
2	B	828	ALA	N-CA-C	10.02	124.59	108.76
2	B	583	ASN	CA-C-N	-10.02	108.24	122.86
2	B	583	ASN	C-N-CA	-10.02	108.24	122.86
3	C	245	VAL	N-CA-C	-9.95	100.15	111.00
1	A	969	GLN	N-CA-C	-9.95	99.45	112.68
9	K	79	GLU	N-CA-C	-9.95	95.04	109.96
1	A	893	PHE	N-CA-C	-9.93	100.53	111.36
1	A	107	CYS	N-CA-C	-9.92	92.99	109.46
5	F	72	LYS	CA-C-N	9.91	140.48	121.54
5	F	72	LYS	C-N-CA	9.91	140.48	121.54
1	A	1158	PRO	CA-C-O	-9.91	105.91	118.99
3	C	66	ARG	NE-CZ-NH1	-9.89	111.61	121.50
2	B	1183	LYS	CA-C-N	-9.88	112.82	123.30
2	B	1183	LYS	C-N-CA	-9.88	112.82	123.30
3	C	49	VAL	CA-C-O	-9.86	110.49	120.25
2	B	365	THR	N-CA-C	-9.86	93.51	108.99
1	A	1219	THR	N-CA-C	9.85	123.04	111.71
1	A	557	ASP	O-C-N	-9.85	110.21	122.82
2	B	1097	HIS	CA-CB-CG	-9.85	103.95	113.80
1	A	1385	THR	N-CA-CB	-9.83	94.78	111.50
1	A	566	ILE	N-CA-C	9.82	121.99	111.58
7	I	75	CYS	N-CA-CB	9.81	121.90	110.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	J	21	TYR	N-CA-C	-9.81	99.44	111.40
2	B	56	ASP	N-CA-C	9.80	125.08	112.34
1	A	885	THR	CA-CB-CG2	9.79	127.15	110.50
1	A	1166	ASP	N-CA-C	-9.79	101.56	112.72
1	A	223	GLY	N-CA-C	9.77	127.91	115.21
1	A	922	ASP	N-CA-C	9.77	124.20	109.25
10	L	48	CYS	N-CA-C	9.75	120.74	108.45
1	A	347	PHE	N-CA-C	9.74	124.46	112.58
2	B	787	VAL	N-CA-CB	-9.73	101.50	112.21
1	A	1280	GLU	CB-CG-CD	9.71	129.11	112.60
2	B	605	ARG	NE-CZ-NH2	9.71	127.94	119.20
1	A	704	ALA	CA-C-N	-9.70	108.30	123.23
1	A	704	ALA	C-N-CA	-9.70	108.30	123.23
2	B	102	VAL	N-CA-C	9.68	122.88	108.46
9	K	85	ASP	N-CA-C	-9.68	100.04	112.23
4	E	14	ARG	CA-C-N	-9.65	105.64	120.31
4	E	14	ARG	C-N-CA	-9.65	105.64	120.31
2	B	731	VAL	N-CA-C	-9.64	93.68	107.75
10	L	68	GLU	CB-CG-CD	9.64	128.98	112.60
1	A	782	ARG	CA-C-O	-9.63	110.20	120.99
1	A	1014	ALA	CA-C-O	9.63	130.98	120.10
1	A	782	ARG	N-CA-C	9.63	124.11	108.99
9	K	95	ILE	O-C-N	9.60	131.60	121.90
2	B	734	HIS	N-CA-C	-9.58	99.22	112.25
3	C	155	LEU	CB-CA-C	-9.57	90.72	109.68
2	B	165	VAL	CB-CA-C	-9.54	95.64	111.29
2	B	1165	ILE	N-CA-C	-9.53	103.36	111.56
3	C	239	PRO	CA-C-O	9.54	134.28	122.08
7	I	118	ARG	N-CA-C	9.53	124.60	110.30
1	A	466	SER	N-CA-C	9.53	125.17	112.88
1	A	1116	LEU	N-CA-C	-9.52	93.88	109.40
7	I	75	CYS	CA-C-O	-9.52	112.03	120.60
3	C	86	CYS	CA-CB-SG	9.51	136.27	114.40
1	A	986	ILE	N-CA-C	9.48	119.50	110.30
1	A	434	ARG	NE-CZ-NH2	-9.48	110.67	119.20
1	A	999	VAL	N-CA-C	-9.47	104.14	111.62
5	F	120	ILE	N-CA-C	-9.47	101.16	110.72
1	A	744	LYS	N-CA-C	-9.46	99.30	112.45
2	B	604	ARG	NE-CZ-NH1	9.45	130.95	121.50
1	A	659	HIS	CB-CG-CD2	9.44	143.47	131.20
1	A	537	ARG	CB-CG-CD	9.43	132.98	111.30
4	E	66	GLU	N-CA-CB	9.42	124.11	110.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	709	ASP	N-CA-C	-9.42	101.79	113.28
1	A	352	VAL	CG1-CB-CG2	-9.38	90.16	110.80
4	E	11	ARG	NE-CZ-NH1	-9.38	112.12	121.50
1	A	389	THR	OG1-CB-CG2	-9.37	90.56	109.30
1	A	108	MET	N-CA-C	9.37	124.34	113.19
2	B	1207	LEU	N-CA-C	9.36	121.57	111.36
1	A	795	GLU	CB-CG-CD	9.35	128.49	112.60
3	C	172	PRO	N-CD-CG	9.34	117.21	103.20
1	A	377	PRO	CA-C-O	-9.32	111.04	121.11
2	B	1086	PHE	N-CA-C	-9.32	94.94	109.76
1	A	1291	VAL	N-CA-C	-9.32	101.55	109.19
1	A	1154	TYR	N-CA-C	-9.30	94.17	108.96
1	A	492	PRO	CA-C-O	-9.29	110.16	121.31
2	B	337	ARG	CG-CD-NE	-9.29	91.57	112.00
1	A	749	ALA	N-CA-C	9.28	122.38	111.71
9	K	110	ASN	N-CA-C	-9.27	99.56	112.45
9	K	114	LEU	CB-CG-CD2	9.27	138.51	110.70
1	A	826	ASP	N-CA-C	-9.24	101.29	111.36
1	A	938	LYS	CB-CA-C	-9.24	95.45	110.79
1	A	970	THR	N-CA-C	9.23	122.32	111.71
2	B	598	GLU	CB-CG-CD	9.22	128.27	112.60
1	A	999	VAL	N-CA-CB	-9.21	104.08	111.64
1	A	821	ARG	CG-CD-NE	-9.21	91.74	112.00
1	A	1438	THR	N-CA-CB	-9.21	93.56	110.32
5	F	125	LEU	N-CA-C	-9.19	100.39	111.69
1	A	832	ALA	CA-C-N	9.19	132.95	120.54
1	A	832	ALA	C-N-CA	9.19	132.95	120.54
1	A	283	GLY	N-CA-C	-9.18	91.42	113.18
3	C	33	LEU	N-CA-C	-9.17	100.41	111.69
1	A	1013	ASP	N-CA-C	-9.16	101.25	111.14
1	A	1271	ILE	N-CA-CB	9.16	123.54	111.64
1	A	146	MET	N-CA-CB	-9.14	96.11	110.46
1	A	1062	GLU	CB-CG-CD	9.14	128.13	112.60
2	B	622	LYS	CA-CB-CG	9.13	132.37	114.10
1	A	1006	ILE	CG1-CB-CG2	-9.13	83.31	110.70
1	A	446	ARG	NE-CZ-NH2	-9.12	110.99	119.20
1	A	1222	ASN	CA-C-O	-9.13	110.88	120.55
4	E	47	CYS	N-CA-C	9.12	123.77	108.90
2	B	567	GLU	O-C-N	-9.12	111.81	122.20
9	K	26	LYS	CA-C-O	9.11	130.40	120.10
9	K	83	PRO	N-CD-CG	-9.11	89.54	103.20
1	A	982	THR	CA-CB-CG2	9.10	125.97	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	150	GLY	CA-C-O	9.10	129.07	118.97
2	B	531	GLN	N-CA-C	-9.09	101.27	111.82
4	E	153	HIS	CA-CB-CG	9.09	122.89	113.80
1	A	1103	GLU	CB-CA-C	9.08	126.28	110.85
1	A	1239	ARG	CB-CA-C	9.08	126.13	109.70
1	A	916	GLY	N-CA-C	9.07	123.61	112.73
1	A	218	ASP	N-CA-C	-9.06	100.35	111.40
1	A	934	LYS	N-CA-C	-9.05	101.41	111.28
5	F	114	GLU	CA-C-O	-9.03	111.98	121.55
3	C	53	THR	OG1-CB-CG2	-9.03	91.24	109.30
2	B	65	GLU	N-CA-C	-9.02	99.32	110.41
3	C	39	ALA	N-CA-C	9.02	124.97	113.88
7	I	32	CYS	N-CA-C	-9.01	96.71	109.69
2	B	1097	HIS	CB-CG-CD2	9.01	142.91	131.20
1	A	858	ASN	CA-C-O	-9.01	111.70	121.88
1	A	495	GLU	N-CA-CB	-9.00	96.89	110.12
1	A	1349	TYR	N-CA-C	-8.98	101.58	111.36
9	K	14	GLU	CB-CA-C	8.98	125.69	109.62
1	A	709	THR	OG1-CB-CG2	-8.97	91.35	109.30
1	A	1370	LEU	CD1-CG-CD2	-8.96	91.09	110.80
2	B	168	GLY	N-CA-C	8.96	123.00	111.09
3	C	14	SER	O-C-N	-8.96	114.33	123.29
1	A	491	VAL	N-CA-C	8.95	116.41	107.55
1	A	492	PRO	O-C-N	8.95	133.84	123.10
3	C	24	ASN	N-CA-C	8.95	123.59	111.24
1	A	793	SER	N-CA-C	8.95	124.37	109.87
1	A	596	THR	CB-CA-C	-8.94	92.63	110.42
1	A	1062	GLU	CA-CB-CG	8.94	131.98	114.10
1	A	295	LEU	N-CA-C	-8.92	100.72	111.69
1	A	1226	VAL	CB-CA-C	-8.92	96.19	110.28
2	B	1099	VAL	CB-CA-C	-8.92	96.66	111.29
1	A	163	SER	N-CA-CB	8.91	124.94	110.41
2	B	1075	GLY	N-CA-C	8.91	123.70	112.83
1	A	706	HIS	N-CA-CB	8.90	125.53	110.49
2	B	595	ARG	N-CA-CB	8.89	122.90	110.01
1	A	493	GLN	CB-CG-CD	8.88	127.70	112.60
1	A	940	ARG	NE-CZ-NH1	8.87	130.37	121.50
4	E	204	THR	CA-CB-OG1	8.87	122.91	109.60
2	B	747	MET	CG-SD-CE	-8.87	81.39	100.90
5	F	150	GLU	N-CA-CB	-8.87	96.65	110.30
1	A	1100	ARG	NE-CZ-NH1	8.86	130.36	121.50
2	B	904	ARG	NE-CZ-NH2	8.86	127.17	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I	27	PHE	N-CA-C	8.85	123.15	108.73
1	A	288	ALA	CA-C-N	8.82	131.73	120.70
1	A	288	ALA	C-N-CA	8.82	131.73	120.70
1	A	1014	ALA	N-CA-C	8.82	121.85	111.71
2	B	1042	GLY	O-C-N	8.81	130.39	123.61
9	K	94	ILE	N-CA-C	-8.78	102.17	110.42
1	A	1406	VAL	O-C-N	8.77	130.51	121.91
7	I	38	ALA	CA-C-N	8.77	129.50	119.94
7	I	38	ALA	C-N-CA	8.77	129.50	119.94
1	A	1368	MET	N-CA-C	-8.77	101.18	112.23
2	B	589	VAL	CB-CA-C	8.76	125.87	110.71
2	B	1097	HIS	CB-CA-C	8.76	127.84	110.42
1	A	982	THR	N-CA-C	8.75	122.37	110.55
8	J	2	ILE	CB-CA-C	-8.75	95.44	111.18
1	A	1158	PRO	N-CA-C	-8.74	103.71	114.20
1	A	1072	ILE	N-CA-C	-8.74	103.32	111.45
2	B	1196	ILE	N-CA-C	8.74	116.36	109.19
7	I	106	CYS	CA-C-N	8.74	136.77	123.05
7	I	106	CYS	C-N-CA	8.74	136.77	123.05
6	H	127	GLY	N-CA-C	8.73	133.88	113.18
1	A	607	ILE	CA-C-O	-8.73	111.30	120.64
3	C	44	LEU	CA-C-O	-8.73	111.28	120.70
2	B	653	VAL	CB-CA-C	-8.72	99.24	111.28
1	A	843	LYS	CB-CG-CD	8.72	131.36	111.30
2	B	644	GLU	CB-CG-CD	-8.71	97.79	112.60
3	C	183	TRP	N-CA-C	-8.70	96.87	110.36
1	A	1238	ILE	CA-C-O	-8.70	111.26	120.48
1	A	475	THR	N-CA-CB	-8.68	97.36	110.12
1	A	1278	ASN	CA-C-N	-8.68	111.57	122.93
1	A	1278	ASN	C-N-CA	-8.68	111.57	122.93
3	C	27	LEU	CA-C-N	-8.68	109.16	120.44
3	C	27	LEU	C-N-CA	-8.68	109.16	120.44
7	I	31	THR	CA-C-N	8.67	139.62	123.32
7	I	31	THR	C-N-CA	8.67	139.62	123.32
1	A	916	GLY	CA-C-N	8.67	131.71	120.44
1	A	916	GLY	C-N-CA	8.67	131.71	120.44
2	B	217	ARG	CB-CG-CD	8.66	131.22	111.30
8	J	7	CYS	N-CA-CB	8.66	122.90	109.48
8	J	1	MET	CG-SD-CE	-8.66	81.86	100.90
2	B	967	ARG	NE-CZ-NH1	-8.65	112.85	121.50
2	B	642	ASP	CA-C-N	-8.64	105.04	121.54
2	B	642	ASP	C-N-CA	-8.64	105.04	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1284	MET	CA-CB-CG	-8.64	96.82	114.10
1	A	649	ILE	CA-CB-CG1	8.63	125.07	110.40
1	A	739	ASP	N-CA-C	8.63	123.56	112.34
1	A	982	THR	OG1-CB-CG2	-8.63	92.04	109.30
2	B	852	ARG	N-CA-CB	-8.63	97.28	109.97
3	C	240	VAL	CB-CA-C	-8.61	100.68	111.70
10	L	68	GLU	CG-CD-OE1	8.61	138.21	118.40
1	A	1054	LEU	CA-C-O	8.61	129.87	119.97
1	A	27	VAL	N-CA-C	8.60	119.39	110.62
3	C	75	MET	N-CA-C	-8.60	101.91	111.28
1	A	589	GLN	CA-C-O	-8.59	111.06	121.11
1	A	29	ALA	N-CA-C	8.58	122.73	111.75
6	H	120	GLY	N-CA-C	8.57	126.36	115.21
2	B	129	PHE	N-CA-C	8.57	122.86	108.20
3	C	11	ARG	CB-CA-C	-8.57	94.98	109.38
2	B	513	GLN	CA-CB-CG	8.56	131.23	114.10
1	A	61	ILE	N-CA-C	-8.56	91.53	109.34
2	B	137	TYR	CA-CB-CG	8.56	129.31	113.90
9	K	79	GLU	CB-CA-C	8.55	123.56	109.89
1	A	885	THR	OG1-CB-CG2	-8.54	92.22	109.30
2	B	368	GLU	N-CA-C	8.54	120.36	111.14
8	J	5	VAL	N-CA-C	8.54	119.32	110.36
9	K	52	ASN	N-CA-C	-8.52	102.66	113.23
7	I	13	MET	N-CA-CB	-8.49	97.54	110.45
4	E	175	LEU	N-CA-C	-8.49	99.36	110.39
1	A	1015	VAL	N-CA-CB	-8.48	101.00	112.28
2	B	851	PHE	N-CA-C	8.47	122.97	112.47
3	C	252	GLN	CB-CA-C	8.46	124.84	110.79
2	B	465	ASN	N-CA-C	8.46	122.67	108.20
4	E	61	GLN	N-CA-C	-8.46	96.55	109.41
8	J	6	ARG	CA-C-O	-8.46	111.55	121.11
2	B	412	LEU	N-CA-C	-8.46	102.06	111.28
1	A	708	MET	N-CA-CB	-8.44	96.40	110.32
2	B	354	ASP	N-CA-C	-8.43	102.17	111.36
3	C	38	ILE	N-CA-C	8.43	119.21	110.36
2	B	104	GLU	N-CA-C	8.42	122.38	110.50
6	H	107	VAL	N-CA-C	-8.42	91.82	109.34
2	B	518	HIS	CA-CB-CG	8.42	122.22	113.80
7	I	53	GLY	N-CA-C	8.42	127.93	115.64
2	B	452	THR	OG1-CB-CG2	-8.41	92.48	109.30
2	B	329	THR	OG1-CB-CG2	-8.41	92.48	109.30
2	B	1166	CYS	O-C-N	-8.40	111.41	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	600	PRO	N-CD-CG	-8.40	90.60	103.20
2	B	1108	ARG	N-CA-C	8.40	128.69	110.80
2	B	612	GLU	CB-CG-CD	8.37	126.84	112.60
1	A	134	ARG	N-CA-C	-8.37	101.19	111.40
4	E	106	GLN	N-CA-C	-8.37	102.85	113.23
1	A	1280	GLU	O-C-N	-8.36	111.47	122.59
8	J	2	ILE	CB-CG1-CD1	-8.36	96.25	113.80
4	E	103	LYS	N-CA-CB	8.35	123.14	110.70
1	A	962	ARG	N-CA-C	-8.35	100.85	112.45
1	A	603	ASN	N-CA-CB	-8.34	97.55	110.56
2	B	781	PHE	N-CA-C	8.34	121.30	111.71
1	A	182	VAL	CA-C-N	-8.34	113.38	122.38
1	A	182	VAL	C-N-CA	-8.34	113.38	122.38
8	J	45	CYS	O-C-N	-8.33	113.36	122.03
1	A	907	THR	CB-CA-C	-8.33	93.33	113.15
1	A	1209	MET	CA-C-N	-8.32	109.64	120.13
1	A	1209	MET	C-N-CA	-8.32	109.64	120.13
2	B	798	TYR	CA-C-N	8.32	128.39	119.90
2	B	798	TYR	C-N-CA	8.32	128.39	119.90
1	A	301	ALA	N-CA-C	8.32	120.04	110.97
1	A	895	LYS	N-CA-CB	8.32	123.03	110.22
1	A	549	MET	CG-SD-CE	8.31	119.19	100.90
1	A	567	LYS	CA-C-O	-8.31	108.78	120.16
9	K	64	GLU	N-CA-C	8.31	121.46	111.82
3	C	79	GLN	N-CA-C	-8.30	101.62	112.41
2	B	336	ARG	N-CA-C	8.29	121.24	111.71
2	B	962	LYS	N-CA-C	-8.29	97.53	109.96
1	A	243	PRO	N-CD-CG	-8.28	90.78	103.20
1	A	461	LYS	CB-CA-C	-8.28	96.90	110.14
7	I	106	CYS	CA-CB-SG	8.26	133.41	114.40
1	A	411	ASP	CA-C-O	-8.26	111.51	120.92
2	B	418	LYS	N-CA-C	-8.25	100.60	111.24
2	B	552	MET	CG-SD-CE	8.25	119.05	100.90
1	A	1241	ARG	NE-CZ-NH2	-8.23	111.79	119.20
1	A	859	SER	N-CA-C	-8.23	102.28	111.82
2	B	1185	CYS	CA-CB-SG	8.23	133.32	114.40
10	L	63	ARG	N-CA-CB	8.23	122.23	109.48
1	A	884	ASP	CA-C-O	-8.22	111.75	120.55
2	B	267	ARG	O-C-N	-8.20	112.85	122.93
2	B	1085	ILE	N-CA-C	8.20	119.92	108.12
1	A	557	ASP	CA-C-N	-8.19	105.35	121.41
1	A	557	ASP	C-N-CA	-8.19	105.35	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	589	VAL	N-CA-CB	-8.19	98.02	111.45
1	A	873	MET	N-CA-C	8.19	122.64	110.52
1	A	1348	LEU	N-CA-C	-8.19	102.36	111.28
2	B	362	PRO	CA-C-O	-8.18	107.57	118.86
6	H	23	VAL	CA-C-O	-8.18	111.51	120.67
1	A	801	GLU	OE1-CD-OE2	8.17	142.52	122.90
1	A	941	LYS	CD-CE-NZ	-8.17	85.74	111.90
1	A	1275	GLY	N-CA-C	-8.17	101.24	111.70
1	A	1135	ARG	NE-CZ-NH1	-8.16	113.34	121.50
1	A	531	ILE	N-CA-C	-8.16	100.51	111.44
1	A	896	ARG	NH1-CZ-NH2	8.15	129.90	119.30
1	A	962	ARG	O-C-N	-8.15	110.30	122.28
3	C	108	GLU	N-CA-C	-8.15	101.46	111.40
2	B	646	LEU	N-CA-C	8.14	128.15	110.80
3	C	97	VAL	CA-C-O	-8.14	110.68	121.02
1	A	1064	VAL	N-CA-C	8.14	124.14	113.07
7	I	42	LEU	N-CA-C	8.14	120.87	109.15
2	B	639	ILE	CA-CB-CG1	8.13	124.22	110.40
1	A	465	TYR	O-C-N	-8.12	111.78	122.59
1	A	184	SER	N-CA-C	8.12	123.11	107.44
2	B	1007	VAL	N-CA-CB	-8.12	99.84	111.21
1	A	111	GLY	CA-C-O	8.12	128.40	119.06
9	K	26	LYS	CG-CD-CE	8.11	129.94	111.30
2	B	1166	CYS	N-CA-CB	-8.10	96.80	110.49
2	B	342	GLY	CA-C-O	-8.10	112.52	119.56
2	B	981	ALA	N-CA-C	8.09	121.70	108.99
2	B	100	PRO	N-CD-CG	-8.09	91.06	103.20
6	H	12	VAL	N-CA-C	8.09	120.34	107.73
10	L	34	CYS	CA-CB-SG	-8.08	95.81	114.40
2	B	678	GLU	CB-CG-CD	8.08	126.33	112.60
1	A	244	PRO	N-CA-C	8.08	120.55	110.70
2	B	165	VAL	N-CA-CB	8.08	124.56	111.23
1	A	1341	ILE	N-CA-C	8.07	118.86	110.62
2	B	940	PRO	N-CD-CG	-8.07	91.10	103.20
2	B	836	GLU	O-C-N	8.07	132.51	122.91
1	A	1384	VAL	N-CA-C	8.06	118.74	111.81
1	A	979	SER	CA-C-O	-8.05	112.22	121.72
2	B	963	PHE	CB-CA-C	-8.05	93.47	109.33
1	A	548	ASN	N-CA-C	-8.04	101.80	111.69
2	B	225	VAL	N-CA-C	8.04	121.43	108.97
2	B	942	ARG	CB-CA-C	-8.04	98.54	109.71
5	F	119	ARG	N-CA-C	8.04	120.95	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	498	ARG	NE-CZ-NH1	-8.03	113.47	121.50
1	A	793	SER	N-CA-CB	-8.04	99.35	110.04
2	B	1106	ARG	N-CA-C	8.03	123.03	108.17
2	B	501	PRO	O-C-N	8.03	131.54	123.03
1	A	641	VAL	N-CA-C	-8.03	102.61	110.72
3	C	248	ILE	CB-CA-C	-8.03	101.61	111.88
7	I	43	VAL	N-CA-C	8.01	123.08	113.22
1	A	1012	ARG	CG-CD-NE	-8.01	94.38	112.00
1	A	961	ARG	NE-CZ-NH2	8.01	126.41	119.20
1	A	866	PHE	N-CA-C	-8.01	102.96	112.89
2	B	372	SER	CA-C-O	8.01	129.04	120.55
4	E	204	THR	N-CA-CB	-8.00	99.95	110.59
2	B	684	LEU	N-CA-C	8.00	121.01	111.33
2	B	1183	LYS	N-CA-C	-7.99	93.77	110.80
1	A	170	THR	OG1-CB-CG2	-7.99	93.32	109.30
1	A	649	ILE	N-CA-C	-7.98	102.66	110.72
2	B	1071	VAL	N-CA-C	-7.98	98.36	109.21
3	C	78	GLU	CB-CG-CD	7.98	126.16	112.60
4	E	63	ASN	N-CA-C	7.98	122.31	110.10
2	B	381	MET	CB-CA-C	-7.97	97.30	110.85
1	A	1146	VAL	N-CA-CB	-7.96	99.96	112.07
3	C	14	SER	N-CA-C	-7.96	96.04	108.14
3	C	164	ALA	CA-C-O	-7.96	111.11	120.10
2	B	63	ILE	O-C-N	-7.96	113.86	121.90
3	C	84	ARG	N-CA-C	-7.94	103.38	113.23
1	A	138	ILE	CA-CB-CG2	7.94	124.00	110.50
7	I	55	THR	N-CA-CB	-7.93	98.63	110.61
1	A	1124	HIS	N-CA-C	-7.92	104.57	112.97
1	A	1195	LEU	CA-C-O	7.92	129.25	120.70
4	E	98	ILE	CB-CA-C	7.91	122.84	112.24
1	A	1064	VAL	N-CA-CB	-7.91	90.16	111.75
9	K	6	ARG	N-CA-CB	-7.91	98.03	110.28
4	E	168	TYR	CA-C-O	7.90	128.59	119.35
1	A	1162	VAL	N-CA-C	-7.90	103.71	112.80
2	B	883	LEU	CA-CB-CG	7.90	143.94	116.30
1	A	127	ALA	N-CA-C	7.89	120.79	111.71
1	A	1415	SER	CB-CA-C	-7.89	94.57	109.72
1	A	740	LEU	N-CA-C	-7.89	103.65	113.28
2	B	767	ASN	N-CA-C	-7.89	102.67	111.82
1	A	205	GLU	CB-CA-C	7.88	124.07	110.68
7	I	111	THR	OG1-CB-CG2	-7.88	93.55	109.30
2	B	1064	TYR	CA-C-N	-7.87	108.87	120.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1064	TYR	C-N-CA	-7.87	108.87	120.75
2	B	764	SER	N-CA-CB	-7.87	98.24	110.43
1	A	830	LYS	CB-CA-C	-7.86	98.43	110.92
10	L	25	ALA	CA-C-N	7.86	136.54	121.54
10	L	25	ALA	C-N-CA	7.86	136.54	121.54
2	B	997	GLU	CA-CB-CG	-7.85	98.39	114.10
1	A	640	GLN	O-C-N	-7.84	113.21	122.15
2	B	287	ARG	NE-CZ-NH2	-7.84	112.14	119.20
2	B	1026	LEU	CA-C-O	-7.84	112.11	120.42
1	A	56	PRO	O-C-N	7.83	133.21	122.64
2	B	246	LYS	N-CA-C	7.83	122.58	110.20
1	A	856	THR	N-CA-CB	-7.83	98.28	110.57
1	A	913	LEU	N-CA-CB	-7.82	96.97	111.13
2	B	368	GLU	CA-C-N	-7.82	106.09	121.41
2	B	368	GLU	C-N-CA	-7.82	106.09	121.41
9	K	95	ILE	CA-C-N	7.82	133.77	120.71
9	K	95	ILE	C-N-CA	7.82	133.77	120.71
3	C	185	LYS	N-CA-C	-7.81	103.88	113.41
1	A	1281	ARG	CB-CA-C	-7.81	95.17	109.54
8	J	3	VAL	CB-CA-C	-7.81	97.15	111.36
2	B	461	LEU	N-CA-C	7.80	120.69	111.71
1	A	1170	ILE	N-CA-C	-7.80	102.50	111.00
1	A	890	ASP	N-CA-C	-7.80	102.86	111.36
2	B	642	ASP	CB-CA-C	7.80	124.55	111.30
1	A	562	THR	CA-C-O	-7.79	113.27	119.66
2	B	272	THR	OG1-CB-CG2	-7.79	93.72	109.30
2	B	1192	TYR	CA-C-O	7.79	130.20	121.40
4	E	162	ARG	CB-CG-CD	7.79	129.21	111.30
3	C	3	GLU	CA-C-N	7.77	136.38	121.54
3	C	3	GLU	C-N-CA	7.77	136.38	121.54
2	B	766	ARG	NE-CZ-NH1	-7.77	113.73	121.50
4	E	12	LEU	N-CA-C	-7.77	102.81	111.28
1	A	50	ILE	N-CA-C	7.77	119.47	108.36
10	L	58	LYS	N-CA-C	7.76	127.33	110.80
2	B	712	PRO	N-CD-CG	-7.76	91.56	103.20
7	I	107	SER	CA-C-O	7.75	129.47	120.32
1	A	752	LYS	CG-CD-CE	-7.74	93.50	111.30
1	A	1106	ASN	N-CA-C	7.74	122.30	113.01
2	B	484	ASN	CB-CA-C	-7.74	96.87	109.72
3	C	24	ASN	CB-CA-C	-7.74	100.18	112.09
1	A	81	PHE	CA-C-O	7.73	128.63	120.36
8	J	42	LYS	CA-C-N	-7.72	110.38	121.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	J	42	LYS	C-N-CA	-7.72	110.38	121.42
6	H	77	ARG	NE-CZ-NH1	7.72	129.22	121.50
1	A	917	SER	CA-CB-OG	-7.71	95.67	111.10
2	B	447	ALA	CA-C-N	7.71	132.75	123.19
2	B	447	ALA	C-N-CA	7.71	132.75	123.19
2	B	633	VAL	CB-CA-C	-7.70	99.68	111.31
3	C	230	MET	N-CA-C	7.70	122.29	110.36
7	I	45	ARG	CA-CB-CG	7.69	129.49	114.10
6	H	80	ARG	N-CA-C	-7.69	96.56	108.55
1	A	468	PHE	N-CA-C	-7.68	98.06	110.20
7	I	4	PHE	N-CA-C	7.68	127.16	110.80
1	A	1385	THR	N-CA-C	7.67	132.48	111.00
2	B	463	THR	N-CA-C	7.67	123.11	112.45
8	J	25	LEU	N-CA-C	7.67	121.12	111.69
4	E	80	VAL	CB-CA-C	-7.67	98.90	110.55
9	K	75	ILE	CA-CB-CG1	7.67	123.43	110.40
10	L	41	SER	N-CA-C	7.67	127.13	110.80
1	A	33	ALA	N-CA-C	7.66	121.62	110.28
2	B	691	GLU	CA-CB-CG	7.66	129.43	114.10
1	A	1357	ALA	N-CA-C	7.66	121.89	112.54
9	K	1	MET	CG-SD-CE	7.66	117.75	100.90
3	C	23	SER	N-CA-C	-7.66	96.15	108.55
1	A	1417	GLU	N-CA-C	-7.65	98.48	109.96
1	A	203	SER	N-CA-CB	7.65	121.18	110.17
8	J	17	LYS	CA-C-N	-7.65	109.43	120.29
8	J	17	LYS	C-N-CA	-7.65	109.43	120.29
1	A	110	CYS	CB-CA-C	-7.65	97.85	110.85
6	H	91	ASP	N-CA-C	7.65	120.87	108.41
4	E	21	GLU	CB-CG-CD	7.64	125.60	112.60
8	J	43	ARG	N-CA-C	7.64	122.28	110.20
1	A	932	GLU	CB-CG-CD	7.64	125.59	112.60
1	A	1077	THR	O-C-N	-7.64	113.28	122.22
1	A	170	THR	N-CA-C	-7.64	100.24	110.55
1	A	1111	MET	N-CA-CB	-7.64	98.24	110.46
2	B	21	GLU	N-CA-C	-7.63	103.95	113.18
2	B	988	GLY	CA-C-O	-7.62	112.77	121.68
2	B	106	ASP	CB-CG-OD2	7.62	135.92	118.40
2	B	1129	ARG	CG-CD-NE	-7.62	95.25	112.00
1	A	827	THR	N-CA-C	7.61	119.21	111.07
2	B	1047	PHE	CA-C-O	-7.60	111.55	120.98
10	L	58	LYS	O-C-N	-7.60	112.48	122.59
1	A	876	ALA	N-CA-C	7.60	121.81	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1037	LEU	N-CA-C	7.60	121.25	110.23
1	A	377	PRO	CB-CA-C	-7.59	105.49	111.87
3	C	26	ASP	CA-C-O	7.59	129.66	121.16
1	A	673	GLY	N-CA-C	-7.59	105.58	115.22
2	B	297	ILE	CA-CB-CG1	7.59	123.30	110.40
2	B	1223	ASP	CA-C-N	7.59	135.35	121.70
2	B	1223	ASP	C-N-CA	7.59	135.35	121.70
2	B	1050	ILE	CG1-CB-CG2	-7.58	87.94	110.70
2	B	620	ARG	CA-C-O	7.58	127.48	119.14
1	A	59	GLY	N-CA-C	7.58	131.15	113.18
2	B	435	THR	OG1-CB-CG2	-7.58	94.14	109.30
2	B	996	ARG	N-CA-C	7.58	119.54	111.28
1	A	856	THR	OG1-CB-CG2	-7.58	94.15	109.30
2	B	858	SER	CA-CB-OG	-7.56	95.97	111.10
2	B	336	ARG	CB-CA-C	-7.56	96.64	110.63
2	B	607	GLY	N-CA-C	-7.55	104.66	114.85
2	B	1212	ILE	CA-CB-CG1	-7.55	97.57	110.40
2	B	996	ARG	NE-CZ-NH1	-7.55	113.95	121.50
1	A	1055	ARG	CG-CD-NE	-7.54	95.41	112.00
1	A	1130	GLN	N-CA-C	-7.53	103.90	113.23
2	B	525	ALA	N-CA-C	7.53	122.53	113.12
6	H	140	ALA	N-CA-C	7.53	120.82	107.80
7	I	55	THR	CA-CB-CG2	7.53	123.30	110.50
1	A	99	ILE	N-CA-C	-7.53	102.94	110.62
2	B	245	GLU	CA-CB-CG	7.53	129.15	114.10
10	L	27	LEU	CA-CB-CG	7.53	142.64	116.30
1	A	294	SER	N-CA-C	7.52	121.56	112.38
1	A	655	PHE	CA-C-N	-7.52	109.45	120.28
1	A	655	PHE	C-N-CA	-7.52	109.45	120.28
3	C	4	GLU	O-C-N	7.52	132.59	122.59
4	E	88	VAL	CB-CA-C	7.52	120.23	110.91
1	A	1425	SER	N-CA-C	7.51	119.11	111.07
2	B	1161	HIS	CB-CA-C	7.51	122.97	109.83
2	B	522	VAL	N-CA-CB	-7.51	98.33	111.39
4	E	198	ILE	CA-C-N	-7.50	113.36	123.12
4	E	198	ILE	C-N-CA	-7.50	113.36	123.12
7	I	98	VAL	CA-C-O	-7.49	114.09	121.58
1	A	980	ASP	CB-CA-C	-7.49	97.91	110.56
1	A	1404	GLU	N-CA-C	7.49	122.23	110.17
2	B	899	ILE	N-CA-C	-7.49	101.75	110.21
4	E	180	ARG	N-CA-C	-7.48	103.13	111.28
1	A	98	LYS	CG-CD-CE	-7.48	94.11	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	252	GLN	N-CA-C	-7.47	103.13	111.28
2	B	616	ILE	CA-C-N	-7.47	112.41	122.72
2	B	616	ILE	C-N-CA	-7.47	112.41	122.72
1	A	656	TRP	N-CA-C	7.46	120.29	111.71
7	I	70	ARG	NE-CZ-NH2	-7.46	112.48	119.20
1	A	646	PHE	CA-C-N	-7.46	110.75	120.22
1	A	646	PHE	C-N-CA	-7.46	110.75	120.22
2	B	982	SER	CA-C-O	-7.46	113.45	121.88
1	A	1218	GLN	N-CA-C	-7.46	104.21	113.38
2	B	496	ARG	NE-CZ-NH2	-7.45	112.50	119.20
1	A	495	GLU	CB-CG-CD	7.45	125.26	112.60
1	A	1377	THR	CB-CA-C	-7.45	94.43	109.99
2	B	125	SER	CB-CA-C	7.45	124.10	109.66
2	B	960	GLY	N-CA-C	7.44	125.58	115.32
7	I	6	PHE	CA-C-N	7.44	131.69	121.05
7	I	6	PHE	C-N-CA	7.44	131.69	121.05
2	B	732	SER	CA-C-O	-7.44	113.67	121.55
1	A	514	PRO	CA-C-O	7.43	129.12	118.86
7	I	3	THR	O-C-N	7.42	133.15	123.06
2	B	986	GLN	CA-CB-CG	-7.42	99.27	114.10
2	B	1127	GLY	N-CA-C	7.42	134.81	113.30
5	F	81	THR	N-CA-C	7.42	119.53	110.41
7	I	93	LYS	N-CA-C	-7.42	103.22	111.82
1	A	771	GLU	CG-CD-OE1	-7.41	101.36	118.40
1	A	1299	VAL	N-CA-CB	-7.41	98.66	112.36
1	A	1077	THR	N-CA-C	7.40	120.22	111.71
2	B	412	LEU	N-CA-CB	7.40	121.00	110.12
2	B	642	ASP	N-CA-CB	7.40	121.37	110.35
4	E	162	ARG	CB-CA-C	7.40	123.07	110.79
8	J	7	CYS	CB-CA-C	-7.39	98.75	109.84
2	B	90	ILE	N-CA-C	7.39	124.71	109.34
8	J	48	ARG	CA-CB-CG	7.39	128.88	114.10
3	C	34	ARG	NE-CZ-NH1	7.38	128.88	121.50
1	A	1326	ARG	NH1-CZ-NH2	-7.38	109.71	119.30
4	E	76	GLY	N-CA-C	-7.38	99.93	112.77
1	A	1299	VAL	CB-CA-C	7.37	122.75	110.30
1	A	503	GLN	N-CA-C	-7.35	104.33	113.38
2	B	167	ILE	CB-CA-C	-7.35	99.23	111.29
2	B	654	ARG	NE-CZ-NH1	-7.35	114.15	121.50
1	A	670	ILE	CB-CA-C	-7.35	102.06	110.96
6	H	96	VAL	N-CA-CB	-7.35	100.79	111.52
1	A	497	THR	N-CA-CB	-7.35	99.32	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1010	LEU	CB-CG-CD1	-7.35	88.66	110.70
1	A	646	PHE	CB-CA-C	-7.34	98.37	110.85
1	A	498	ARG	CD-NE-CZ	-7.34	114.12	124.40
2	B	1071	VAL	CA-C-N	-7.34	109.94	123.01
2	B	1071	VAL	C-N-CA	-7.34	109.94	123.01
2	B	866	TYR	N-CA-C	7.34	121.65	113.21
4	E	100	ILE	CB-CA-C	-7.34	102.40	111.87
1	A	90	VAL	N-CA-CB	-7.34	100.11	112.44
1	A	1308	THR	CA-C-O	-7.34	112.68	121.56
2	B	983	ARG	CA-CB-CG	7.34	128.77	114.10
5	F	72	LYS	N-CA-C	7.34	131.54	111.00
1	A	1265	ASN	N-CA-C	7.33	119.91	111.11
1	A	1345	ARG	N-CA-C	-7.33	103.29	111.28
2	B	559	SER	N-CA-C	-7.33	104.14	113.23
4	E	201	LYS	CD-CE-NZ	-7.33	88.44	111.90
1	A	226	GLU	N-CA-CB	7.33	121.72	110.14
10	L	50	ASP	CA-C-N	7.33	134.03	122.74
10	L	50	ASP	C-N-CA	7.33	134.03	122.74
6	H	38	LEU	CB-CA-C	-7.33	98.42	110.14
3	C	66	ARG	CD-NE-CZ	-7.33	114.14	124.40
4	E	125	PRO	N-CA-C	-7.32	98.20	110.21
5	F	135	ARG	CA-C-O	-7.32	112.74	120.58
2	B	170	LEU	CB-CA-C	-7.32	101.50	109.85
1	A	479	ASN	N-CA-C	7.31	121.48	111.54
1	A	1375	MET	CG-SD-CE	7.30	116.96	100.90
2	B	94	LYS	N-CA-C	7.29	120.27	110.35
1	A	855	THR	N-CA-C	-7.29	99.73	110.52
3	C	248	ILE	CB-CG1-CD1	-7.29	98.50	113.80
4	E	181	ALA	N-CA-C	7.28	121.02	112.72
2	B	807	ARG	CG-CD-NE	-7.28	95.99	112.00
7	I	75	CYS	CA-CB-SG	7.28	131.14	114.40
1	A	1199	ARG	O-C-N	7.28	129.59	122.03
6	H	27	GLU	N-CA-C	7.27	120.79	107.99
4	E	28	TYR	N-CA-C	-7.27	98.25	109.52
2	B	400	HIS	N-CA-C	-7.27	98.91	109.59
1	A	410	GLY	N-CA-C	-7.26	105.30	115.32
2	B	605	ARG	NE-CZ-NH1	-7.26	114.23	121.50
3	C	184	ASN	CA-C-N	-7.26	109.10	122.09
3	C	184	ASN	C-N-CA	-7.26	109.10	122.09
1	A	1234	GLU	CA-CB-CG	7.25	128.61	114.10
1	A	615	GLY	O-C-N	-7.25	115.57	122.75
2	B	667	GLN	N-CA-C	7.25	120.91	109.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1019	SER	CA-C-N	-7.25	107.45	121.58
2	B	1019	SER	C-N-CA	-7.25	107.45	121.58
1	A	174	ILE	CG1-CB-CG2	-7.24	88.98	110.70
4	E	96	PHE	N-CA-C	-7.24	102.57	111.40
2	B	1135	ARG	NE-CZ-NH2	-7.23	112.69	119.20
2	B	118	ARG	CD-NE-CZ	7.23	134.52	124.40
2	B	457	LEU	N-CA-C	-7.23	99.83	111.04
3	C	100	THR	OG1-CB-CG2	-7.23	94.84	109.30
7	I	80	SER	N-CA-C	7.23	119.64	110.24
1	A	96	ILE	CA-C-O	7.22	128.56	121.05
1	A	948	VAL	CA-C-N	7.22	133.78	121.14
1	A	948	VAL	C-N-CA	7.22	133.78	121.14
7	I	75	CYS	CB-CA-C	-7.22	98.46	108.86
7	I	7	CYS	CA-CB-SG	7.22	131.01	114.40
1	A	1069	ALA	CA-C-N	7.22	130.54	120.29
1	A	1069	ALA	C-N-CA	7.22	130.54	120.29
1	A	1046	LEU	N-CA-C	7.21	119.22	111.36
4	E	119	SER	CA-C-O	7.21	126.83	118.90
1	A	197	PRO	CA-C-O	-7.21	112.63	122.15
2	B	589	VAL	O-C-N	-7.21	115.05	123.05
1	A	518	LYS	CD-CE-NZ	-7.20	88.85	111.90
2	B	552	MET	CA-CB-CG	7.20	128.50	114.10
6	H	110	ASP	CA-C-N	7.20	134.37	122.07
6	H	110	ASP	C-N-CA	7.20	134.37	122.07
7	I	119	THR	CB-CA-C	-7.19	98.70	110.79
1	A	673	GLY	CA-C-O	-7.19	114.83	119.65
1	A	980	ASP	N-CA-C	7.19	121.76	112.92
2	B	586	TRP	CB-CA-C	7.19	122.78	110.77
2	B	1005	GLY	N-CA-C	7.19	125.66	115.30
3	C	125	MET	CG-SD-CE	7.19	116.71	100.90
5	F	79	ARG	CB-CG-CD	-7.18	94.79	111.30
7	I	55	THR	CA-CB-OG1	-7.18	98.83	109.60
1	A	1136	SER	CB-CA-C	7.17	124.11	109.55
9	K	96	ASN	N-CA-CB	7.17	120.75	110.13
9	K	78	THR	N-CA-CB	7.17	121.40	109.92
1	A	292	ALA	CA-C-O	-7.17	112.82	120.42
1	A	1267	MET	CG-SD-CE	-7.17	85.13	100.90
4	E	21	GLU	CB-CA-C	-7.16	98.50	110.68
2	B	597	MET	CA-C-O	-7.16	113.24	120.90
1	A	621	THR	N-CA-C	7.16	120.49	111.69
1	A	720	ARG	CG-CD-NE	7.16	127.74	112.00
1	A	1445	ILE	O-C-N	7.16	130.75	122.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1405	THR	CA-C-N	7.15	129.57	120.56
1	A	1405	THR	C-N-CA	7.15	129.57	120.56
2	B	402	GLY	CA-C-O	7.15	127.89	119.45
1	A	709	THR	CA-CB-CG2	7.15	122.65	110.50
3	C	142	VAL	N-CA-C	7.14	118.93	109.21
2	B	66	ASP	CA-C-N	7.14	129.72	120.44
2	B	66	ASP	C-N-CA	7.14	129.72	120.44
1	A	1325	THR	N-CA-CB	-7.14	98.76	110.40
5	F	87	LYS	N-CA-C	-7.14	103.54	111.82
1	A	162	VAL	CA-C-O	-7.14	113.71	121.28
1	A	14	VAL	CA-C-O	-7.14	112.94	120.57
6	H	86	ASP	CB-CA-C	7.14	124.62	110.42
2	B	95	ILE	CG1-CB-CG2	-7.13	89.32	110.70
1	A	1203	ASN	CB-CA-C	7.12	122.96	110.85
2	B	1183	LYS	CG-CD-CE	7.12	127.69	111.30
1	A	938	LYS	CG-CD-CE	-7.12	94.92	111.30
7	I	118	ARG	CA-CB-CG	7.12	128.35	114.10
1	A	961	ARG	NE-CZ-NH1	-7.12	114.38	121.50
2	B	1202	LEU	N-CA-C	7.12	118.69	111.07
2	B	523	CYS	CA-C-N	7.12	127.73	120.04
2	B	523	CYS	C-N-CA	7.12	127.73	120.04
1	A	1241	ARG	CG-CD-NE	-7.11	96.35	112.00
2	B	120	ARG	NE-CZ-NH1	-7.11	114.39	121.50
1	A	1202	MET	CG-SD-CE	7.11	116.54	100.90
4	E	17	ARG	CA-C-O	7.11	128.50	120.90
2	B	297	ILE	CA-CB-CG2	-7.11	98.42	110.50
1	A	411	ASP	N-CA-CB	7.10	120.56	109.69
2	B	250	PHE	CA-C-N	7.10	134.75	121.97
2	B	250	PHE	C-N-CA	7.10	134.75	121.97
8	J	7	CYS	N-CA-C	-7.10	99.80	110.24
8	J	18	TRP	N-CA-C	7.10	119.10	111.36
1	A	246	VAL	N-CA-C	7.09	117.86	110.62
1	A	622	VAL	N-CA-CB	-7.09	103.14	112.36
1	A	1329	THR	OG1-CB-CG2	-7.09	95.11	109.30
9	K	16	GLU	CA-C-O	-7.09	113.01	121.66
1	A	1273	LEU	N-CA-C	7.09	120.39	111.24
2	B	266	ALA	CA-C-N	-7.09	111.02	120.95
2	B	266	ALA	C-N-CA	-7.09	111.02	120.95
8	J	64	ASN	CB-CA-C	7.09	123.57	110.10
2	B	880	THR	N-CA-C	7.08	120.18	108.49
3	C	207	CYS	N-CA-C	7.08	118.79	111.14
4	E	150	VAL	O-C-N	-7.08	116.91	121.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	346	GLU	CB-CG-CD	7.08	124.64	112.60
2	B	109	THR	N-CA-C	7.08	125.88	110.80
1	A	992	ASP	N-CA-CB	-7.08	99.69	110.16
4	E	136	ASN	CA-C-O	-7.08	114.05	121.55
2	B	564	GLU	OE1-CD-OE2	7.07	139.88	122.90
3	C	176	ILE	CA-C-O	-7.07	113.08	120.51
7	I	95	THR	N-CA-C	7.07	119.97	110.35
1	A	829	VAL	CA-C-N	7.07	130.62	120.79
1	A	829	VAL	C-N-CA	7.07	130.62	120.79
1	A	593	GLU	N-CA-C	7.07	119.84	111.71
1	A	159	THR	CB-CA-C	-7.07	97.56	110.63
7	I	91	ARG	NE-CZ-NH2	-7.07	112.84	119.20
1	A	728	LYS	CB-CG-CD	7.07	127.55	111.30
3	C	16	ASP	CB-CG-OD2	7.06	134.63	118.40
5	F	107	VAL	CA-C-N	-7.05	111.60	122.60
5	F	107	VAL	C-N-CA	-7.05	111.60	122.60
1	A	855	THR	N-CA-CB	7.05	121.74	110.46
2	B	429	PHE	N-CA-CB	-7.05	100.35	110.57
2	B	217	ARG	CG-CD-NE	-7.04	96.51	112.00
1	A	1433	MET	N-CA-CB	7.03	121.62	110.23
1	A	218	ASP	CA-C-O	-7.03	113.03	120.55
6	H	115	TYR	N-CA-C	7.03	122.03	112.68
1	A	27	VAL	CB-CA-C	-7.03	102.66	112.14
2	B	705	MET	CG-SD-CE	-7.03	85.44	100.90
3	C	207	CYS	CB-CA-C	-7.02	99.80	110.90
1	A	475	THR	CB-CA-C	7.02	122.44	110.79
1	A	1094	VAL	N-CA-C	7.02	118.75	109.21
3	C	198	ALA	N-CA-C	7.02	119.01	111.36
1	A	596	THR	CA-C-O	-7.02	110.48	120.51
1	A	198	GLU	CA-C-O	-7.01	112.96	120.46
1	A	1227	ILE	N-CA-C	-7.01	98.48	108.65
1	A	779	PHE	N-CA-C	-7.01	101.49	110.53
2	B	346	GLU	CA-C-O	-7.01	113.12	120.55
2	B	391	ASP	N-CA-C	-7.01	104.03	112.58
8	J	48	ARG	NE-CZ-NH1	7.01	128.51	121.50
10	L	57	LEU	CB-CA-C	-7.01	99.56	110.78
3	C	192	TRP	O-C-N	-7.00	114.74	123.01
1	A	72	GLU	N-CA-C	7.00	125.72	110.80
2	B	990	ILE	CB-CA-C	-7.00	100.89	111.33
1	A	1271	ILE	CA-CB-CG2	-7.00	98.60	110.50
1	A	1384	VAL	CB-CA-C	-7.00	103.50	111.55
2	B	619	ILE	CA-C-O	-7.00	112.69	120.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	391	ASP	OD1-CG-OD2	-6.99	106.12	122.90
7	I	30	ARG	CG-CD-NE	-6.99	96.62	112.00
10	L	55	ILE	CA-C-N	-6.99	113.14	122.99
10	L	55	ILE	C-N-CA	-6.99	113.14	122.99
1	A	743	VAL	N-CA-C	-6.99	103.49	110.62
2	B	1002	THR	OG1-CB-CG2	-6.99	95.33	109.30
1	A	948	VAL	N-CA-CB	-6.98	96.95	110.78
1	A	917	SER	CB-CA-C	-6.98	99.92	110.88
1	A	620	LYS	CD-CE-NZ	6.98	134.23	111.90
2	B	230	ALA	N-CA-C	6.98	125.23	109.81
1	A	504	LEU	N-CA-CB	-6.98	98.70	110.49
1	A	761	MET	CA-C-O	-6.98	113.02	120.42
6	H	128	ASN	N-CA-C	6.98	125.66	110.80
1	A	419	LYS	CD-CE-NZ	-6.97	89.60	111.90
2	B	598	GLU	CG-CD-OE2	6.97	134.43	118.40
2	B	1176	ASN	CA-C-O	-6.96	112.87	121.02
4	E	153	HIS	O-C-N	-6.96	115.04	123.19
4	E	46	TYR	CA-C-N	-6.96	113.17	122.99
4	E	46	TYR	C-N-CA	-6.96	113.17	122.99
5	F	73	ALA	N-CA-C	6.96	125.62	110.80
3	C	139	GLY	CA-C-O	6.96	128.38	120.03
2	B	1043	ASP	CB-CG-OD2	6.96	134.40	118.40
1	A	728	LYS	CD-CE-NZ	6.95	134.15	111.90
2	B	820	GLY	CA-C-O	-6.95	114.78	121.87
4	E	137	GLU	N-CA-C	-6.95	103.63	111.14
2	B	353	LYS	CD-CE-NZ	6.95	134.14	111.90
10	L	53	HIS	N-CA-C	6.95	121.00	109.46
1	A	923	LEU	N-CA-CB	6.95	121.00	110.30
1	A	1176	LEU	N-CA-C	-6.95	91.54	111.00
2	B	178	ASN	N-CA-C	6.95	121.21	112.87
3	C	165	LYS	CD-CE-NZ	6.94	134.12	111.90
4	E	33	GLU	N-CA-C	-6.94	104.55	113.16
1	A	651	LYS	CB-CA-C	6.94	122.26	110.74
3	C	233	GLU	CA-C-O	-6.94	112.68	120.66
1	A	669	THR	CB-CA-C	-6.93	98.45	110.17
2	B	730	ARG	NE-CZ-NH2	6.93	125.44	119.20
3	C	210	GLU	O-C-N	-6.93	115.50	123.33
1	A	351	THR	N-CA-C	6.93	118.63	108.86
1	A	806	ARG	NE-CZ-NH1	-6.93	114.57	121.50
9	K	63	VAL	CB-CA-C	6.92	120.81	111.19
2	B	228	LYS	CA-C-O	-6.92	113.01	121.11
2	B	990	ILE	CA-CB-CG1	6.92	122.17	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	386	LEU	CA-C-O	-6.92	113.21	120.55
2	B	790	ASP	CB-CA-C	6.92	123.25	110.24
3	C	42	PRO	N-CA-CB	-6.92	97.33	103.35
1	A	393	ARG	CA-C-O	-6.92	112.56	120.24
2	B	895	ASP	N-CA-CB	6.92	121.67	110.40
1	A	1377	THR	N-CA-CB	6.91	121.67	110.40
2	B	267	ARG	N-CA-C	6.91	120.33	109.96
7	I	111	THR	CB-CA-C	-6.91	95.73	109.33
2	B	945	GLU	N-CA-C	6.90	121.30	110.32
1	A	946	VAL	CB-CA-C	-6.90	102.70	112.22
2	B	63	ILE	N-CA-CB	-6.90	99.71	110.54
3	C	78	GLU	O-C-N	-6.90	113.25	122.43
4	E	179	GLN	CG-CD-NE2	-6.90	106.05	116.40
2	B	777	ALA	N-CA-C	-6.90	100.59	110.59
8	J	38	ARG	NE-CZ-NH1	6.90	128.40	121.50
2	B	165	VAL	N-CA-C	6.90	123.68	109.34
1	A	1382	THR	OG1-CB-CG2	-6.89	95.51	109.30
2	B	315	LYS	CB-CA-C	-6.89	99.94	112.76
1	A	1378	GLN	CA-C-N	-6.89	112.80	122.86
1	A	1378	GLN	C-N-CA	-6.89	112.80	122.86
1	A	1165	GLU	CA-C-N	-6.89	111.64	122.73
1	A	1165	GLU	C-N-CA	-6.89	111.64	122.73
1	A	1269	GLU	N-CA-C	6.88	121.72	113.12
2	B	701	ILE	N-CA-C	6.88	123.66	109.34
7	I	45	ARG	N-CA-C	6.88	120.76	109.06
2	B	642	ASP	CA-CB-CG	6.88	119.48	112.60
1	A	664	THR	CB-CA-C	-6.88	95.29	109.94
2	B	723	VAL	N-CA-CB	6.88	122.53	110.49
6	H	21	ASN	N-CA-C	6.87	122.33	113.88
1	A	1137	ALA	CA-C-N	-6.87	115.99	122.66
1	A	1137	ALA	C-N-CA	-6.87	115.99	122.66
1	A	81	PHE	N-CA-C	6.87	119.92	108.73
1	A	843	LYS	CB-CA-C	6.87	121.66	110.88
2	B	408	LEU	N-CA-CB	-6.87	98.33	110.14
3	C	64	ALA	CA-C-O	6.86	127.89	120.20
10	L	55	ILE	CB-CA-C	-6.86	101.03	110.77
1	A	932	GLU	N-CA-C	-6.86	103.73	111.14
2	B	436	VAL	CB-CA-C	6.86	122.54	111.29
3	C	163	ILE	CB-CA-C	6.85	121.66	110.69
1	A	519	PRO	CA-C-O	-6.84	113.62	121.56
2	B	889	THR	CB-CA-C	-6.84	98.24	109.53
3	C	221	TYR	N-CA-C	6.84	120.73	112.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1213	THR	CB-CA-C	-6.84	102.21	110.08
1	A	940	ARG	CG-CD-NE	-6.84	96.95	112.00
7	I	3	THR	CA-C-N	6.84	134.60	121.54
7	I	3	THR	C-N-CA	6.84	134.60	121.54
1	A	751	SER	N-CA-C	6.83	121.36	112.89
1	A	413	ILE	CB-CG1-CD1	-6.83	99.46	113.80
1	A	576	GLN	CA-C-N	-6.83	110.72	120.42
1	A	576	GLN	C-N-CA	-6.83	110.72	120.42
1	A	731	ARG	NH1-CZ-NH2	6.83	128.18	119.30
1	A	738	LYS	CA-C-O	-6.83	113.66	121.72
1	A	66	LYS	CA-CB-CG	6.82	127.73	114.10
2	B	959	ASP	N-CA-C	-6.81	104.72	113.16
1	A	828	ALA	N-CA-C	6.81	118.35	111.07
2	B	204	ILE	CA-C-N	6.81	132.25	123.13
2	B	204	ILE	C-N-CA	6.81	132.25	123.13
5	F	115	THR	OG1-CB-CG2	-6.80	95.69	109.30
2	B	972	LYS	CD-CE-NZ	-6.80	90.14	111.90
3	C	100	THR	CA-CB-OG1	-6.80	99.40	109.60
4	E	73	PRO	CA-C-O	-6.80	108.23	120.60
1	A	1311	VAL	CA-C-O	-6.79	113.16	120.36
2	B	416	LEU	CA-C-O	-6.79	113.91	120.90
3	C	183	TRP	O-C-N	-6.79	113.78	122.20
7	I	30	ARG	NE-CZ-NH1	-6.79	114.71	121.50
9	K	78	THR	N-CA-C	6.79	119.06	110.24
10	L	48	CYS	N-CA-CB	-6.79	98.68	110.76
7	I	120	GLN	N-CA-C	6.78	125.25	110.80
2	B	135	ARG	N-CA-C	-6.78	98.34	108.99
1	A	149	GLU	N-CA-C	6.78	119.57	110.35
9	K	4	PRO	CA-C-O	-6.78	113.35	121.48
1	A	985	ASP	CB-CG-OD1	-6.78	102.82	118.40
2	B	53	GLN	CA-CB-CG	6.78	127.65	114.10
5	F	140	ASP	N-CA-C	6.77	125.22	110.80
10	L	68	GLU	OE1-CD-OE2	-6.77	106.64	122.90
2	B	1103	ILE	N-CA-CB	6.77	122.40	111.23
1	A	295	LEU	CA-C-O	-6.77	112.73	120.24
1	A	918	GLU	N-CA-C	6.76	121.13	113.01
1	A	1284	MET	CA-C-O	-6.76	113.14	120.92
7	I	57	GLY	CA-C-N	-6.76	113.91	122.43
7	I	57	GLY	C-N-CA	-6.76	113.91	122.43
2	B	612	GLU	CA-CB-CG	-6.76	100.57	114.10
1	A	1214	GLU	O-C-N	6.76	131.39	122.33
1	A	70	CYS	CA-CB-SG	6.76	129.94	114.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	181	LEU	N-CA-C	-6.76	104.85	113.23
1	A	119	ASN	N-CA-C	6.76	121.84	112.45
1	A	1317	MET	N-CA-CB	-6.76	99.81	110.22
3	C	263	THR	CA-CB-OG1	-6.75	99.47	109.60
1	A	1015	VAL	O-C-N	-6.75	114.96	122.05
1	A	159	THR	N-CA-CB	6.75	120.62	110.22
1	A	833	GLU	CB-CG-CD	6.75	124.08	112.60
2	B	117	ALA	CA-C-N	-6.75	109.43	120.71
2	B	117	ALA	C-N-CA	-6.75	109.43	120.71
1	A	554	PRO	CA-C-N	-6.75	112.75	122.67
1	A	554	PRO	C-N-CA	-6.75	112.75	122.67
2	B	185	THR	OG1-CB-CG2	-6.75	95.81	109.30
4	E	202	SER	CB-CA-C	-6.75	98.49	109.89
2	B	1168	LEU	CA-C-N	-6.74	112.07	122.05
2	B	1168	LEU	C-N-CA	-6.74	112.07	122.05
1	A	806	ARG	N-CA-C	6.74	119.64	111.82
1	A	857	ARG	NE-CZ-NH1	-6.74	114.76	121.50
1	A	383	TYR	CA-C-O	6.74	127.16	119.27
3	C	15	LYS	CG-CD-CE	6.74	126.80	111.30
2	B	132	VAL	N-CA-C	6.74	119.41	108.97
7	I	54	GLU	CG-CD-OE2	-6.74	102.91	118.40
1	A	964	ILE	CA-C-O	-6.73	112.95	120.96
4	E	84	ASP	N-CA-C	6.73	119.63	111.82
1	A	346	ASP	CA-CB-CG	6.73	119.33	112.60
1	A	1293	SER	N-CA-C	6.73	119.89	110.20
2	B	362	PRO	N-CA-C	6.73	122.31	114.03
2	B	788	ARG	CA-C-N	-6.73	113.26	122.95
2	B	788	ARG	C-N-CA	-6.73	113.26	122.95
9	K	28	PRO	CB-CA-C	6.73	120.77	110.21
2	B	1002	THR	N-CA-CB	-6.73	100.06	110.29
2	B	1135	ARG	NH1-CZ-NH2	6.72	128.04	119.30
7	I	5	ARG	CB-CG-CD	6.72	126.75	111.30
4	E	20	LYS	CA-CB-CG	6.72	127.54	114.10
1	A	930	ASP	N-CA-C	-6.72	104.04	111.36
2	B	652	LYS	CD-CE-NZ	6.71	133.38	111.90
2	B	952	VAL	O-C-N	6.71	130.50	123.05
1	A	277	GLU	CA-CB-CG	6.71	127.52	114.10
2	B	496	ARG	CD-NE-CZ	6.71	133.79	124.40
1	A	451	HIS	CB-CG-CD2	-6.71	122.48	131.20
1	A	128	ILE	CA-CB-CG1	6.71	121.80	110.40
1	A	1161	THR	OG1-CB-CG2	-6.71	95.88	109.30
1	A	1422	ARG	NE-CZ-NH1	6.71	128.21	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	926	GLN	CA-C-O	-6.70	112.53	120.10
2	B	130	VAL	N-CA-C	6.70	123.28	109.34
1	A	393	ARG	NE-CZ-NH2	6.70	125.23	119.20
9	K	93	SER	N-CA-CB	6.70	120.72	110.14
9	K	23	PRO	CA-C-N	-6.69	112.68	122.65
9	K	23	PRO	C-N-CA	-6.69	112.68	122.65
1	A	1211	GLN	N-CA-CB	6.69	120.03	110.13
1	A	1138	ILE	CB-CG1-CD1	-6.69	99.76	113.80
2	B	1184	GLY	N-CA-C	-6.68	106.43	113.58
2	B	527	THR	CB-CA-C	6.68	119.14	109.45
3	C	251	LEU	CB-CA-C	-6.68	100.12	110.81
2	B	1205	GLN	N-CA-C	-6.68	104.07	111.82
6	H	3	ASN	CA-C-N	6.68	133.04	122.36
6	H	3	ASN	C-N-CA	6.68	133.04	122.36
5	F	122	MET	CB-CA-C	-6.67	99.51	110.85
1	A	107	CYS	CA-CB-SG	6.67	129.74	114.40
1	A	926	GLN	O-C-N	6.67	130.03	122.22
2	B	239	GLU	CB-CG-CD	6.67	123.94	112.60
9	K	45	LEU	N-CA-C	-6.67	103.26	111.40
7	I	93	LYS	CA-CB-CG	6.67	127.43	114.10
1	A	1138	ILE	N-CA-C	6.67	117.30	111.90
2	B	1130	PHE	CA-C-N	6.67	128.87	122.27
2	B	1130	PHE	C-N-CA	6.67	128.87	122.27
1	A	96	ILE	CA-CB-CG1	6.66	121.72	110.40
2	B	359	GLU	CB-CA-C	-6.66	99.19	110.64
2	B	285	ILE	CA-C-O	6.66	127.88	120.95
8	J	50	ILE	CB-CA-C	6.66	120.33	111.94
1	A	419	LYS	O-C-N	-6.65	113.74	122.39
2	B	1019	SER	N-CA-CB	6.65	120.54	110.30
6	H	139	ASN	CA-C-N	-6.65	112.80	122.44
6	H	139	ASN	C-N-CA	-6.65	112.80	122.44
1	A	93	VAL	N-CA-C	6.65	117.44	110.72
1	A	935	GLN	CA-C-O	-6.65	112.32	119.97
2	B	615	MET	N-CA-CB	-6.65	99.64	110.81
7	I	84	VAL	CB-CA-C	6.65	120.47	110.90
1	A	1274	ARG	CG-CD-NE	-6.65	97.38	112.00
2	B	942	ARG	CG-CD-NE	-6.64	97.38	112.00
1	A	1067	LEU	N-CA-C	6.64	119.37	111.33
2	B	753	ALA	N-CA-C	-6.64	105.14	113.18
1	A	49	LYS	CB-CG-CD	6.64	126.57	111.30
1	A	351	THR	CA-C-N	6.64	130.38	120.69
1	A	351	THR	C-N-CA	6.64	130.38	120.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	702	LEU	CD1-CG-CD2	-6.64	96.19	110.80
7	I	107	SER	N-CA-C	6.64	120.96	112.86
1	A	1345	ARG	NE-CZ-NH2	-6.63	113.23	119.20
1	A	396	PRO	N-CD-CG	-6.63	93.25	103.20
1	A	1281	ARG	N-CA-C	6.63	119.85	110.50
1	A	1161	THR	N-CA-C	6.63	119.23	108.76
2	B	328	GLU	CA-CB-CG	-6.63	100.85	114.10
4	E	16	PHE	CA-C-O	6.63	127.59	119.97
6	H	102	TYR	N-CA-CB	-6.62	101.41	110.95
1	A	1046	LEU	CA-C-O	6.62	127.44	120.42
8	J	34	THR	N-CA-C	-6.62	103.25	112.45
1	A	829	VAL	CA-C-O	-6.62	114.39	121.27
1	A	524	VAL	N-CA-C	6.61	116.88	108.82
1	A	1284	MET	CG-SD-CE	-6.61	86.37	100.90
7	I	88	SER	CB-CA-C	-6.61	99.93	109.84
1	A	157	ASP	OD1-CG-OD2	-6.60	107.05	122.90
2	B	252	SER	N-CA-CB	6.60	119.79	109.69
2	B	936	ASP	CA-C-O	-6.59	113.12	120.70
6	H	135	LEU	CA-CB-CG	6.59	139.36	116.30
7	I	13	MET	CG-SD-CE	-6.59	86.40	100.90
2	B	780	VAL	N-CA-CB	-6.58	106.06	112.65
1	A	455	MET	CG-SD-CE	-6.58	86.42	100.90
2	B	370	PHE	CB-CA-C	6.58	123.52	110.42
1	A	354	SER	CA-CB-OG	6.58	124.26	111.10
2	B	1181	GLU	CA-CB-CG	6.58	127.26	114.10
6	H	103	LYS	CA-C-O	-6.58	111.10	120.51
1	A	373	THR	N-CA-C	6.58	119.78	111.69
3	C	18	VAL	N-CA-C	-6.58	95.66	109.34
1	A	1239	ARG	N-CA-C	-6.57	97.65	108.76
3	C	161	LYS	N-CA-C	-6.57	101.68	110.55
9	K	78	THR	CB-CA-C	-6.57	98.02	109.64
1	A	400	PRO	CB-CA-C	6.56	122.39	111.56
1	A	144	THR	CA-CB-CG2	6.56	121.66	110.50
1	A	296	LEU	CA-C-N	6.56	130.66	120.82
1	A	296	LEU	C-N-CA	6.56	130.66	120.82
2	B	1055	ILE	CA-CB-CG1	6.56	121.55	110.40
1	A	462	VAL	O-C-N	6.55	130.17	122.83
6	H	80	ARG	NE-CZ-NH2	6.55	125.10	119.20
1	A	581	ALA	N-CA-C	6.55	121.35	113.23
1	A	565	ILE	CG1-CB-CG2	-6.55	91.06	110.70
3	C	20	PHE	CA-C-O	-6.55	114.13	121.40
8	J	43	ARG	CG-CD-NE	-6.55	97.59	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	957	ASN	N-CA-CB	-6.55	99.43	110.49
1	A	421	ALA	CA-C-O	-6.54	113.56	120.63
7	I	3	THR	CB-CA-C	-6.54	102.79	111.82
7	I	98	VAL	CA-CB-CG2	-6.54	99.27	110.40
2	B	20	ASP	N-CA-CB	6.54	119.94	110.06
2	B	774	GLY	N-CA-C	-6.54	104.57	113.27
1	A	1241	ARG	NE-CZ-NH1	6.54	128.04	121.50
6	H	116	TYR	N-CA-C	6.54	124.73	110.80
2	B	205	ILE	CA-C-N	6.53	131.41	122.07
2	B	205	ILE	C-N-CA	6.53	131.41	122.07
2	B	1053	GLU	N-CA-C	-6.53	104.09	111.14
8	J	34	THR	OG1-CB-CG2	-6.53	96.24	109.30
1	A	1006	ILE	CA-CB-CG1	6.53	121.50	110.40
2	B	983	ARG	NE-CZ-NH2	-6.53	113.32	119.20
1	A	592	ASP	CA-C-O	-6.53	111.17	120.51
1	A	710	LEU	O-C-N	-6.53	115.30	122.09
4	E	154	ILE	CB-CA-C	-6.53	101.61	110.42
7	I	109	ILE	CG1-CB-CG2	-6.53	91.12	110.70
3	C	252	GLN	CA-CB-CG	6.53	127.15	114.10
1	A	602	ASP	CA-C-N	6.52	134.61	122.74
1	A	602	ASP	C-N-CA	6.52	134.61	122.74
1	A	545	GLN	N-CA-C	-6.52	104.25	111.36
1	A	1321	GLY	O-C-N	-6.52	113.88	122.42
5	F	119	ARG	NE-CZ-NH2	-6.52	113.33	119.20
2	B	836	GLU	CA-C-O	-6.52	113.89	122.03
1	A	582	ILE	CA-C-O	6.51	122.99	119.15
2	B	209	GLU	N-CA-C	6.51	119.16	109.59
7	I	75	CYS	N-CA-C	6.51	119.27	110.29
1	A	852	TYR	CA-C-O	-6.50	110.59	119.05
1	A	1411	GLU	CA-C-O	6.50	127.31	120.42
2	B	89	GLU	N-CA-C	6.50	129.21	111.00
9	K	40	HIS	CA-C-O	6.50	127.44	119.97
8	J	26	GLN	N-CA-C	-6.50	105.00	113.12
2	B	56	ASP	O-C-N	-6.50	113.89	122.33
1	A	652	VAL	CG1-CB-CG2	-6.49	96.52	110.80
3	C	147	LEU	N-CA-C	6.49	120.11	109.72
7	I	76	PRO	N-CA-C	6.49	123.22	113.81
1	A	1296	GLY	N-CA-C	6.49	120.52	113.58
2	B	242	SER	CB-CA-C	6.49	121.40	109.46
2	B	434	ARG	CG-CD-NE	6.49	126.28	112.00
2	B	1167	GLY	N-CA-C	6.49	128.56	113.18
7	I	52	ILE	CA-C-O	6.49	128.96	120.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I	74	GLU	CA-CB-CG	6.49	127.07	114.10
1	A	1005	GLU	CG-CD-OE1	6.48	133.31	118.40
2	B	736	THR	N-CA-CB	6.48	120.77	110.73
4	E	136	ASN	CA-C-N	6.48	129.25	120.44
4	E	136	ASN	C-N-CA	6.48	129.25	120.44
1	A	1143	LEU	N-CA-C	-6.47	104.26	111.71
2	B	1182	CYS	CA-CB-SG	6.47	129.29	114.40
8	J	50	ILE	N-CA-C	-6.47	104.72	111.58
1	A	733	ALA	CA-C-N	6.47	128.85	120.44
1	A	733	ALA	C-N-CA	6.47	128.85	120.44
1	A	207	ILE	CB-CA-C	-6.46	103.70	111.97
2	B	889	THR	N-CA-CB	6.46	120.70	110.23
2	B	911	ILE	CA-CB-CG2	6.46	121.49	110.50
1	A	205	GLU	CB-CG-CD	6.46	123.59	112.60
5	F	82	THR	N-CA-CB	6.46	119.54	110.11
6	H	131	ASN	N-CA-CB	6.46	119.38	110.01
1	A	1197	LEU	CA-C-O	6.46	129.54	121.66
1	A	790	ASP	CA-C-O	-6.46	114.05	121.54
1	A	1241	ARG	N-CA-C	-6.46	99.26	109.07
9	K	26	LYS	O-C-N	-6.46	114.67	122.22
2	B	910	VAL	CB-CA-C	-6.45	102.73	111.63
2	B	41	LYS	N-CA-C	-6.45	105.57	113.50
2	B	986	GLN	CG-CD-NE2	6.45	126.08	116.40
2	B	593	PRO	N-CA-C	-6.44	105.47	113.84
1	A	586	ILE	CB-CG1-CD1	-6.44	100.28	113.80
1	A	11	LEU	CD1-CG-CD2	-6.44	96.64	110.80
7	I	45	ARG	CD-NE-CZ	-6.44	115.39	124.40
8	J	6	ARG	O-C-N	6.44	131.56	123.19
3	C	172	PRO	O-C-N	6.44	131.33	122.64
4	E	25	ASP	OD1-CG-OD2	-6.44	107.45	122.90
2	B	36	ALA	N-CA-C	-6.43	104.35	111.36
2	B	68	THR	OG1-CB-CG2	-6.43	96.43	109.30
1	A	910	PRO	N-CD-CG	-6.43	93.55	103.20
1	A	1042	PHE	N-CA-C	-6.43	104.19	111.07
2	B	945	GLU	CG-CD-OE2	-6.43	103.60	118.40
2	B	1013	ASN	CB-CA-C	6.43	117.22	109.31
3	C	84	ARG	NE-CZ-NH2	6.43	124.99	119.20
2	B	574	SER	N-CA-C	6.43	120.25	108.94
1	A	1005	GLU	CG-CD-OE2	-6.42	103.62	118.40
1	A	291	GLU	N-CA-C	-6.42	103.79	111.69
2	B	298	LEU	N-CA-C	-6.42	104.14	112.23
2	B	357	GLN	N-CA-C	-6.42	104.93	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	97	ARG	CG-CD-NE	-6.42	97.87	112.00
2	B	373	ARG	N-CA-C	6.42	118.28	111.28
2	B	398	ARG	CB-CA-C	-6.42	97.65	110.42
1	A	1003	LYS	CA-CB-CG	-6.42	101.27	114.10
2	B	530	GLY	N-CA-C	6.42	120.80	111.24
1	A	235	ILE	CB-CA-C	6.41	119.56	110.84
2	B	97	VAL	CB-CA-C	6.41	119.87	110.77
2	B	999	MET	CG-SD-CE	-6.41	86.80	100.90
4	E	167	ARG	NE-CZ-NH1	-6.41	115.09	121.50
2	B	451	LYS	O-C-N	-6.41	114.07	122.59
10	L	55	ILE	N-CA-C	6.41	117.11	107.75
9	K	111	LEU	CD1-CG-CD2	6.41	124.89	110.80
1	A	369	SER	N-CA-C	6.40	119.07	111.71
5	F	107	VAL	O-C-N	-6.40	116.31	123.03
7	I	66	PRO	CB-CA-C	-6.40	101.77	111.44
1	A	491	VAL	O-C-N	-6.40	117.34	121.37
1	A	1163	ILE	O-C-N	6.40	126.81	120.92
2	B	876	LYS	CA-C-O	-6.40	111.39	120.16
1	A	446	ARG	NE-CZ-NH1	-6.40	115.10	121.50
2	B	194	GLU	CB-CA-C	6.40	120.30	109.75
3	C	68	GLY	CA-C-N	-6.40	110.16	122.06
3	C	68	GLY	C-N-CA	-6.40	110.16	122.06
1	A	1228	TRP	CA-CB-CG	6.39	125.75	113.60
2	B	996	ARG	NE-CZ-NH2	-6.39	113.45	119.20
1	A	788	SER	CB-CA-C	6.39	120.34	109.80
3	C	75	MET	CB-CA-C	6.39	121.40	110.79
4	E	53	PRO	N-CD-CG	-6.39	93.61	103.20
2	B	1131	GLY	N-CA-C	6.39	121.99	112.41
2	B	1183	LYS	CB-CA-C	6.39	123.13	110.42
1	A	291	GLU	CA-CB-CG	6.38	126.87	114.10
1	A	459	ARG	NE-CZ-NH1	6.38	127.88	121.50
2	B	968	VAL	CA-C-O	-6.38	113.29	121.40
1	A	857	ARG	NE-CZ-NH2	6.38	124.94	119.20
1	A	1004	ASN	N-CA-CB	-6.38	101.61	110.29
2	B	896	ASP	N-CA-CB	6.38	120.40	110.44
1	A	364	VAL	CA-CB-CG1	6.38	121.25	110.40
2	B	529	GLU	CA-C-O	6.38	128.81	121.47
8	J	48	ARG	CD-NE-CZ	6.38	133.33	124.40
1	A	926	GLN	N-CA-CB	6.38	120.04	110.22
7	I	18	GLU	CB-CA-C	6.38	120.26	109.80
2	B	416	LEU	N-CA-CB	6.37	119.22	109.98
3	C	172	PRO	CB-CA-C	-6.37	101.05	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	204	SER	N-CA-CB	-6.37	101.00	110.17
2	B	983	ARG	NE-CZ-NH1	6.37	127.87	121.50
4	E	10	SER	CB-CA-C	-6.37	101.15	110.96
1	A	613	ILE	CA-CB-CG2	6.37	121.32	110.50
9	K	26	LYS	N-CA-C	6.37	119.03	111.71
1	A	123	ARG	N-CA-CB	6.36	120.14	110.28
2	B	477	ALA	CB-CA-C	6.36	120.05	110.50
3	C	248	ILE	O-C-N	-6.36	115.58	121.94
6	H	32	THR	OG1-CB-CG2	-6.36	96.58	109.30
1	A	207	ILE	CA-CB-CG1	6.36	121.21	110.40
1	A	285	PRO	CA-C-N	6.36	133.69	121.54
1	A	285	PRO	C-N-CA	6.36	133.69	121.54
4	E	11	ARG	NH1-CZ-NH2	6.36	127.57	119.30
6	H	139	ASN	CA-CB-CG	6.36	118.96	112.60
1	A	1267	MET	CB-CA-C	6.36	121.39	110.84
2	B	643	ASP	CA-CB-CG	6.36	118.96	112.60
10	L	58	LYS	CA-C-N	-6.36	109.40	121.54
10	L	58	LYS	C-N-CA	-6.36	109.40	121.54
6	H	16	ASP	CB-CA-C	-6.36	99.11	109.41
1	A	1280	GLU	CG-CD-OE2	6.35	133.01	118.40
1	A	1073	GLY	N-CA-C	6.35	119.87	112.50
2	B	1028	GLU	CB-CA-C	-6.35	100.05	110.85
1	A	1003	LYS	CB-CG-CD	6.35	125.90	111.30
1	A	1316	VAL	N-CA-C	6.35	118.98	111.05
2	B	106	ASP	CA-CB-CG	6.34	118.94	112.60
1	A	52	GLY	CA-C-O	-6.34	109.53	120.57
2	B	706	GLN	CG-CD-NE2	6.34	125.91	116.40
2	B	1183	LYS	O-C-N	-6.34	114.16	122.59
2	B	538	ASN	N-CA-CB	-6.34	100.16	110.81
3	C	7	GLN	N-CA-C	6.34	120.16	109.76
1	A	474	VAL	N-CA-CB	-6.34	101.44	112.08
2	B	780	VAL	CB-CA-C	-6.34	104.83	111.23
1	A	984	LYS	N-CA-C	6.33	119.17	111.82
7	I	25	LEU	N-CA-C	6.33	119.03	108.96
2	B	119	LEU	O-C-N	6.33	129.37	122.15
4	E	98	ILE	CA-C-N	6.33	129.09	120.54
4	E	98	ILE	C-N-CA	6.33	129.09	120.54
2	B	657	HIS	N-CA-C	-6.33	104.46	111.36
1	A	1136	SER	N-CA-CB	-6.33	100.57	110.44
1	A	1291	VAL	N-CA-CB	-6.33	104.87	111.64
1	A	203	SER	N-CA-C	-6.33	101.58	110.50
1	A	351	THR	CB-CA-C	-6.33	96.47	111.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	968	GLN	CA-CB-CG	-6.33	101.45	114.10
4	E	189	GLY	N-CA-C	6.33	122.72	113.48
9	K	71	PHE	N-CA-CB	6.33	121.87	111.62
9	K	107	THR	O-C-N	6.33	128.86	122.03
2	B	950	ASP	N-CA-CB	-6.32	102.59	111.00
9	K	96	ASN	N-CA-C	-6.32	103.69	111.40
1	A	861	GLY	N-CA-C	-6.32	106.52	115.43
2	B	566	LEU	N-CA-C	6.32	118.17	111.28
1	A	96	ILE	CG1-CB-CG2	-6.32	91.75	110.70
2	B	216	GLU	CA-C-O	-6.31	113.49	120.69
1	A	416	ARG	NE-CZ-NH2	-6.31	113.52	119.20
2	B	365	THR	OG1-CB-CG2	-6.31	96.67	109.30
2	B	710	LEU	N-CA-C	6.31	119.10	111.40
2	B	962	LYS	N-CA-CB	6.31	119.26	109.85
2	B	1210	MET	CA-C-N	-6.31	113.77	124.31
2	B	1210	MET	C-N-CA	-6.31	113.77	124.31
2	B	552	MET	O-C-N	-6.31	114.86	120.48
7	I	119	THR	N-CA-CB	6.31	119.47	110.13
1	A	226	GLU	CA-C-O	-6.30	113.14	120.20
5	F	97	ARG	CB-CG-CD	6.30	125.80	111.30
1	A	53	LEU	CA-CB-CG	6.30	138.35	116.30
1	A	413	ILE	N-CA-C	6.30	117.56	107.73
1	A	1080	THR	CA-CB-CG2	6.30	121.21	110.50
2	B	969	ARG	N-CA-C	6.30	119.21	109.07
1	A	5	GLN	N-CA-CB	6.30	119.36	110.36
1	A	129	LYS	N-CA-CB	-6.30	101.27	110.40
2	B	108	VAL	CB-CA-C	6.30	121.62	111.29
1	A	407	ARG	NE-CZ-NH2	-6.29	113.54	119.20
1	A	413	ILE	CB-CA-C	-6.29	103.26	111.25
1	A	720	ARG	NE-CZ-NH2	6.29	124.86	119.20
3	C	94	LYS	CA-CB-CG	6.29	126.69	114.10
3	C	235	VAL	CA-C-O	6.29	126.47	119.42
4	E	55	ARG	N-CA-C	6.29	117.94	111.14
9	K	23	PRO	CA-C-O	-6.29	114.24	121.98
1	A	285	PRO	CA-C-O	-6.29	114.25	121.36
2	B	626	ILE	N-CA-CB	-6.29	100.29	111.93
1	A	446	ARG	CG-CD-NE	6.29	125.83	112.00
1	A	894	GLU	CA-C-O	-6.29	112.74	119.97
1	A	979	SER	N-CA-C	-6.29	101.21	110.52
2	B	209	GLU	N-CA-CB	-6.29	100.03	109.71
4	E	107	THR	N-CA-C	6.29	119.74	109.24
1	A	1265	ASN	O-C-N	-6.29	115.55	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	J	45	CYS	CA-CB-SG	6.29	128.85	114.40
10	L	28	LYS	O-C-N	-6.29	114.23	122.59
1	A	1360	GLY	N-CA-C	6.28	123.72	115.36
1	A	830	LYS	N-CA-CB	6.28	119.37	109.82
1	A	1427	ASN	N-CA-C	6.28	118.93	111.71
2	B	852	ARG	NH1-CZ-NH2	-6.28	111.14	119.30
1	A	1420	ASP	N-CA-C	6.28	120.40	112.87
2	B	407	ASP	CA-C-O	6.28	127.23	120.32
3	C	96	SER	CA-CB-OG	6.28	123.65	111.10
1	A	512	VAL	CA-CB-CG1	6.28	121.07	110.40
1	A	1135	ARG	CA-C-N	-6.28	110.61	121.66
1	A	1135	ARG	C-N-CA	-6.28	110.61	121.66
1	A	854	ASN	N-CA-CB	-6.27	102.93	113.15
2	B	1043	ASP	N-CA-CB	6.27	119.33	110.24
4	E	121	MET	N-CA-C	-6.27	104.73	112.38
1	A	435	HIS	CA-C-O	-6.27	114.90	121.55
9	K	94	ILE	O-C-N	6.27	128.65	121.94
1	A	1445	ILE	CA-C-O	-6.27	113.70	120.85
2	B	1212	ILE	N-CA-C	6.27	117.82	108.23
2	B	213	ILE	N-CA-C	-6.26	99.40	108.36
2	B	1158	PHE	N-CA-C	6.26	124.14	110.80
2	B	203	PHE	N-CA-CB	-6.26	100.83	110.85
4	E	108	GLY	CA-C-O	6.26	131.47	120.57
2	B	1065	GLN	CA-C-O	-6.26	114.91	121.55
1	A	454	SER	N-CA-C	-6.26	105.64	113.28
2	B	201	GLY	CA-C-O	6.26	126.26	119.06
2	B	452	THR	CA-C-N	6.26	133.23	121.97
2	B	452	THR	C-N-CA	6.26	133.23	121.97
2	B	1041	GLU	N-CA-CB	6.26	118.82	109.19
1	A	934	LYS	N-CA-CB	6.25	119.31	110.12
1	A	1235	LYS	CB-CA-C	6.25	120.64	109.38
1	A	742	ASN	N-CA-C	-6.25	104.35	112.23
3	C	10	ILE	CB-CA-C	-6.25	101.04	111.29
2	B	1055	ILE	CB-CG1-CD1	-6.25	100.68	113.80
2	B	348	ARG	N-CA-C	6.25	118.61	111.11
4	E	161	LYS	CA-CB-CG	6.25	126.59	114.10
8	J	20	SER	N-CA-C	6.25	118.90	111.71
1	A	1233	ASP	N-CA-C	-6.25	105.62	113.18
2	B	105	SER	CA-CB-OG	6.25	123.59	111.10
2	B	482	VAL	N-CA-C	6.24	117.10	109.30
7	I	119	THR	O-C-N	6.24	129.72	122.17
1	A	365	GLY	O-C-N	-6.24	116.59	122.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1141	THR	OG1-CB-CG2	-6.24	96.82	109.30
1	A	1309	ASP	CB-CA-C	-6.24	100.79	110.78
6	H	18	GLY	O-C-N	-6.24	114.58	122.70
1	A	412	ARG	CA-C-O	-6.24	114.05	120.54
1	A	74	MET	CG-SD-CE	6.24	114.62	100.90
2	B	660	LYS	N-CA-C	-6.24	104.54	111.71
6	H	17	PRO	N-CA-C	-6.24	106.69	114.68
1	A	207	ILE	N-CA-CB	6.24	117.85	110.55
1	A	420	ARG	NE-CZ-NH1	6.23	127.73	121.50
2	B	497	ARG	NE-CZ-NH2	-6.23	113.59	119.20
2	B	498	THR	CA-CB-OG1	6.23	118.95	109.60
2	B	968	VAL	N-CA-C	6.23	118.36	108.89
7	I	110	PHE	CA-C-O	-6.23	114.53	121.51
2	B	579	ARG	NE-CZ-NH1	-6.23	115.27	121.50
6	H	56	THR	N-CA-C	-6.23	97.55	108.20
2	B	242	SER	O-C-N	-6.23	115.92	122.96
2	B	1078	GLY	N-CA-C	6.23	127.94	113.18
1	A	1316	VAL	CB-CA-C	-6.22	102.51	112.16
4	E	17	ARG	CG-CD-NE	-6.22	98.31	112.00
8	J	36	LEU	N-CA-C	-6.22	104.58	111.36
2	B	103	ASN	CA-CB-CG	6.22	118.82	112.60
1	A	241	VAL	O-C-N	6.22	125.29	121.37
3	C	124	LEU	CA-C-O	-6.22	111.27	119.10
1	A	1215	ARG	N-CA-CB	6.21	119.33	110.13
3	C	113	VAL	O-C-N	-6.21	115.83	123.10
1	A	919	ILE	N-CA-C	-6.21	106.66	113.43
2	B	1098	MET	CG-SD-CE	6.21	114.56	100.90
2	B	1151	LEU	O-C-N	-6.21	114.89	122.34
9	K	46	ILE	O-C-N	-6.21	115.83	121.91
1	A	172	PRO	CA-C-O	6.21	129.24	121.67
2	B	171	PRO	N-CD-CG	-6.21	93.89	103.20
9	K	22	ASP	CB-CG-OD1	6.21	132.67	118.40
2	B	1018	PRO	CA-C-O	-6.20	110.22	119.34
5	F	113	GLY	N-CA-C	6.20	122.07	114.69
7	I	83	ASN	CB-CA-C	-6.20	97.62	109.66
1	A	1242	VAL	N-CA-CB	-6.20	101.00	111.23
1	A	921	GLY	CA-C-N	-6.20	112.73	121.72
1	A	921	GLY	C-N-CA	-6.20	112.73	121.72
7	I	91	ARG	NE-CZ-NH1	6.20	127.70	121.50
1	A	694	THR	N-CA-C	6.20	117.70	111.07
1	A	1326	ARG	NE-CZ-NH2	6.20	124.78	119.20
5	F	94	LEU	CA-C-N	-6.20	109.26	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	94	LEU	C-N-CA	-6.20	109.26	121.41
1	A	1053	PHE	CA-C-N	-6.20	110.89	120.31
1	A	1053	PHE	C-N-CA	-6.20	110.89	120.31
1	A	1015	VAL	CB-CA-C	6.20	119.72	111.85
4	E	75	MET	CB-CA-C	6.20	120.45	110.29
2	B	97	VAL	N-CA-C	-6.19	98.71	107.75
4	E	139	ALA	CA-C-O	-6.19	111.76	119.38
2	B	1064	TYR	O-C-N	-6.19	115.98	123.10
6	H	110	ASP	O-C-N	6.19	129.89	122.21
1	A	415	LEU	CA-C-N	-6.19	111.01	122.09
1	A	415	LEU	C-N-CA	-6.19	111.01	122.09
1	A	1208	THR	CB-CA-C	-6.19	99.04	109.50
2	B	802	PRO	O-C-N	6.19	130.02	123.03
6	H	87	ARG	CA-CB-CG	6.19	126.48	114.10
1	A	12	ARG	NE-CZ-NH2	-6.19	113.63	119.20
1	A	991	LYS	O-C-N	-6.19	115.10	122.15
6	H	117	SER	CB-CA-C	-6.19	100.61	110.14
1	A	815	PHE	N-CA-C	-6.19	104.64	111.82
1	A	1019	CYS	CA-C-O	-6.19	113.11	120.10
4	E	99	HIS	N-CA-CB	6.18	119.16	109.94
1	A	1445	ILE	CA-C-N	6.18	131.43	122.16
1	A	1445	ILE	C-N-CA	6.18	131.43	122.16
4	E	16	PHE	CB-CA-C	6.18	122.54	110.67
9	K	18	LYS	N-CA-CB	6.18	118.97	110.01
1	A	35	ILE	N-CA-C	6.18	122.19	109.34
6	H	106	GLU	CB-CA-C	6.18	122.26	110.27
1	A	1318	THR	CB-CA-C	6.18	120.40	109.65
2	B	1139	ILE	CA-C-O	-6.18	114.30	120.85
6	H	81	PRO	N-CA-C	6.18	118.23	110.70
6	H	130	ARG	NE-CZ-NH1	-6.18	115.32	121.50
1	A	844	ALA	CA-C-O	-6.17	113.96	120.63
1	A	1403	GLU	N-CA-C	6.17	123.95	110.80
2	B	1006	ILE	CG1-CB-CG2	-6.17	92.19	110.70
1	A	704	ALA	CA-C-O	-6.17	114.53	121.81
1	A	1160	SER	N-CA-C	-6.17	100.68	108.45
2	B	907	GLY	N-CA-C	-6.17	100.12	111.34
3	C	63	ILE	CB-CG1-CD1	-6.17	100.85	113.80
1	A	1033	GLN	CA-C-O	-6.16	112.39	119.60
2	B	939	THR	N-CA-C	6.16	118.82	110.31
5	F	79	ARG	CA-CB-CG	6.16	126.43	114.10
9	K	114	LEU	CA-CB-CG	6.16	137.87	116.30
10	L	70	ARG	NE-CZ-NH1	6.16	127.66	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	567	LYS	CD-CE-NZ	6.16	131.62	111.90
1	A	1171	GLN	N-CA-C	-6.16	104.62	111.71
1	A	1259	MET	CA-C-N	-6.16	112.43	120.44
1	A	1259	MET	C-N-CA	-6.16	112.43	120.44
1	A	1328	TYR	N-CA-C	6.16	118.78	109.23
2	B	789	MET	CB-CA-C	-6.16	101.69	111.17
2	B	955	THR	CB-CA-C	-6.15	99.47	112.82
1	A	974	ASP	O-C-N	6.15	130.20	123.13
1	A	1069	ALA	N-CA-C	6.15	118.06	111.36
3	C	33	LEU	CB-CA-C	6.15	121.95	110.70
3	C	260	LEU	CA-C-O	6.15	126.94	119.38
8	J	28	ASP	CB-CA-C	-6.15	100.11	110.44
8	J	29	GLU	N-CA-C	6.14	120.10	112.24
2	B	909	ASP	CB-CG-OD2	6.14	132.53	118.40
10	L	47	ARG	NE-CZ-NH2	6.14	124.73	119.20
1	A	941	LYS	N-CA-CB	6.14	118.89	109.98
9	K	110	ASN	CB-CA-C	6.14	121.72	110.11
1	A	229	SER	O-C-N	-6.14	114.71	123.06
1	A	778	GLY	N-CA-C	6.14	122.27	114.66
1	A	590	ARG	NE-CZ-NH2	-6.14	113.68	119.20
1	A	607	ILE	N-CA-C	-6.13	99.87	108.27
7	I	24	ARG	N-CA-CB	6.13	122.37	111.69
1	A	1285	MET	CG-SD-CE	6.13	114.39	100.90
1	A	586	ILE	O-C-N	6.13	129.88	123.26
6	H	103	LYS	CB-CG-CD	6.13	125.40	111.30
1	A	751	SER	CA-C-O	-6.13	111.71	119.31
1	A	833	GLU	CG-CD-OE1	6.13	132.50	118.40
2	B	222	ILE	N-CA-CB	-6.13	102.92	111.25
2	B	680	THR	OG1-CB-CG2	-6.13	97.04	109.30
4	E	98	ILE	N-CA-C	-6.13	104.32	111.00
2	B	463	THR	CB-CA-C	-6.13	98.53	110.11
2	B	900	ALA	O-C-N	-6.13	115.90	121.66
7	I	35	VAL	CA-C-O	6.12	127.58	121.45
1	A	189	ARG	N-CA-C	6.12	120.06	112.59
1	A	7	SER	N-CA-C	6.12	118.38	108.34
6	H	126	GLU	CA-C-O	-6.12	114.90	121.94
2	B	795	ILE	CB-CA-C	-6.12	101.08	110.50
1	A	636	GLU	CA-C-N	-6.12	112.75	122.29
1	A	636	GLU	C-N-CA	-6.12	112.75	122.29
6	H	11	GLN	CB-CA-C	-6.12	100.16	110.19
9	K	18	LYS	N-CA-C	6.12	117.62	111.07
2	B	644	GLU	N-CA-CB	-6.12	100.15	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	35	SER	CB-CA-C	-6.12	99.32	110.63
2	B	888	GLY	CA-C-O	-6.12	113.59	122.52
1	A	788	SER	CA-CB-OG	-6.11	98.87	111.10
2	B	1008	PRO	CA-C-O	6.11	128.81	121.48
8	J	26	GLN	CB-CA-C	6.11	119.65	109.56
10	L	26	THR	CA-CB-CG2	6.11	120.89	110.50
2	B	710	LEU	CD1-CG-CD2	-6.11	97.36	110.80
6	H	130	ARG	CA-C-N	6.11	128.38	120.44
6	H	130	ARG	C-N-CA	6.11	128.38	120.44
2	B	265	SER	CA-CB-OG	6.11	123.31	111.10
5	F	149	GLU	N-CA-CB	6.11	119.04	109.94
1	A	478	TYR	N-CA-C	-6.10	105.83	113.28
2	B	847	ASP	N-CA-C	-6.10	104.63	111.28
6	H	5	LEU	N-CA-C	6.10	123.80	110.80
1	A	811	GLN	N-CA-C	-6.10	104.63	111.28
2	B	975	GLN	CB-CA-C	-6.10	97.33	110.45
1	A	748	MET	N-CA-C	6.10	118.01	111.36
2	B	25	ILE	CB-CG1-CD1	-6.10	100.99	113.80
1	A	305	ASP	N-CA-C	6.10	128.07	111.00
1	A	469	ARG	CG-CD-NE	-6.09	98.59	112.00
2	B	964	VAL	CA-CB-CG2	-6.09	100.04	110.40
1	A	105	CYS	CA-C-O	6.09	125.49	118.97
1	A	1266	THR	CB-CA-C	6.09	120.56	110.81
2	B	41	LYS	CB-CA-C	6.09	120.38	109.29
3	C	123	ASN	O-C-N	-6.09	114.90	122.82
2	B	896	ASP	N-CA-C	-6.09	105.68	113.23
1	A	1134	ILE	CG1-CB-CG2	-6.09	92.44	110.70
3	C	93	ASP	N-CA-C	-6.08	105.86	113.28
2	B	1183	LYS	CA-CB-CG	6.08	126.26	114.10
7	I	54	GLU	N-CA-C	-6.08	104.66	111.28
2	B	1201	LYS	CA-C-N	-6.08	112.54	120.44
2	B	1201	LYS	C-N-CA	-6.08	112.54	120.44
2	B	448	ILE	N-CA-C	6.07	116.67	108.17
4	E	212	ARG	NE-CZ-NH2	-6.07	113.73	119.20
1	A	685	GLU	N-CA-C	-6.06	104.59	112.23
1	A	1236	LEU	N-CA-C	6.06	118.57	108.20
9	K	48	ALA	N-CA-C	6.06	118.85	111.82
2	B	120	ARG	N-CA-C	6.06	120.54	113.20
2	B	576	ASP	N-CA-C	-6.06	105.75	113.02
2	B	1047	PHE	N-CA-C	6.06	120.04	111.92
2	B	728	ARG	N-CA-C	6.06	118.59	110.35
1	A	411	ASP	O-C-N	6.06	130.46	122.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	253	LYS	N-CA-C	6.06	118.85	111.82
2	B	796	LEU	N-CA-CB	-6.06	101.08	110.29
1	A	93	VAL	N-CA-CB	6.05	119.66	110.58
1	A	1424	VAL	CB-CA-C	-6.05	103.86	112.22
2	B	268	THR	CA-CB-CG2	6.05	120.79	110.50
2	B	649	LYS	N-CA-C	-6.05	99.79	109.96
9	K	49	GLU	CA-C-O	-6.05	114.46	120.82
1	A	472	LEU	CA-CB-CG	-6.05	95.12	116.30
8	J	36	LEU	CA-C-N	-6.04	109.85	121.94
8	J	36	LEU	C-N-CA	-6.04	109.85	121.94
5	F	153	VAL	CA-C-O	-6.04	113.78	120.97
7	I	1	MET	CG-SD-CE	6.04	114.19	100.90
1	A	79	GLY	N-CA-C	-6.04	98.87	113.18
2	B	728	ARG	NE-CZ-NH1	-6.04	115.46	121.50
1	A	32	VAL	N-CA-CB	-6.04	101.27	111.23
1	A	102	VAL	O-C-N	6.04	127.83	121.91
1	A	591	PHE	CB-CA-C	6.04	120.16	109.72
2	B	41	LYS	CB-CG-CD	6.04	125.18	111.30
2	B	627	PHE	CB-CA-C	-6.04	100.85	110.14
7	I	68	LEU	CA-C-N	-6.04	114.06	120.03
7	I	68	LEU	C-N-CA	-6.04	114.06	120.03
2	B	840	ILE	O-C-N	-6.03	116.07	122.83
1	A	586	ILE	CA-C-N	6.03	132.46	122.33
1	A	586	ILE	C-N-CA	6.03	132.46	122.33
1	A	80	HIS	CB-CA-C	6.03	120.56	109.71
4	E	154	ILE	CG1-CB-CG2	-6.03	92.61	110.70
1	A	109	HIS	CB-CA-C	6.03	122.79	112.00
1	A	563	PRO	CA-C-O	6.03	128.54	121.31
1	A	476	SER	CA-CB-OG	-6.03	99.04	111.10
1	A	1198	ASP	N-CA-C	6.03	118.54	108.96
2	B	49	ASP	CA-C-O	6.03	126.91	120.10
6	H	54	SER	N-CA-C	6.03	118.34	109.24
4	E	109	ILE	CB-CA-C	-6.03	101.64	110.62
6	H	58	THR	N-CA-C	6.03	118.66	107.99
1	A	481	ASP	CA-C-O	-6.02	114.21	121.32
1	A	1017	LEU	CA-C-N	-6.02	112.21	120.28
1	A	1017	LEU	C-N-CA	-6.02	112.21	120.28
3	C	222	LYS	N-CA-CB	6.02	119.50	110.53
2	B	394	ASP	CB-CG-OD2	6.02	132.24	118.40
5	F	135	ARG	NE-CZ-NH1	-6.02	115.48	121.50
3	C	15	LYS	N-CA-C	-6.02	105.43	112.89
2	B	1220	ARG	NE-CZ-NH2	6.01	124.61	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	437	MET	CB-CA-C	-6.01	97.44	111.09
2	B	664	THR	CA-C-N	6.01	128.66	120.54
2	B	664	THR	C-N-CA	6.01	128.66	120.54
2	B	706	GLN	CB-CG-CD	6.01	122.82	112.60
2	B	969	ARG	CD-NE-CZ	-6.01	115.99	124.40
7	I	39	GLY	CA-C-O	-6.01	114.17	120.90
9	K	52	ASN	CA-C-N	6.01	131.03	121.66
9	K	52	ASN	C-N-CA	6.01	131.03	121.66
1	A	377	PRO	CA-N-CD	-6.01	103.59	112.00
1	A	919	ILE	CA-C-O	-6.01	113.25	118.96
8	J	51	LEU	N-CA-C	6.00	119.87	112.54
3	C	35	ARG	N-CA-C	-6.00	104.31	111.69
1	A	486	GLU	CG-CD-OE1	6.00	132.20	118.40
2	B	106	ASP	N-CA-C	6.00	123.58	110.80
1	A	22	PHE	N-CA-C	-6.00	99.38	108.67
1	A	516	SER	N-CA-CB	-6.00	101.53	111.49
1	A	770	VAL	CA-C-N	5.99	130.64	122.19
1	A	770	VAL	C-N-CA	5.99	130.64	122.19
2	B	284	ILE	CA-CB-CG1	5.99	120.59	110.40
2	B	399	ASP	N-CA-CB	-5.99	101.63	110.49
1	A	633	VAL	CA-C-N	-5.99	112.65	120.44
1	A	633	VAL	C-N-CA	-5.99	112.65	120.44
1	A	978	PRO	CB-CG-CD	-5.99	86.94	106.10
2	B	222	ILE	N-CA-C	5.99	116.55	108.17
8	J	62	ARG	CG-CD-NE	-5.99	98.83	112.00
1	A	1206	ASP	N-CA-C	-5.99	103.13	111.39
4	E	57	MET	N-CA-CB	5.99	119.52	110.30
1	A	1198	ASP	CB-CA-C	-5.98	100.23	110.22
3	C	90	ASP	N-CA-C	5.98	123.54	110.80
2	B	606	LYS	CG-CD-CE	5.98	125.05	111.30
2	B	419	THR	OG1-CB-CG2	-5.98	97.34	109.30
6	H	131	ASN	CA-CB-CG	5.98	118.58	112.60
1	A	174	ILE	CA-CB-CG1	5.97	120.56	110.40
2	B	316	PRO	N-CD-CG	-5.97	94.24	103.20
4	E	87	SER	CB-CA-C	5.97	119.99	110.19
2	B	63	ILE	N-CA-C	5.97	119.41	111.17
3	C	142	VAL	CB-CA-C	-5.97	102.86	111.34
1	A	1054	LEU	N-CA-C	5.97	118.75	111.82
2	B	43	LEU	N-CA-C	5.97	120.72	113.38
2	B	1082	MET	CA-C-N	-5.97	113.26	122.87
2	B	1082	MET	C-N-CA	-5.97	113.26	122.87
5	F	131	PRO	CA-C-N	-5.97	113.22	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	131	PRO	C-N-CA	-5.97	113.22	122.59
1	A	528	LEU	N-CA-C	5.97	117.58	111.14
3	C	263	THR	N-CA-CB	-5.97	100.41	110.49
4	E	49	SER	N-CA-C	5.97	119.20	107.98
8	J	13	VAL	N-CA-C	-5.97	101.88	109.58
1	A	174	ILE	O-C-N	-5.96	116.82	123.26
1	A	1227	ILE	CA-CB-CG1	5.96	120.54	110.40
2	B	389	ALA	N-CA-C	5.96	118.56	111.71
5	F	116	ASP	N-CA-CB	5.96	118.04	110.23
1	A	1379	GLY	CA-C-O	5.96	125.65	119.27
2	B	1154	ALA	N-CA-C	-5.95	105.51	112.89
5	F	77	ASP	CA-C-N	-5.95	110.17	121.54
5	F	77	ASP	C-N-CA	-5.95	110.17	121.54
2	B	68	THR	CB-CA-C	5.95	119.56	109.50
2	B	916	THR	N-CA-C	5.95	127.66	111.00
3	C	131	HIS	N-CA-C	-5.95	102.16	109.65
3	C	248	ILE	CA-C-O	5.95	127.46	121.27
7	I	114	GLN	N-CA-C	5.95	119.64	112.38
10	L	61	THR	CA-CB-CG2	5.95	120.61	110.50
1	A	1321	GLY	CA-C-O	5.95	125.58	119.10
2	B	547	VAL	CG1-CB-CG2	5.95	123.88	110.80
4	E	179	GLN	CB-CG-CD	-5.95	102.49	112.60
1	A	209	ASN	N-CA-CB	5.95	119.12	110.26
1	A	1047	SER	N-CA-C	-5.94	104.92	111.82
3	C	3	GLU	CA-CB-CG	-5.94	102.21	114.10
1	A	708	MET	O-C-N	-5.94	115.89	123.26
2	B	22	SER	CA-C-O	5.94	126.60	119.59
2	B	799	PRO	N-CD-CG	-5.94	94.29	103.20
1	A	740	LEU	CB-CG-CD1	5.94	128.52	110.70
1	A	1172	LEU	N-CA-C	5.94	121.28	113.20
4	E	113	GLN	CA-C-N	-5.94	110.28	121.63
4	E	113	GLN	C-N-CA	-5.94	110.28	121.63
2	B	318	VAL	N-CA-C	5.94	116.12	110.42
1	A	1240	CYS	N-CA-CB	-5.94	101.58	111.20
9	K	6	ARG	NE-CZ-NH2	-5.94	113.86	119.20
1	A	15	LYS	N-CA-C	-5.93	106.00	113.72
1	A	470	LEU	CB-CA-C	-5.93	97.30	109.94
2	B	304	ASP	N-CA-CB	5.93	120.52	110.49
2	B	550	ASP	CB-CA-C	5.93	117.24	108.87
9	K	73	LEU	CB-CG-CD1	-5.93	92.91	110.70
3	C	79	GLN	CA-CB-CG	5.93	125.96	114.10
3	C	133	ILE	N-CA-C	5.93	117.27	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	157	ASP	CB-CG-OD1	5.93	132.03	118.40
3	C	123	ASN	CB-CA-C	5.93	120.67	110.77
8	J	3	VAL	N-CA-CB	5.93	119.51	111.21
1	A	717	ASN	CB-CG-ND2	-5.92	107.52	116.40
1	A	19	PHE	N-CA-C	5.92	119.25	110.48
1	A	1103	GLU	N-CA-CB	-5.92	101.40	110.16
2	B	1178	ASN	N-CA-C	5.92	119.73	111.74
2	B	1198	TYR	N-CA-C	-5.92	104.17	111.33
7	I	61	ASP	N-CA-CB	-5.92	102.39	110.56
1	A	544	ASP	CA-C-N	5.92	128.69	120.29
1	A	544	ASP	C-N-CA	5.92	128.69	120.29
2	B	711	GLU	CB-CA-C	-5.92	98.51	110.17
7	I	92	ARG	NE-CZ-NH1	-5.92	115.58	121.50
1	A	470	LEU	CA-C-O	5.92	127.61	120.99
1	A	561	PRO	CB-CA-C	-5.91	103.49	111.12
2	B	169	ARG	CA-C-O	5.91	126.63	120.30
2	B	261	ARG	N-CA-C	-5.91	101.71	110.46
2	B	722	ASP	OD1-CG-OD2	-5.91	108.71	122.90
6	H	16	ASP	N-CA-C	5.91	117.10	109.65
1	A	1001	ARG	CG-CD-NE	-5.91	99.00	112.00
2	B	136	THR	CA-C-N	5.91	132.83	121.54
2	B	136	THR	C-N-CA	5.91	132.83	121.54
2	B	249	ARG	CD-NE-CZ	5.91	132.67	124.40
4	E	70	SER	CA-C-O	-5.91	114.29	120.55
1	A	475	THR	CA-C-O	5.90	126.81	120.55
3	C	55	THR	N-CA-C	-5.90	105.73	113.17
1	A	280	GLU	N-CA-C	-5.90	104.92	111.71
2	B	1017	ILE	CA-CB-CG1	-5.90	100.37	110.40
4	E	148	GLU	CB-CG-CD	5.90	122.63	112.60
7	I	59	VAL	O-C-N	-5.90	116.69	123.00
1	A	919	ILE	N-CA-CB	5.90	118.70	112.21
2	B	606	LYS	N-CA-CB	-5.90	102.47	110.67
6	H	121	LEU	CD1-CG-CD2	-5.90	97.82	110.80
1	A	247	ARG	CB-CA-C	5.90	116.57	109.85
6	H	104	PHE	N-CA-C	5.90	123.36	110.80
7	I	91	ARG	N-CA-C	-5.89	95.35	107.67
1	A	1199	ARG	CA-C-O	-5.89	114.81	121.00
1	A	1377	THR	CA-CB-CG2	5.89	120.52	110.50
2	B	1097	HIS	CA-C-O	5.89	128.94	120.51
7	I	70	ARG	CA-C-O	-5.89	114.45	121.11
1	A	1275	GLY	CA-C-O	5.89	128.09	122.26
1	A	858	ASN	N-CA-C	5.89	118.48	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	354	ASP	CA-C-O	-5.89	114.18	120.42
2	B	106	ASP	N-CA-CB	-5.89	100.54	110.49
2	B	477	ALA	N-CA-CB	5.89	119.23	110.40
6	H	139	ASN	N-CA-C	-5.89	98.26	110.80
10	L	38	LEU	N-CA-C	-5.89	100.86	109.63
10	L	50	ASP	N-CA-CB	5.89	120.44	110.49
2	B	1166	CYS	CA-CB-SG	5.88	127.93	114.40
7	I	118	ARG	CD-NE-CZ	5.88	132.64	124.40
9	K	13	GLY	N-CA-C	-5.88	104.37	112.25
7	I	68	LEU	CA-C-O	-5.88	115.25	120.19
1	A	1207	LEU	CB-CG-CD1	-5.88	93.07	110.70
7	I	70	ARG	NH1-CZ-NH2	5.88	126.94	119.30
4	E	198	ILE	O-C-N	-5.88	116.97	123.20
1	A	364	VAL	CG1-CB-CG2	-5.88	97.87	110.80
2	B	106	ASP	CB-CG-OD1	-5.87	104.89	118.40
2	B	739	THR	CB-CA-C	-5.87	99.20	109.07
8	J	48	ARG	NE-CZ-NH2	-5.87	113.92	119.20
1	A	691	LEU	N-CA-C	5.87	118.46	111.71
1	A	674	PRO	N-CD-CG	5.87	112.00	103.20
2	B	852	ARG	NE-CZ-NH2	5.87	124.48	119.20
3	C	57	VAL	N-CA-CB	-5.87	98.67	111.81
6	H	112	ILE	CB-CA-C	5.87	120.92	111.29
1	A	1234	GLU	CB-CA-C	-5.87	98.75	110.42
2	B	1099	VAL	N-CA-C	5.87	121.54	109.34
1	A	1021	LEU	N-CA-C	-5.86	104.48	111.69
2	B	499	ASN	CA-C-O	-5.86	113.57	120.60
1	A	605	MET	CG-SD-CE	-5.86	88.01	100.90
1	A	1139	GLU	CB-CA-C	-5.86	100.76	109.90
2	B	204	ILE	CA-CB-CG1	5.86	120.36	110.40
2	B	577	ALA	O-C-N	5.86	129.96	123.16
2	B	371	GLU	N-CA-C	-5.86	106.27	113.41
1	A	229	SER	N-CA-C	5.85	119.49	107.37
3	C	250	THR	OG1-CB-CG2	-5.85	97.60	109.30
1	A	244	PRO	N-CD-CG	-5.85	94.43	103.20
1	A	366	VAL	O-C-N	-5.85	114.44	121.10
1	A	666	ILE	CA-C-N	-5.85	113.57	120.00
1	A	666	ILE	C-N-CA	-5.85	113.57	120.00
10	L	28	LYS	N-CA-C	5.84	123.25	110.80
2	B	707	PRO	CA-C-O	5.84	128.43	119.55
3	C	202	PRO	N-CA-C	5.84	119.62	110.80
2	B	431	TYR	CB-CA-C	-5.84	102.00	111.06
8	J	49	MET	N-CA-CB	-5.84	101.52	110.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1278	ASN	N-CA-C	5.84	123.23	110.80
2	B	249	ARG	CA-C-N	5.84	129.65	121.24
2	B	249	ARG	C-N-CA	5.84	129.65	121.24
2	B	1179	GLN	CA-C-O	5.84	126.74	120.38
9	K	17	SER	CB-CA-C	-5.84	99.20	109.71
1	A	1318	THR	N-CA-C	-5.84	106.20	113.38
1	A	229	SER	CA-CB-OG	-5.83	99.43	111.10
1	A	944	ARG	NH1-CZ-NH2	-5.83	111.72	119.30
2	B	325	GLN	CA-C-N	-5.83	112.30	121.87
2	B	325	GLN	C-N-CA	-5.83	112.30	121.87
2	B	1015	HIS	N-CA-C	-5.83	106.01	113.01
1	A	920	LEU	CA-C-O	5.83	127.57	120.92
2	B	264	SER	N-CA-C	-5.83	100.82	109.86
9	K	64	GLU	CG-CD-OE1	5.83	131.80	118.40
4	E	116	ILE	CB-CA-C	5.83	119.52	111.19
2	B	630	ALA	CB-CA-C	-5.82	97.74	109.68
5	F	120	ILE	CB-CG1-CD1	-5.82	101.57	113.80
6	H	38	LEU	CD1-CG-CD2	-5.82	97.99	110.80
1	A	1104	ILE	CB-CA-C	-5.82	104.53	111.81
2	B	1020	ARG	CA-CB-CG	5.82	125.74	114.10
2	B	393	LYS	CG-CD-CE	5.82	124.69	111.30
5	F	129	LYS	N-CA-C	5.82	119.15	112.57
1	A	895	LYS	CD-CE-NZ	-5.82	93.28	111.90
4	E	66	GLU	CB-CG-CD	5.82	122.49	112.60
1	A	913	LEU	O-C-N	-5.81	116.61	123.41
1	A	925	LEU	N-CA-C	-5.81	105.02	111.36
2	B	244	LEU	N-CA-C	5.81	118.98	108.69
8	J	3	VAL	CG1-CB-CG2	5.81	123.59	110.80
1	A	418	SER	N-CA-C	5.81	123.18	110.80
1	A	685	GLU	N-CA-CB	-5.81	101.35	110.30
1	A	1012	ARG	CA-CB-CG	5.81	125.72	114.10
1	A	1135	ARG	CG-CD-NE	-5.81	99.22	112.00
1	A	1352	VAL	CA-C-O	5.81	127.50	121.05
7	I	11	ASN	CB-CA-C	-5.81	102.33	111.51
9	K	92	ASN	CB-CA-C	5.81	120.49	110.84
2	B	122	LEU	N-CA-C	5.81	118.37	110.35
4	E	131	THR	CA-CB-CG2	5.81	120.38	110.50
1	A	1376	THR	CA-CB-OG1	5.81	118.31	109.60
6	H	121	LEU	N-CA-C	-5.81	100.36	109.25
9	K	1	MET	CB-CG-SD	-5.81	95.27	112.70
1	A	414	ASP	OD1-CG-OD2	-5.81	108.96	122.90
2	B	1033	LYS	CD-CE-NZ	-5.80	93.32	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1107	ALA	CA-C-N	5.80	132.63	121.54
2	B	1107	ALA	C-N-CA	5.80	132.63	121.54
4	E	31	THR	CA-C-N	-5.80	112.43	120.38
4	E	31	THR	C-N-CA	-5.80	112.43	120.38
9	K	74	ARG	CB-CG-CD	5.80	124.65	111.30
1	A	1359	ASP	CA-C-O	-5.80	112.21	120.51
2	B	1074	ASN	CA-C-O	5.80	127.31	120.58
2	B	598	GLU	O-C-N	-5.80	115.97	122.12
2	B	732	SER	N-CA-C	5.80	118.24	110.35
1	A	367	PRO	CA-C-O	5.80	127.92	121.43
1	A	1122	PRO	CA-C-N	-5.80	110.05	121.41
1	A	1122	PRO	C-N-CA	-5.80	110.05	121.41
2	B	860	MET	CB-CA-C	-5.80	100.04	110.36
1	A	303	TYR	N-CA-C	-5.80	104.96	111.28
2	B	403	LYS	CA-CB-CG	-5.80	102.51	114.10
2	B	1201	LYS	N-CA-C	-5.80	104.15	111.11
1	A	664	THR	N-CA-CB	5.79	122.30	111.52
4	E	72	PHE	O-C-N	5.79	126.72	121.04
1	A	984	LYS	CA-CB-CG	5.79	125.68	114.10
7	I	4	PHE	CA-C-O	-5.79	112.23	120.51
4	E	103	LYS	CA-CB-CG	5.79	125.68	114.10
1	A	75	ASN	N-CA-C	5.79	123.13	110.80
9	K	14	GLU	N-CA-C	-5.79	102.48	110.35
1	A	1274	ARG	CB-CA-C	-5.79	96.72	109.56
1	A	1299	VAL	CA-C-O	5.78	127.36	121.63
2	B	903	VAL	CB-CA-C	-5.78	103.63	111.15
9	K	17	SER	CA-C-O	-5.78	114.56	121.56
2	B	435	THR	N-CA-CB	5.78	118.99	110.49
2	B	1163	CYS	CB-CA-C	5.78	119.54	109.65
2	B	735	ALA	O-C-N	5.78	130.68	123.28
1	A	608	ILE	CA-CB-CG1	5.78	120.22	110.40
2	B	344	LYS	N-CA-C	5.78	118.61	110.23
2	B	462	ALA	N-CA-C	-5.78	104.42	112.45
1	A	1325	THR	CA-CB-CG2	5.78	120.32	110.50
2	B	114	PRO	N-CD-CG	5.78	111.86	103.20
3	C	106	GLU	O-C-N	5.78	129.00	122.19
3	C	182	PRO	N-CD-CG	-5.78	94.54	103.20
1	A	630	ILE	N-CA-C	-5.77	103.87	111.09
2	B	678	GLU	CA-CB-CG	-5.77	102.55	114.10
1	A	583	PRO	CA-C-O	-5.77	114.17	122.31
1	A	853	ASP	N-CA-C	5.77	121.34	113.37
1	A	671	ALA	CA-C-N	5.77	132.56	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	671	ALA	C-N-CA	5.77	132.56	121.54
4	E	172	GLU	N-CA-C	-5.77	104.99	111.28
1	A	285	PRO	N-CA-CB	5.77	108.33	103.25
1	A	1022	LEU	N-CA-C	5.77	118.03	111.11
2	B	460	ALA	CA-C-O	-5.77	114.31	120.42
4	E	95	THR	CB-CA-C	-5.77	98.61	110.38
1	A	659	HIS	CG-CD2-NE2	-5.77	101.43	107.20
3	C	40	GLU	N-CA-CB	-5.77	101.69	111.20
1	A	1158	PRO	CB-CA-C	5.76	121.07	111.21
2	B	509	ALA	CB-CA-C	5.76	119.15	110.50
1	A	1040	GLN	N-CA-C	-5.76	104.37	111.40
1	A	1190	PRO	N-CA-C	-5.76	106.17	114.18
2	B	900	ALA	CA-C-O	5.76	126.95	120.04
1	A	235	ILE	N-CA-CB	-5.76	104.08	110.99
1	A	503	GLN	CA-C-N	-5.76	110.54	121.54
1	A	503	GLN	C-N-CA	-5.76	110.54	121.54
1	A	683	ILE	CG1-CB-CG2	-5.76	93.42	110.70
2	B	629	ASP	N-CA-C	5.76	119.00	110.48
4	E	31	THR	CA-CB-CG2	5.76	120.29	110.50
7	I	78	CYS	N-CA-C	-5.76	105.75	112.89
1	A	861	GLY	CA-C-N	-5.75	111.91	120.94
1	A	861	GLY	C-N-CA	-5.75	111.91	120.94
4	E	91	LYS	CA-C-N	5.75	128.30	120.54
4	E	91	LYS	C-N-CA	5.75	128.30	120.54
1	A	475	THR	CA-CB-CG2	5.75	120.27	110.50
1	A	1127	ASP	CA-CB-CG	5.75	118.35	112.60
1	A	1432	GLN	N-CA-C	5.75	117.92	109.24
2	B	1135	ARG	N-CA-CB	-5.75	101.74	110.07
6	H	47	PHE	CA-C-N	-5.75	114.69	120.21
6	H	47	PHE	C-N-CA	-5.75	114.69	120.21
2	B	790	ASP	CB-CG-OD2	-5.74	105.19	118.40
2	B	822	ASN	CA-C-O	-5.74	114.11	120.60
2	B	228	LYS	N-CA-C	-5.74	100.43	109.50
10	L	61	THR	N-CA-CB	5.74	118.57	110.36
1	A	698	GLN	N-CA-C	5.74	118.31	111.71
1	A	1259	MET	N-CA-CB	5.74	118.56	110.12
1	A	1258	HIS	N-CA-CB	5.74	118.62	110.13
2	B	494	HIS	CB-CA-C	5.74	120.61	110.85
2	B	282	ILE	CA-CB-CG1	5.74	120.15	110.40
3	C	106	GLU	N-CA-C	-5.74	103.87	111.96
1	A	1154	TYR	CA-C-O	-5.73	114.01	120.43
2	B	1162	ILE	CA-CB-CG2	5.73	120.25	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	632	ARG	CA-C-N	-5.73	113.42	122.64
2	B	632	ARG	C-N-CA	-5.73	113.42	122.64
7	I	17	ARG	CB-CG-CD	5.73	124.48	111.30
1	A	912	LEU	CA-C-N	-5.73	111.86	121.94
1	A	912	LEU	C-N-CA	-5.73	111.86	121.94
3	C	50	GLU	CB-CG-CD	5.73	122.34	112.60
6	H	114	VAL	CG1-CB-CG2	-5.73	98.20	110.80
1	A	396	PRO	CA-C-O	-5.72	110.99	119.00
1	A	411	ASP	CA-CB-CG	-5.72	106.88	112.60
2	B	954	VAL	CB-CA-C	-5.72	101.69	110.50
3	C	196	ASP	CA-CB-CG	5.72	118.32	112.60
7	I	54	GLU	OE1-CD-OE2	5.72	136.62	122.90
1	A	37	PHE	CA-C-O	-5.72	114.22	120.17
1	A	1296	GLY	CA-C-O	5.72	124.69	119.83
6	H	93	TYR	N-CA-C	5.72	118.54	110.14
7	I	35	VAL	CB-CA-C	-5.72	100.19	110.48
2	B	326	ASP	CB-CG-OD2	5.71	131.54	118.40
2	B	910	VAL	CA-C-O	-5.71	114.57	121.54
2	B	650	GLU	CG-CD-OE1	-5.71	105.26	118.40
2	B	107	GLY	CA-C-N	5.71	132.25	121.97
2	B	107	GLY	C-N-CA	5.71	132.25	121.97
2	B	257	LYS	CD-CE-NZ	-5.71	93.64	111.90
1	A	398	GLU	N-CA-C	-5.70	99.11	108.41
2	B	1103	ILE	O-C-N	5.70	129.70	122.57
1	A	1066	VAL	CA-C-N	-5.70	112.57	120.38
1	A	1066	VAL	C-N-CA	-5.70	112.57	120.38
1	A	1222	ASN	O-C-N	5.70	128.16	122.12
2	B	346	GLU	OE1-CD-OE2	-5.70	109.22	122.90
3	C	228	PHE	N-CA-C	5.70	117.70	108.41
6	H	53	ASP	CA-C-N	-5.70	112.98	122.21
6	H	53	ASP	C-N-CA	-5.70	112.98	122.21
1	A	15	LYS	O-C-N	-5.70	115.34	122.35
1	A	706	HIS	N-CA-C	-5.70	98.66	110.80
2	B	404	LYS	CG-CD-CE	5.70	124.41	111.30
2	B	555	ILE	CA-C-O	5.70	126.88	120.95
1	A	1272	THR	N-CA-C	-5.70	99.90	108.96
1	A	922	ASP	CB-CA-C	-5.70	100.95	110.29
1	A	1064	VAL	CA-CB-CG1	5.70	120.08	110.40
1	A	1226	VAL	N-CA-C	5.70	116.49	108.17
4	E	127	ILE	O-C-N	5.70	127.59	121.10
9	K	113	THR	CA-C-N	5.70	131.95	121.70
9	K	113	THR	C-N-CA	5.70	131.95	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	95	PHE	N-CA-CB	-5.69	101.59	110.98
1	A	384	ASN	N-CA-CB	-5.69	101.82	111.27
1	A	915	SER	CA-C-N	-5.69	113.66	119.98
1	A	915	SER	C-N-CA	-5.69	113.66	119.98
2	B	735	ALA	CA-C-O	-5.69	113.26	120.20
2	B	995	ARG	CB-CG-CD	-5.69	98.21	111.30
7	I	14	LEU	CA-C-O	-5.69	114.48	120.80
1	A	1165	GLU	N-CA-C	5.69	119.74	112.34
3	C	21	ILE	CB-CA-C	-5.69	102.38	110.12
2	B	312	GLU	N-CA-CB	-5.69	101.46	110.22
2	B	711	GLU	N-CA-C	5.69	122.38	109.81
1	A	326	ARG	CA-CB-CG	5.69	125.47	114.10
1	A	504	LEU	CA-C-O	-5.68	112.38	120.51
1	A	1138	ILE	O-C-N	5.68	127.98	122.07
2	B	1021	MET	N-CA-CB	-5.68	103.29	111.70
2	B	482	VAL	CB-CA-C	-5.68	102.86	111.33
2	B	806	THR	OG1-CB-CG2	5.68	120.67	109.30
1	A	522	GLY	CA-C-O	-5.68	114.93	121.46
1	A	761	MET	CG-SD-CE	5.68	113.39	100.90
2	B	1022	THR	CA-CB-OG1	-5.68	101.08	109.60
1	A	1120	LEU	N-CA-C	5.68	118.92	110.52
1	A	362	ASP	N-CA-C	5.67	119.90	112.92
1	A	646	PHE	N-CA-C	-5.67	105.18	111.36
2	B	386	LEU	N-CA-C	5.67	117.46	111.28
1	A	786	HIS	N-CA-C	-5.67	106.13	113.16
3	C	268	ASP	CA-C-O	-5.67	111.16	120.80
1	A	85	ASP	N-CA-CB	5.67	118.30	109.97
1	A	575	LYS	N-CA-C	5.67	120.72	111.37
1	A	618	GLU	CG-CD-OE1	-5.67	105.36	118.40
2	B	60	GLN	O-C-N	-5.67	116.11	122.12
9	K	103	THR	CA-C-O	-5.67	112.40	120.51
1	A	239	LEU	CA-C-O	5.67	125.30	119.86
1	A	1269	GLU	CB-CA-C	-5.67	100.21	109.56
2	B	995	ARG	NH1-CZ-NH2	5.67	126.67	119.30
1	A	1031	VAL	CB-CA-C	-5.66	104.49	112.14
2	B	1155	SER	CA-CB-OG	5.66	122.43	111.10
7	I	118	ARG	CA-C-N	5.66	130.17	120.71
7	I	118	ARG	C-N-CA	5.66	130.17	120.71
3	C	254	LYS	O-C-N	5.66	127.92	122.03
1	A	682	THR	CA-C-N	5.66	128.84	120.74
1	A	682	THR	C-N-CA	5.66	128.84	120.74
2	B	96	TYR	CA-C-N	-5.66	115.57	123.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	96	TYR	C-N-CA	-5.66	115.57	123.10
8	J	17	LYS	N-CA-C	-5.66	105.12	113.61
8	J	28	ASP	N-CA-CB	5.66	120.67	111.27
7	I	74	GLU	CA-C-O	-5.66	114.77	121.16
1	A	44	THR	N-CA-CB	5.66	120.05	110.49
1	A	1354	ASN	CA-CB-CG	-5.66	106.94	112.60
1	A	1425	SER	CA-CB-OG	-5.66	99.79	111.10
2	B	512	ARG	CA-C-O	5.66	126.32	119.31
7	I	5	ARG	NH1-CZ-NH2	-5.66	111.95	119.30
1	A	372	LYS	CD-CE-NZ	-5.65	93.81	111.90
4	E	52	ARG	CA-C-O	5.65	126.00	120.23
1	A	1285	MET	CA-C-N	-5.65	115.14	123.05
1	A	1285	MET	C-N-CA	-5.65	115.14	123.05
1	A	84	ILE	CA-C-O	-5.65	113.72	120.78
2	B	177	LYS	N-CA-C	-5.65	105.20	111.36
2	B	771	SER	N-CA-CB	5.65	119.03	110.28
9	K	34	THR	CA-C-O	5.65	126.53	120.32
1	A	896	ARG	CD-NE-CZ	-5.64	116.50	124.40
7	I	40	SER	N-CA-C	5.64	122.28	109.81
4	E	81	GLU	N-CA-CB	-5.64	101.00	110.99
1	A	1271	ILE	CG1-CB-CG2	-5.64	93.78	110.70
9	K	78	THR	O-C-N	5.64	130.04	122.82
1	A	647	GLY	N-CA-C	5.64	120.93	113.37
1	A	1301	GLU	N-CA-CB	5.64	120.40	110.37
2	B	91	SER	CA-C-N	5.63	129.56	121.50
2	B	91	SER	C-N-CA	5.63	129.56	121.50
2	B	205	ILE	CB-CA-C	-5.63	103.67	110.99
4	E	187	TYR	N-CA-C	5.63	118.19	111.71
1	A	764	CYS	N-CA-CB	-5.63	101.02	110.99
7	I	41	PRO	CA-C-O	5.63	124.74	118.38
3	C	267	GLN	N-CA-C	5.63	122.79	110.80
6	H	132	LEU	N-CA-C	-5.63	101.97	110.70
2	B	294	ASP	CB-CG-OD2	5.63	131.34	118.40
1	A	941	LYS	CB-CA-C	-5.62	102.23	110.95
1	A	352	VAL	CA-CB-CG1	5.62	119.96	110.40
2	B	911	ILE	CG1-CB-CG2	-5.62	93.83	110.70
2	B	978	ASP	CA-CB-CG	5.62	118.22	112.60
6	H	131	ASN	CA-C-N	5.62	130.53	122.21
6	H	131	ASN	C-N-CA	5.62	130.53	122.21
9	K	45	LEU	CA-C-O	-5.62	114.54	120.55
2	B	518	HIS	CB-CA-C	-5.62	99.90	110.01
3	C	57	VAL	CG1-CB-CG2	5.62	123.16	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	214	ASN	N-CA-C	5.62	117.67	108.52
7	I	74	GLU	N-CA-CB	-5.62	101.87	110.85
2	B	101	MET	CG-SD-CE	5.61	113.25	100.90
2	B	446	LEU	CB-CA-C	5.61	120.77	110.10
1	A	1282	VAL	O-C-N	-5.61	117.14	123.20
8	J	14	VAL	O-C-N	-5.61	115.56	122.57
9	K	70	ARG	NE-CZ-NH2	5.61	124.25	119.20
1	A	393	ARG	N-CA-C	-5.61	104.79	111.69
2	B	555	ILE	CA-CB-CG1	5.61	119.94	110.40
10	L	70	ARG	N-CA-C	5.61	126.71	111.00
1	A	12	ARG	O-C-N	-5.61	116.65	123.10
1	A	948	VAL	CA-C-O	5.61	126.81	120.03
1	A	1194	ARG	CB-CA-C	-5.61	101.17	110.14
1	A	1407	GLU	CB-CA-C	5.61	121.58	110.42
2	B	186	GLU	N-CA-C	-5.61	104.56	111.40
2	B	703	ILE	CA-C-O	5.61	127.23	120.67
3	C	186	LEU	N-CA-CB	-5.61	100.79	110.32
2	B	892	LYS	N-CA-C	-5.60	106.44	113.72
4	E	12	LEU	CB-CA-C	5.60	120.09	110.79
3	C	163	ILE	N-CA-CB	-5.60	101.57	111.93
1	A	1449	SER	CA-C-N	5.60	131.78	121.70
1	A	1449	SER	C-N-CA	5.60	131.78	121.70
2	B	887	HIS	CA-CB-CG	5.60	119.40	113.80
3	C	116	LYS	CD-CE-NZ	-5.60	93.99	111.90
2	B	53	GLN	CB-CG-CD	-5.59	103.09	112.60
7	I	113	ASP	OD1-CG-OD2	-5.59	109.47	122.90
1	A	12	ARG	CG-CD-NE	-5.59	99.70	112.00
1	A	1196	GLU	CG-CD-OE2	-5.59	105.54	118.40
1	A	776	ALA	CB-CA-C	-5.59	99.94	110.51
2	B	885	MET	CA-C-O	-5.59	114.51	121.55
2	B	1188	LYS	CA-C-O	-5.59	112.26	118.69
6	H	77	ARG	NH1-CZ-NH2	-5.59	112.03	119.30
1	A	826	ASP	CB-CG-OD2	5.59	131.25	118.40
1	A	1134	ILE	CB-CA-C	5.59	119.12	111.97
1	A	1166	ASP	CA-CB-CG	5.59	118.19	112.60
2	B	394	ASP	N-CA-CB	-5.59	101.80	110.29
2	B	619	ILE	N-CA-C	-5.59	103.95	111.44
2	B	853	SER	CB-CA-C	-5.59	97.78	110.07
1	A	549	MET	CA-C-O	-5.58	114.63	120.55
2	B	252	SER	CB-CA-C	-5.58	101.19	109.90
1	A	550	LEU	N-CA-C	-5.58	105.27	111.36
1	A	630	ILE	CG1-CB-CG2	-5.58	93.95	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	51	PHE	CA-C-O	-5.58	114.50	120.42
1	A	1188	GLN	CB-CA-C	-5.58	101.15	110.19
2	B	875	GLU	CA-C-O	-5.58	114.00	120.31
3	C	119	VAL	CA-CB-CG2	5.58	119.89	110.40
4	E	3	GLN	N-CA-CB	5.58	119.92	110.49
2	B	485	ARG	CD-NE-CZ	5.58	132.21	124.40
2	B	848	ARG	CG-CD-NE	-5.58	99.73	112.00
1	A	386	ASP	N-CA-C	5.58	117.22	111.03
1	A	1301	GLU	N-CA-C	-5.58	97.49	109.81
2	B	806	THR	N-CA-C	-5.58	100.88	109.52
2	B	1210	MET	CB-CA-C	-5.58	102.42	111.06
2	B	646	LEU	CB-CG-CD2	5.57	127.42	110.70
1	A	164	ARG	CD-NE-CZ	5.57	132.20	124.40
2	B	689	LEU	N-CA-CB	-5.57	101.97	110.33
1	A	949	ASP	CB-CG-OD2	5.57	131.21	118.40
2	B	1186	ASP	CB-CA-C	5.57	119.21	111.63
4	E	183	PRO	O-C-N	-5.57	115.43	122.17
1	A	612	ILE	CA-C-O	-5.57	114.48	121.11
3	C	109	SER	N-CA-CB	-5.57	102.68	110.25
1	A	1165	GLU	O-C-N	-5.57	115.09	122.33
2	B	729	ILE	N-CA-C	5.57	116.19	108.84
3	C	15	LYS	CA-C-N	5.57	131.24	122.11
3	C	15	LYS	C-N-CA	5.57	131.24	122.11
8	J	1	MET	CA-CB-CG	5.57	125.23	114.10
1	A	1102	LYS	N-CA-CB	-5.57	101.94	110.12
2	B	284	ILE	N-CA-C	-5.57	104.94	110.62
2	B	322	PHE	CA-C-O	-5.57	113.97	120.20
2	B	764	SER	N-CA-C	5.57	121.06	113.16
6	H	41	ASP	CB-CG-OD1	5.57	131.20	118.40
9	K	46	ILE	N-CA-C	-5.57	105.08	110.42
8	J	9	SER	N-CA-C	5.56	120.19	112.90
8	J	63	TYR	CA-C-O	-5.56	114.87	121.66
2	B	184	ALA	N-CA-C	5.56	117.92	110.35
2	B	391	ASP	CB-CG-OD2	5.56	131.19	118.40
6	H	4	THR	O-C-N	-5.56	115.95	122.96
2	B	324	ILE	CB-CG1-CD1	-5.56	102.12	113.80
5	F	72	LYS	N-CA-CB	-5.56	101.05	110.50
1	A	37	PHE	CA-CB-CG	5.56	119.36	113.80
1	A	912	LEU	N-CA-CB	5.56	118.90	110.28
1	A	187	LYS	CA-C-N	5.56	132.16	121.54
1	A	187	LYS	C-N-CA	5.56	132.16	121.54
8	J	39	LEU	N-CA-C	-5.56	106.82	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	576	GLN	CB-CA-C	-5.55	100.01	110.67
5	F	142	SER	CA-C-O	-5.55	115.43	121.87
9	K	62	LYS	CA-C-N	-5.55	115.56	123.11
9	K	62	LYS	C-N-CA	-5.55	115.56	123.11
2	B	391	ASP	N-CA-CB	5.55	120.91	112.47
4	E	107	THR	O-C-N	-5.55	116.50	123.27
1	A	436	ILE	CA-CB-CG1	5.55	119.84	110.40
1	A	466	SER	N-CA-CB	5.55	119.34	110.73
2	B	723	VAL	O-C-N	5.55	129.42	122.59
1	A	1225	PHE	O-C-N	-5.55	116.83	123.27
2	B	531	GLN	CA-C-N	-5.55	112.34	122.38
2	B	531	GLN	C-N-CA	-5.55	112.34	122.38
4	E	98	ILE	CA-C-O	-5.55	114.77	120.71
2	B	171	PRO	O-C-N	-5.55	116.63	123.01
1	A	204	THR	CA-C-N	5.55	127.98	120.38
1	A	204	THR	C-N-CA	5.55	127.98	120.38
1	A	616	VAL	N-CA-CB	-5.55	101.48	110.13
1	A	1356	ILE	CG1-CB-CG2	-5.55	94.06	110.70
7	I	10	CYS	CA-C-O	5.55	126.19	119.31
2	B	489	SER	CA-CB-OG	-5.54	100.01	111.10
1	A	7	SER	CA-C-O	5.54	126.12	120.24
2	B	212	LEU	CD1-CG-CD2	-5.54	98.61	110.80
2	B	912	ILE	N-CA-C	5.54	116.09	107.28
7	I	69	PRO	CA-C-O	-5.54	114.98	122.08
1	A	393	ARG	NE-CZ-NH1	-5.54	115.96	121.50
2	B	175	ARG	CB-CG-CD	5.54	124.05	111.30
3	C	29	MET	CG-SD-CE	5.54	113.09	100.90
2	B	735	ALA	N-CA-C	5.54	117.46	108.26
1	A	382	PRO	N-CA-C	-5.54	107.22	114.03
1	A	1046	LEU	O-C-N	-5.54	115.84	122.15
2	B	239	GLU	CB-CA-C	5.54	120.62	109.38
2	B	342	GLY	O-C-N	5.54	127.98	122.77
4	E	152	LYS	CG-CD-CE	5.54	124.04	111.30
1	A	1046	LEU	CB-CA-C	-5.54	101.44	110.85
1	A	139	TRP	CA-C-O	5.54	126.61	120.63
1	A	618	GLU	CB-CG-CD	5.53	122.01	112.60
2	B	711	GLU	OE1-CD-OE2	-5.53	109.62	122.90
2	B	42	GLY	N-CA-C	5.53	124.95	112.01
9	K	69	ALA	CA-C-O	-5.53	115.39	121.58
7	I	87	GLN	N-CA-C	5.53	117.66	110.53
2	B	168	GLY	CA-C-O	5.53	127.60	121.96
2	B	957	ASN	N-CA-C	5.53	122.57	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	238	ILE	CA-C-O	-5.53	112.55	119.95
4	E	14	ARG	NE-CZ-NH2	-5.53	114.23	119.20
1	A	469	ARG	CA-CB-CG	5.52	125.15	114.10
1	A	547	LEU	N-CA-C	-5.52	106.04	112.89
1	A	504	LEU	CA-CB-CG	5.52	135.63	116.30
2	B	286	PHE	CA-C-O	-5.52	115.02	120.82
2	B	879	ARG	CB-CA-C	-5.52	99.43	110.42
6	H	60	ALA	CA-C-N	-5.52	110.99	121.54
6	H	60	ALA	C-N-CA	-5.52	110.99	121.54
1	A	176	LYS	O-C-N	-5.52	116.73	123.19
1	A	399	HIS	C-N-CD	-5.52	102.37	125.00
6	H	40	LEU	CD1-CG-CD2	-5.52	98.66	110.80
2	B	739	THR	N-CA-CB	5.51	118.33	110.67
2	B	1035	ALA	CA-C-N	-5.51	112.46	120.29
2	B	1035	ALA	C-N-CA	-5.51	112.46	120.29
6	H	26	ILE	CB-CG1-CD1	-5.51	102.22	113.80
9	K	46	ILE	CA-C-O	5.51	127.02	121.17
1	A	21	LEU	N-CA-C	5.51	118.71	109.95
2	B	120	ARG	NE-CZ-NH2	5.51	124.16	119.20
2	B	364	ILE	O-C-N	-5.51	115.68	122.57
1	A	1196	GLU	OE1-CD-OE2	5.51	136.12	122.90
2	B	992	ILE	CA-C-O	-5.51	116.97	120.66
3	C	105	GLY	N-CA-C	-5.51	100.13	113.18
1	A	151	ASP	N-CA-C	-5.50	100.15	108.46
1	A	1008	GLN	N-CA-C	5.50	117.28	111.28
2	B	327	ARG	NE-CZ-NH1	-5.50	116.00	121.50
1	A	620	LYS	N-CA-C	5.50	117.28	111.28
1	A	1379	GLY	N-CA-C	5.50	121.24	114.69
4	E	207	ARG	NH1-CZ-NH2	-5.50	112.15	119.30
1	A	620	LYS	O-C-N	-5.50	116.29	122.12
9	K	67	PHE	N-CA-C	-5.50	106.41	113.23
1	A	114	LEU	CD1-CG-CD2	-5.50	98.70	110.80
2	B	593	PRO	CB-CG-CD	-5.50	88.51	106.10
3	C	55	THR	OG1-CB-CG2	-5.50	98.30	109.30
1	A	1194	ARG	CA-CB-CG	5.50	125.09	114.10
2	B	284	ILE	CB-CG1-CD1	5.50	125.34	113.80
2	B	630	ALA	N-CA-C	5.50	117.78	110.53
2	B	827	ILE	CA-C-O	5.49	127.11	120.74
2	B	1050	ILE	N-CA-C	5.49	120.77	109.34
4	E	32	GLN	CA-C-N	-5.49	112.44	122.38
4	E	32	GLN	C-N-CA	-5.49	112.44	122.38
2	B	390	LEU	CA-C-N	5.49	130.64	122.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	390	LEU	C-N-CA	5.49	130.64	122.74
2	B	814	PHE	N-CA-C	-5.49	104.94	111.69
2	B	962	LYS	CG-CD-CE	5.49	123.92	111.30
2	B	1023	VAL	CA-CB-CG2	-5.49	101.07	110.40
5	F	84	TYR	N-CA-C	5.49	118.19	109.96
1	A	206	GLU	N-CA-CB	5.48	118.43	110.26
1	A	863	VAL	CB-CA-C	-5.48	104.02	111.15
3	C	54	ASN	O-C-N	-5.48	117.20	123.40
3	C	138	GLU	CB-CG-CD	-5.48	103.28	112.60
1	A	884	ASP	CB-CG-OD2	5.48	131.01	118.40
1	A	1418	LEU	CB-CA-C	-5.48	102.10	111.31
1	A	1436	ILE	O-C-N	-5.48	117.26	123.18
2	B	273	LEU	CB-CA-C	-5.48	100.97	108.86
2	B	662	MET	CA-CB-CG	-5.48	103.14	114.10
2	B	806	THR	N-CA-CB	-5.48	102.01	111.55
2	B	1193	GLN	CB-CG-CD	-5.48	103.28	112.60
4	E	68	SER	N-CA-C	5.48	116.94	111.07
1	A	1048	ASN	CA-C-O	-5.48	115.06	120.70
2	B	1185	CYS	CB-CA-C	5.48	120.67	109.55
1	A	790	ASP	N-CA-C	5.47	118.98	111.54
3	C	38	ILE	CB-CA-C	-5.47	104.87	111.88
4	E	72	PHE	CG-CD2-CE2	-5.47	111.39	120.70
1	A	434	ARG	CD-NE-CZ	5.47	132.06	124.40
1	A	503	GLN	CG-CD-NE2	-5.47	108.19	116.40
1	A	912	LEU	O-C-N	-5.47	115.54	122.27
1	A	923	LEU	CB-CA-C	-5.47	99.22	110.38
2	B	98	THR	CA-C-O	-5.47	115.75	121.55
2	B	276	ILE	N-CA-C	-5.47	100.60	108.48
2	B	463	THR	OG1-CB-CG2	-5.47	98.36	109.30
4	E	65	THR	CA-C-N	-5.47	112.52	120.29
4	E	65	THR	C-N-CA	-5.47	112.52	120.29
1	A	39	GLU	N-CA-C	5.47	118.00	109.52
1	A	1118	VAL	CA-CB-CG1	5.47	119.69	110.40
1	A	1411	GLU	N-CA-C	-5.47	105.40	111.36
2	B	398	ARG	NE-CZ-NH1	-5.47	116.03	121.50
2	B	914	LYS	O-C-N	5.47	129.48	123.25
6	H	11	GLN	CA-C-N	-5.47	115.54	122.43
6	H	11	GLN	C-N-CA	-5.47	115.54	122.43
1	A	850	VAL	N-CA-C	5.46	117.17	108.87
3	C	105	GLY	O-C-N	5.46	129.80	122.70
9	K	2	ASN	N-CA-CB	-5.46	102.58	110.56
2	B	737	THR	N-CA-C	5.46	119.25	112.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	751	SER	CA-CB-OG	5.46	122.02	111.10
2	B	884	ARG	CG-CD-NE	-5.46	99.98	112.00
4	E	212	ARG	N-CA-CB	-5.46	101.43	111.37
3	C	175	ALA	N-CA-CB	-5.46	102.55	110.36
7	I	57	GLY	O-C-N	-5.46	116.44	122.50
2	B	277	LYS	N-CA-CB	-5.46	102.41	110.49
3	C	183	TRP	CA-C-O	-5.46	115.22	121.82
9	K	94	ILE	CA-C-N	5.46	129.57	120.62
9	K	94	ILE	C-N-CA	5.46	129.57	120.62
6	H	132	LEU	CA-CB-CG	5.46	135.39	116.30
3	C	211	ASP	N-CA-C	-5.45	102.90	109.72
2	B	1051	THR	O-C-N	-5.45	116.53	123.24
6	H	110	ASP	CB-CG-OD2	5.45	130.94	118.40
7	I	45	ARG	NE-CZ-NH1	-5.45	116.05	121.50
9	K	88	LYS	N-CA-C	-5.45	105.24	111.07
1	A	1109	LYS	CB-CA-C	5.45	121.70	110.31
2	B	771	SER	N-CA-C	-5.45	105.50	111.82
2	B	184	ALA	CA-C-O	-5.45	115.78	121.55
2	B	115	GLN	N-CA-C	5.45	118.72	111.75
2	B	34	ILE	N-CA-C	-5.45	105.22	110.72
3	C	93	ASP	CA-C-N	-5.45	111.93	122.06
3	C	93	ASP	C-N-CA	-5.45	111.93	122.06
9	K	26	LYS	N-CA-CB	-5.44	101.84	110.22
2	B	65	GLU	CB-CG-CD	5.44	121.85	112.60
2	B	904	ARG	N-CA-C	5.44	118.12	110.23
1	A	101	LYS	CG-CD-CE	-5.44	98.79	111.30
1	A	280	GLU	CA-CB-CG	5.44	124.98	114.10
4	E	14	ARG	NE-CZ-NH1	5.44	126.94	121.50
2	B	512	ARG	N-CA-CB	-5.44	101.54	110.40
1	A	403	LYS	CA-CB-CG	5.43	124.97	114.10
1	A	524	VAL	N-CA-CB	-5.43	106.36	112.45
2	B	478	GLY	N-CA-C	-5.43	107.77	115.43
2	B	559	SER	CA-C-O	-5.43	112.91	119.27
9	K	5	ASP	CB-CG-OD1	-5.43	105.90	118.40
1	A	451	HIS	CA-C-O	-5.43	115.64	121.45
1	A	465	TYR	CA-C-N	-5.43	114.13	122.60
1	A	465	TYR	C-N-CA	-5.43	114.13	122.60
1	A	717	ASN	N-CA-C	5.43	117.28	111.36
1	A	1030	ARG	CB-CA-C	-5.43	102.32	110.90
2	B	853	SER	N-CA-C	5.43	117.44	109.24
4	E	32	GLN	N-CA-C	5.43	117.90	111.33
1	A	516	SER	CA-C-O	5.43	126.08	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	434	ARG	CG-CD-NE	-5.43	100.06	112.00
1	A	957	PRO	N-CA-C	-5.43	103.32	111.57
2	B	555	ILE	CB-CG1-CD1	-5.43	102.40	113.80
2	B	944	THR	CB-CA-C	-5.42	99.31	109.72
2	B	995	ARG	NE-CZ-NH1	5.42	126.92	121.50
1	A	4	GLN	CA-C-N	5.42	130.84	120.97
1	A	4	GLN	C-N-CA	5.42	130.84	120.97
7	I	30	ARG	N-CA-C	5.42	119.59	112.92
1	A	1108	ALA	N-CA-CB	-5.42	101.55	109.95
2	B	488	TYR	CA-C-O	5.42	126.48	120.63
1	A	153	PRO	CA-C-N	-5.42	111.25	121.66
1	A	153	PRO	C-N-CA	-5.42	111.25	121.66
4	E	36	GLU	CB-CG-CD	5.42	121.81	112.60
7	I	104	LEU	N-CA-C	-5.42	106.34	113.17
1	A	217	LYS	CA-C-O	5.42	126.70	120.90
1	A	1076	ALA	N-CA-C	5.42	117.94	111.71
2	B	367	LEU	CB-CG-CD2	5.42	126.96	110.70
2	B	995	ARG	CD-NE-CZ	5.42	131.99	124.40
3	C	69	LEU	N-CA-C	5.42	119.89	113.28
2	B	870	ILE	CB-CG1-CD1	5.41	125.17	113.80
1	A	291	GLU	OE1-CD-OE2	-5.41	109.91	122.90
1	A	25	GLU	CB-CG-CD	5.41	121.80	112.60
1	A	387	ARG	O-C-N	-5.41	116.47	122.09
3	C	116	LYS	CA-C-O	-5.41	114.14	120.20
1	A	1374	VAL	N-CA-CB	5.41	117.23	110.47
2	B	724	ASP	N-CA-C	5.41	121.76	109.81
1	A	199	LEU	CA-CB-CG	5.40	135.22	116.30
1	A	705	LYS	N-CA-CB	5.40	120.82	110.82
4	E	24	LYS	N-CA-C	5.40	117.17	111.28
9	K	35	PHE	CA-C-O	-5.40	114.38	120.43
1	A	69	THR	CA-C-N	5.40	131.46	121.52
1	A	69	THR	C-N-CA	5.40	131.46	121.52
1	A	1267	MET	CA-C-N	-5.40	111.34	120.58
1	A	1267	MET	C-N-CA	-5.40	111.34	120.58
3	C	35	ARG	CG-CD-NE	-5.40	100.12	112.00
3	C	195	GLN	CB-CG-CD	-5.40	103.42	112.60
4	E	38	PRO	O-C-N	5.40	129.93	122.64
1	A	960	ILE	CG1-CB-CG2	-5.40	94.50	110.70
7	I	24	ARG	CA-CB-CG	5.40	124.90	114.10
1	A	1376	THR	CB-CA-C	5.40	119.03	109.75
1	A	193	ASP	N-CA-CB	5.40	119.61	110.49
1	A	820	GLY	CA-C-N	-5.40	112.63	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	820	GLY	C-N-CA	-5.40	112.63	120.29
1	A	276	LEU	N-CA-C	-5.39	105.43	112.23
2	B	1129	ARG	NE-CZ-NH1	5.39	126.89	121.50
3	C	155	LEU	CA-C-N	-5.39	114.19	122.87
3	C	155	LEU	C-N-CA	-5.39	114.19	122.87
6	H	82	PRO	CA-C-O	-5.39	110.78	120.60
2	B	942	ARG	CA-CB-CG	5.39	124.88	114.10
4	E	47	CYS	N-CA-CB	-5.39	101.62	110.68
1	A	126	LEU	O-C-N	5.39	128.29	122.15
1	A	858	ASN	CB-CG-OD1	-5.39	110.02	120.80
1	A	1187	GLN	CA-C-N	5.39	129.94	122.77
1	A	1187	GLN	C-N-CA	5.39	129.94	122.77
2	B	118	ARG	CB-CG-CD	5.39	123.70	111.30
2	B	191	LYS	N-CA-CB	5.39	118.04	110.12
2	B	213	ILE	CB-CG1-CD1	-5.39	102.48	113.80
2	B	313	MET	N-CA-C	5.39	119.48	113.01
6	H	115	TYR	CA-C-N	-5.39	111.25	121.54
6	H	115	TYR	C-N-CA	-5.39	111.25	121.54
1	A	677	ARG	CA-C-N	5.39	127.50	120.28
1	A	677	ARG	C-N-CA	5.39	127.50	120.28
2	B	1129	ARG	NE-CZ-NH2	-5.39	114.35	119.20
1	A	598	LEU	N-CA-CB	-5.38	102.34	111.17
2	B	465	ASN	CA-C-N	5.38	131.82	121.54
2	B	465	ASN	C-N-CA	5.38	131.82	121.54
2	B	825	VAL	CB-CA-C	-5.38	103.15	110.42
7	I	1	MET	CA-CB-CG	5.38	124.86	114.10
1	A	878	ILE	N-CA-CB	-5.38	102.03	111.39
1	A	907	THR	CA-CB-CG2	5.38	119.65	110.50
1	A	935	GLN	CA-C-N	5.38	127.49	120.28
1	A	935	GLN	C-N-CA	5.38	127.49	120.28
5	F	78	GLN	O-C-N	-5.38	115.43	122.59
9	K	93	SER	CB-CA-C	-5.38	100.02	110.46
2	B	1103	ILE	CB-CA-C	-5.38	102.47	111.29
4	E	74	ASP	N-CA-C	5.38	122.26	110.80
4	E	80	VAL	CA-C-O	-5.38	116.02	121.67
1	A	1277	GLU	CG-CD-OE2	5.38	130.77	118.40
1	A	894	GLU	N-CA-C	-5.38	105.58	111.82
2	B	620	ARG	NE-CZ-NH2	-5.38	114.36	119.20
1	A	391	LEU	N-CA-CB	5.38	118.11	110.16
4	E	121	MET	CB-CG-SD	5.38	128.82	112.70
9	K	84	LYS	CA-C-O	5.38	125.99	119.49
1	A	360	GLU	N-CA-C	5.37	117.66	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	549	THR	N-CA-C	-5.37	100.57	108.79
4	E	58	MET	N-CA-C	5.37	117.83	111.33
6	H	19	ARG	CD-NE-CZ	5.37	131.92	124.40
1	A	408	ASP	CA-CB-CG	-5.37	107.23	112.60
9	K	29	ASN	N-CA-C	-5.37	103.88	111.56
1	A	1286	LYS	CA-C-O	-5.37	114.41	120.32
1	A	293	GLU	N-CA-CB	5.37	118.53	109.78
1	A	906	HIS	CA-C-O	5.37	126.45	119.95
9	K	36	GLU	N-CA-C	5.37	118.81	110.17
1	A	364	VAL	CA-CB-CG2	5.36	119.52	110.40
7	I	16	PRO	N-CD-CG	-5.36	95.16	103.20
1	A	1208	THR	CA-CB-OG1	5.36	117.64	109.60
1	A	914	GLU	CA-C-O	-5.36	115.16	120.90
6	H	61	SER	CA-C-O	-5.36	112.84	120.51
1	A	561	PRO	CA-C-O	-5.36	115.25	121.95
4	E	9	ILE	CB-CA-C	-5.36	105.06	112.24
4	E	132	ILE	N-CA-C	5.36	115.83	108.12
3	C	194	GLU	CA-C-O	-5.36	112.85	120.51
6	H	41	ASP	OD1-CG-OD2	-5.36	110.05	122.90
1	A	1024	SER	CA-CB-OG	5.35	121.81	111.10
4	E	141	VAL	CA-CB-CG1	5.35	119.50	110.40
2	B	742	GLU	CA-C-O	-5.35	115.88	121.55
6	H	145	ARG	O-C-N	5.35	129.82	123.24
9	K	51	LEU	N-CA-CB	-5.35	102.25	110.44
1	A	457	ALA	CA-C-O	-5.35	114.77	120.92
2	B	284	ILE	CG1-CB-CG2	-5.35	94.65	110.70
6	H	107	VAL	CA-CB-CG1	5.35	119.50	110.40
2	B	567	GLU	CB-CG-CD	5.35	121.69	112.60
1	A	32	VAL	CG1-CB-CG2	-5.34	99.04	110.80
2	B	190	TYR	CA-C-O	-5.34	115.21	120.82
6	H	115	TYR	CA-C-O	-5.34	112.65	120.13
7	I	8	ARG	N-CA-C	-5.34	105.62	111.82
1	A	391	LEU	CB-CG-CD2	-5.34	94.68	110.70
1	A	811	GLN	CB-CG-CD	5.34	121.68	112.60
3	C	158	VAL	N-CA-C	5.34	115.55	107.80
1	A	420	ARG	NH1-CZ-NH2	-5.34	112.36	119.30
2	B	566	LEU	O-C-N	-5.34	116.46	122.12
2	B	1075	GLY	CA-C-O	5.34	126.03	120.80
5	F	143	PHE	O-C-N	-5.34	117.16	123.25
7	I	3	THR	OG1-CB-CG2	-5.34	98.62	109.30
2	B	598	GLU	OE1-CD-OE2	-5.34	110.09	122.90
3	C	35	ARG	CD-NE-CZ	5.34	131.87	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	389	THR	N-CA-CB	5.33	117.89	109.94
1	A	1326	ARG	CG-CD-NE	-5.33	100.26	112.00
2	B	129	PHE	N-CA-CB	-5.33	101.57	110.37
7	I	90	GLN	O-C-N	-5.33	116.51	122.75
1	A	93	VAL	O-C-N	5.33	127.32	121.83
1	A	299	HIS	N-CA-C	-5.33	105.91	112.90
1	A	837	ILE	CA-CB-CG1	-5.33	101.33	110.40
2	B	645	SER	N-CA-C	5.33	122.16	110.80
4	E	112	TYR	OH-CZ-CE2	5.33	135.90	119.90
1	A	966	ASN	CA-C-O	-5.33	115.41	120.90
8	J	45	CYS	CA-C-O	5.33	126.60	121.00
2	B	249	ARG	NE-CZ-NH1	5.33	126.83	121.50
6	H	40	LEU	CA-C-N	5.33	129.71	122.19
6	H	40	LEU	C-N-CA	5.33	129.71	122.19
1	A	562	THR	CA-C-N	5.33	125.09	119.76
1	A	562	THR	C-N-CA	5.33	125.09	119.76
1	A	600	PRO	CA-N-CD	5.33	119.46	112.00
1	A	666	ILE	CG1-CB-CG2	5.33	126.68	110.70
1	A	1277	GLU	CG-CD-OE1	-5.33	106.14	118.40
2	B	354	ASP	N-CA-CB	5.33	118.05	110.16
2	B	222	ILE	CA-C-O	-5.33	114.84	120.48
9	K	19	LEU	N-CA-CB	-5.33	101.97	111.08
1	A	9	ALA	O-C-N	5.32	126.13	121.18
1	A	70	CYS	N-CA-CB	5.32	118.31	110.33
1	A	808	LEU	N-CA-C	5.32	118.78	110.32
1	A	840	ARG	CG-CD-NE	-5.32	100.29	112.00
2	B	434	ARG	CA-CB-CG	5.32	124.75	114.10
2	B	578	THR	CA-C-O	-5.32	114.31	120.49
3	C	25	VAL	CB-CA-C	-5.32	100.90	110.48
3	C	199	LYS	CA-CB-CG	-5.32	103.45	114.10
2	B	457	LEU	CD1-CG-CD2	5.32	122.51	110.80
1	A	412	ARG	CB-CG-CD	5.32	123.54	111.30
1	A	821	ARG	NH1-CZ-NH2	5.32	126.22	119.30
2	B	738	PHE	CA-C-O	5.32	127.04	121.19
3	C	50	GLU	CA-C-N	-5.32	115.87	123.11
3	C	50	GLU	C-N-CA	-5.32	115.87	123.11
3	C	145	CYS	N-CA-CB	-5.32	102.33	111.21
1	A	613	ILE	CG1-CB-CG2	-5.32	94.75	110.70
2	B	136	THR	O-C-N	5.32	129.28	123.27
2	B	728	ARG	NE-CZ-NH2	5.32	123.98	119.20
2	B	599	THR	CA-C-O	-5.31	114.86	120.55
4	E	53	PRO	CA-C-N	-5.31	115.47	122.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	53	PRO	C-N-CA	-5.31	115.47	122.85
2	B	1076	HIS	CA-CB-CG	5.31	119.11	113.80
4	E	191	LYS	O-C-N	-5.31	116.28	123.19
1	A	285	PRO	O-C-N	5.31	129.63	122.89
9	K	107	THR	OG1-CB-CG2	5.31	119.92	109.30
2	B	232	SER	N-CA-C	-5.31	102.49	110.24
3	C	158	VAL	O-C-N	-5.31	116.89	123.10
7	I	77	LYS	CA-C-N	5.31	130.43	121.14
7	I	77	LYS	C-N-CA	5.31	130.43	121.14
9	K	24	ASP	CB-CA-C	-5.31	100.56	109.48
10	L	58	LYS	CA-C-O	-5.31	112.92	120.51
6	H	55	LEU	CA-C-N	-5.31	115.94	122.84
6	H	55	LEU	C-N-CA	-5.31	115.94	122.84
4	E	178	ILE	N-CA-C	-5.30	100.43	108.17
1	A	987	VAL	CB-CA-C	-5.30	105.18	111.97
3	C	258	ILE	CB-CG1-CD1	-5.30	102.67	113.80
1	A	156	ASP	N-CA-C	5.30	122.09	110.80
1	A	1214	GLU	N-CA-CB	5.30	118.46	110.30
5	F	90	ARG	NE-CZ-NH1	-5.30	116.20	121.50
4	E	156	LEU	CD1-CG-CD2	5.30	122.46	110.80
1	A	1419	ASP	N-CA-CB	5.30	118.63	110.21
10	L	33	GLU	N-CA-C	5.30	122.08	110.80
1	A	1344	GLY	CA-C-O	5.29	126.12	120.30
2	B	956	THR	CB-CA-C	-5.29	100.02	109.71
1	A	46	THR	CB-CA-C	-5.29	103.53	111.73
1	A	1135	ARG	CD-NE-CZ	5.29	131.81	124.40
8	J	28	ASP	O-C-N	5.29	128.87	122.20
1	A	225	ASN	CB-CG-ND2	-5.29	108.46	116.40
3	C	187	LYS	N-CA-CB	-5.29	104.05	111.62
1	A	1167	GLU	CB-CA-C	5.29	119.19	110.88
2	B	118	ARG	N-CA-C	-5.29	104.95	111.40
2	B	479	VAL	N-CA-C	-5.29	104.36	111.44
4	E	185	ALA	CA-C-O	-5.29	114.81	120.42
1	A	1172	LEU	CA-C-O	-5.29	112.12	120.37
2	B	21	GLU	CB-CA-C	5.29	120.47	109.95
2	B	362	PRO	CB-CA-C	-5.29	103.46	111.44
6	H	6	PHE	N-CA-C	-5.29	101.03	109.07
9	K	48	ALA	CA-C-N	5.29	127.31	120.44
9	K	48	ALA	C-N-CA	5.29	127.31	120.44
9	K	101	LEU	N-CA-C	5.29	117.79	111.71
7	I	32	CYS	CB-CA-C	-5.28	100.55	111.22
1	A	825	ILE	N-CA-C	5.28	116.06	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	579	ARG	NH1-CZ-NH2	5.28	126.17	119.30
4	E	165	LEU	CD1-CG-CD2	-5.28	99.18	110.80
1	A	766	GLY	N-CA-C	5.28	122.33	112.77
2	B	485	ARG	CA-C-N	-5.28	112.79	120.29
2	B	485	ARG	C-N-CA	-5.28	112.79	120.29
6	H	52	GLN	O-C-N	-5.28	115.57	122.59
1	A	367	PRO	O-C-N	-5.28	116.28	122.99
1	A	535	THR	N-CA-CB	-5.28	102.55	110.73
7	I	57	GLY	N-CA-C	5.28	123.35	115.64
1	A	267	ALA	CA-C-N	5.28	127.88	120.28
1	A	267	ALA	C-N-CA	5.28	127.88	120.28
1	A	917	SER	N-CA-CB	-5.28	102.36	110.01
1	A	1318	THR	CA-CB-CG2	5.28	119.47	110.50
4	E	130	ALA	N-CA-C	-5.28	102.04	109.96
1	A	1074	GLU	CB-CG-CD	5.28	121.57	112.60
3	C	202	PRO	CA-C-O	-5.27	115.02	121.03
2	B	974	PRO	CA-C-N	5.27	130.87	121.75
2	B	974	PRO	C-N-CA	5.27	130.87	121.75
5	F	75	PRO	CA-C-O	-5.27	115.33	121.34
2	B	892	LYS	CB-CG-CD	5.27	123.42	111.30
1	A	151	ASP	O-C-N	-5.27	117.72	123.52
1	A	514	PRO	N-CA-CB	-5.27	98.46	103.41
2	B	788	ARG	CA-C-O	-5.27	115.72	121.89
1	A	487	MET	CG-SD-CE	-5.27	89.31	100.90
1	A	651	LYS	CG-CD-CE	5.27	123.42	111.30
1	A	914	GLU	CG-CD-OE2	-5.27	106.29	118.40
1	A	1277	GLU	N-CA-CB	5.27	117.78	110.04
1	A	1412	ALA	O-C-N	5.27	127.50	122.07
2	B	316	PRO	O-C-N	5.27	129.30	122.24
3	C	68	GLY	N-CA-C	-5.27	107.25	113.99
1	A	15	LYS	N-CA-CB	-5.26	102.91	110.65
1	A	462	VAL	CB-CA-C	5.26	117.24	111.08
1	A	1428	VAL	N-CA-CB	-5.26	104.70	110.65
2	B	166	PHE	CA-C-O	-5.26	115.26	121.16
2	B	651	LEU	CA-C-N	5.26	127.59	120.38
2	B	651	LEU	C-N-CA	5.26	127.59	120.38
4	E	73	PRO	CB-CA-C	5.26	120.25	111.56
4	E	92	THR	CA-C-N	5.26	127.28	120.44
4	E	92	THR	C-N-CA	5.26	127.28	120.44
1	A	891	ALA	CA-C-O	5.26	126.35	120.82
4	E	71	LYS	N-CA-C	5.26	119.70	113.12
3	C	77	ILE	CA-C-O	-5.26	114.15	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	135	GLN	CA-CB-CG	5.26	124.62	114.10
1	A	287	HIS	N-CA-C	5.26	122.00	110.80
1	A	194	ALA	N-CA-C	5.26	116.14	107.20
2	B	979	LYS	N-CA-C	5.26	118.63	110.17
4	E	199	ILE	N-CA-CB	-5.26	104.84	111.46
1	A	1155	ASP	OD1-CG-OD2	-5.25	110.29	122.90
5	F	112	GLU	CA-CB-CG	-5.25	103.59	114.10
1	A	451	HIS	CB-CG-ND1	5.25	130.58	122.70
2	B	1164	GLY	CA-C-N	-5.25	117.78	123.08
2	B	1164	GLY	C-N-CA	-5.25	117.78	123.08
1	A	36	ARG	CA-C-O	-5.25	113.00	120.51
1	A	1141	THR	N-CA-CB	-5.25	102.21	110.77
1	A	1310	GLY	O-C-N	5.25	128.73	122.64
4	E	172	GLU	CG-CD-OE1	-5.25	106.32	118.40
6	H	145	ARG	CA-C-N	5.25	131.15	121.70
6	H	145	ARG	C-N-CA	5.25	131.15	121.70
10	L	40	LEU	N-CA-C	-5.25	100.98	108.23
1	A	192	GLY	N-CA-C	-5.25	105.38	112.57
1	A	239	LEU	CA-CB-CG	5.25	134.68	116.30
1	A	656	TRP	CB-CA-C	-5.25	100.92	110.63
2	B	432	MET	CA-C-O	-5.25	113.00	120.51
2	B	914	LYS	CB-CA-C	-5.25	99.17	110.45
6	H	97	MET	N-CA-CB	-5.25	102.88	110.70
7	I	47	GLU	N-CA-CB	5.25	118.99	110.17
8	J	46	CYS	CA-CB-SG	-5.25	102.33	114.40
9	K	70	ARG	CB-CA-C	5.25	121.12	109.94
1	A	764	CYS	CA-CB-SG	5.25	126.47	114.40
1	A	829	VAL	N-CA-C	5.25	115.87	110.36
2	B	857	ARG	CA-CB-CG	-5.25	103.61	114.10
1	A	229	SER	CB-CA-C	-5.25	104.58	111.82
2	B	131	ASP	O-C-N	5.25	129.85	123.14
7	I	47	GLU	O-C-N	-5.25	117.10	123.13
1	A	706	HIS	O-C-N	5.24	129.56	122.59
1	A	894	GLU	CA-C-N	-5.24	112.73	120.28
1	A	894	GLU	C-N-CA	-5.24	112.73	120.28
2	B	479	VAL	CG1-CB-CG2	-5.24	99.27	110.80
1	A	1108	ALA	N-CA-C	5.24	118.09	109.76
2	B	95	ILE	CB-CA-C	-5.24	102.85	110.81
4	E	192	ARG	CA-C-O	5.24	127.10	121.44
5	F	120	ILE	CA-CB-CG1	5.24	119.30	110.40
1	A	479	ASN	CA-C-N	5.24	130.79	122.94
1	A	479	ASN	C-N-CA	5.24	130.79	122.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	736	ASN	CA-C-N	-5.24	113.74	122.64
1	A	736	ASN	C-N-CA	-5.24	113.74	122.64
2	B	268	THR	CB-CA-C	5.24	120.08	110.24
2	B	477	ALA	O-C-N	-5.24	114.62	123.00
6	H	135	LEU	CA-C-N	5.24	131.54	121.54
6	H	135	LEU	C-N-CA	5.24	131.54	121.54
2	B	653	VAL	CA-CB-CG1	5.23	119.29	110.40
2	B	784	ASN	CA-C-N	-5.23	111.78	120.68
2	B	784	ASN	C-N-CA	-5.23	111.78	120.68
8	J	14	VAL	N-CA-CB	-5.23	102.59	111.23
1	A	1237	ILE	N-CA-C	-5.23	100.71	108.45
4	E	74	ASP	CA-C-O	5.23	127.99	120.51
9	K	110	ASN	N-CA-CB	5.23	118.05	110.26
4	E	84	ASP	CA-C-N	5.23	128.52	121.20
4	E	84	ASP	C-N-CA	5.23	128.52	121.20
7	I	40	SER	CA-CB-OG	5.23	121.56	111.10
1	A	982	THR	CA-CB-OG1	-5.23	101.76	109.60
1	A	443	LEU	N-CA-C	-5.22	100.88	109.40
1	A	611	GLN	N-CA-CB	5.22	119.38	110.71
2	B	510	LYS	CB-CG-CD	-5.22	99.28	111.30
2	B	566	LEU	CA-C-O	5.22	126.09	120.55
7	I	110	PHE	N-CA-CB	-5.22	103.16	111.62
9	K	39	ASP	OD1-CG-OD2	-5.22	110.36	122.90
1	A	166	GLY	N-CA-C	5.22	119.83	110.95
1	A	295	LEU	CB-CA-C	-5.22	101.14	110.70
1	A	1274	ARG	CB-CG-CD	5.22	123.31	111.30
1	A	632	VAL	N-CA-C	5.22	115.36	110.30
1	A	1127	ASP	CB-CA-C	-5.22	102.96	111.68
2	B	845	SER	CA-C-O	5.22	126.00	120.10
2	B	899	ILE	CA-C-O	-5.22	116.34	122.13
2	B	1054	GLY	CA-C-O	-5.22	115.38	120.75
4	E	50	MET	CG-SD-CE	5.22	112.38	100.90
6	H	40	LEU	N-CA-C	5.22	117.00	108.55
2	B	848	ARG	NE-CZ-NH1	-5.21	116.28	121.50
7	I	92	ARG	CA-C-N	5.21	128.24	120.31
7	I	92	ARG	C-N-CA	5.21	128.24	120.31
2	B	484	ASN	N-CA-C	5.21	117.79	110.23
1	A	1300	LYS	CG-CD-CE	-5.21	99.32	111.30
1	A	460	VAL	CA-C-N	5.21	130.11	122.77
1	A	460	VAL	C-N-CA	5.21	130.11	122.77
2	B	645	SER	O-C-N	-5.21	115.66	122.59
2	B	408	LEU	N-CA-C	5.21	118.19	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	680	THR	CA-CB-CG2	5.21	119.35	110.50
2	B	965	LYS	CG-CD-CE	5.21	123.27	111.30
2	B	1094	ARG	NE-CZ-NH2	5.21	123.89	119.20
1	A	85	ASP	N-CA-C	-5.20	102.58	110.28
1	A	1415	SER	CA-CB-OG	-5.20	100.69	111.10
2	B	292	ILE	N-CA-C	5.20	120.12	108.88
1	A	709	THR	N-CA-C	5.20	117.42	110.35
2	B	1201	LYS	CA-C-O	-5.20	115.33	120.90
4	E	66	GLU	CA-C-N	-5.20	112.90	120.29
4	E	66	GLU	C-N-CA	-5.20	112.90	120.29
9	K	6	ARG	CD-NE-CZ	5.20	131.68	124.40
2	B	446	LEU	CA-C-N	5.20	131.47	121.54
2	B	446	LEU	C-N-CA	5.20	131.47	121.54
1	A	666	ILE	CA-C-O	5.20	126.30	119.85
1	A	753	GLY	N-CA-C	5.20	119.41	112.65
2	B	1031	LEU	CD1-CG-CD2	-5.20	99.36	110.80
1	A	301	ALA	CA-C-N	5.20	127.50	120.38
1	A	301	ALA	C-N-CA	5.20	127.50	120.38
1	A	959	ASN	CA-CB-CG	-5.20	107.40	112.60
1	A	243	PRO	CB-CA-C	-5.20	104.58	110.92
1	A	850	VAL	CB-CA-C	-5.20	104.09	111.21
5	F	108	PHE	O-C-N	-5.19	116.07	122.25
1	A	1446	ASP	CA-CB-CG	5.19	117.79	112.60
2	B	164	LYS	CA-C-O	-5.19	111.97	120.80
9	K	6	ARG	CG-CD-NE	-5.19	100.58	112.00
1	A	574	GLY	CA-C-N	-5.19	113.03	120.82
1	A	574	GLY	C-N-CA	-5.19	113.03	120.82
2	B	830	TYR	CA-C-O	5.19	126.08	120.63
2	B	1141	HIS	CE1-NE2-CD2	-5.19	103.81	109.00
2	B	1222	ARG	CA-C-N	5.19	131.45	121.54
2	B	1222	ARG	C-N-CA	5.19	131.45	121.54
6	H	44	VAL	CG1-CB-CG2	5.19	122.22	110.80
1	A	557	ASP	OD1-CG-OD2	-5.19	110.45	122.90
1	A	1130	GLN	CB-CA-C	5.19	120.08	109.55
2	B	601	ARG	NE-CZ-NH1	-5.19	116.31	121.50
2	B	959	ASP	OD1-CG-OD2	-5.19	110.44	122.90
1	A	491	VAL	CB-CA-C	-5.19	104.92	111.04
2	B	91	SER	O-C-N	5.19	129.92	123.28
2	B	944	THR	O-C-N	5.19	129.78	122.41
9	K	110	ASN	CA-C-O	-5.19	113.67	120.00
1	A	219	PHE	CA-C-N	5.18	127.18	120.44
1	A	219	PHE	C-N-CA	5.18	127.18	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1138	ILE	N-CA-CB	-5.18	103.16	111.82
4	E	23	VAL	CA-C-O	5.18	126.67	121.17
4	E	165	LEU	CA-C-N	-5.18	113.39	120.44
4	E	165	LEU	C-N-CA	-5.18	113.39	120.44
2	B	291	ILE	N-CA-C	-5.18	99.49	106.85
1	A	225	ASN	N-CA-CB	-5.18	102.11	110.81
1	A	938	LYS	N-CA-CB	5.18	117.73	110.12
7	I	63	GLY	O-C-N	-5.18	115.97	122.70
2	B	28	GLU	N-CA-CB	-5.18	102.25	110.22
2	B	757	PRO	CB-CA-C	-5.18	105.05	111.11
6	H	116	TYR	CB-CA-C	-5.17	100.12	110.42
2	B	303	TYR	CB-CA-C	-5.17	104.83	111.50
6	H	82	PRO	N-CA-C	-5.17	101.82	112.47
8	J	25	LEU	CD1-CG-CD2	5.17	122.17	110.80
8	J	59	LYS	N-CA-C	-5.17	107.10	113.41
10	L	63	ARG	CG-CD-NE	5.17	123.37	112.00
1	A	419	LYS	CB-CG-CD	5.17	123.19	111.30
3	C	109	SER	O-C-N	-5.17	115.44	122.36
4	E	47	CYS	CB-CA-C	5.17	119.17	109.71
2	B	542	MET	CG-SD-CE	-5.16	89.54	100.90
9	K	37	LYS	N-CA-C	5.16	118.32	111.30
2	B	1084	GLN	CA-C-N	5.16	130.16	122.99
2	B	1084	GLN	C-N-CA	5.16	130.16	122.99
8	J	17	LYS	CD-CE-NZ	-5.16	95.38	111.90
9	K	5	ASP	CB-CA-C	-5.16	101.39	109.70
9	K	46	ILE	CA-CB-CG1	5.16	119.17	110.40
2	B	629	ASP	CB-CG-OD2	5.16	130.26	118.40
3	C	219	PHE	O-C-N	5.16	129.26	122.97
1	A	287	HIS	O-C-N	-5.16	115.73	122.59
1	A	1203	ASN	N-CA-C	5.16	116.98	111.36
1	A	712	GLU	CA-C-O	-5.16	114.04	119.97
1	A	808	LEU	N-CA-CB	-5.16	102.01	110.41
2	B	766	ARG	NH1-CZ-NH2	5.16	126.00	119.30
2	B	817	LEU	CB-CA-C	-5.16	103.10	111.14
2	B	1023	VAL	CA-C-O	-5.16	115.05	120.57
6	H	126	GLU	CA-CB-CG	5.16	124.41	114.10
1	A	1158	PRO	N-CD-CG	5.15	110.93	103.20
4	E	152	LYS	CB-CG-CD	-5.15	99.45	111.30
4	E	190	LEU	CB-CA-C	-5.15	100.06	109.54
1	A	1384	VAL	CA-C-O	-5.15	114.66	120.32
9	K	76	GLN	CB-CA-C	-5.15	100.11	109.38
2	B	371	GLU	N-CA-CB	5.15	117.99	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	617	ARG	CA-C-O	-5.15	114.82	120.43
2	B	1197	PRO	CA-C-O	5.15	127.21	121.34
8	J	6	ARG	CA-C-N	5.15	128.41	121.05
8	J	6	ARG	C-N-CA	5.15	128.41	121.05
2	B	395	GLN	N-CA-CB	5.15	118.16	109.92
8	J	59	LYS	CD-CE-NZ	-5.15	95.43	111.90
1	A	242	PRO	N-CA-CB	-5.15	100.31	103.19
1	A	1036	ARG	NE-CZ-NH2	-5.15	114.57	119.20
1	A	65	LEU	CA-CB-CG	5.14	134.30	116.30
1	A	931	GLU	CA-C-N	5.14	127.44	120.44
1	A	931	GLU	C-N-CA	5.14	127.44	120.44
2	B	452	THR	CA-CB-CG2	5.14	119.25	110.50
4	E	98	ILE	CA-CB-CG1	5.14	119.15	110.40
1	A	1402	PHE	CA-CB-CG	-5.14	108.66	113.80
2	B	1044	ALA	CA-C-N	-5.14	112.80	121.03
2	B	1044	ALA	C-N-CA	-5.14	112.80	121.03
4	E	116	ILE	CB-CG1-CD1	-5.14	103.01	113.80
7	I	32	CYS	CA-C-O	5.14	127.82	121.60
2	B	723	VAL	CA-C-O	-5.14	115.27	121.54
1	A	264	PHE	CA-CB-CG	5.14	118.94	113.80
2	B	612	GLU	CB-CA-C	5.14	119.24	110.56
1	A	1418	LEU	N-CA-C	5.13	117.30	107.75
2	B	1040	ASN	CA-CB-CG	-5.13	107.47	112.60
4	E	17	ARG	NE-CZ-NH2	5.13	123.82	119.20
8	J	16	ASP	N-CA-CB	-5.13	103.06	110.56
1	A	793	SER	CA-CB-OG	5.13	121.36	111.10
2	B	40	GLU	N-CA-C	5.13	116.95	111.36
2	B	238	ALA	CA-C-O	-5.13	115.16	120.70
2	B	842	ASN	N-CA-C	-5.13	101.40	109.25
9	K	66	PRO	CA-N-CD	-5.13	104.82	112.00
1	A	997	LEU	CD1-CG-CD2	-5.13	99.51	110.80
1	A	361	LEU	CB-CA-C	-5.13	101.96	110.68
2	B	599	THR	CB-CA-C	-5.13	102.17	110.79
1	A	1039	LYS	CA-C-O	5.13	125.98	120.55
2	B	785	TYR	CA-C-N	-5.13	112.40	120.60
2	B	785	TYR	C-N-CA	-5.13	112.40	120.60
2	B	938	SER	CB-CA-C	5.13	119.16	109.37
4	E	132	ILE	CB-CA-C	-5.13	102.85	110.33
2	B	496	ARG	CB-CG-CD	5.12	123.08	111.30
2	B	546	SER	CA-C-O	-5.12	115.98	121.56
2	B	974	PRO	N-CA-CB	-5.12	99.02	103.32
3	C	16	ASP	CA-C-N	5.12	130.27	121.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	16	ASP	C-N-CA	5.12	130.27	121.87
8	J	46	CYS	CA-C-O	-5.12	115.10	120.63
9	K	51	LEU	CB-CG-CD1	-5.12	95.34	110.70
1	A	407	ARG	NH1-CZ-NH2	5.12	125.96	119.30
2	B	517	THR	N-CA-CB	5.12	119.43	110.42
2	B	1188	LYS	O-C-N	5.12	127.46	122.19
3	C	35	ARG	CA-CB-CG	5.12	124.34	114.10
2	B	109	THR	CA-C-N	5.12	130.34	121.64
2	B	109	THR	C-N-CA	5.12	130.34	121.64
3	C	19	ASP	N-CA-CB	-5.12	101.72	110.16
4	E	192	ARG	CD-NE-CZ	5.12	131.56	124.40
1	A	234	MET	CG-SD-CE	5.11	112.15	100.90
2	B	1136	ASP	N-CA-C	5.11	117.52	111.33
2	B	351	TYR	N-CA-C	-5.11	105.60	111.07
4	E	147	HIS	CA-CB-CG	5.11	118.91	113.80
4	E	43	LYS	CA-C-N	5.11	131.29	121.54
4	E	43	LYS	C-N-CA	5.11	131.29	121.54
5	F	150	GLU	CG-CD-OE1	-5.11	106.66	118.40
6	H	121	LEU	N-CA-CB	-5.11	101.55	109.87
1	A	1019	CYS	N-CA-C	5.10	117.58	111.71
3	C	176	ILE	N-CA-C	5.10	115.70	106.61
2	B	92	PHE	N-CA-CB	5.10	117.86	109.95
2	B	699	GLU	CB-CA-C	-5.10	99.64	110.31
9	K	64	GLU	O-C-N	-5.10	115.99	122.27
2	B	396	ASP	O-C-N	5.10	128.88	122.86
1	A	161	LEU	CA-C-O	-5.10	115.66	121.68
6	H	80	ARG	CA-CB-CG	5.10	124.30	114.10
1	A	21	LEU	N-CA-CB	-5.10	102.69	110.85
1	A	406	ILE	CB-CA-C	-5.10	102.89	110.33
1	A	1157	ASP	O-C-N	5.10	126.23	120.83
5	F	92	ARG	NE-CZ-NH1	5.10	126.60	121.50
1	A	416	ARG	CG-CD-NE	-5.10	100.79	112.00
2	B	628	THR	OG1-CB-CG2	-5.10	99.11	109.30
1	A	959	ASN	N-CA-C	-5.09	98.75	108.17
2	B	561	TRP	CA-C-N	-5.09	114.15	122.40
2	B	561	TRP	C-N-CA	-5.09	114.15	122.40
8	J	17	LYS	CA-CB-CG	-5.09	103.91	114.10
9	K	62	LYS	N-CA-C	5.09	116.81	108.76
10	L	49	LYS	N-CA-C	5.09	116.92	107.60
1	A	634	THR	CA-CB-CG2	-5.09	101.85	110.50
2	B	94	LYS	CA-C-O	-5.09	116.15	121.55
6	H	48	PRO	CB-CA-C	5.09	118.91	111.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	K	85	ASP	N-CA-CB	5.09	118.14	110.30
1	A	346	ASP	CA-C-N	-5.09	115.41	122.74
1	A	346	ASP	C-N-CA	-5.09	115.41	122.74
1	A	1217	LYS	CA-C-N	-5.09	113.46	122.26
1	A	1217	LYS	C-N-CA	-5.09	113.46	122.26
2	B	893	LEU	CD1-CG-CD2	-5.09	99.61	110.80
2	B	904	ARG	CG-CD-NE	-5.09	100.80	112.00
1	A	1010	ALA	CA-C-O	5.09	125.81	120.42
2	B	393	LYS	N-CA-CB	5.09	120.99	111.53
3	C	254	LYS	CA-C-O	-5.09	115.66	121.00
6	H	124	ARG	CG-CD-NE	-5.09	100.81	112.00
1	A	834	THR	OG1-CB-CG2	-5.09	99.12	109.30
2	B	260	GLY	N-CA-C	-5.09	101.13	113.18
3	C	202	PRO	CA-C-N	5.08	128.32	121.05
3	C	202	PRO	C-N-CA	5.08	128.32	121.05
1	A	598	LEU	CB-CA-C	-5.08	102.95	111.13
1	A	721	PHE	CA-C-O	5.08	126.12	120.63
1	A	1357	ALA	CB-CA-C	-5.08	99.68	110.31
4	E	155	ARG	O-C-N	5.08	128.99	123.04
5	F	74	ILE	CA-CB-CG1	5.08	119.04	110.40
6	H	144	ILE	N-CA-C	-5.08	101.31	108.27
3	C	211	ASP	CB-CA-C	5.08	116.65	109.08
4	E	207	ARG	NE-CZ-NH1	5.08	126.58	121.50
1	A	164	ARG	O-C-N	-5.08	115.98	122.94
1	A	931	GLU	N-CA-C	5.08	117.55	111.71
9	K	45	LEU	CB-CA-C	5.08	119.33	110.79
1	A	919	ILE	CA-CB-CG1	5.08	119.03	110.40
2	B	1096	ARG	NE-CZ-NH2	-5.08	114.63	119.20
1	A	479	ASN	CA-CB-CG	-5.08	107.53	112.60
1	A	817	ALA	CA-C-N	-5.08	113.95	120.65
1	A	817	ALA	C-N-CA	-5.08	113.95	120.65
2	B	567	GLU	CB-CA-C	5.08	120.31	110.46
8	J	47	ARG	N-CA-C	-5.08	105.75	111.28
1	A	98	LYS	CB-CA-C	-5.07	102.37	110.79
1	A	549	MET	CA-CB-CG	-5.07	103.96	114.10
1	A	780	VAL	CB-CA-C	-5.07	105.82	111.35
6	H	84	ALA	N-CA-C	-5.07	103.00	111.37
1	A	1316	VAL	CA-C-O	5.07	125.99	120.57
2	B	979	LYS	CB-CA-C	-5.07	100.93	109.50
4	E	1	MET	CG-SD-CE	5.07	112.05	100.90
1	A	686	ALA	N-CA-CB	5.07	117.63	110.13
6	H	103	LYS	N-CA-CB	5.07	119.06	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	158	PRO	CA-C-N	-5.07	112.99	120.28
1	A	158	PRO	C-N-CA	-5.07	112.99	120.28
1	A	881	GLN	OE1-CD-NE2	5.07	127.67	122.60
1	A	1055	ARG	CA-C-O	-5.07	113.03	119.31
2	B	384	ARG	NE-CZ-NH1	5.07	126.57	121.50
2	B	497	ARG	CG-CD-NE	-5.07	100.86	112.00
2	B	766	ARG	N-CA-C	5.07	117.70	111.82
9	K	24	ASP	N-CA-C	5.07	118.07	109.76
1	A	932	GLU	CA-CB-CG	5.06	124.23	114.10
4	E	149	LEU	CA-C-O	-5.06	113.15	119.28
1	A	1025	ARG	N-CA-CB	5.06	117.92	110.33
4	E	31	THR	N-CA-C	-5.06	101.46	109.96
7	I	61	ASP	N-CA-C	5.06	118.60	112.93
7	I	114	GLN	CA-C-O	-5.06	113.36	119.49
1	A	1062	GLU	OE1-CD-OE2	5.06	135.04	122.90
3	C	143	LEU	CB-CG-CD2	-5.06	95.52	110.70
4	E	158	SER	CA-CB-OG	-5.06	100.98	111.10
1	A	76	GLU	CA-C-N	5.06	128.28	121.20
1	A	76	GLU	C-N-CA	5.06	128.28	121.20
1	A	439	ASN	O-C-N	-5.06	116.47	121.88
1	A	586	ILE	N-CA-C	-5.06	101.03	108.11
1	A	1337	GLU	CA-C-O	-5.06	113.82	119.79
1	A	1377	THR	O-C-N	-5.06	115.48	122.46
2	B	20	ASP	CA-C-O	-5.06	115.28	121.05
2	B	654	ARG	N-CA-CB	-5.06	102.86	111.31
2	B	797	TYR	N-CA-CB	5.06	117.51	109.82
6	H	56	THR	CB-CA-C	5.06	118.87	110.78
7	I	45	ARG	CB-CA-C	-5.06	99.11	109.38
1	A	895	LYS	CA-C-O	5.06	125.81	120.10
1	A	1209	MET	CB-CA-C	-5.06	102.72	110.81
1	A	92	HIS	CB-CA-C	-5.05	102.68	110.26
1	A	621	THR	CA-C-O	5.05	125.85	120.24
2	B	741	CYS	N-CA-C	5.05	117.06	109.23
3	C	136	ASP	CA-CB-CG	5.05	117.66	112.60
8	J	2	ILE	CA-C-O	-5.05	115.99	121.19
1	A	206	GLU	N-CA-C	-5.05	105.43	112.45
1	A	645	LEU	O-C-N	-5.05	116.77	122.12
4	E	207	ARG	CB-CG-CD	5.05	122.92	111.30
6	H	50	ALA	N-CA-C	5.05	117.97	110.14
1	A	372	LYS	N-CA-C	5.05	119.29	113.18
1	A	1241	ARG	CD-NE-CZ	5.05	131.47	124.40
1	A	1383	SER	N-CA-C	5.05	117.95	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	117	SER	O-C-N	5.05	129.74	123.28
1	A	891	ALA	O-C-N	-5.05	116.87	122.07
1	A	1262	LYS	N-CA-CB	5.05	117.30	109.98
2	B	284	ILE	CA-C-N	-5.05	113.55	120.46
2	B	284	ILE	C-N-CA	-5.05	113.55	120.46
2	B	789	MET	CG-SD-CE	-5.05	89.80	100.90
1	A	591	PHE	CA-C-O	-5.04	114.88	120.38
2	B	137	TYR	CA-C-N	5.04	130.78	121.70
2	B	137	TYR	C-N-CA	5.04	130.78	121.70
1	A	501	LEU	CA-C-N	-5.04	112.31	121.14
1	A	501	LEU	C-N-CA	-5.04	112.31	121.14
1	A	839	ARG	CB-CG-CD	-5.04	99.70	111.30
1	A	1111	MET	O-C-N	-5.04	117.29	122.94
3	C	184	ASN	CB-CA-C	5.04	119.17	111.76
1	A	474	VAL	CB-CA-C	5.04	119.84	111.37
2	B	599	THR	CA-C-N	-5.04	113.26	120.82
2	B	599	THR	C-N-CA	-5.04	113.26	120.82
2	B	778	MET	N-CA-C	-5.04	101.47	109.59
1	A	1434	ALA	N-CA-C	5.04	116.18	109.93
3	C	104	PHE	N-CA-C	-5.04	101.08	108.99
1	A	683	ILE	CA-CB-CG1	5.04	118.96	110.40
1	A	237	THR	N-CA-C	-5.04	100.07	110.80
1	A	446	ARG	CD-NE-CZ	-5.04	117.35	124.40
1	A	846	GLU	N-CA-CB	-5.04	102.46	110.22
1	A	1432	GLN	CA-C-N	-5.04	114.64	122.09
1	A	1432	GLN	C-N-CA	-5.04	114.64	122.09
1	A	46	THR	CA-C-O	-5.04	115.33	121.58
1	A	412	ARG	NE-CZ-NH1	-5.04	116.46	121.50
1	A	416	ARG	CA-CB-CG	5.04	124.17	114.10
7	I	111	THR	N-CA-C	5.04	117.78	109.72
1	A	202	LEU	CD1-CG-CD2	-5.03	99.73	110.80
1	A	440	ASP	N-CA-C	-5.03	103.44	109.83
1	A	1210	GLY	N-CA-C	5.03	119.96	113.27
3	C	38	ILE	CG1-CB-CG2	-5.03	95.60	110.70
2	B	285	ILE	N-CA-C	5.03	115.75	110.62
6	H	24	CYS	CB-CA-C	-5.03	99.63	110.45
9	K	49	GLU	CB-CA-C	-5.03	102.98	110.88
1	A	32	VAL	CB-CA-C	5.03	119.54	111.29
3	C	32	SER	N-CA-C	5.03	117.50	111.71
4	E	81	GLU	OE1-CD-OE2	5.03	134.97	122.90
5	F	130	ILE	N-CA-C	5.03	112.53	107.55
2	B	291	ILE	N-CA-CB	-5.03	105.64	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	112	TYR	CE1-CZ-CE2	-5.03	110.24	120.30
2	B	875	GLU	CB-CG-CD	5.03	121.15	112.60
2	B	1074	ASN	N-CA-C	5.03	116.98	109.59
1	A	548	ASN	O-C-N	-5.03	115.70	122.23
1	A	1259	MET	CG-SD-CE	5.03	111.96	100.90
2	B	843	GLN	N-CA-C	5.03	116.84	111.36
2	B	217	ARG	NE-CZ-NH2	5.02	123.72	119.20
1	A	425	GLN	CB-CA-C	-5.02	102.60	110.79
1	A	682	THR	O-C-N	5.02	127.44	122.12
2	B	1189	ILE	N-CA-C	5.02	119.79	109.34
8	J	24	LEU	CB-CA-C	-5.02	101.03	110.67
2	B	952	VAL	N-CA-C	-5.02	101.02	108.45
2	B	1150	ARG	N-CA-C	5.02	117.64	111.82
9	K	74	ARG	CG-CD-NE	-5.02	100.95	112.00
2	B	705	MET	CB-CG-SD	-5.02	97.64	112.70
1	A	46	THR	CA-CB-CG2	5.02	119.03	110.50
1	A	432	VAL	N-CA-C	5.02	115.08	107.75
1	A	596	THR	CA-CB-CG2	-5.02	101.97	110.50
2	B	48	LEU	CA-C-O	-5.02	115.15	121.02
1	A	413	ILE	CA-C-O	-5.02	114.63	120.75
2	B	389	ALA	N-CA-CB	-5.02	102.50	110.22
1	A	274	ILE	N-CA-C	-5.01	105.66	110.72
1	A	486	GLU	OE1-CD-OE2	-5.01	110.86	122.90
1	A	1000	LEU	N-CA-C	5.01	117.58	109.40
1	A	1351	GLU	CA-CB-CG	-5.01	104.07	114.10
2	B	21	GLU	N-CA-CB	5.01	118.83	110.41
2	B	113	TYR	O-C-N	-5.01	115.92	121.53
3	C	196	ASP	CB-CA-C	-5.01	100.88	109.65
1	A	1150	SER	CA-C-O	-5.01	115.50	121.16
1	A	1201	ALA	N-CA-CB	-5.01	102.54	110.06
2	B	58	THR	OG1-CB-CG2	-5.01	99.27	109.30
3	C	75	MET	CA-C-N	-5.01	113.70	122.62
3	C	75	MET	C-N-CA	-5.01	113.70	122.62
4	E	110	PHE	CB-CA-C	-5.01	102.42	110.14
4	E	167	ARG	N-CA-C	5.01	118.50	112.38
7	I	35	VAL	CA-CB-CG2	-5.01	101.88	110.40
2	B	773	MET	O-C-N	-5.01	116.81	122.12
3	C	125	MET	CB-CG-SD	5.01	127.74	112.70
6	H	111	LEU	N-CA-C	5.01	118.29	110.32
1	A	212	LYS	CA-CB-CG	5.01	124.12	114.10
2	B	611	PRO	CA-N-CD	-5.01	104.99	112.00
9	K	104	ASN	N-CA-CB	5.01	119.20	110.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	519	PRO	N-CD-CG	5.01	110.71	103.20
4	E	62	ALA	CA-C-O	-5.01	114.52	120.43
4	E	128	PRO	N-CA-C	5.01	116.81	110.70
1	A	1262	LYS	CA-C-O	-5.01	115.74	120.90
2	B	272	THR	CA-C-O	-5.01	115.10	120.46
1	A	325	ILE	CG1-CB-CG2	-5.00	95.69	110.70
2	B	459	TYR	O-C-N	-5.00	116.89	122.09
7	I	31	THR	N-CA-C	5.00	120.03	113.88
1	A	174	ILE	N-CA-C	-5.00	101.11	108.11
1	A	1292	PRO	O-C-N	5.00	128.70	123.10
2	B	271	ALA	CA-C-N	5.00	130.21	123.11
2	B	271	ALA	C-N-CA	5.00	130.21	123.11
2	B	755	ILE	N-CA-CB	-5.00	104.47	112.07
7	I	102	VAL	N-CA-CB	5.00	118.50	112.10
10	L	63	ARG	N-CA-C	-5.00	102.89	110.24

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	E	204	THR	CB

All (124) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1015	VAL	Mainchain
1	A	1027	ALA	Mainchain
1	A	1035	TYR	Sidechain
1	A	1046	LEU	Mainchain
1	A	1093	LYS	Peptide
1	A	1119	TYR	Sidechain
1	A	1155	ASP	Peptide,Mainchain
1	A	1218	GLN	Peptide
1	A	1232	ASN	Peptide
1	A	1301	GLU	Mainchain
1	A	1366	ARG	Sidechain
1	A	1375	MET	Mainchain
1	A	1384	VAL	Peptide
1	A	158	PRO	Peptide
1	A	165	GLY	Peptide
1	A	187	LYS	Peptide
1	A	191	THR	Peptide
1	A	194	ALA	Peptide

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Mol	Chain	Res	Type	Group
1	A	325	ILE	Peptide
1	A	377	PRO	Mainchain
1	A	399	HIS	Peptide,Mainchain
1	A	434	ARG	Sidechain
1	A	44	THR	Peptide
1	A	460	VAL	Peptide
1	A	464	PRO	Peptide,Mainchain
1	A	469	ARG	Mainchain
1	A	555	ASP	Peptide
1	A	60	SER	Peptide
1	A	631	HIS	Sidechain
1	A	659	HIS	Sidechain
1	A	705	LYS	Peptide
1	A	706	HIS	Peptide
1	A	74	MET	Peptide
1	A	741	ASN	Mainchain
1	A	759	ALA	Mainchain
1	A	920	LEU	Mainchain
1	A	936	LEU	Mainchain
1	A	941	LYS	Mainchain
2	B	1009	ASP	Mainchain
2	B	1025	HIS	Sidechain
2	B	104	GLU	Peptide
2	B	107	GLY	Peptide
2	B	109	THR	Peptide
2	B	1097	HIS	Sidechain
2	B	1101	ASP	Peptide
2	B	1102	LYS	Peptide
2	B	1109	GLY	Peptide
2	B	1152	MET	Peptide
2	B	1155	SER	Peptide
2	B	1157	ALA	Peptide
2	B	1166	CYS	Mainchain
2	B	1181	GLU	Peptide
2	B	1221	SER	Peptide
2	B	1222	ARG	Peptide
2	B	199	MET	Mainchain
2	B	202	TYR	Sidechain
2	B	292	ILE	Mainchain
2	B	337	ARG	Sidechain
2	B	369	GLY	Peptide
2	B	431	TYR	Peptide

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Mol	Chain	Res	Type	Group
2	B	501	PRO	Peptide
2	B	517	THR	Mainchain
2	B	518	HIS	Sidechain
2	B	601	ARG	Sidechain
2	B	604	ARG	Sidechain
2	B	642	ASP	Peptide
2	B	643	ASP	Peptide
2	B	644	GLU	Peptide
2	B	667	GLN	Peptide
2	B	732	SER	Peptide
2	B	742	GLU	Mainchain
2	B	808	ALA	Mainchain
2	B	863	GLU	Peptide
2	B	868	MET	Peptide
2	B	882	THR	Peptide
2	B	884	ARG	Peptide
2	B	98	THR	Peptide
2	B	984	HIS	Sidechain
3	C	126	GLY	Peptide
3	C	156	THR	Mainchain
3	C	163	ILE	Mainchain
3	C	184	ASN	Peptide
3	C	190	ASP	Peptide
3	C	194	GLU	Mainchain
3	C	238	ILE	Mainchain
3	C	240	VAL	Mainchain
3	C	261	ALA	Peptide
3	C	267	GLN	Peptide
3	C	34	ARG	Sidechain
3	C	35	ARG	Sidechain
3	C	4	GLU	Peptide
4	E	125	PRO	Peptide
4	E	128	PRO	Peptide
4	E	170	LEU	Peptide
4	E	207	ARG	Mainchain
4	E	212	ARG	Sidechain
4	E	77	SER	Peptide
5	F	122	MET	Mainchain
5	F	144	GLU	Mainchain
6	H	102	TYR	Peptide
6	H	103	LYS	Peptide
6	H	127	GLY	Peptide

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Mol	Chain	Res	Type	Group
6	H	135	LEU	Peptide
6	H	136	LYS	Peptide
6	H	17	PRO	Peptide
6	H	26	ILE	Peptide
6	H	61	SER	Peptide
6	H	62	SER	Peptide
6	H	86	ASP	Peptide
6	H	87	ARG	Peptide
6	H	94	ASP	Peptide
7	I	26	LEU	Peptide
7	I	3	THR	Peptide
7	I	39	GLY	Mainchain
7	I	41	PRO	Mainchain
7	I	43	VAL	Mainchain
7	I	83	ASN	Peptide
8	J	21	TYR	Sidechain
9	K	70	ARG	Mainchain
10	L	35	SER	Peptide
10	L	59	ALA	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10635	0	10691	722	0
2	B	8690	0	8715	529	0
3	C	2095	0	2053	164	0
4	E	1760	0	1788	135	0
5	F	670	0	690	47	0
6	H	1068	0	1040	168	0
7	I	990	0	949	69	0
8	J	525	0	537	49	0
9	K	919	0	929	77	0
10	L	364	0	388	67	0
11	A	2	0	0	0	0
12	A	2	0	0	1	0
12	B	1	0	0	1	0
12	C	1	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	I	2	0	0	0	0
12	J	1	0	0	2	0
12	L	1	0	0	2	0
13	A	31	0	12	0	0
All	All	27757	0	27792	1902	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 35.

All (1902) 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:1057:LYS:CE	2:B:1057:LYS:CD	1.75	1.65
1:A:368:LYS:CD	1:A:368:LYS:CE	1.75	1.65
1:A:919:ILE:CD1	1:A:919:ILE:CG1	1.75	1.64
4:E:37:LEU:CD1	4:E:37:LEU:CG	1.75	1.64
1:A:1112:LYS:CD	1:A:1112:LYS:CE	1.74	1.64
3:C:116:LYS:CD	3:C:116:LYS:CE	1.75	1.64
4:E:71:LYS:CD	4:E:71:LYS:CG	1.75	1.64
1:A:174:ILE:CA	1:A:174:ILE:CB	1.75	1.64
2:B:436:VAL:CA	2:B:436:VAL:CB	1.76	1.64
1:A:1385:THR:CB	1:A:1385:THR:CG2	1.76	1.63
4:E:90:VAL:CG1	4:E:90:VAL:CB	1.75	1.63
10:L:64:LEU:CD1	10:L:64:LEU:CG	1.75	1.63
1:A:61:ILE:CA	1:A:61:ILE:CB	1.77	1.63
1:A:1102:LYS:CD	1:A:1102:LYS:CE	1.75	1.63
2:B:883:LEU:CA	2:B:883:LEU:CB	1.75	1.63
1:A:1445:ILE:CB	1:A:1445:ILE:CG2	1.74	1.63
2:B:353:LYS:CG	2:B:353:LYS:CD	1.74	1.62
3:C:205:LYS:CB	3:C:205:LYS:CG	1.74	1.62
1:A:237:THR:CB	1:A:237:THR:CG2	1.75	1.62
1:A:1239:ARG:CG	1:A:1239:ARG:CD	1.75	1.62
1:A:1261:LYS:CD	1:A:1261:LYS:CE	1.77	1.62
1:A:1350:LYS:CG	1:A:1350:LYS:CD	1.76	1.62
2:B:343:ILE:CD1	2:B:343:ILE:CG1	1.75	1.62
1:A:710:LEU:CD2	1:A:710:LEU:CG	1.75	1.62
4:E:129:PRO:CG	4:E:129:PRO:CD	1.76	1.61
7:I:1:MET:CB	7:I:1:MET:CG	1.76	1.61
1:A:1003:LYS:CG	1:A:1003:LYS:CD	1.76	1.61
8:J:38:ARG:CG	8:J:38:ARG:CB	1.75	1.61
2:B:118:ARG:CG	2:B:118:ARG:CD	1.76	1.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:THR:CA	1:A:46:THR:CB	1.77	1.61
1:A:123:ARG:CD	1:A:123:ARG:CG	1.76	1.61
2:B:347:LYS:CD	2:B:347:LYS:CE	1.77	1.61
3:C:199:LYS:CG	3:C:199:LYS:CD	1.75	1.61
4:E:45:LYS:CD	4:E:45:LYS:CE	1.75	1.61
9:K:25:THR:CB	9:K:25:THR:CG2	1.75	1.61
2:B:882:THR:CB	2:B:882:THR:CG2	1.75	1.61
10:L:65:VAL:CB	10:L:65:VAL:CG2	1.78	1.61
1:A:843:LYS:CG	1:A:843:LYS:CD	1.76	1.60
2:B:1163:CYS:CA	2:B:1163:CYS:CB	1.74	1.60
1:A:217:LYS:CD	1:A:217:LYS:CG	1.80	1.60
2:B:358:LYS:CB	2:B:358:LYS:CG	1.75	1.60
1:A:1215:ARG:CB	1:A:1215:ARG:CG	1.75	1.60
3:C:9:LYS:CE	3:C:9:LYS:CD	1.75	1.60
7:I:93:LYS:CG	7:I:93:LYS:CD	1.76	1.60
1:A:74:MET:CB	1:A:74:MET:CG	1.80	1.60
1:A:571:LEU:CD2	1:A:571:LEU:CG	1.78	1.60
2:B:425:THR:CB	2:B:425:THR:CG2	1.75	1.60
4:E:52:ARG:CB	4:E:52:ARG:CG	1.75	1.60
2:B:712:PRO:CG	2:B:712:PRO:CD	1.76	1.60
1:A:175:ARG:CB	1:A:175:ARG:CG	1.74	1.59
2:B:706:GLN:CG	2:B:706:GLN:CD	1.75	1.59
4:E:98:ILE:CA	4:E:98:ILE:CB	1.81	1.59
9:K:102:LYS:CE	9:K:102:LYS:CD	1.74	1.59
1:A:121:LEU:CG	1:A:121:LEU:CD1	1.75	1.59
1:A:840:ARG:CG	1:A:840:ARG:CD	1.76	1.59
1:A:1222:ASN:CG	1:A:1222:ASN:CB	1.76	1.59
2:B:399:ASP:CG	2:B:399:ASP:CB	1.75	1.59
3:C:94:LYS:CB	3:C:94:LYS:CG	1.75	1.59
6:H:136:LYS:C	6:H:136:LYS:CA	1.75	1.59
10:L:62:LYS:CD	10:L:62:LYS:CE	1.80	1.59
2:B:616:ILE:CG1	2:B:616:ILE:CD1	1.79	1.59
10:L:43:THR:CB	10:L:43:THR:CG2	1.75	1.59
1:A:1235:LYS:CD	1:A:1235:LYS:CE	1.79	1.59
2:B:305:VAL:CG1	2:B:305:VAL:CB	1.79	1.59
2:B:775:LYS:CB	2:B:775:LYS:CG	1.77	1.59
3:C:154:LYS:CB	3:C:154:LYS:CG	1.77	1.59
6:H:144:ILE:CD1	6:H:144:ILE:CG1	1.75	1.59
10:L:28:LYS:CA	10:L:28:LYS:C	1.76	1.59
2:B:167:ILE:CG1	2:B:167:ILE:CD1	1.81	1.58
6:H:107:VAL:CA	6:H:107:VAL:CB	1.76	1.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:THR:CB	1:A:144:THR:CG2	1.78	1.58
1:A:689:LYS:CD	1:A:689:LYS:CE	1.74	1.58
1:A:941:LYS:CD	1:A:941:LYS:CG	1.75	1.58
2:B:961:LEU:CG	2:B:961:LEU:CD1	1.77	1.58
3:C:199:LYS:CD	3:C:199:LYS:CE	1.80	1.58
4:E:103:LYS:CD	4:E:103:LYS:CE	1.75	1.58
2:B:1165:ILE:CG1	2:B:1165:ILE:CD1	1.75	1.58
4:E:161:LYS:CD	4:E:161:LYS:CE	1.82	1.58
6:H:19:ARG:CB	6:H:19:ARG:CG	1.77	1.58
5:F:72:LYS:CD	5:F:72:LYS:CE	1.75	1.58
10:L:54:ARG:CG	10:L:54:ARG:CD	1.77	1.58
1:A:1003:LYS:CD	1:A:1003:LYS:CE	1.81	1.57
2:B:418:LYS:CD	2:B:418:LYS:CE	1.74	1.57
3:C:9:LYS:CD	3:C:9:LYS:CG	1.76	1.57
3:C:163:ILE:CB	3:C:163:ILE:CG2	1.74	1.57
1:A:157:ASP:CB	1:A:157:ASP:CG	1.77	1.57
1:A:1236:LEU:CD2	1:A:1236:LEU:CG	1.78	1.57
2:B:1057:LYS:CD	2:B:1057:LYS:CG	1.80	1.57
3:C:169:LYS:CE	3:C:169:LYS:CD	1.75	1.57
6:H:77:ARG:CB	6:H:77:ARG:CG	1.81	1.57
9:K:111:LEU:CD1	9:K:111:LEU:CG	1.81	1.57
4:E:129:PRO:CG	4:E:129:PRO:CB	1.75	1.57
4:E:191:LYS:CD	4:E:191:LYS:CE	1.75	1.57
9:K:88:LYS:CG	9:K:88:LYS:CD	1.76	1.57
1:A:728:LYS:CE	1:A:728:LYS:NZ	1.67	1.57
1:A:973:ILE:CB	1:A:973:ILE:CG2	1.74	1.57
6:H:52:GLN:CG	6:H:52:GLN:CD	1.76	1.57
1:A:66:LYS:CB	1:A:66:LYS:CG	1.76	1.56
1:A:720:ARG:CG	1:A:720:ARG:CD	1.78	1.56
2:B:434:ARG:CG	2:B:434:ARG:CB	1.77	1.56
3:C:15:LYS:CB	3:C:15:LYS:CG	1.75	1.56
3:C:267:GLN:C	3:C:267:GLN:CA	1.75	1.56
7:I:30:ARG:CG	7:I:30:ARG:CD	1.76	1.56
1:A:1102:LYS:CD	1:A:1102:LYS:CG	1.77	1.56
2:B:231:PRO:CB	2:B:231:PRO:CG	1.83	1.56
2:B:646:LEU:CD1	2:B:646:LEU:CG	1.79	1.56
6:H:91:ASP:CA	6:H:91:ASP:C	1.75	1.56
4:E:54:GLN:CG	4:E:54:GLN:CB	1.78	1.56
8:J:26:GLN:CB	8:J:26:GLN:CG	1.75	1.56
1:A:5:GLN:CG	1:A:5:GLN:CB	1.76	1.56
1:A:123:ARG:CG	1:A:123:ARG:CB	1.74	1.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:344:LYS:CB	2:B:344:LYS:CG	1.83	1.56
2:B:428:ILE:CG1	2:B:428:ILE:CD1	1.80	1.56
4:E:41:ASP:CB	4:E:41:ASP:CG	1.76	1.56
6:H:131:ASN:CB	6:H:131:ASN:CG	1.74	1.56
2:B:164:LYS:CE	2:B:164:LYS:CD	1.83	1.56
2:B:959:ASP:CB	2:B:959:ASP:CG	1.78	1.56
6:H:9:ILE:CB	6:H:9:ILE:CA	1.78	1.56
1:A:191:THR:CB	1:A:191:THR:CA	1.75	1.55
1:A:387:ARG:CG	1:A:387:ARG:CD	1.79	1.55
1:A:518:LYS:CE	1:A:518:LYS:CD	1.81	1.55
2:B:1097:HIS:CB	2:B:1097:HIS:CA	1.82	1.55
6:H:9:ILE:CG1	6:H:9:ILE:CD1	1.84	1.55
1:A:795:GLU:CG	1:A:795:GLU:CD	1.79	1.55
1:A:895:LYS:CG	1:A:895:LYS:CD	1.82	1.55
1:A:941:LYS:CD	1:A:941:LYS:CE	1.84	1.55
1:A:1223:ASP:CB	1:A:1223:ASP:CG	1.75	1.55
1:A:1280:GLU:CG	1:A:1280:GLU:CD	1.75	1.55
2:B:641:GLU:CG	2:B:641:GLU:CD	1.79	1.55
2:B:706:GLN:CG	2:B:706:GLN:CB	1.84	1.55
5:F:129:LYS:CD	5:F:129:LYS:CE	1.78	1.55
10:L:61:THR:CB	10:L:61:THR:CG2	1.83	1.55
1:A:295:LEU:CD2	1:A:295:LEU:CG	1.83	1.55
1:A:1112:LYS:CE	1:A:1112:LYS:NZ	1.70	1.55
5:F:76:LYS:NZ	5:F:76:LYS:CE	1.67	1.55
9:K:26:LYS:CB	9:K:26:LYS:CG	1.78	1.55
1:A:1187:GLN:CB	1:A:1187:GLN:CG	1.81	1.55
2:B:870:ILE:CA	2:B:870:ILE:CB	1.81	1.55
1:A:49:LYS:CD	1:A:49:LYS:CE	1.79	1.54
1:A:274:ILE:CA	1:A:274:ILE:CB	1.80	1.54
1:A:1144:LYS:CD	1:A:1144:LYS:CE	1.82	1.54
2:B:246:LYS:CA	2:B:246:LYS:C	1.79	1.54
4:E:152:LYS:CG	4:E:152:LYS:CD	1.81	1.54
10:L:26:THR:CB	10:L:26:THR:CG2	1.79	1.54
10:L:48:CYS:C	10:L:48:CYS:CA	1.78	1.54
1:A:830:LYS:CD	1:A:830:LYS:CG	1.85	1.54
1:A:1132:LYS:CG	1:A:1132:LYS:CD	1.78	1.54
1:A:695:LYS:CE	1:A:695:LYS:CD	1.84	1.54
7:I:120:GLN:CG	7:I:120:GLN:CB	1.79	1.54
10:L:62:LYS:CE	10:L:62:LYS:NZ	1.68	1.54
1:A:601:LYS:NZ	1:A:601:LYS:CE	1.70	1.54
1:A:1132:LYS:CD	1:A:1132:LYS:CE	1.81	1.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:915:THR:CA	2:B:915:THR:CB	1.74	1.54
6:H:139:ASN:CB	6:H:139:ASN:CG	1.81	1.54
2:B:115:GLN:CG	2:B:115:GLN:CD	1.76	1.54
1:A:555:ASP:CB	1:A:555:ASP:CG	1.81	1.53
1:A:1445:ILE:CG1	1:A:1445:ILE:CD1	1.82	1.53
3:C:154:LYS:CG	3:C:154:LYS:CD	1.85	1.53
7:I:49:ILE:CG1	7:I:49:ILE:CD1	1.84	1.53
1:A:601:LYS:CE	1:A:601:LYS:CD	1.85	1.53
1:A:843:LYS:CD	1:A:843:LYS:CE	1.80	1.53
2:B:346:GLU:CG	2:B:346:GLU:CD	1.79	1.53
2:B:1154:ALA:CA	2:B:1154:ALA:CB	1.83	1.53
9:K:26:LYS:CG	9:K:26:LYS:CD	1.80	1.53
1:A:1446:ASP:CB	1:A:1446:ASP:CG	1.77	1.53
2:B:895:ASP:CB	2:B:895:ASP:CG	1.81	1.53
2:B:1101:ASP:CB	2:B:1101:ASP:CG	1.78	1.53
1:A:44:THR:CA	1:A:44:THR:CB	1.81	1.53
1:A:1109:LYS:CD	1:A:1109:LYS:CG	1.87	1.53
2:B:962:LYS:CD	2:B:962:LYS:CE	1.85	1.53
2:B:620:ARG:CG	2:B:620:ARG:CD	1.81	1.53
1:A:1171:GLN:CG	1:A:1171:GLN:CD	1.76	1.52
2:B:227:LYS:CD	2:B:227:LYS:CE	1.79	1.52
2:B:1097:HIS:CA	2:B:1097:HIS:C	1.81	1.52
10:L:45:ALA:CA	10:L:45:ALA:CB	1.81	1.52
1:A:346:ASP:CB	1:A:346:ASP:CG	1.81	1.52
1:A:423:ASP:CB	1:A:423:ASP:CG	1.81	1.52
2:B:434:ARG:CG	2:B:434:ARG:CD	1.83	1.52
3:C:102:GLN:CB	3:C:102:GLN:CG	1.86	1.52
2:B:595:ARG:CD	2:B:595:ARG:CG	1.82	1.52
1:A:1290:LYS:NZ	1:A:1290:LYS:CE	1.71	1.52
2:B:415:GLN:CG	2:B:415:GLN:CB	1.83	1.52
1:A:368:LYS:CD	1:A:368:LYS:CG	1.84	1.52
1:A:199:LEU:CG	1:A:199:LEU:CD1	1.81	1.51
7:I:45:ARG:CG	7:I:45:ARG:CD	1.85	1.51
1:A:566:ILE:CB	1:A:566:ILE:CG2	1.84	1.51
1:A:1109:LYS:CG	1:A:1109:LYS:CB	1.82	1.51
4:E:191:LYS:CE	4:E:191:LYS:NZ	1.72	1.51
1:A:248:PRO:CB	1:A:248:PRO:CG	1.77	1.51
2:B:227:LYS:CE	2:B:227:LYS:NZ	1.71	1.51
2:B:646:LEU:CG	2:B:646:LEU:CD2	1.88	1.51
1:A:1132:LYS:CE	1:A:1132:LYS:NZ	1.68	1.51
2:B:509:ALA:CA	2:B:509:ALA:CB	1.87	1.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:531:GLN:CB	2:B:531:GLN:CG	1.83	1.51
1:A:69:THR:C	1:A:69:THR:CA	1.78	1.51
1:A:1135:ARG:CG	1:A:1135:ARG:CD	1.85	1.51
2:B:227:LYS:CD	2:B:227:LYS:CG	1.82	1.51
5:F:87:LYS:NZ	5:F:87:LYS:CE	1.69	1.50
6:H:19:ARG:CG	6:H:19:ARG:CD	1.84	1.50
1:A:1039:LYS:NZ	1:A:1039:LYS:CE	1.68	1.50
1:A:895:LYS:CD	1:A:895:LYS:CE	1.87	1.50
2:B:502:ILE:CA	2:B:502:ILE:CB	1.90	1.50
9:K:20:LYS:CG	9:K:20:LYS:CD	1.85	1.50
2:B:1102:LYS:CB	2:B:1102:LYS:CG	1.83	1.50
1:A:217:LYS:CD	1:A:217:LYS:CE	1.90	1.50
2:B:723:VAL:CB	2:B:723:VAL:CG1	1.85	1.50
3:C:160:LYS:NZ	3:C:160:LYS:CE	1.70	1.49
1:A:644:LYS:NZ	1:A:644:LYS:CE	1.69	1.49
2:B:870:ILE:CG1	2:B:870:ILE:CD1	1.86	1.49
1:A:1235:LYS:CE	1:A:1235:LYS:NZ	1.71	1.49
2:B:736:THR:CB	2:B:736:THR:CG2	1.89	1.49
2:B:477:ALA:CA	2:B:477:ALA:CB	1.89	1.49
7:I:1:MET:CE	7:I:1:MET:SD	2.01	1.48
1:A:705:LYS:CB	1:A:705:LYS:CG	1.87	1.48
10:L:26:THR:CB	10:L:26:THR:CA	1.89	1.48
2:B:531:GLN:CG	2:B:531:GLN:CD	1.84	1.48
3:C:260:LEU:CD2	3:C:260:LEU:CG	1.86	1.48
1:A:620:LYS:CD	1:A:620:LYS:CE	1.92	1.48
2:B:652:LYS:NZ	2:B:652:LYS:CE	1.73	1.48
4:E:50:MET:SD	4:E:50:MET:CG	2.02	1.48
1:A:1263:ILE:CD1	1:A:1263:ILE:CG1	1.92	1.47
3:C:15:LYS:CG	3:C:15:LYS:CD	1.90	1.47
4:E:121:MET:SD	4:E:121:MET:CG	2.01	1.47
2:B:315:LYS:NZ	2:B:315:LYS:CE	1.70	1.47
4:E:152:LYS:CD	4:E:152:LYS:CE	1.93	1.47
1:A:752:LYS:CE	1:A:752:LYS:CD	1.93	1.47
4:E:162:ARG:CB	4:E:162:ARG:CG	1.92	1.47
6:H:104:PHE:C	6:H:104:PHE:CA	1.86	1.47
1:A:1111:MET:SD	1:A:1111:MET:CG	2.02	1.47
4:E:131:THR:CB	4:E:131:THR:CG2	1.89	1.47
2:B:432:MET:CE	2:B:432:MET:SD	2.02	1.46
2:B:962:LYS:CD	2:B:962:LYS:CG	1.91	1.46
6:H:123:MET:SD	6:H:123:MET:CG	2.03	1.46
1:A:597:LEU:CD1	1:A:597:LEU:CG	1.93	1.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:934:LYS:CD	1:A:934:LYS:CE	1.91	1.46
1:A:941:LYS:CE	1:A:941:LYS:NZ	1.76	1.46
1:A:74:MET:CE	1:A:74:MET:SD	2.03	1.46
10:L:68:GLU:CG	10:L:68:GLU:CD	1.85	1.46
1:A:938:LYS:CD	1:A:938:LYS:CE	1.87	1.46
4:E:215:MET:CE	4:E:215:MET:SD	2.04	1.45
2:B:233:PRO:CB	2:B:233:PRO:CG	1.75	1.45
2:B:1210:MET:CE	2:B:1210:MET:SD	2.04	1.44
2:B:1169:MET:CE	2:B:1169:MET:SD	2.03	1.44
2:B:598:GLU:CG	2:B:598:GLU:CD	1.87	1.44
2:B:347:LYS:CD	2:B:347:LYS:CG	1.96	1.43
2:B:999:MET:CG	2:B:999:MET:SD	2.06	1.43
7:I:17:ARG:CG	7:I:17:ARG:CD	1.94	1.43
3:C:154:LYS:CD	3:C:154:LYS:CE	1.95	1.43
1:A:728:LYS:CG	1:A:728:LYS:CD	1.93	1.43
2:B:593:PRO:CG	2:B:593:PRO:CB	1.84	1.43
5:F:129:LYS:CE	5:F:129:LYS:NZ	1.78	1.42
1:A:978:PRO:CB	1:A:978:PRO:CG	1.88	1.42
2:B:986:GLN:CG	2:B:986:GLN:CD	1.92	1.42
2:B:987:LYS:NZ	2:B:987:LYS:CE	1.79	1.42
1:A:620:LYS:CE	1:A:620:LYS:NZ	1.80	1.41
2:B:1097:HIS:ND1	2:B:1097:HIS:HA	1.29	1.41
1:A:676:MET:SD	1:A:676:MET:CG	2.09	1.40
1:A:1232:ASN:CG	1:A:1232:ASN:CB	1.92	1.40
1:A:1444:MET:CE	1:A:1444:MET:SD	2.10	1.40
3:C:29:MET:CE	3:C:29:MET:SD	2.09	1.40
1:A:1294:PRO:CB	1:A:1294:PRO:CG	1.85	1.39
4:E:20:LYS:NZ	4:E:20:LYS:CE	1.84	1.39
4:E:201:LYS:CG	4:E:201:LYS:CD	1.99	1.39
1:A:41:MET:CE	1:A:41:MET:SD	2.10	1.39
1:A:1259:MET:SD	1:A:1259:MET:CG	2.12	1.38
2:B:1189:ILE:CG1	2:B:1189:ILE:CD1	2.00	1.38
7:I:1:MET:CG	7:I:1:MET:SD	2.11	1.38
1:A:1302:PRO:CG	1:A:1302:PRO:CB	1.90	1.37
4:E:121:MET:SD	4:E:121:MET:CE	2.11	1.36
4:E:162:ARG:CG	4:E:162:ARG:CD	2.06	1.33
1:A:1202:MET:CE	1:A:1202:MET:SD	2.17	1.32
6:H:104:PHE:O	6:H:106:GLU:N	1.62	1.32
1:A:369:SER:OG	9:K:2:ASN:ND2	1.61	1.31
7:I:55:THR:CB	7:I:55:THR:CG2	2.08	1.31
2:B:999:MET:SD	2:B:999:MET:CE	1.20	1.30

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:265:MET:CE	3:C:265:MET:SD	2.19	1.29
7:I:4:PHE:CE1	7:I:13:MET:HE2	1.66	1.29
1:A:728:LYS:CE	1:A:728:LYS:CD	2.11	1.29
8:J:1:MET:CE	8:J:1:MET:SD	2.21	1.28
4:E:93:MET:CE	4:E:93:MET:SD	2.23	1.27
4:E:1:MET:CE	4:E:1:MET:SD	2.23	1.26
1:A:752:LYS:CE	1:A:752:LYS:NZ	1.98	1.25
2:B:1097:HIS:CA	2:B:1097:HIS:ND1	1.97	1.25
1:A:156:ASP:O	1:A:158:PRO:HD3	1.34	1.25
1:A:70:CYS:SG	1:A:80:HIS:NE2	2.12	1.22
1:A:1259:MET:SD	1:A:1259:MET:CE	2.27	1.22
1:A:437:MET:CE	1:A:437:MET:SD	2.28	1.22
3:C:75:MET:CE	3:C:75:MET:SD	2.28	1.22
2:B:792:MET:SD	2:B:792:MET:CE	2.29	1.21
1:A:487:MET:CE	1:A:487:MET:CG	2.18	1.20
2:B:662:MET:CE	2:B:662:MET:SD	2.30	1.19
2:B:999:MET:SD	2:B:999:MET:HE1	1.78	1.19
3:C:165:LYS:NZ	3:C:165:LYS:CE	2.06	1.18
7:I:45:ARG:HG2	7:I:45:ARG:HH11	1.03	1.18
3:C:54:ASN:OD1	3:C:56:THR:HB	1.42	1.17
5:F:103:MET:CE	5:F:103:MET:SD	2.31	1.17
1:A:1402:PHE:O	1:A:1403:GLU:HB2	1.37	1.17
1:A:708:MET:CE	1:A:708:MET:SD	2.33	1.16
6:H:106:GLU:O	6:H:107:VAL:C	1.82	1.16
7:I:45:ARG:CG	7:I:45:ARG:HH11	1.56	1.16
2:B:999:MET:SD	2:B:999:MET:HE2	1.78	1.15
1:A:535:THR:HG21	1:A:617:VAL:H	1.10	1.14
6:H:63:LEU:C	6:H:90:ALA:HB3	1.73	1.12
1:A:567:LYS:HB3	6:H:96:VAL:H	1.15	1.11
6:H:138:GLU:O	6:H:139:ASN:C	1.93	1.11
3:C:125:MET:CE	3:C:125:MET:SD	2.40	1.10
9:K:1:MET:SD	9:K:1:MET:CE	2.40	1.09
2:B:552:MET:CE	2:B:552:MET:SD	2.40	1.09
2:B:955:THR:HG22	10:L:54:ARG:O	1.51	1.08
2:B:999:MET:SD	2:B:999:MET:HE3	1.78	1.08
1:A:42:ASP:OD2	1:A:47:ARG:N	1.86	1.08
1:A:487:MET:CE	1:A:487:MET:SD	0.98	1.08
2:B:101:MET:SD	2:B:101:MET:CE	2.44	1.06
2:B:999:MET:CG	2:B:999:MET:CE	2.32	1.06
1:A:567:LYS:HE2	6:H:95:TYR:CE2	1.88	1.05
2:B:100:PRO:HD2	2:B:180:TYR:CE1	1.92	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1285:MET:CE	1:A:1285:MET:SD	2.46	1.04
1:A:304:MET:CE	1:A:304:MET:SD	2.45	1.04
7:I:4:PHE:HE1	7:I:13:MET:CE	1.71	1.02
6:H:128:ASN:O	6:H:131:ASN:ND2	1.92	1.02
7:I:16:PRO:O	7:I:17:ARG:HD3	1.59	1.02
2:B:552:MET:SD	2:B:552:MET:CG	2.49	1.01
6:H:106:GLU:O	6:H:107:VAL:O	1.77	1.01
1:A:518:LYS:CD	1:A:518:LYS:NZ	2.23	1.00
1:A:567:LYS:HB3	6:H:96:VAL:N	1.76	1.00
1:A:567:LYS:HD3	6:H:95:TYR:HA	1.41	0.99
1:A:487:MET:SD	1:A:487:MET:HE1	1.59	0.99
2:B:1190:ASP:O	2:B:1191:ILE:HG13	1.63	0.99
1:A:567:LYS:HD3	6:H:95:TYR:CG	1.97	0.98
1:A:1385:THR:O	1:A:1385:THR:HG22	1.61	0.98
2:B:1051:THR:HG22	2:B:1053:GLU:H	1.25	0.98
1:A:487:MET:SD	1:A:487:MET:HE3	1.59	0.97
2:B:620:ARG:CG	2:B:620:ARG:NE	2.27	0.97
1:A:487:MET:SD	1:A:487:MET:HE2	1.59	0.97
1:A:752:LYS:HZ3	2:B:1019:SER:H	1.09	0.97
9:K:110:ASN:O	9:K:112:GLN:N	1.98	0.97
2:B:313:MET:HE3	2:B:386:LEU:HD22	1.45	0.97
2:B:428:ILE:HG12	2:B:448:ILE:HD11	1.46	0.97
2:B:885:MET:CE	2:B:885:MET:SD	2.52	0.97
3:C:95:CYS:HG	12:C:3002:ZN:ZN	0.77	0.96
1:A:1079:MET:SD	1:A:1359:ASP:OD2	2.25	0.95
1:A:1233:ASP:O	1:A:1234:GLU:HB3	1.64	0.95
4:E:12:LEU:HD21	4:E:58:MET:SD	2.07	0.94
2:B:1220:ARG:O	2:B:1222:ARG:HD3	1.66	0.94
2:B:643:ASP:O	2:B:644:GLU:HB2	1.64	0.93
3:C:172:PRO:O	3:C:235:VAL:HG12	1.67	0.93
1:A:347:PHE:H	2:B:1107:ALA:HA	1.33	0.93
3:C:163:ILE:CG2	3:C:163:ILE:HB	1.98	0.93
1:A:567:LYS:HD3	6:H:95:TYR:CA	1.98	0.92
1:A:567:LYS:HG3	1:A:568:PRO:CD	1.98	0.92
1:A:1364:ASN:ND2	1:A:1366:ARG:HD2	1.85	0.92
4:E:100:ILE:HG22	4:E:101:GLN:N	1.85	0.92
8:J:7:CYS:HG	12:J:3001:ZN:ZN	0.60	0.92
9:K:93:SER:O	9:K:97:LYS:HG3	1.70	0.91
4:E:63:ASN:O	4:E:64:PRO:O	1.88	0.91
7:I:45:ARG:HG2	7:I:45:ARG:NH1	1.85	0.91
1:A:1111:MET:CG	1:A:1111:MET:CE	2.48	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1097:HIS:CA	2:B:1097:HIS:CG	2.52	0.90
1:A:35:ILE:H	1:A:35:ILE:HD12	1.37	0.90
1:A:567:LYS:CG	1:A:568:PRO:CD	2.48	0.90
6:H:130:ARG:HD2	6:H:130:ARG:C	1.95	0.90
7:I:45:ARG:CG	7:I:45:ARG:NH1	2.35	0.90
5:F:81:THR:CG2	5:F:136:ARG:HH11	1.84	0.90
1:A:567:LYS:CD	6:H:95:TYR:HA	2.02	0.90
1:A:567:LYS:CB	6:H:96:VAL:H	1.85	0.89
3:C:86:CYS:HG	3:C:95:CYS:HG	1.15	0.89
4:E:57:MET:CE	4:E:57:MET:SD	2.60	0.89
1:A:122:MET:HE1	1:A:138:ILE:HD13	1.54	0.89
1:A:148:CYS:HG	12:A:3006:ZN:ZN	0.60	0.89
1:A:567:LYS:HG3	1:A:568:PRO:HD2	1.51	0.89
8:J:1:MET:CE	8:J:1:MET:CG	2.51	0.89
2:B:846:ILE:HD12	2:B:974:PRO:HB2	1.53	0.89
2:B:431:TYR:HD2	2:B:431:TYR:O	1.56	0.88
2:B:431:TYR:O	2:B:431:TYR:CD2	2.26	0.88
6:H:63:LEU:C	6:H:90:ALA:CB	2.46	0.88
1:A:156:ASP:O	1:A:158:PRO:CD	2.20	0.88
1:A:1402:PHE:O	1:A:1403:GLU:CB	2.18	0.88
6:H:103:LYS:HB3	6:H:105:GLU:OE1	1.73	0.88
1:A:567:LYS:HD2	1:A:568:PRO:HD3	1.55	0.88
10:L:48:CYS:HG	12:L:3005:ZN:ZN	0.77	0.88
6:H:123:MET:HE1	6:H:142:LEU:HD13	1.54	0.88
1:A:247:ARG:NH1	1:A:263:THR:HG23	1.90	0.87
1:A:187:LYS:HB2	1:A:194:ALA:HB3	1.57	0.87
6:H:104:PHE:O	6:H:106:GLU:CA	2.22	0.86
2:B:100:PRO:HD2	2:B:180:TYR:CZ	2.10	0.86
4:E:147:HIS:HD2	4:E:149:LEU:H	1.18	0.86
5:F:111:LEU:O	5:F:113:GLY:N	2.08	0.86
6:H:104:PHE:O	6:H:105:GLU:C	2.19	0.86
2:B:1051:THR:HG22	2:B:1053:GLU:N	1.90	0.86
2:B:104:GLU:OE1	10:L:54:ARG:NE	2.09	0.86
6:H:93:TYR:HB3	6:H:144:ILE:O	1.76	0.86
4:E:36:GLU:O	4:E:37:LEU:C	2.17	0.86
2:B:561:TRP:O	2:B:590:HIS:HE1	1.57	0.85
2:B:680:THR:HG22	2:B:682:SER:H	1.39	0.85
3:C:116:LYS:CD	3:C:116:LYS:NZ	2.37	0.85
10:L:64:LEU:CD1	10:L:64:LEU:HG	2.06	0.85
3:C:18:VAL:HG23	3:C:240:VAL:HG11	1.59	0.85
1:A:752:LYS:CE	1:A:752:LYS:CG	2.54	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:99:LEU:HD12	3:C:99:LEU:N	1.92	0.85
1:A:1242:VAL:HG11	1:A:1259:MET:HE3	1.59	0.85
1:A:369:SER:H	9:K:2:ASN:HD21	1.19	0.85
2:B:1097:HIS:C	2:B:1097:HIS:HA	2.00	0.85
1:A:1079:MET:HG2	1:A:1359:ASP:OD2	1.76	0.84
2:B:1084:GLN:HE22	3:C:192:TRP:H	1.21	0.84
2:B:879:ARG:NH2	2:B:885:MET:CE	2.41	0.84
4:E:79:TRP:HB2	4:E:105:PHE:CE1	2.13	0.84
2:B:169:ARG:HB2	2:B:454:THR:HG23	1.60	0.83
1:A:72:GLU:OE2	2:B:1175:LEU:HD11	1.78	0.83
1:A:871:ASP:HB3	4:E:204:THR:HG23	1.59	0.83
7:I:4:PHE:HE1	7:I:13:MET:HE2	0.76	0.83
2:B:1182:CYS:HG	2:B:1185:CYS:HB2	1.43	0.83
1:A:73:GLY:O	1:A:75:ASN:N	2.10	0.82
1:A:23:SER:O	1:A:27:VAL:HG23	1.78	0.82
1:A:172:PRO:HG2	1:A:174:ILE:HD11	1.61	0.82
2:B:251:ILE:O	2:B:251:ILE:HG22	1.79	0.82
1:A:64:ASN:OD1	1:A:64:ASN:O	1.96	0.82
2:B:542:MET:HG3	2:B:747:MET:HE3	1.62	0.82
1:A:61:ILE:CB	1:A:61:ILE:HA	2.07	0.82
1:A:1364:ASN:HD22	1:A:1366:ARG:H	1.24	0.82
4:E:50:MET:SD	4:E:50:MET:CE	2.68	0.82
6:H:5:LEU:O	6:H:133:ASN:ND2	2.12	0.82
5:F:77:ASP:O	5:F:78:GLN:HB2	1.79	0.82
7:I:30:ARG:CG	7:I:30:ARG:NE	2.41	0.82
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.45	0.82
1:A:938:LYS:CE	1:A:938:LYS:CG	2.58	0.81
1:A:70:CYS:HG	1:A:80:HIS:CE1	1.97	0.81
2:B:1065:GLN:HE22	2:B:1067:ARG:HB2	1.44	0.81
6:H:138:GLU:O	6:H:140:ALA:N	2.13	0.81
2:B:775:LYS:CB	2:B:775:LYS:CD	2.58	0.81
2:B:1084:GLN:NE2	3:C:192:TRP:H	1.77	0.81
3:C:8:VAL:HG12	3:C:9:LYS:H	1.46	0.81
2:B:542:MET:HE2	2:B:747:MET:HG3	1.62	0.81
2:B:498:THR:CG2	2:B:537:LYS:HB2	2.11	0.81
1:A:903:ASN:C	1:A:903:ASN:HD22	1.88	0.80
1:A:55:ASP:O	1:A:57:ARG:N	2.11	0.80
1:A:107:CYS:SG	1:A:148:CYS:SG	2.79	0.80
1:A:120:GLU:HG2	1:A:123:ARG:HH22	1.45	0.80
8:J:14:VAL:HG13	8:J:50:ILE:HD11	1.63	0.80
2:B:294:ASP:H	7:I:12:ASN:ND2	1.79	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:THR:C	1:A:69:THR:HA	2.05	0.79
1:A:596:THR:HG22	1:A:597:LEU:H	1.47	0.79
2:B:542:MET:HG3	2:B:747:MET:CE	2.12	0.79
3:C:255:VAL:O	3:C:255:VAL:HG12	1.82	0.79
1:A:1385:THR:CG2	1:A:1385:THR:C	2.56	0.79
1:A:941:LYS:CD	1:A:941:LYS:NZ	2.45	0.79
1:A:1364:ASN:ND2	1:A:1366:ARG:H	1.81	0.79
1:A:108:MET:H	1:A:171:GLN:HE22	1.27	0.79
4:E:98:ILE:CB	4:E:98:ILE:HA	2.05	0.79
1:A:187:LYS:HG3	1:A:194:ALA:CB	2.13	0.79
4:E:129:PRO:CG	4:E:129:PRO:CA	2.61	0.79
1:A:588:LEU:HD23	1:A:588:LEU:C	2.08	0.79
1:A:711:ARG:HE	7:I:95:THR:HG22	1.48	0.79
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.31	0.78
1:A:46:THR:CA	1:A:46:THR:HB	2.10	0.78
1:A:567:LYS:CD	1:A:568:PRO:HD3	2.13	0.78
1:A:55:ASP:N	1:A:56:PRO:CD	2.46	0.78
1:A:1079:MET:CG	1:A:1359:ASP:OD2	2.31	0.78
1:A:174:ILE:CA	1:A:174:ILE:HB	2.09	0.78
1:A:247:ARG:HH11	1:A:263:THR:HG23	1.42	0.78
1:A:1445:ILE:CG2	1:A:1445:ILE:CA	2.61	0.78
2:B:428:ILE:CG1	2:B:448:ILE:HD11	2.14	0.78
2:B:1128:LEU:HD12	2:B:1128:LEU:C	2.06	0.78
6:H:89:LEU:O	6:H:91:ASP:N	2.16	0.78
10:L:28:LYS:C	10:L:28:LYS:HA	2.03	0.78
2:B:1182:CYS:SG	2:B:1185:CYS:HB2	2.24	0.78
1:A:901:LEU:H	1:A:926:GLN:NE2	1.82	0.78
1:A:535:THR:HG21	1:A:617:VAL:N	1.95	0.77
1:A:1259:MET:SD	1:A:1259:MET:CB	2.71	0.77
2:B:643:ASP:O	2:B:644:GLU:CB	2.32	0.77
2:B:839:MET:HE3	2:B:1010:LEU:HD11	1.66	0.77
2:B:877:PRO:O	2:B:878:GLN:HG2	1.84	0.77
3:C:167:HIS:HD2	3:C:169:LYS:H	1.30	0.77
9:K:111:LEU:CD1	9:K:111:LEU:CB	2.62	0.77
6:H:89:LEU:HB3	6:H:91:ASP:OD1	1.85	0.77
1:A:369:SER:CB	9:K:2:ASN:ND2	2.46	0.77
2:B:879:ARG:HH21	2:B:885:MET:HE1	1.47	0.77
1:A:110:CYS:SG	1:A:167:CYS:SG	2.82	0.77
2:B:119:LEU:O	2:B:965:LYS:NZ	2.17	0.77
2:B:1077:THR:HG22	2:B:1079:LYS:H	1.47	0.77
1:A:571:LEU:CD2	1:A:571:LEU:CD1	2.59	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:909:ASP:OD1	1:A:911:SER:N	2.16	0.77
2:B:217:ARG:HD3	2:B:407:ASP:OD2	1.84	0.77
2:B:246:LYS:C	2:B:246:LYS:HA	2.06	0.77
5:F:75:PRO:O	5:F:77:ASP:O	2.03	0.77
2:B:114:PRO:HD3	2:B:124:TYR:CE1	2.20	0.77
4:E:90:VAL:CG1	4:E:90:VAL:HB	2.11	0.77
10:L:47:ARG:HG2	10:L:48:CYS:H	1.50	0.77
1:A:199:LEU:CD1	1:A:199:LEU:CD2	2.61	0.77
2:B:417:PHE:CD2	2:B:417:PHE:O	2.39	0.77
2:B:593:PRO:HG2	2:B:617:ARG:NH2	1.99	0.77
9:K:35:PHE:HE1	9:K:73:LEU:HD12	1.48	0.77
3:C:120:ILE:H	3:C:120:ILE:HD12	1.48	0.76
1:A:413:ILE:HD13	1:A:413:ILE:N	2.00	0.76
1:A:555:ASP:OD1	9:K:26:LYS:HE3	1.86	0.76
6:H:105:GLU:HB3	6:H:107:VAL:HG23	1.67	0.76
1:A:849:MET:HE2	1:A:1061:GLY:HA2	1.66	0.76
2:B:879:ARG:NH2	2:B:885:MET:HE1	1.99	0.76
3:C:196:ASP:HB3	3:C:199:LYS:HG3	1.67	0.76
4:E:79:TRP:HB2	4:E:105:PHE:CD1	2.20	0.76
7:I:4:PHE:CE1	7:I:13:MET:CE	2.56	0.76
1:A:555:ASP:OD1	9:K:26:LYS:CE	2.34	0.76
1:A:1350:LYS:CD	1:A:1350:LYS:CB	2.63	0.76
2:B:1163:CYS:CB	2:B:1163:CYS:HA	2.11	0.76
1:A:567:LYS:CD	6:H:95:TYR:CG	2.68	0.76
1:A:1385:THR:CG2	1:A:1385:THR:CA	2.62	0.76
1:A:32:VAL:HG23	1:A:33:ALA:H	1.49	0.76
1:A:446:ARG:CG	1:A:446:ARG:HH11	1.99	0.76
1:A:61:ILE:O	1:A:62:ASP:HB2	1.87	0.75
3:C:73:GLN:HE21	3:C:75:MET:H	1.32	0.75
1:A:752:LYS:HZ3	2:B:1019:SER:N	1.83	0.75
1:A:1233:ASP:O	1:A:1234:GLU:CB	2.29	0.75
2:B:393:LYS:NZ	2:B:621:GLU:OE2	2.17	0.75
2:B:477:ALA:CB	2:B:477:ALA:HA	2.13	0.75
10:L:34:CYS:CB	10:L:51:CYS:HB3	2.17	0.75
1:A:567:LYS:CG	1:A:568:PRO:HD3	2.17	0.75
1:A:567:LYS:CE	6:H:95:TYR:CE2	2.63	0.75
1:A:1161:THR:CG2	1:A:1163:ILE:H	1.99	0.75
2:B:1025:HIS:HE1	2:B:1090:THR:HG21	1.50	0.75
3:C:167:HIS:HE1	10:L:70:ARG:O	1.69	0.75
6:H:6:PHE:CD2	6:H:7:ASP:N	2.55	0.75
1:A:541:ILE:HD12	1:A:541:ILE:N	2.02	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:571:LEU:CD2	1:A:571:LEU:HG	2.12	0.75
10:L:34:CYS:HB3	10:L:51:CYS:CB	2.16	0.75
3:C:169:LYS:CE	3:C:169:LYS:CG	2.64	0.75
1:A:973:ILE:CG2	1:A:973:ILE:HB	2.11	0.75
6:H:91:ASP:CA	6:H:92:ASP:N	2.48	0.75
2:B:515:HIS:H	2:B:518:HIS:HD2	1.33	0.74
2:B:955:THR:HG23	10:L:55:ILE:HA	1.69	0.74
2:B:1166:CYS:O	2:B:1168:LEU:N	2.20	0.74
1:A:351:THR:CG2	2:B:1103:ILE:CG1	2.66	0.74
1:A:369:SER:N	9:K:2:ASN:HD21	1.85	0.74
5:F:81:THR:HG23	5:F:136:ARG:HH11	1.50	0.74
6:H:91:ASP:C	6:H:91:ASP:CG	2.56	0.74
6:H:107:VAL:CB	6:H:107:VAL:HA	2.10	0.74
2:B:90:ILE:N	2:B:90:ILE:HD12	2.03	0.74
2:B:595:ARG:CD	2:B:595:ARG:CB	2.64	0.74
1:A:1404:GLU:HG3	1:A:1405:THR:HB	1.69	0.74
3:C:169:LYS:CD	3:C:169:LYS:NZ	2.51	0.74
6:H:77:ARG:O	6:H:78:SER:O	2.04	0.74
3:C:163:ILE:CG2	3:C:163:ILE:CG1	2.65	0.74
9:K:82:ASP:OD1	9:K:83:PRO:HG2	1.86	0.74
1:A:710:LEU:CD2	1:A:710:LEU:HG	2.13	0.74
2:B:305:VAL:CG1	2:B:305:VAL:CA	2.65	0.74
3:C:267:GLN:C	3:C:267:GLN:HA	2.06	0.74
1:A:895:LYS:CD	1:A:895:LYS:NZ	2.50	0.74
3:C:18:VAL:HG23	3:C:240:VAL:CG1	2.17	0.74
1:A:174:ILE:CA	1:A:174:ILE:CG2	2.62	0.73
1:A:282:ASN:C	1:A:283:GLY:O	2.21	0.73
2:B:282:ILE:HD13	2:B:282:ILE:H	1.53	0.73
7:I:32:CYS:HB2	7:I:34:TYR:H	1.52	0.73
1:A:237:THR:CG2	1:A:237:THR:CA	2.64	0.73
2:B:531:GLN:CD	2:B:531:GLN:H	1.95	0.73
8:J:1:MET:C	8:J:2:ILE:HD12	2.14	0.73
8:J:7:CYS:SG	8:J:10:CYS:SG	2.86	0.73
1:A:243:PRO:HB2	1:A:245:PRO:HD2	1.69	0.73
1:A:555:ASP:OD1	9:K:26:LYS:NZ	2.21	0.73
2:B:484:ASN:OD1	2:B:486:TYR:CE1	2.41	0.73
5:F:73:ALA:HB2	5:F:143:PHE:CZ	2.23	0.73
2:B:498:THR:HG21	2:B:537:LYS:HB2	1.71	0.73
6:H:96:VAL:HG22	6:H:143:LEU:HD23	1.70	0.73
2:B:357:GLN:NE2	2:B:368:GLU:HG2	2.04	0.73
8:J:38:ARG:CB	8:J:38:ARG:CD	2.64	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:213:ILE:HD12	2:B:213:ILE:N	2.03	0.73
1:A:353:ILE:HD13	1:A:487:MET:HE3	1.69	0.72
10:L:48:CYS:C	10:L:48:CYS:HA	2.03	0.72
2:B:744:HIS:HD2	2:B:746:SER:H	1.37	0.72
7:I:30:ARG:CD	7:I:30:ARG:CB	2.67	0.72
1:A:121:LEU:CD1	1:A:121:LEU:HG	2.10	0.72
1:A:351:THR:CG2	2:B:1103:ILE:HG12	2.19	0.72
1:A:547:LEU:HB3	9:K:58:PHE:CE1	2.25	0.72
2:B:251:ILE:O	2:B:251:ILE:CG2	2.37	0.72
2:B:1222:ARG:HH11	2:B:1222:ARG:HB2	1.53	0.72
7:I:116:ASN:HD21	7:I:118:ARG:HB2	1.54	0.72
1:A:46:THR:CB	1:A:46:THR:C	2.63	0.72
6:H:89:LEU:C	6:H:91:ASP:H	1.97	0.72
1:A:605:MET:HE2	1:A:607:ILE:HD11	1.72	0.72
10:L:58:LYS:O	10:L:59:ALA:HB3	1.90	0.72
1:A:31:SER:CB	1:A:83:HIS:HD2	2.02	0.72
2:B:915:THR:CA	2:B:915:THR:HB	2.11	0.72
4:E:127:ILE:N	4:E:128:PRO:CD	2.53	0.72
1:A:709:THR:HG22	1:A:712:GLU:H	1.54	0.71
10:L:65:VAL:CG2	10:L:65:VAL:CA	2.67	0.71
1:A:119:ASN:O	1:A:120:GLU:HB2	1.91	0.71
1:A:351:THR:HG21	2:B:1103:ILE:HG12	1.71	0.71
2:B:1154:ALA:CB	2:B:1154:ALA:HA	2.14	0.71
1:A:206:GLU:O	1:A:210:ILE:HD13	1.91	0.71
1:A:1151:GLU:OE2	7:I:45:ARG:HD3	1.90	0.71
2:B:90:ILE:HA	2:B:133:LYS:O	1.91	0.71
3:C:50:GLU:HB3	10:L:64:LEU:HD13	1.70	0.71
8:J:7:CYS:SG	8:J:46:CYS:SG	2.89	0.71
2:B:58:THR:O	2:B:62:ILE:HG12	1.90	0.71
3:C:8:VAL:CG1	3:C:9:LYS:H	2.04	0.71
5:F:109:VAL:CG1	5:F:110:ASP:N	2.53	0.71
2:B:1177:HIS:HB2	2:B:1179:GLN:NE2	2.06	0.71
2:B:654:ARG:H	2:B:657:HIS:HD2	1.37	0.70
4:E:98:ILE:CA	4:E:98:ILE:HB	2.15	0.70
1:A:265:LYS:HD3	1:A:302:THR:HG22	1.72	0.70
1:A:566:ILE:CG2	1:A:566:ILE:CA	2.69	0.70
2:B:883:LEU:CA	2:B:883:LEU:HB2	2.15	0.70
2:B:549:THR:HG22	2:B:628:THR:HB	1.70	0.70
2:B:883:LEU:CA	2:B:883:LEU:HB3	2.15	0.70
6:H:105:GLU:H	6:H:105:GLU:CD	1.99	0.70
1:A:120:GLU:HG2	1:A:123:ARG:NH2	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:587:HIS:HD2	1:A:966:ASN:OD1	1.73	0.70
1:A:636:GLU:OE1	1:A:966:ASN:ND2	2.24	0.70
4:E:37:LEU:CD1	4:E:37:LEU:HG	2.11	0.70
1:A:1151:GLU:CG	7:I:45:ARG:HD2	2.22	0.70
2:B:167:ILE:HG22	2:B:167:ILE:O	1.91	0.70
1:A:523:ILE:HB	1:A:622:VAL:HG13	1.74	0.70
2:B:417:PHE:CD2	2:B:417:PHE:C	2.69	0.70
2:B:644:GLU:OE1	2:B:646:LEU:HB2	1.92	0.70
3:C:241:ASP:HB3	9:K:109:TRP:CE2	2.26	0.70
6:H:91:ASP:C	6:H:91:ASP:CB	2.64	0.70
1:A:120:GLU:CG	1:A:123:ARG:HH22	2.03	0.70
1:A:840:ARG:CG	1:A:840:ARG:NE	2.53	0.70
5:F:93:ILE:HD11	5:F:134:ILE:HD11	1.73	0.70
6:H:91:ASP:OD1	6:H:91:ASP:O	2.08	0.70
2:B:1084:GLN:HE22	3:C:192:TRP:N	1.87	0.70
1:A:535:THR:CG2	1:A:617:VAL:H	1.97	0.69
1:A:1348:LEU:HG	1:A:1372:VAL:HG22	1.74	0.69
1:A:446:ARG:HH11	1:A:446:ARG:HG2	1.57	0.69
1:A:693:VAL:HG21	1:A:721:PHE:HE1	1.56	0.69
4:E:152:LYS:CD	4:E:152:LYS:CB	2.70	0.69
1:A:567:LYS:HD2	1:A:568:PRO:CD	2.22	0.69
2:B:914:LYS:H	2:B:938:SER:HB2	1.57	0.69
2:B:1222:ARG:HG2	2:B:1222:ARG:NH1	2.07	0.69
1:A:184:SER:HB2	1:A:199:LEU:HD23	1.74	0.69
1:A:795:GLU:HG2	2:B:731:VAL:HG21	1.74	0.69
2:B:879:ARG:NH2	2:B:885:MET:HE2	2.06	0.69
2:B:1065:GLN:NE2	2:B:1067:ARG:H	1.91	0.69
1:A:1135:ARG:CG	1:A:1135:ARG:NE	2.54	0.69
1:A:1385:THR:CG2	1:A:1385:THR:O	2.39	0.69
2:B:424:LEU:HD23	2:B:424:LEU:C	2.18	0.69
2:B:663:ALA:O	2:B:667:GLN:HG3	1.92	0.69
6:H:26:ILE:HD12	6:H:42:ILE:HD12	1.74	0.69
2:B:294:ASP:H	7:I:12:ASN:HD22	1.40	0.69
2:B:436:VAL:CA	2:B:436:VAL:HB	2.16	0.69
3:C:8:VAL:HG12	3:C:9:LYS:N	2.08	0.69
2:B:487:THR:HG22	2:B:490:SER:H	1.59	0.68
1:A:886:ILE:HD12	1:A:943:LEU:HB3	1.76	0.68
2:B:99:LYS:HB3	2:B:100:PRO:HD3	1.75	0.68
1:A:567:LYS:CG	6:H:96:VAL:H	2.07	0.68
5:F:76:LYS:O	5:F:79:ARG:HD2	1.93	0.68
6:H:123:MET:CG	6:H:123:MET:CE	2.72	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:834:THR:HG21	1:A:1077:THR:OG1	1.94	0.68
2:B:315:LYS:NZ	2:B:315:LYS:CD	2.51	0.68
2:B:620:ARG:CG	2:B:620:ARG:HE	2.05	0.68
2:B:915:THR:CB	2:B:915:THR:C	2.63	0.68
2:B:1220:ARG:O	2:B:1222:ARG:CD	2.41	0.68
2:B:1166:CYS:HB3	2:B:1185:CYS:SG	2.33	0.68
3:C:260:LEU:HD12	3:C:260:LEU:O	1.92	0.68
6:H:107:VAL:CA	6:H:107:VAL:HB	2.15	0.68
1:A:849:MET:CE	1:A:1061:GLY:HA2	2.24	0.68
1:A:752:LYS:HG3	1:A:753:GLY:N	2.09	0.67
2:B:358:LYS:CG	2:B:358:LYS:CA	2.70	0.67
3:C:199:LYS:CD	3:C:199:LYS:NZ	2.56	0.67
9:K:35:PHE:CE1	9:K:73:LEU:HD12	2.30	0.67
1:A:1039:LYS:NZ	1:A:1039:LYS:CD	2.56	0.67
2:B:787:VAL:O	2:B:787:VAL:CG1	2.42	0.67
1:A:503:GLN:NE2	5:F:90:ARG:NH2	2.43	0.67
1:A:1259:MET:SD	1:A:1259:MET:HB2	2.35	0.67
2:B:227:LYS:CD	2:B:227:LYS:CB	2.69	0.67
2:B:399:ASP:CG	2:B:399:ASP:CA	2.67	0.67
4:E:96:PHE:CZ	4:E:100:ILE:HD11	2.29	0.67
9:K:88:LYS:CD	9:K:88:LYS:CB	2.72	0.67
1:A:941:LYS:CD	1:A:941:LYS:CB	2.67	0.67
2:B:1182:CYS:HG	2:B:1185:CYS:CB	2.07	0.67
3:C:209:TYR:HD1	3:C:209:TYR:H	1.43	0.67
6:H:106:GLU:O	6:H:108:SER:N	2.27	0.67
1:A:535:THR:O	1:A:575:LYS:HE2	1.94	0.67
1:A:587:HIS:CE1	1:A:969:GLN:HG2	2.29	0.67
2:B:118:ARG:HH22	2:B:194:GLU:CD	2.01	0.67
1:A:174:ILE:CB	1:A:174:ILE:HA	2.15	0.67
1:A:537:ARG:NH2	1:A:600:PRO:O	2.27	0.67
2:B:1222:ARG:NH1	2:B:1222:ARG:CG	2.57	0.67
6:H:130:ARG:HB2	6:H:133:ASN:HB3	1.76	0.67
9:K:102:LYS:CE	9:K:102:LYS:CG	2.72	0.67
3:C:86:CYS:HG	12:C:3002:ZN:ZN	1.07	0.67
8:J:2:ILE:O	8:J:3:VAL:C	2.38	0.67
5:F:77:ASP:O	5:F:78:GLN:CB	2.41	0.67
2:B:1008:PRO:HG2	2:B:1011:ILE:HD11	1.77	0.66
1:A:596:THR:HG22	1:A:597:LEU:HD12	1.78	0.66
1:A:1162:VAL:O	1:A:1162:VAL:HG12	1.94	0.66
1:A:1195:LEU:HD11	1:A:1267:MET:CE	2.24	0.66
1:A:1350:LYS:CG	1:A:1350:LYS:CE	2.72	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:884:ARG:O	2:B:936:ASP:HB3	1.95	0.66
1:A:901:LEU:HD22	1:A:919:ILE:HD13	1.77	0.66
6:H:89:LEU:C	6:H:91:ASP:N	2.53	0.66
9:K:65:HIS:HD2	9:K:67:PHE:H	1.44	0.66
2:B:883:LEU:CB	2:B:883:LEU:HA	2.15	0.66
5:F:109:VAL:HG12	5:F:110:ASP:N	2.09	0.66
1:A:11:LEU:HD11	2:B:1195:HIS:CD2	2.31	0.66
2:B:645:SER:OG	2:B:646:LEU:N	2.28	0.66
5:F:129:LYS:CE	5:F:129:LYS:CG	2.70	0.66
1:A:35:ILE:HD12	1:A:35:ILE:N	2.10	0.66
2:B:515:HIS:H	2:B:518:HIS:CD2	2.12	0.66
4:E:71:LYS:NZ	4:E:160:GLU:OE2	2.23	0.66
6:H:123:MET:CE	6:H:142:LEU:HD22	2.26	0.66
6:H:131:ASN:H	6:H:131:ASN:HD22	1.43	0.66
5:F:81:THR:HG23	5:F:136:ARG:NH1	2.11	0.66
6:H:104:PHE:C	6:H:104:PHE:HA	2.10	0.66
1:A:369:SER:CB	9:K:2:ASN:HD21	2.07	0.66
1:A:531:ILE:O	1:A:535:THR:HB	1.94	0.66
2:B:789:MET:HE3	2:B:965:LYS:HB3	1.76	0.66
2:B:1166:CYS:O	2:B:1167:GLY:C	2.36	0.66
10:L:40:LEU:HD22	10:L:44:ASP:OD1	1.95	0.66
1:A:567:LYS:HB2	1:A:568:PRO:HD3	1.78	0.65
2:B:1222:ARG:HH11	2:B:1222:ARG:CG	2.08	0.65
1:A:14:VAL:H	1:A:1432:GLN:NE2	1.94	0.65
1:A:427:GLN:HB2	1:A:430:TRP:CE2	2.31	0.65
1:A:534:LEU:O	1:A:574:GLY:HA3	1.96	0.65
1:A:144:THR:CG2	1:A:144:THR:HB	2.17	0.65
1:A:73:GLY:C	1:A:75:ASN:N	2.54	0.65
2:B:431:TYR:CE1	2:B:447:ALA:HB1	2.31	0.65
2:B:643:ASP:HB3	2:B:644:GLU:C	2.22	0.65
2:B:757:PRO:HG2	2:B:984:HIS:CE1	2.32	0.65
2:B:806:THR:HG23	2:B:808:ALA:H	1.61	0.65
2:B:870:ILE:CB	2:B:870:ILE:HA	2.15	0.65
3:C:114:TYR:CD2	3:C:140:ASN:HB3	2.32	0.65
4:E:83:CYS:O	4:E:113:GLN:NE2	2.30	0.65
5:F:81:THR:CG2	5:F:136:ARG:NH1	2.59	0.65
4:E:117:THR:O	4:E:119:SER:N	2.30	0.65
6:H:19:ARG:CG	6:H:19:ARG:CA	2.73	0.65
6:H:27:GLU:OE1	6:H:39:THR:OG1	2.07	0.65
1:A:869:GLY:O	4:E:204:THR:HG21	1.96	0.65
4:E:116:ILE:HG22	4:E:120:ALA:HB3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:605:MET:HE3	1:A:607:ILE:HG13	1.79	0.64
2:B:1025:HIS:CE1	2:B:1090:THR:HG21	2.31	0.64
2:B:515:HIS:HD2	2:B:517:THR:OG1	1.80	0.64
3:C:209:TYR:N	3:C:209:TYR:CD1	2.65	0.64
1:A:567:LYS:HD3	6:H:95:TYR:CD2	2.31	0.64
2:B:313:MET:CE	2:B:386:LEU:HD22	2.22	0.64
2:B:436:VAL:CB	2:B:436:VAL:HA	2.17	0.64
1:A:274:ILE:CB	1:A:274:ILE:C	2.70	0.64
1:A:503:GLN:NE2	5:F:90:ARG:HH21	1.96	0.64
1:A:636:GLU:OE2	1:A:962:ARG:HD2	1.97	0.64
3:C:169:LYS:NZ	10:L:69:ALA:O	2.31	0.64
6:H:6:PHE:CG	6:H:7:ASP:N	2.65	0.64
6:H:130:ARG:HB2	6:H:133:ASN:CB	2.27	0.64
2:B:754:SER:O	2:B:806:THR:HG21	1.97	0.64
2:B:792:MET:SD	2:B:857:ARG:NH2	2.71	0.64
2:B:99:LYS:HB3	2:B:100:PRO:CD	2.28	0.64
2:B:118:ARG:CG	2:B:118:ARG:NE	2.53	0.64
3:C:252:GLN:HE22	9:K:99:GLY:HA2	1.62	0.64
4:E:147:HIS:CD2	4:E:149:LEU:H	2.08	0.64
1:A:567:LYS:CB	1:A:568:PRO:CD	2.76	0.64
2:B:906:SER:O	2:B:907:GLY:C	2.40	0.64
4:E:153:HIS:CE1	4:E:184:VAL:HG11	2.32	0.64
7:I:120:GLN:O	7:I:121:PHE:HB2	1.98	0.64
1:A:741:ASN:HD22	1:A:741:ASN:C	2.06	0.64
6:H:123:MET:SD	6:H:123:MET:CB	2.84	0.64
1:A:903:ASN:C	1:A:903:ASN:ND2	2.56	0.64
2:B:531:GLN:HE21	2:B:532:ALA:H	1.44	0.64
1:A:144:THR:O	1:A:146:MET:HG2	1.99	0.63
1:A:1198:ASP:OD1	1:A:1200:ALA:HB3	1.97	0.63
6:H:63:LEU:HB2	6:H:90:ALA:HB2	1.79	0.63
2:B:132:VAL:HG12	2:B:133:LYS:N	2.13	0.63
6:H:123:MET:HE3	6:H:142:LEU:HD22	1.79	0.63
1:A:567:LYS:CB	6:H:95:TYR:HA	2.29	0.63
1:A:589:GLN:HB2	1:A:961:ARG:HH22	1.61	0.63
4:E:191:LYS:CD	4:E:191:LYS:NZ	2.62	0.63
1:A:472:LEU:O	1:A:475:THR:HB	1.98	0.63
2:B:916:THR:N	2:B:935:ARG:O	2.32	0.63
1:A:41:MET:O	1:A:50:ILE:HD11	1.99	0.63
1:A:596:THR:HG22	1:A:597:LEU:N	2.13	0.63
1:A:844:ALA:HB2	1:A:1384:VAL:HG12	1.81	0.63
2:B:916:THR:HB	2:B:935:ARG:HB2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:64:SER:O	7:I:66:PRO:HD3	1.99	0.63
1:A:369:SER:H	9:K:2:ASN:ND2	1.93	0.63
1:A:567:LYS:CD	1:A:568:PRO:CD	2.76	0.63
2:B:1222:ARG:HH11	2:B:1222:ARG:CB	2.10	0.63
9:K:49:GLU:HG2	9:K:94:ILE:HD11	1.79	0.63
2:B:846:ILE:CD1	2:B:974:PRO:HB2	2.28	0.62
6:H:103:LYS:O	6:H:115:TYR:HD1	1.81	0.62
10:L:34:CYS:SG	10:L:36:SER:OG	2.57	0.62
1:A:172:PRO:HG2	1:A:174:ILE:CD1	2.29	0.62
1:A:644:LYS:NZ	1:A:644:LYS:CD	2.62	0.62
1:A:744:LYS:HD3	1:A:748:MET:CE	2.29	0.62
1:A:1077:THR:HG22	1:A:1078:GLN:NE2	2.13	0.62
2:B:1002:THR:HG22	2:B:1006:ILE:H	1.63	0.62
3:C:152:GLU:OE2	3:C:154:LYS:HD2	1.99	0.62
8:J:1:MET:CE	8:J:1:MET:CB	2.77	0.62
1:A:858:ASN:HD21	1:A:860:LEU:HB2	1.64	0.62
9:K:49:GLU:CG	9:K:94:ILE:HD11	2.29	0.62
3:C:40:GLU:OE2	3:C:254:LYS:NZ	2.32	0.62
1:A:744:LYS:HD3	1:A:748:MET:SD	2.39	0.62
3:C:54:ASN:OD1	3:C:56:THR:CB	2.35	0.62
1:A:265:LYS:CD	1:A:302:THR:HG22	2.30	0.62
1:A:535:THR:CG2	1:A:616:VAL:HA	2.29	0.62
2:B:435:THR:HG23	2:B:437:GLU:HB2	1.81	0.62
1:A:265:LYS:HZ2	1:A:302:THR:HG21	1.64	0.62
9:K:12:LEU:N	9:K:12:LEU:HD12	2.14	0.62
8:J:53:HIS:HE1	8:J:55:ASP:HA	1.65	0.62
1:A:533:LYS:NZ	1:A:745:GLN:HE22	1.97	0.61
1:A:1144:LYS:CD	1:A:1144:LYS:NZ	2.60	0.61
2:B:498:THR:HG22	2:B:537:LYS:HB2	1.81	0.61
6:H:123:MET:HE1	6:H:142:LEU:CD1	2.28	0.61
1:A:804:TYR:O	2:B:761:HIS:ND1	2.31	0.61
2:B:242:SER:HG	2:B:363:HIS:HD1	1.48	0.61
2:B:269:ILE:HB	2:B:282:ILE:HD12	1.82	0.61
3:C:252:GLN:HE22	9:K:99:GLY:CA	2.13	0.61
6:H:105:GLU:C	6:H:107:VAL:N	2.57	0.61
3:C:209:TYR:HD1	3:C:209:TYR:N	1.99	0.61
5:F:87:LYS:NZ	5:F:87:LYS:CD	2.62	0.61
1:A:689:LYS:CE	1:A:689:LYS:CG	2.74	0.61
3:C:116:LYS:CE	3:C:116:LYS:CG	2.75	0.61
6:H:144:ILE:CD1	6:H:144:ILE:CB	2.72	0.61
1:A:518:LYS:CE	1:A:518:LYS:CG	2.78	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:129:PRO:CG	4:E:129:PRO:N	2.62	0.61
1:A:26:GLU:HA	1:A:29:ALA:HB3	1.83	0.61
1:A:164:ARG:O	1:A:166:GLY:N	2.33	0.61
1:A:1236:LEU:C	1:A:1237:ILE:HD12	2.25	0.61
4:E:36:GLU:O	4:E:38:PRO:N	2.32	0.61
1:A:715:GLU:OE1	1:A:774:ARG:HD3	2.01	0.61
1:A:973:ILE:HD11	1:A:1038:THR:HG23	1.82	0.61
1:A:982:THR:HG22	1:A:985:ASP:H	1.64	0.61
2:B:561:TRP:O	2:B:590:HIS:CE1	2.48	0.61
2:B:1051:THR:CG2	2:B:1053:GLU:H	2.05	0.61
2:B:1097:HIS:CE1	2:B:1102:LYS:HG3	2.35	0.61
1:A:57:ARG:O	1:A:68:GLN:NE2	2.32	0.61
1:A:187:LYS:CB	1:A:194:ALA:HB3	2.29	0.61
2:B:757:PRO:HD2	2:B:984:HIS:HE1	1.66	0.60
1:A:752:LYS:CE	1:A:752:LYS:HG2	2.30	0.60
2:B:1152:MET:HA	2:B:1152:MET:CE	2.31	0.60
1:A:351:THR:CG2	2:B:1103:ILE:HG13	2.29	0.60
1:A:492:PRO:HB2	1:A:497:THR:HG22	1.82	0.60
4:E:98:ILE:O	4:E:101:GLN:HB3	2.01	0.60
1:A:42:ASP:OD2	1:A:47:ARG:CA	2.50	0.60
1:A:567:LYS:CD	6:H:95:TYR:CD1	2.84	0.60
1:A:1239:ARG:CG	1:A:1239:ARG:NE	2.61	0.60
4:E:45:LYS:CE	4:E:45:LYS:CG	2.79	0.60
6:H:115:TYR:O	6:H:123:MET:O	2.19	0.60
8:J:53:HIS:ND1	8:J:54:VAL:N	2.48	0.60
2:B:955:THR:CG2	10:L:55:ILE:HA	2.31	0.60
1:A:752:LYS:HE2	2:B:1019:SER:OG	2.01	0.60
1:A:982:THR:HB	1:A:985:ASP:OD2	2.01	0.60
1:A:351:THR:HG21	2:B:1103:ILE:CG1	2.30	0.60
2:B:25:ILE:HD11	2:B:651:LEU:HD12	1.83	0.60
2:B:357:GLN:HE21	2:B:368:GLU:HG2	1.66	0.60
8:J:7:CYS:HA	8:J:49:MET:HE3	1.84	0.60
2:B:98:THR:HB	2:B:99:LYS:O	2.02	0.60
2:B:999:MET:CG	2:B:999:MET:HE3	2.27	0.60
6:H:127:GLY:O	6:H:128:ASN:HB2	2.00	0.60
1:A:46:THR:HB	1:A:46:THR:O	2.02	0.60
1:A:535:THR:HG23	1:A:616:VAL:HA	1.83	0.60
2:B:206:ASN:OD1	2:B:458:LYS:CE	2.50	0.60
8:J:45:CYS:HG	12:J:3001:ZN:ZN	1.13	0.60
1:A:858:ASN:C	1:A:858:ASN:HD22	2.10	0.60
2:B:616:ILE:CD1	2:B:616:ILE:CB	2.73	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:63:ILE:HG12	2:B:95:ILE:HD11	1.83	0.59
3:C:181:ASP:OD2	3:C:186:LEU:HB2	2.02	0.59
3:C:196:ASP:CB	3:C:199:LYS:HG3	2.32	0.59
6:H:105:GLU:HG2	6:H:136:LYS:NZ	2.17	0.59
1:A:63:ARG:HA	1:A:74:MET:SD	2.42	0.59
2:B:566:LEU:HD13	2:B:588:GLY:HA2	1.82	0.59
1:A:72:GLU:OE2	2:B:1175:LEU:CD1	2.51	0.59
2:B:418:LYS:CE	2:B:418:LYS:CG	2.80	0.59
3:C:131:HIS:O	3:C:132:PRO:C	2.44	0.59
1:A:63:ARG:HA	1:A:74:MET:HG2	1.84	0.59
1:A:1112:LYS:CE	1:A:1112:LYS:CG	2.79	0.59
6:H:107:VAL:CA	6:H:107:VAL:CG2	2.78	0.59
1:A:1265:ASN:O	1:A:1266:THR:C	2.42	0.59
1:A:1282:VAL:HG22	1:A:1308:THR:HG22	1.84	0.59
1:A:1315:GLU:O	1:A:1318:THR:HG22	2.02	0.59
10:L:26:THR:CG2	10:L:27:LEU:H	2.16	0.59
1:A:956:LEU:HB3	1:A:957:PRO:HD2	1.84	0.59
1:A:1287:TYR:CD1	1:A:1305:VAL:HG21	2.37	0.59
2:B:118:ARG:HH22	2:B:194:GLU:CG	2.14	0.59
6:H:136:LYS:C	6:H:136:LYS:HA	2.11	0.59
1:A:55:ASP:O	1:A:55:ASP:OD1	2.21	0.59
2:B:185:THR:HG23	2:B:188:ASP:OD2	2.03	0.59
7:I:55:THR:CG2	7:I:55:THR:HB	2.26	0.59
1:A:1385:THR:HG22	1:A:1385:THR:C	2.23	0.59
2:B:425:THR:CG2	2:B:425:THR:HB	2.17	0.59
2:B:531:GLN:NE2	2:B:532:ALA:H	2.00	0.59
10:L:26:THR:CA	10:L:26:THR:HB	2.19	0.59
1:A:673:GLY:N	1:A:674:PRO:HD2	2.17	0.59
1:A:844:ALA:CB	1:A:1384:VAL:HG12	2.32	0.59
6:H:47:PHE:CZ	6:H:146:ARG:HD2	2.38	0.59
8:J:2:ILE:HD11	8:J:57:ILE:HD12	1.83	0.59
9:K:46:ILE:O	9:K:47:ARG:C	2.35	0.59
2:B:999:MET:CG	2:B:999:MET:HE2	2.27	0.58
1:A:446:ARG:CG	1:A:446:ARG:NH1	2.65	0.58
1:A:567:LYS:CB	1:A:568:PRO:HD3	2.31	0.58
8:J:26:GLN:CG	8:J:26:GLN:CA	2.75	0.58
1:A:351:THR:HG23	2:B:1103:ILE:CG1	2.33	0.58
1:A:518:LYS:CD	1:A:518:LYS:HZ2	2.15	0.58
1:A:903:ASN:ND2	1:A:905:ASP:H	2.02	0.58
2:B:900:ALA:O	2:B:901:PRO:C	2.44	0.58
2:B:995:ARG:HD2	2:B:997:GLU:OE2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1198:TYR:CE1	2:B:1201:LYS:HD2	2.38	0.58
9:K:12:LEU:HD12	9:K:12:LEU:H	1.69	0.58
1:A:295:LEU:CD2	1:A:295:LEU:CB	2.78	0.58
2:B:775:LYS:CG	2:B:775:LYS:CA	2.73	0.58
3:C:133:ILE:C	3:C:134:ILE:HG12	2.28	0.58
4:E:55:ARG:O	4:E:56:LYS:C	2.46	0.58
1:A:174:ILE:CB	1:A:174:ILE:N	2.59	0.58
1:A:265:LYS:NZ	1:A:302:THR:HG21	2.17	0.58
1:A:1172:LEU:O	1:A:1173:HIS:CD2	2.56	0.58
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.37	0.58
1:A:587:HIS:NE2	1:A:969:GLN:HG2	2.18	0.58
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.85	0.58
3:C:205:LYS:CG	3:C:205:LYS:CA	2.74	0.58
6:H:76:THR:O	6:H:76:THR:HG22	2.04	0.58
8:J:53:HIS:HE1	8:J:55:ASP:CA	2.16	0.58
1:A:42:ASP:OD2	1:A:46:THR:C	2.45	0.58
6:H:9:ILE:CB	6:H:9:ILE:C	2.73	0.58
1:A:487:MET:CG	1:A:487:MET:HE3	2.13	0.58
1:A:744:LYS:HD3	1:A:748:MET:HE2	1.84	0.58
3:C:252:GLN:NE2	9:K:99:GLY:N	2.52	0.58
1:A:123:ARG:CG	1:A:123:ARG:CA	2.76	0.58
2:B:1162:ILE:HD11	2:B:1169:MET:HG2	1.85	0.58
1:A:55:ASP:C	1:A:57:ARG:H	2.04	0.58
2:B:1002:THR:HG21	2:B:1006:ILE:HB	1.85	0.57
2:B:1077:THR:CG2	2:B:1079:LYS:H	2.15	0.57
4:E:6:GLU:OE2	4:E:43:LYS:NZ	2.37	0.57
6:H:81:PRO:HB2	6:H:82:PRO:HD2	1.86	0.57
1:A:365:GLY:HA2	1:A:461:LYS:O	2.04	0.57
2:B:95:ILE:HG22	2:B:96:TYR:N	2.18	0.57
3:C:11:ARG:NE	3:C:209:TYR:CE2	2.72	0.57
3:C:29:MET:CE	3:C:29:MET:HB2	2.34	0.57
2:B:127:GLY:HA2	2:B:168:GLY:O	2.05	0.57
2:B:1002:THR:CG2	2:B:1006:ILE:HB	2.33	0.57
6:H:93:TYR:CD1	6:H:93:TYR:N	2.72	0.57
1:A:567:LYS:HD3	6:H:95:TYR:CB	2.34	0.57
2:B:134:LYS:O	2:B:135:ARG:HG3	2.05	0.57
3:C:8:VAL:CG1	3:C:9:LYS:N	2.67	0.57
3:C:162:GLY:HA3	3:C:170:TRP:CE2	2.40	0.57
2:B:862:GLN:HE22	2:B:961:LEU:HD13	1.70	0.57
1:A:567:LYS:HE2	6:H:95:TYR:CD2	2.40	0.57
2:B:101:MET:HA	2:B:110:HIS:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:341:LEU:HD12	2:B:342:GLY:H	1.69	0.57
1:A:1215:ARG:CB	1:A:1215:ARG:CD	2.76	0.57
2:B:914:LYS:CD	2:B:937:ALA:HB3	2.35	0.57
3:C:252:GLN:HE22	9:K:99:GLY:N	2.02	0.57
6:H:47:PHE:CB	6:H:95:TYR:HD1	2.18	0.57
6:H:98:TYR:C	6:H:118:PHE:HD2	2.13	0.57
1:A:567:LYS:CG	1:A:568:PRO:HD2	2.22	0.57
2:B:210:LYS:HE3	2:B:461:LEU:O	2.04	0.57
2:B:249:ARG:CZ	2:B:415:GLN:HG3	2.34	0.57
5:F:114:GLU:HB2	5:F:120:ILE:CD1	2.35	0.57
10:L:51:CYS:SG	10:L:53:HIS:HB2	2.44	0.57
1:A:103:CYS:SG	1:A:207:ILE:HD12	2.45	0.57
1:A:858:ASN:ND2	1:A:862:ASN:H	2.01	0.57
1:A:1404:GLU:HG3	1:A:1404:GLU:O	2.00	0.57
2:B:955:THR:CG2	10:L:54:ARG:O	2.40	0.57
3:C:208:GLU:O	3:C:210:GLU:N	2.38	0.57
1:A:941:LYS:NZ	1:A:941:LYS:HD3	2.19	0.57
2:B:261:ARG:O	2:B:264:SER:N	2.38	0.57
2:B:360:PHE:O	2:B:361:LEU:C	2.48	0.57
2:B:916:THR:HB	2:B:935:ARG:CB	2.34	0.57
1:A:1202:MET:HE2	1:A:1209:MET:SD	2.45	0.56
2:B:228:LYS:O	2:B:261:ARG:NH2	2.28	0.56
2:B:680:THR:HG22	2:B:682:SER:N	2.16	0.56
4:E:103:LYS:CE	4:E:103:LYS:CG	2.76	0.56
9:K:78:THR:HG22	9:K:79:GLU:H	1.70	0.56
1:A:346:ASP:O	1:A:347:PHE:HB2	2.05	0.56
2:B:1198:TYR:OH	2:B:1201:LYS:NZ	2.37	0.56
3:C:40:GLU:CD	3:C:254:LYS:NZ	2.64	0.56
3:C:56:THR:HG22	3:C:58:LEU:H	1.69	0.56
1:A:57:ARG:HB3	1:A:68:GLN:HG2	1.86	0.56
1:A:175:ARG:CG	1:A:175:ARG:CA	2.74	0.56
1:A:187:LYS:CG	1:A:194:ALA:CB	2.83	0.56
2:B:68:THR:HG23	2:B:91:SER:HB3	1.86	0.56
7:I:10:CYS:SG	7:I:29:CYS:SG	3.04	0.56
1:A:741:ASN:C	1:A:741:ASN:ND2	2.62	0.56
1:A:1151:GLU:HG3	7:I:45:ARG:HD2	1.88	0.56
4:E:39:LEU:O	4:E:42:PHE:HB3	2.05	0.56
6:H:103:LYS:HG2	6:H:105:GLU:OE2	2.05	0.56
1:A:599:SER:HB2	1:A:602:ASP:H	1.70	0.56
2:B:293:PRO:HA	7:I:12:ASN:HD21	1.71	0.56
3:C:15:LYS:CB	3:C:15:LYS:CD	2.84	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:103:LYS:NZ	6:H:105:GLU:OE2	2.27	0.56
7:I:98:VAL:HG22	7:I:99:LEU:N	2.19	0.56
1:A:200:ARG:NH2	1:A:206:GLU:OE2	2.39	0.56
3:C:255:VAL:O	3:C:255:VAL:CG1	2.51	0.56
1:A:261:ASP:N	1:A:261:ASP:OD1	2.39	0.56
2:B:120:ARG:NH2	2:B:956:THR:O	2.35	0.56
6:H:91:ASP:C	6:H:91:ASP:OD1	2.48	0.56
4:E:2:ASP:HB3	4:E:6:GLU:HB2	1.88	0.56
9:K:20:LYS:CG	9:K:20:LYS:CE	2.82	0.56
1:A:487:MET:CG	1:A:487:MET:HE2	2.13	0.56
1:A:1263:ILE:CD1	1:A:1263:ILE:CB	2.79	0.56
2:B:425:THR:CG2	2:B:425:THR:CA	2.77	0.56
2:B:864:LYS:O	2:B:961:LEU:HD23	2.06	0.56
2:B:882:THR:CG2	2:B:882:THR:HB	2.18	0.56
7:I:49:ILE:HG22	7:I:49:ILE:O	2.06	0.56
1:A:1261:LYS:CD	1:A:1261:LYS:NZ	2.66	0.55
2:B:787:VAL:O	2:B:787:VAL:HG12	2.06	0.55
2:B:841:MET:SD	2:B:846:ILE:HD11	2.46	0.55
2:B:999:MET:HB3	2:B:1000:PRO:HD2	1.88	0.55
6:H:44:VAL:O	6:H:44:VAL:HG13	2.05	0.55
9:K:55:LYS:HB3	9:K:81:TYR:HD1	1.71	0.55
10:L:68:GLU:O	10:L:69:ALA:HB3	2.06	0.55
1:A:606:LEU:HD11	1:A:608:ILE:HD11	1.88	0.55
1:A:982:THR:HB	1:A:985:ASP:CG	2.32	0.55
1:A:1132:LYS:CD	1:A:1132:LYS:CB	2.78	0.55
3:C:15:LYS:O	3:C:240:VAL:CG2	2.55	0.55
3:C:252:GLN:NE2	9:K:99:GLY:H	2.05	0.55
4:E:161:LYS:CE	4:E:161:LYS:CG	2.75	0.55
1:A:768:GLN:NE2	1:A:816:HIS:HA	2.22	0.55
1:A:1151:GLU:CG	7:I:45:ARG:CD	2.83	0.55
2:B:961:LEU:CD1	2:B:961:LEU:CD2	2.81	0.55
3:C:239:PRO:O	3:C:242:GLN:HB2	2.06	0.55
4:E:116:ILE:H	4:E:116:ILE:HD12	1.71	0.55
4:E:117:THR:OG1	4:E:120:ALA:CB	2.55	0.55
1:A:31:SER:HB3	1:A:83:HIS:HD2	1.71	0.55
2:B:167:ILE:CG2	2:B:424:LEU:HD13	2.36	0.55
6:H:142:LEU:HG	6:H:143:LEU:N	2.17	0.55
7:I:116:ASN:ND2	7:I:118:ARG:HB2	2.21	0.55
2:B:1128:LEU:HG	2:B:1128:LEU:O	2.07	0.55
6:H:118:PHE:O	6:H:119:GLY:C	2.44	0.55
2:B:46:GLN:HG3	2:B:47:GLN:H	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:550:ASP:OD1	2:B:551:PRO:HD2	2.06	0.55
2:B:642:ASP:HB3	2:B:649:LYS:HG3	1.89	0.55
2:B:1195:HIS:C	2:B:1196:ILE:HG23	2.31	0.55
3:C:56:THR:CG2	3:C:58:LEU:H	2.19	0.55
9:K:24:ASP:OD1	9:K:74:ARG:NH1	2.40	0.55
10:L:38:LEU:HG	10:L:39:SER:H	1.72	0.55
1:A:150:THR:HA	1:A:166:GLY:HA2	1.89	0.55
1:A:279:LEU:HB3	1:A:289:ILE:HD11	1.87	0.55
1:A:494:SER:OG	1:A:497:THR:HB	2.07	0.55
1:A:1224:LEU:HG	1:A:1225:PHE:N	2.21	0.55
2:B:353:LYS:CD	2:B:353:LYS:CB	2.77	0.55
4:E:14:ARG:O	4:E:15:ALA:C	2.46	0.55
6:H:27:GLU:OE1	6:H:39:THR:CG2	2.54	0.55
2:B:910:VAL:C	2:B:911:ILE:HD12	2.32	0.55
2:B:1002:THR:HG22	2:B:1006:ILE:N	2.21	0.55
3:C:40:GLU:OE1	3:C:254:LYS:NZ	2.40	0.55
8:J:42:LYS:HG3	8:J:43:ARG:N	2.22	0.55
1:A:150:THR:HG22	1:A:151:ASP:OD2	2.07	0.54
1:A:175:ARG:CB	1:A:175:ARG:CD	2.83	0.54
1:A:843:LYS:CG	1:A:843:LYS:CE	2.85	0.54
4:E:116:ILE:HG22	4:E:120:ALA:CB	2.36	0.54
10:L:47:ARG:HG2	10:L:48:CYS:N	2.19	0.54
1:A:562:THR:CG2	6:H:98:TYR:CD2	2.90	0.54
1:A:1161:THR:HG22	1:A:1163:ILE:N	2.20	0.54
1:A:1258:HIS:O	1:A:1259:MET:C	2.50	0.54
2:B:956:THR:HA	2:B:961:LEU:O	2.07	0.54
3:C:178:PHE:C	3:C:178:PHE:CD2	2.86	0.54
3:C:240:VAL:C	3:C:242:GLN:N	2.64	0.54
8:J:2:ILE:HD11	8:J:57:ILE:CD1	2.37	0.54
1:A:89:PRO:HB2	1:A:204:THR:HG21	1.90	0.54
6:H:32:THR:HG22	6:H:33:GLN:CD	2.32	0.54
1:A:1325:THR:O	4:E:148:GLU:HG2	2.06	0.54
2:B:282:ILE:HD13	2:B:282:ILE:N	2.22	0.54
2:B:744:HIS:CD2	2:B:746:SER:H	2.21	0.54
4:E:71:LYS:CG	4:E:71:LYS:CE	2.80	0.54
7:I:109:ILE:HD12	7:I:109:ILE:N	2.21	0.54
2:B:435:THR:O	2:B:435:THR:HG22	2.07	0.54
3:C:47:ASP:CG	3:C:47:ASP:O	2.49	0.54
2:B:1163:CYS:CA	2:B:1163:CYS:SG	2.95	0.54
2:B:1163:CYS:CB	2:B:1182:CYS:SG	2.96	0.54
2:B:1163:CYS:HB2	2:B:1182:CYS:SG	2.48	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:33:LEU:HD13	3:C:248:ILE:HD13	1.88	0.54
4:E:61:GLN:HB2	4:E:79:TRP:HE3	1.71	0.54
1:A:507:VAL:N	1:A:508:PRO:CD	2.70	0.54
2:B:1182:CYS:SG	2:B:1185:CYS:SG	3.06	0.54
8:J:4:PRO:HD3	8:J:53:HIS:HD2	1.72	0.54
9:K:49:GLU:C	9:K:51:LEU:N	2.65	0.54
1:A:1203:ASN:O	1:A:1205:LYS:N	2.41	0.54
2:B:509:ALA:CB	2:B:509:ALA:N	2.65	0.54
4:E:47:CYS:SG	4:E:52:ARG:O	2.66	0.54
6:H:95:TYR:HE2	6:H:97:MET:HG3	1.73	0.54
10:L:32:ALA:HB2	10:L:55:ILE:HG22	1.90	0.54
10:L:65:VAL:CG2	10:L:65:VAL:HB	2.17	0.54
1:A:1122:PRO:O	1:A:1123:GLY:C	2.48	0.54
4:E:61:GLN:HB2	4:E:79:TRP:CE3	2.43	0.54
6:H:95:TYR:CE2	6:H:97:MET:HG3	2.43	0.54
10:L:51:CYS:HG	12:L:3005:ZN:ZN	1.21	0.54
1:A:217:LYS:CD	1:A:217:LYS:CB	2.81	0.54
3:C:15:LYS:CG	3:C:15:LYS:CA	2.80	0.54
4:E:117:THR:O	4:E:118:PRO:C	2.51	0.54
6:H:47:PHE:CG	6:H:95:TYR:HD1	2.26	0.54
1:A:55:ASP:N	1:A:56:PRO:HD2	2.22	0.53
1:A:846:GLU:HA	1:A:1066:VAL:HG23	1.88	0.53
1:A:1146:VAL:HG12	1:A:1197:LEU:HD22	1.90	0.53
2:B:463:THR:HG21	2:B:465:ASN:OD1	2.08	0.53
6:H:44:VAL:O	6:H:44:VAL:CG1	2.56	0.53
8:J:53:HIS:CE1	8:J:54:VAL:C	2.86	0.53
10:L:54:ARG:CG	10:L:54:ARG:NE	2.62	0.53
1:A:852:TYR:CD2	5:F:136:ARG:HD3	2.43	0.53
1:A:1318:THR:HG23	4:E:11:ARG:HH12	1.73	0.53
2:B:984:HIS:CD2	2:B:1025:HIS:HA	2.42	0.53
2:B:1097:HIS:C	2:B:1097:HIS:ND1	2.67	0.53
2:B:1177:HIS:HB2	2:B:1179:GLN:HE21	1.71	0.53
1:A:672:ASP:HB3	1:A:674:PRO:HG2	1.89	0.53
4:E:60:PHE:CD1	4:E:60:PHE:C	2.87	0.53
9:K:98:LEU:O	9:K:99:GLY:C	2.51	0.53
1:A:897:TYR:CD2	1:A:936:LEU:HD13	2.44	0.53
1:A:1111:MET:HE3	1:A:1111:MET:CB	2.39	0.53
2:B:89:GLU:HB2	2:B:137:TYR:HB2	1.90	0.53
2:B:243:ALA:C	2:B:244:LEU:HG	2.32	0.53
2:B:436:VAL:CA	2:B:436:VAL:CG1	2.78	0.53
10:L:48:CYS:HB3	10:L:51:CYS:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:9:ILE:CB	6:H:9:ILE:HA	2.17	0.53
1:A:191:THR:CB	1:A:191:THR:HA	2.18	0.53
1:A:1445:ILE:CG2	1:A:1445:ILE:HA	2.36	0.53
2:B:1190:ASP:C	2:B:1191:ILE:HG13	2.32	0.53
5:F:111:LEU:C	5:F:113:GLY:N	2.66	0.53
6:H:9:ILE:CA	6:H:9:ILE:HB	2.17	0.53
7:I:16:PRO:O	7:I:17:ARG:CD	2.46	0.53
1:A:919:ILE:CD1	1:A:919:ILE:CB	2.81	0.53
1:A:1298:TYR:O	1:A:1299:VAL:HG23	2.08	0.53
2:B:755:ILE:CG2	2:B:755:ILE:O	2.56	0.53
4:E:116:ILE:HD12	4:E:116:ILE:N	2.24	0.53
6:H:31:THR:O	6:H:32:THR:OG1	2.20	0.53
6:H:100:THR:O	6:H:116:TYR:HA	2.08	0.53
8:J:6:ARG:HD2	8:J:11:GLY:O	2.08	0.53
6:H:138:GLU:HG2	6:H:139:ASN:N	2.23	0.53
8:J:26:GLN:CB	8:J:26:GLN:CD	2.77	0.53
1:A:1166:ASP:OD2	1:A:1239:ARG:NH2	2.22	0.53
1:A:1209:MET:O	1:A:1210:GLY:C	2.48	0.53
1:A:1362:TYR:C	1:A:1362:TYR:CD2	2.85	0.53
2:B:98:THR:OG1	2:B:127:GLY:O	2.26	0.53
2:B:169:ARG:O	2:B:457:LEU:HD12	2.08	0.53
4:E:63:ASN:O	4:E:64:PRO:C	2.46	0.53
6:H:6:PHE:CD2	6:H:6:PHE:C	2.87	0.53
2:B:103:ASN:HB2	2:B:169:ARG:HH22	1.73	0.52
6:H:130:ARG:HD2	6:H:130:ARG:O	2.07	0.52
7:I:120:GLN:O	7:I:121:PHE:CB	2.56	0.52
1:A:1162:VAL:O	1:A:1162:VAL:CG1	2.57	0.52
7:I:71:SER:OG	7:I:83:ASN:ND2	2.41	0.52
1:A:476:SER:N	1:A:477:PRO:HD2	2.24	0.52
1:A:1195:LEU:HD11	1:A:1267:MET:HE1	1.91	0.52
2:B:453:ILE:HG22	2:B:454:THR:N	2.23	0.52
3:C:167:HIS:CE1	10:L:70:ARG:O	2.58	0.52
5:F:72:LYS:CE	5:F:72:LYS:CG	2.84	0.52
1:A:274:ILE:CA	1:A:274:ILE:CG1	2.82	0.52
1:A:636:GLU:OE2	1:A:962:ARG:CD	2.57	0.52
1:A:658:LEU:HD12	1:A:658:LEU:O	2.10	0.52
1:A:771:GLU:CD	2:B:510:LYS:NZ	2.68	0.52
1:A:1155:ASP:O	1:A:1241:ARG:NH2	2.42	0.52
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.92	0.52
3:C:19:ASP:C	3:C:19:ASP:OD1	2.48	0.52
6:H:59:ILE:HG22	6:H:60:ALA:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:1:MET:CB	8:J:1:MET:HE3	2.39	0.52
9:K:25:THR:CG2	9:K:25:THR:CA	2.78	0.52
1:A:42:ASP:OD2	1:A:47:ARG:CG	2.58	0.52
1:A:278:THR:O	1:A:278:THR:HG22	2.09	0.52
1:A:387:ARG:O	1:A:388:LEU:C	2.51	0.52
1:A:1293:SER:HB2	1:A:1294:PRO:HD2	1.92	0.52
2:B:516:ASN:HD22	2:B:516:ASN:H	1.55	0.52
2:B:1057:LYS:CD	2:B:1057:LYS:NZ	2.66	0.52
4:E:176:PRO:O	4:E:212:ARG:HA	2.09	0.52
6:H:103:LYS:CB	6:H:105:GLU:OE1	2.51	0.52
6:H:105:GLU:HG2	6:H:136:LYS:HZ2	1.74	0.52
9:K:18:LYS:HE3	9:K:38:GLU:HG2	1.91	0.52
1:A:268:ASP:HB3	1:A:299:HIS:CD2	2.44	0.52
6:H:96:VAL:HA	6:H:142:LEU:O	2.10	0.52
1:A:1172:LEU:C	1:A:1173:HIS:CD2	2.87	0.52
1:A:1323:ASP:OD1	1:A:1325:THR:HB	2.09	0.52
2:B:294:ASP:N	7:I:12:ASN:HD22	2.08	0.52
2:B:658:ILE:HG22	2:B:658:ILE:O	2.10	0.52
4:E:63:ASN:C	4:E:64:PRO:O	2.52	0.52
4:E:127:ILE:H	4:E:128:PRO:HD3	1.74	0.52
1:A:1266:THR:O	1:A:1267:MET:C	2.53	0.52
6:H:37:LYS:O	6:H:125:LEU:HA	2.10	0.52
1:A:1111:MET:HE1	1:A:1331:SER:HB2	1.92	0.52
6:H:114:VAL:HG11	6:H:134:ASN:ND2	2.25	0.52
8:J:53:HIS:ND1	8:J:53:HIS:C	2.66	0.52
4:E:71:LYS:CD	4:E:71:LYS:CB	2.78	0.52
4:E:152:LYS:CD	4:E:152:LYS:NZ	2.70	0.52
8:J:16:ASP:OD1	8:J:17:LYS:HG3	2.10	0.52
1:A:107:CYS:HB2	1:A:148:CYS:HB2	1.92	0.51
2:B:43:LEU:HD11	2:B:811:TYR:O	2.10	0.51
2:B:117:ALA:HA	2:B:122:LEU:HB2	1.91	0.51
2:B:1097:HIS:CB	2:B:1097:HIS:N	2.69	0.51
1:A:901:LEU:H	1:A:926:GLN:HE22	1.54	0.51
1:A:1287:TYR:HD1	1:A:1305:VAL:HG21	1.76	0.51
1:A:1111:MET:SD	1:A:1111:MET:CB	2.89	0.51
2:B:531:GLN:CG	2:B:531:GLN:CA	2.84	0.51
4:E:37:LEU:CD1	4:E:37:LEU:CB	2.79	0.51
3:C:154:LYS:CG	3:C:154:LYS:CA	2.82	0.51
5:F:114:GLU:HB2	5:F:120:ILE:HD11	1.93	0.51
1:A:55:ASP:N	1:A:56:PRO:HD3	2.24	0.51
1:A:356:ASP:OD2	1:A:469:ARG:HD3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:GLU:OE2	1:A:1438:THR:HG21	2.10	0.51
2:B:46:GLN:HG3	2:B:47:GLN:N	2.25	0.51
1:A:567:LYS:HB2	6:H:95:TYR:HA	1.92	0.51
1:A:588:LEU:C	1:A:588:LEU:CD2	2.82	0.51
2:B:1152:MET:HA	2:B:1152:MET:HE2	1.92	0.51
1:A:378:GLU:OE1	1:A:434:ARG:HD3	2.10	0.51
1:A:562:THR:HG22	6:H:98:TYR:CD2	2.45	0.51
1:A:567:LYS:CE	6:H:95:TYR:CD2	2.94	0.51
1:A:1172:LEU:O	1:A:1173:HIS:CG	2.64	0.51
3:C:180:TYR:CD1	3:C:180:TYR:C	2.88	0.51
4:E:79:TRP:HE1	4:E:81:GLU:HB2	1.76	0.51
1:A:852:TYR:CE2	5:F:136:ARG:HD3	2.45	0.51
1:A:1146:VAL:O	1:A:1146:VAL:CG1	2.53	0.51
2:B:424:LEU:C	2:B:424:LEU:CD2	2.82	0.51
2:B:864:LYS:O	2:B:961:LEU:CD2	2.59	0.51
6:H:95:TYR:CD2	6:H:95:TYR:C	2.88	0.51
2:B:113:TYR:CD2	2:B:192:LEU:HD22	2.46	0.51
2:B:377:PHE:CE2	2:B:381:MET:HE2	2.45	0.51
2:B:788:ARG:HD3	2:B:790:ASP:OD1	2.10	0.51
3:C:8:VAL:O	3:C:9:LYS:HB2	2.11	0.51
3:C:124:LEU:N	3:C:124:LEU:HD23	2.26	0.51
1:A:237:THR:CG2	1:A:237:THR:HB	2.18	0.51
2:B:353:LYS:CG	2:B:353:LYS:CE	2.82	0.51
2:B:424:LEU:O	2:B:428:ILE:HG13	2.09	0.51
1:A:247:ARG:HH11	1:A:263:THR:CG2	2.19	0.50
5:F:109:VAL:HG11	5:F:123:LYS:HG2	1.93	0.50
8:J:2:ILE:HD12	8:J:2:ILE:N	2.18	0.50
9:K:101:LEU:HD13	9:K:101:LEU:C	2.36	0.50
1:A:191:THR:CA	1:A:191:THR:HB	2.18	0.50
1:A:741:ASN:HD21	1:A:743:VAL:HB	1.75	0.50
3:C:7:GLN:OE1	9:K:104:ASN:ND2	2.44	0.50
4:E:127:ILE:N	4:E:128:PRO:HD3	2.24	0.50
1:A:597:LEU:H	1:A:597:LEU:HD12	1.76	0.50
1:A:1166:ASP:O	1:A:1170:ILE:HD13	2.11	0.50
2:B:502:ILE:HA	2:B:502:ILE:HD13	1.93	0.50
2:B:775:LYS:CB	2:B:775:LYS:HD2	2.39	0.50
8:J:3:VAL:HA	8:J:53:HIS:CD2	2.46	0.50
8:J:7:CYS:HG	8:J:45:CYS:HG	1.59	0.50
1:A:237:THR:CG2	1:A:237:THR:C	2.84	0.50
2:B:592:ASN:O	2:B:593:PRO:C	2.52	0.50
6:H:8:ASP:OD2	6:H:9:ILE:N	2.39	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:ARG:HG2	1:A:189:ARG:O	2.11	0.50
1:A:463:ILE:CD1	1:A:469:ARG:HG3	2.42	0.50
1:A:903:ASN:ND2	1:A:905:ASP:N	2.59	0.50
2:B:365:THR:HG22	2:B:367:LEU:H	1.77	0.50
2:B:820:GLY:HA3	2:B:1091:TYR:CZ	2.47	0.50
1:A:61:ILE:CA	1:A:61:ILE:CG1	2.83	0.50
3:C:120:ILE:HD12	3:C:120:ILE:N	2.24	0.50
7:I:41:PRO:HD2	7:I:42:LEU:H	1.77	0.50
10:L:34:CYS:CB	10:L:51:CYS:CB	2.81	0.50
2:B:544:CYS:HB2	2:B:634:TYR:CE1	2.46	0.50
3:C:207:CYS:O	3:C:208:GLU:C	2.55	0.50
10:L:43:THR:CG2	10:L:43:THR:CA	2.82	0.50
6:H:11:GLN:NE2	6:H:52:GLN:HG2	2.27	0.50
7:I:74:GLU:HA	7:I:80:SER:O	2.12	0.50
9:K:102:LYS:O	9:K:106:GLU:HB2	2.12	0.50
1:A:587:HIS:CE1	1:A:609:ASP:H	2.30	0.50
2:B:344:LYS:CG	2:B:344:LYS:CA	2.84	0.50
2:B:428:ILE:HG12	2:B:448:ILE:CD1	2.30	0.50
4:E:31:THR:O	4:E:32:GLN:C	2.52	0.50
6:H:77:ARG:C	6:H:78:SER:O	2.54	0.50
7:I:65:ASP:C	7:I:65:ASP:OD1	2.55	0.50
9:K:26:LYS:CB	9:K:26:LYS:CD	2.89	0.50
10:L:48:CYS:CA	10:L:49:LYS:N	2.67	0.50
1:A:423:ASP:CG	1:A:423:ASP:O	2.55	0.49
1:A:526:ASP:OD1	2:B:1013:ASN:ND2	2.40	0.49
3:C:73:GLN:HE21	3:C:75:MET:N	2.06	0.49
4:E:168:TYR:O	4:E:169:ARG:C	2.51	0.49
8:J:10:CYS:SG	8:J:45:CYS:SG	3.10	0.49
1:A:89:PRO:HB2	1:A:204:THR:CG2	2.42	0.49
1:A:605:MET:CE	1:A:607:ILE:HG13	2.42	0.49
1:A:771:GLU:CD	2:B:510:LYS:HZ3	2.20	0.49
1:A:1127:ASP:HB3	1:A:1130:GLN:H	1.77	0.49
1:A:1336:MET:HE3	1:A:1381:LEU:HD12	1.92	0.49
2:B:773:MET:O	2:B:774:GLY:C	2.53	0.49
2:B:830:TYR:O	2:B:831:SER:CB	2.60	0.49
2:B:1058:LEU:O	2:B:1062:HIS:HD2	1.95	0.49
8:J:53:HIS:C	8:J:53:HIS:HD1	2.20	0.49
2:B:890:TYR:OH	2:B:936:ASP:OD1	2.26	0.49
7:I:16:PRO:HG3	7:I:27:PHE:CE2	2.47	0.49
8:J:1:MET:CE	8:J:1:MET:HG3	2.38	0.49
8:J:53:HIS:HD1	8:J:54:VAL:N	2.09	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:425:THR:CG2	2:B:425:THR:C	2.85	0.49
2:B:516:ASN:H	2:B:516:ASN:ND2	2.11	0.49
5:F:109:VAL:HG22	5:F:127:GLU:OE1	2.11	0.49
9:K:110:ASN:C	9:K:112:GLN:N	2.70	0.49
1:A:247:ARG:NH1	1:A:263:THR:CG2	2.70	0.49
2:B:755:ILE:O	2:B:755:ILE:HG22	2.11	0.49
2:B:957:ASN:OD1	2:B:959:ASP:HB2	2.12	0.49
6:H:138:GLU:CG	6:H:139:ASN:N	2.74	0.49
10:L:43:THR:CG2	10:L:43:THR:HB	2.20	0.49
10:L:47:ARG:CG	10:L:48:CYS:H	2.22	0.49
2:B:1008:PRO:CG	2:B:1011:ILE:HD11	2.43	0.49
8:J:14:VAL:CG1	8:J:50:ILE:HD11	2.39	0.49
1:A:46:THR:O	1:A:48:ALA:N	2.46	0.49
1:A:64:ASN:O	1:A:64:ASN:CG	2.55	0.49
2:B:436:VAL:CA	2:B:436:VAL:CG2	2.80	0.49
2:B:595:ARG:CD	2:B:595:ARG:HB2	2.43	0.49
3:C:53:THR:O	3:C:153:LEU:HA	2.13	0.49
4:E:191:LYS:O	4:E:192:ARG:C	2.49	0.49
1:A:215:SER:OG	1:A:218:ASP:HB2	2.13	0.49
1:A:1383:SER:OG	1:A:1384:VAL:N	2.44	0.49
3:C:244:VAL:O	3:C:248:ILE:HG12	2.13	0.49
4:E:161:LYS:CE	4:E:172:GLU:OE2	2.61	0.49
6:H:99:GLY:N	6:H:118:PHE:CD2	2.81	0.49
9:K:25:THR:CG2	9:K:25:THR:OG1	2.54	0.49
1:A:44:THR:CA	1:A:44:THR:HB	2.20	0.49
1:A:44:THR:CB	1:A:44:THR:C	2.81	0.49
1:A:693:VAL:HG21	1:A:721:PHE:CE1	2.44	0.49
1:A:1445:ILE:CG2	1:A:1445:ILE:HB	2.19	0.49
2:B:1065:GLN:NE2	2:B:1067:ARG:HB2	2.22	0.49
6:H:101:ALA:HB2	6:H:116:TYR:CE2	2.48	0.49
1:A:458:HIS:CE1	1:A:507:VAL:HG21	2.48	0.49
1:A:597:LEU:CD1	1:A:597:LEU:HG	2.24	0.49
1:A:1236:LEU:CD2	1:A:1236:LEU:HG	2.19	0.49
2:B:1051:THR:O	2:B:1055:ILE:HG12	2.13	0.49
9:K:49:GLU:HG3	9:K:94:ILE:CD1	2.43	0.49
9:K:55:LYS:HB2	9:K:81:TYR:CE1	2.48	0.49
1:A:230:ARG:NH1	1:A:232:GLU:OE2	2.43	0.48
2:B:515:HIS:N	2:B:518:HIS:HD2	2.05	0.48
2:B:914:LYS:HD2	2:B:937:ALA:HB3	1.93	0.48
2:B:999:MET:HE2	2:B:999:MET:CB	2.43	0.48
4:E:52:ARG:HG3	4:E:53:PRO:HD3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:VAL:N	1:A:1432:GLN:HE22	2.05	0.48
1:A:59:GLY:C	1:A:60:SER:OG	2.57	0.48
1:A:300:VAL:O	1:A:304:MET:HE2	2.12	0.48
1:A:362:ASP:OD1	1:A:459:ARG:HD3	2.13	0.48
1:A:771:GLU:OE2	2:B:510:LYS:NZ	2.43	0.48
1:A:901:LEU:HB2	1:A:926:GLN:HE21	1.77	0.48
2:B:102:VAL:HG22	2:B:112:LEU:HD22	1.95	0.48
1:A:93:VAL:HG22	1:A:304:MET:HE3	1.94	0.48
1:A:119:ASN:O	1:A:120:GLU:CB	2.58	0.48
1:A:752:LYS:NZ	2:B:1019:SER:H	1.96	0.48
1:A:1290:LYS:HA	1:A:1299:VAL:O	2.12	0.48
2:B:130:VAL:CG2	2:B:167:ILE:HD11	2.44	0.48
2:B:121:ASN:HD21	2:B:965:LYS:NZ	2.11	0.48
2:B:167:ILE:CD1	2:B:167:ILE:CB	2.80	0.48
2:B:286:PHE:HB3	2:B:297:ILE:HD12	1.95	0.48
6:H:103:LYS:HE3	6:H:135:LEU:O	2.13	0.48
1:A:1111:MET:CE	1:A:1111:MET:CB	2.91	0.48
2:B:1163:CYS:SG	2:B:1165:ILE:HG12	2.53	0.48
1:A:110:CYS:SG	1:A:167:CYS:CB	3.02	0.48
1:A:908:LEU:O	1:A:909:ASP:C	2.55	0.48
1:A:1157:ASP:O	1:A:1160:SER:O	2.32	0.48
2:B:724:ASP:O	2:B:725:PRO:C	2.55	0.48
2:B:1057:LYS:CD	2:B:1057:LYS:CB	2.81	0.48
3:C:186:LEU:HA	3:C:186:LEU:HD12	1.53	0.48
5:F:73:ALA:HB2	5:F:143:PHE:CE1	2.49	0.48
6:H:47:PHE:CB	6:H:95:TYR:CD1	2.96	0.48
8:J:38:ARG:CG	8:J:38:ARG:CA	2.82	0.48
9:K:18:LYS:HE3	9:K:36:GLU:O	2.13	0.48
1:A:399:HIS:HE1	1:A:436:ILE:O	1.97	0.48
1:A:464:PRO:O	1:A:465:TYR:O	2.32	0.48
1:A:1226:VAL:HG12	1:A:1227:ILE:N	2.20	0.48
2:B:1085:ILE:N	2:B:1085:ILE:HD12	2.29	0.48
6:H:105:GLU:CD	6:H:105:GLU:N	2.67	0.48
6:H:114:VAL:HG11	6:H:134:ASN:HD22	1.79	0.48
1:A:3:GLY:CA	1:A:76:GLU:HG2	2.43	0.48
1:A:834:THR:HG21	1:A:1077:THR:CA	2.43	0.48
1:A:913:LEU:HD11	1:A:981:LEU:O	2.13	0.48
2:B:436:VAL:CB	2:B:436:VAL:N	2.66	0.48
2:B:69:LEU:O	2:B:70:ILE:HD13	2.13	0.48
2:B:90:ILE:N	2:B:90:ILE:CD1	2.76	0.48
2:B:451:LYS:HA	2:B:454:THR:HB	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:31:THR:OG1	4:E:34:GLU:HB2	2.14	0.48
9:K:110:ASN:C	9:K:112:GLN:H	2.09	0.48
1:A:599:SER:O	1:A:600:PRO:C	2.57	0.48
1:A:1164:PRO:O	1:A:1167:GLU:HG3	2.14	0.48
2:B:1213:THR:HG21	2:B:1215:ARG:NH2	2.29	0.48
4:E:117:THR:C	4:E:119:SER:N	2.71	0.48
1:A:784:LEU:HB3	1:A:786:HIS:HD2	1.79	0.47
1:A:1171:GLN:CG	1:A:1171:GLN:NE2	2.63	0.47
2:B:128:LEU:O	2:B:167:ILE:N	2.43	0.47
3:C:166:GLU:HB2	9:K:10:PHE:HE2	1.79	0.47
6:H:26:ILE:CD1	6:H:42:ILE:HD12	2.44	0.47
10:L:58:LYS:O	10:L:59:ALA:CB	2.44	0.47
2:B:502:ILE:CA	2:B:502:ILE:CG1	2.85	0.47
4:E:7:ARG:O	4:E:8:ASN:C	2.57	0.47
6:H:81:PRO:HB2	6:H:82:PRO:CD	2.43	0.47
6:H:97:MET:HE2	6:H:142:LEU:HD23	1.96	0.47
6:H:105:GLU:C	6:H:107:VAL:H	2.22	0.47
7:I:51:ASN:HB2	7:I:118:ARG:CZ	2.44	0.47
9:K:18:LYS:CE	9:K:38:GLU:OE2	2.62	0.47
9:K:55:LYS:HB3	9:K:81:TYR:CD1	2.49	0.47
10:L:38:LEU:HD13	10:L:48:CYS:HA	1.95	0.47
1:A:35:ILE:HG22	1:A:270:LEU:HD21	1.95	0.47
2:B:531:GLN:HE21	2:B:532:ALA:N	2.11	0.47
2:B:914:LYS:HD3	2:B:937:ALA:HB3	1.94	0.47
10:L:38:LEU:O	10:L:39:SER:HB2	2.13	0.47
1:A:853:ASP:OD2	1:A:857:ARG:NH2	2.47	0.47
2:B:859:TYR:N	2:B:859:TYR:CD1	2.82	0.47
2:B:1012:ILE:C	2:B:1012:ILE:HD12	2.39	0.47
3:C:248:ILE:HD13	3:C:248:ILE:N	2.25	0.47
4:E:36:GLU:O	4:E:38:PRO:CD	2.62	0.47
4:E:43:LYS:O	4:E:47:CYS:HB3	2.13	0.47
4:E:94:LYS:O	4:E:98:ILE:HD13	2.14	0.47
6:H:113:ALA:CB	6:H:124:ARG:HH21	2.28	0.47
8:J:62:ARG:HE	8:J:62:ARG:HB3	1.25	0.47
1:A:35:ILE:H	1:A:35:ILE:CD1	2.16	0.47
1:A:304:MET:CE	1:A:304:MET:HB2	2.44	0.47
1:A:1192:LEU:HD11	1:A:1239:ARG:HB2	1.96	0.47
2:B:94:LYS:HG2	2:B:96:TYR:CE1	2.49	0.47
2:B:128:LEU:HD13	2:B:128:LEU:N	2.29	0.47
1:A:40:THR:HG23	1:A:54:ASN:ND2	2.30	0.47
1:A:66:LYS:CB	1:A:66:LYS:CD	2.86	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:LYS:HG3	1:A:194:ALA:HB3	1.96	0.47
1:A:187:LYS:CG	1:A:194:ALA:HB3	2.43	0.47
1:A:704:ALA:HB1	1:A:708:MET:O	2.15	0.47
2:B:417:PHE:C	2:B:417:PHE:HD2	2.20	0.47
2:B:1004:GLU:HB2	2:B:1006:ILE:HD13	1.96	0.47
4:E:117:THR:C	4:E:119:SER:H	2.22	0.47
4:E:118:PRO:O	4:E:121:MET:SD	2.73	0.47
8:J:1:MET:HG3	8:J:60:PHE:HE2	1.80	0.47
8:J:51:LEU:O	8:J:51:LEU:HG	2.15	0.47
1:A:279:LEU:H	1:A:281:HIS:H	1.61	0.47
1:A:640:GLN:O	1:A:641:VAL:C	2.53	0.47
1:A:840:ARG:CD	1:A:840:ARG:CB	2.86	0.47
1:A:913:LEU:C	1:A:913:LEU:HD12	2.30	0.47
1:A:925:LEU:HD23	1:A:925:LEU:HA	1.72	0.47
1:A:1004:ASN:CG	4:E:167:ARG:HG3	2.40	0.47
1:A:1148:ILE:HD12	1:A:1196:GLU:HG2	1.96	0.47
1:A:1260:LEU:HD12	1:A:1260:LEU:HA	1.68	0.47
2:B:227:LYS:CE	2:B:227:LYS:CG	2.90	0.47
2:B:291:ILE:HG22	2:B:297:ILE:HD13	1.95	0.47
2:B:345:LYS:O	2:B:346:GLU:C	2.50	0.47
2:B:424:LEU:HD21	2:B:428:ILE:HD11	1.96	0.47
2:B:458:LYS:O	2:B:459:TYR:C	2.53	0.47
2:B:529:GLU:O	2:B:531:GLN:NE2	2.48	0.47
2:B:900:ALA:O	2:B:903:VAL:HG23	2.14	0.47
3:C:42:PRO:HG3	3:C:163:ILE:HD11	1.96	0.47
3:C:51:VAL:HG22	3:C:155:LEU:CD2	2.45	0.47
3:C:267:GLN:CA	3:C:268:ASP:N	2.64	0.47
4:E:79:TRP:NE1	4:E:81:GLU:HB2	2.29	0.47
6:H:8:ASP:CG	6:H:9:ILE:H	2.22	0.47
6:H:27:GLU:OE1	6:H:39:THR:HG23	2.12	0.47
10:L:65:VAL:CG2	10:L:65:VAL:N	2.78	0.47
3:C:43:THR:CG2	3:C:44:LEU:N	2.78	0.47
1:A:216:VAL:HG22	1:A:219:PHE:CZ	2.49	0.47
1:A:979:SER:OG	1:A:981:LEU:HB2	2.15	0.47
3:C:181:ASP:CG	3:C:181:ASP:O	2.56	0.47
9:K:77:THR:OG1	9:K:83:PRO:HD3	2.15	0.47
9:K:88:LYS:CG	9:K:88:LYS:CE	2.83	0.47
10:L:48:CYS:HG	10:L:51:CYS:HG	1.61	0.47
1:A:279:LEU:HB3	1:A:289:ILE:CD1	2.45	0.47
1:A:858:ASN:C	1:A:858:ASN:ND2	2.73	0.47
1:A:1151:GLU:HG2	7:I:45:ARG:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:132:VAL:CG1	2:B:133:LYS:N	2.78	0.47
2:B:864:LYS:HG3	2:B:865:LYS:N	2.28	0.47
2:B:914:LYS:N	2:B:938:SER:HB2	2.27	0.47
3:C:63:ILE:HG23	3:C:63:ILE:HD12	1.42	0.47
1:A:664:THR:HG22	1:A:742:ASN:HB3	1.96	0.46
1:A:752:LYS:CE	2:B:1019:SER:OG	2.63	0.46
2:B:737:THR:O	2:B:738:PHE:C	2.55	0.46
5:F:105:ALA:HB1	5:F:106:PRO:HD2	1.97	0.46
6:H:106:GLU:HB2	6:H:113:ALA:HB3	1.96	0.46
10:L:44:ASP:O	10:L:45:ALA:CB	2.63	0.46
2:B:646:LEU:CD1	2:B:646:LEU:CD2	2.90	0.46
2:B:1073:TYR:CE2	2:B:1080:LYS:HG3	2.50	0.46
2:B:1084:GLN:C	2:B:1085:ILE:HD12	2.41	0.46
1:A:62:ASP:C	1:A:64:ASN:H	2.24	0.46
1:A:550:LEU:HD13	1:A:556:TRP:CZ2	2.50	0.46
1:A:896:ARG:HD3	1:A:897:TYR:CE1	2.51	0.46
2:B:431:TYR:CE1	2:B:447:ALA:CB	2.97	0.46
2:B:1002:THR:O	2:B:1003:ALA:C	2.55	0.46
3:C:5:GLY:C	3:C:24:ASN:HD22	2.23	0.46
2:B:167:ILE:CG2	2:B:424:LEU:CD1	2.93	0.46
2:B:451:LYS:O	2:B:452:THR:C	2.59	0.46
3:C:163:ILE:HG21	3:C:163:ILE:HD13	1.96	0.46
3:C:262:LEU:HD23	3:C:262:LEU:HA	1.70	0.46
6:H:76:THR:O	6:H:76:THR:CG2	2.63	0.46
7:I:75:CYS:SG	7:I:106:CYS:SG	3.14	0.46
1:A:54:ASN:C	1:A:56:PRO:HD2	2.41	0.46
1:A:903:ASN:HD21	1:A:905:ASP:HB2	1.80	0.46
1:A:938:LYS:CG	1:A:938:LYS:HE2	2.45	0.46
2:B:26:THR:O	2:B:27:ALA:C	2.57	0.46
1:A:46:THR:CB	1:A:46:THR:O	2.63	0.46
1:A:1449:SER:HB2	5:F:149:GLU:OE2	2.15	0.46
3:C:124:LEU:O	3:C:127:ARG:HG3	2.15	0.46
4:E:129:PRO:CD	4:E:130:ALA:H	2.28	0.46
1:A:217:LYS:O	1:A:221:SER:HB2	2.15	0.46
1:A:565:ILE:HG22	1:A:569:LYS:O	2.16	0.46
1:A:1236:LEU:CD2	1:A:1236:LEU:CD1	2.80	0.46
2:B:1161:HIS:HA	2:B:1192:TYR:O	2.16	0.46
1:A:444:PHE:CE2	1:A:470:LEU:HD21	2.51	0.46
1:A:664:THR:HG21	1:A:746:MET:CE	2.46	0.46
1:A:982:THR:HG22	1:A:984:LYS:N	2.31	0.46
1:A:1151:GLU:HG2	7:I:45:ARG:CD	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:118:ARG:NH2	2:B:194:GLU:CD	2.71	0.46
2:B:254:LEU:HD23	2:B:381:MET:HE1	1.97	0.46
4:E:80:VAL:HG12	4:E:81:GLU:N	2.31	0.46
4:E:118:PRO:HA	4:E:121:MET:SD	2.56	0.46
1:A:64:ASN:O	1:A:66:LYS:N	2.49	0.46
1:A:830:LYS:CD	1:A:830:LYS:CB	2.82	0.46
1:A:837:ILE:O	1:A:838:GLN:C	2.57	0.46
6:H:32:THR:CG2	6:H:33:GLN:CD	2.89	0.46
8:J:1:MET:HE3	8:J:1:MET:CA	2.45	0.46
1:A:920:LEU:HD22	1:A:921:GLY:N	2.30	0.46
3:C:152:GLU:OE2	3:C:154:LYS:CD	2.64	0.46
6:H:93:TYR:N	6:H:93:TYR:HD1	2.12	0.46
1:A:512:VAL:HG11	1:A:635:ARG:HH21	1.81	0.45
1:A:1146:VAL:O	1:A:1146:VAL:HG13	2.17	0.45
2:B:662:MET:CE	2:B:662:MET:CG	2.90	0.45
3:C:29:MET:HB2	3:C:29:MET:HE2	1.97	0.45
6:H:135:LEU:HD13	6:H:139:ASN:O	2.16	0.45
9:K:27:ALA:HB1	9:K:28:PRO:CD	2.46	0.45
1:A:588:LEU:HD23	1:A:589:GLN:N	2.31	0.45
1:A:596:THR:CG2	1:A:597:LEU:N	2.78	0.45
2:B:1153:GLU:HB3	2:B:1155:SER:HB3	1.98	0.45
3:C:56:THR:CG2	3:C:57:VAL:N	2.75	0.45
4:E:36:GLU:O	4:E:38:PRO:HD3	2.16	0.45
6:H:32:THR:CG2	6:H:33:GLN:OE1	2.64	0.45
10:L:28:LYS:O	10:L:59:ALA:HB3	2.15	0.45
1:A:106:VAL:HG21	1:A:214:ILE:HG12	1.99	0.45
1:A:1436:ILE:O	1:A:1437:GLY:C	2.57	0.45
2:B:1182:CYS:HB3	2:B:1185:CYS:HB2	1.97	0.45
1:A:63:ARG:HA	1:A:74:MET:CG	2.45	0.45
1:A:973:ILE:HA	1:A:973:ILE:HD13	1.64	0.45
1:A:1204:ASP:OD1	1:A:1205:LYS:HE2	2.17	0.45
1:A:1224:LEU:HD23	1:A:1226:VAL:CG2	2.47	0.45
3:C:18:VAL:CG2	3:C:240:VAL:CG1	2.91	0.45
4:E:16:PHE:CZ	4:E:20:LYS:HE2	2.51	0.45
9:K:18:LYS:HE2	9:K:38:GLU:OE2	2.15	0.45
1:A:1222:ASN:CB	1:A:1222:ASN:ND2	2.69	0.45
2:B:121:ASN:HD21	2:B:965:LYS:CE	2.30	0.45
2:B:130:VAL:HG23	2:B:167:ILE:HD11	1.99	0.45
1:A:274:ILE:CA	1:A:274:ILE:CD1	2.95	0.45
1:A:351:THR:HG23	2:B:1103:ILE:HG12	1.94	0.45
1:A:884:ASP:O	1:A:885:THR:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1138:ILE:HG21	1:A:1138:ILE:HD13	1.54	0.45
1:A:1263:ILE:CD1	1:A:1263:ILE:HA	2.46	0.45
4:E:37:LEU:C	4:E:38:PRO:O	2.58	0.45
4:E:96:PHE:CZ	4:E:100:ILE:CD1	2.98	0.45
9:K:33:ILE:CD1	9:K:87:LEU:HD22	2.47	0.45
9:K:49:GLU:HG3	9:K:94:ILE:HD11	1.99	0.45
1:A:868:TYR:CE1	1:A:1064:VAL:HG13	2.51	0.45
2:B:95:ILE:CG2	2:B:96:TYR:N	2.80	0.45
4:E:169:ARG:HD3	5:F:140:ASP:OD2	2.17	0.45
1:A:1263:ILE:O	1:A:1267:MET:HG3	2.17	0.45
3:C:102:GLN:CG	3:C:102:GLN:CA	2.84	0.45
5:F:119:ARG:HA	5:F:122:MET:HE2	1.99	0.45
7:I:40:SER:CB	7:I:41:PRO:CD	2.95	0.45
9:K:55:LYS:CB	9:K:81:TYR:CD1	2.99	0.45
1:A:1340:GLY:HA2	4:E:183:PRO:HD2	1.98	0.45
2:B:387:LEU:HA	2:B:387:LEU:HD12	1.68	0.45
2:B:428:ILE:CD1	2:B:448:ILE:HD11	2.47	0.45
2:B:898:LEU:HB2	10:L:58:LYS:HE2	1.98	0.45
4:E:90:VAL:CG1	4:E:90:VAL:CG2	2.81	0.45
6:H:134:ASN:O	6:H:135:LEU:C	2.60	0.45
1:A:633:VAL:O	1:A:634:THR:C	2.58	0.45
1:A:924:LYS:HB2	1:A:924:LYS:HE2	1.81	0.45
1:A:1164:PRO:O	1:A:1167:GLU:CG	2.65	0.45
2:B:197:PHE:O	2:B:198:ASP:C	2.57	0.45
2:B:393:LYS:HZ1	2:B:621:GLU:CD	2.20	0.45
2:B:1097:HIS:CA	2:B:1098:MET:N	2.67	0.45
2:B:1180:PHE:HB3	2:B:1191:ILE:HD13	1.99	0.45
3:C:166:GLU:HB2	9:K:10:PHE:CE2	2.52	0.45
1:A:605:MET:HE2	1:A:607:ILE:CD1	2.45	0.44
1:A:786:HIS:HE1	2:B:742:GLU:OE2	2.00	0.44
1:A:1232:ASN:CB	1:A:1232:ASN:ND2	2.73	0.44
2:B:1212:ILE:O	2:B:1214:PRO:HD3	2.16	0.44
3:C:56:THR:HG23	3:C:57:VAL:N	2.30	0.44
9:K:88:LYS:O	9:K:89:ASN:C	2.59	0.44
1:A:134:ARG:HD2	1:A:221:SER:O	2.17	0.44
1:A:884:ASP:O	1:A:886:ILE:N	2.50	0.44
2:B:294:ASP:N	7:I:12:ASN:ND2	2.57	0.44
4:E:93:MET:CE	4:E:116:ILE:HG21	2.47	0.44
1:A:203:SER:O	1:A:204:THR:C	2.59	0.44
1:A:853:ASP:O	1:A:854:ASN:HB2	2.15	0.44
2:B:102:VAL:O	2:B:109:THR:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:515:HIS:CD2	2:B:517:THR:OG1	2.67	0.44
2:B:882:THR:HG1	2:B:933:SER:N	2.15	0.44
4:E:41:ASP:O	4:E:42:PHE:C	2.59	0.44
6:H:102:TYR:O	6:H:104:PHE:N	2.49	0.44
1:A:540:PHE:C	1:A:541:ILE:HD12	2.41	0.44
1:A:673:GLY:N	1:A:674:PRO:CD	2.80	0.44
2:B:429:PHE:CD2	2:B:429:PHE:O	2.69	0.44
2:B:526:GLU:HG2	2:B:538:ASN:ND2	2.33	0.44
3:C:43:THR:O	3:C:161:LYS:HA	2.17	0.44
4:E:187:TYR:C	4:E:187:TYR:CD2	2.95	0.44
1:A:90:VAL:HG22	1:A:297:GLN:HB2	2.00	0.44
4:E:74:ASP:OD1	4:E:74:ASP:N	2.49	0.44
1:A:148:CYS:SG	1:A:167:CYS:SG	3.16	0.44
1:A:407:ARG:O	1:A:408:ASP:C	2.61	0.44
1:A:896:ARG:HD3	1:A:897:TYR:CZ	2.52	0.44
1:A:903:ASN:HD22	1:A:905:ASP:N	2.15	0.44
1:A:1023:ARG:HH21	1:A:1023:ARG:HD3	1.62	0.44
3:C:260:LEU:CD2	3:C:260:LEU:HG	2.23	0.44
4:E:93:MET:HE3	4:E:116:ILE:HG21	2.00	0.44
4:E:129:PRO:HD2	4:E:130:ALA:H	1.82	0.44
5:F:83:PRO:HA	5:F:146:TRP:CZ3	2.53	0.44
1:A:243:PRO:CB	1:A:245:PRO:HD2	2.42	0.44
1:A:274:ILE:CD1	1:A:274:ILE:HA	2.48	0.44
1:A:304:MET:HE3	1:A:304:MET:HB2	1.98	0.44
1:A:1225:PHE:C	1:A:1226:VAL:HG23	2.43	0.44
2:B:1182:CYS:HG	12:B:3007:ZN:ZN	1.17	0.44
4:E:129:PRO:CD	4:E:130:ALA:N	2.81	0.44
6:H:113:ALA:HA	6:H:125:LEU:O	2.18	0.44
6:H:138:GLU:CG	6:H:139:ASN:H	2.31	0.44
1:A:909:ASP:CG	1:A:910:PRO:HD2	2.43	0.44
1:A:1263:ILE:CD1	1:A:1263:ILE:HG23	2.47	0.44
2:B:215:GLN:HE22	2:B:499:ASN:HD22	1.65	0.44
2:B:282:ILE:HD11	2:B:317:CYS:SG	2.58	0.44
2:B:420:LEU:HB3	2:B:453:ILE:HD13	1.99	0.44
2:B:724:ASP:O	2:B:726:ALA:N	2.51	0.44
4:E:50:MET:HE2	4:E:52:ARG:HH21	1.83	0.44
1:A:567:LYS:HG2	6:H:96:VAL:O	2.18	0.44
1:A:913:LEU:HD12	1:A:913:LEU:HA	1.62	0.44
3:C:86:CYS:SG	3:C:92:CYS:SG	3.16	0.44
4:E:117:THR:OG1	4:E:120:ALA:HB3	2.16	0.44
8:J:1:MET:O	8:J:2:ILE:HD12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:GLN:HE21	5:F:90:ARG:HH21	1.65	0.43
1:A:545:GLN:O	1:A:546:VAL:C	2.53	0.43
1:A:605:MET:CE	1:A:607:ILE:HD11	2.43	0.43
2:B:68:THR:CG2	2:B:91:SER:HB3	2.48	0.43
2:B:307:ASP:C	2:B:309:GLN:N	2.73	0.43
2:B:986:GLN:CD	2:B:986:GLN:HA	2.43	0.43
2:B:1065:GLN:NE2	2:B:1067:ARG:N	2.63	0.43
3:C:52:GLU:HA	10:L:64:LEU:HD21	2.00	0.43
7:I:104:LEU:HD23	7:I:104:LEU:HA	1.80	0.43
1:A:59:GLY:C	1:A:60:SER:HG	2.26	0.43
1:A:846:GLU:HA	1:A:1066:VAL:CG2	2.48	0.43
1:A:916:GLY:O	1:A:919:ILE:HD12	2.18	0.43
1:A:1411:GLU:O	1:A:1412:ALA:C	2.59	0.43
2:B:121:ASN:ND2	2:B:965:LYS:NZ	2.65	0.43
2:B:1153:GLU:OE1	2:B:1153:GLU:HA	2.18	0.43
5:F:143:PHE:CD1	5:F:143:PHE:C	2.96	0.43
1:A:140:THR:HA	1:A:143:LYS:HD3	2.01	0.43
2:B:569:TYR:CE2	2:B:571:PRO:HG3	2.54	0.43
2:B:826:ALA:HB3	2:B:1011:ILE:HD12	2.01	0.43
3:C:260:LEU:CD2	3:C:260:LEU:CD1	2.89	0.43
4:E:117:THR:OG1	4:E:120:ALA:HB2	2.17	0.43
6:H:91:ASP:C	6:H:91:ASP:HA	2.16	0.43
7:I:41:PRO:CD	7:I:42:LEU:H	2.30	0.43
7:I:65:ASP:HA	7:I:66:PRO:HD2	1.81	0.43
1:A:88:LYS:HB3	1:A:89:PRO:HD2	2.01	0.43
1:A:557:ASP:O	1:A:559:VAL:N	2.51	0.43
1:A:793:SER:O	1:A:794:PRO:C	2.59	0.43
1:A:938:LYS:CE	1:A:938:LYS:HG3	2.46	0.43
1:A:1280:GLU:CG	1:A:1280:GLU:OE1	2.53	0.43
3:C:29:MET:CE	3:C:29:MET:CB	2.97	0.43
1:A:101:LYS:O	1:A:102:VAL:C	2.59	0.43
1:A:551:TYR:CD2	9:K:62:LYS:HD3	2.53	0.43
1:A:1293:SER:CB	1:A:1294:PRO:HD2	2.49	0.43
6:H:95:TYR:HB3	6:H:144:ILE:HB	2.00	0.43
8:J:32:GLU:CD	8:J:32:GLU:H	2.26	0.43
9:K:40:HIS:O	9:K:41:THR:C	2.59	0.43
1:A:809:THR:HB	1:A:810:PRO:CD	2.48	0.43
5:F:111:LEU:C	5:F:113:GLY:H	2.16	0.43
6:H:52:GLN:CG	6:H:52:GLN:NE2	2.64	0.43
6:H:55:LEU:HD22	6:H:144:ILE:HG23	2.00	0.43
9:K:82:ASP:HA	9:K:83:PRO:HD2	1.75	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:ILE:HD12	1:A:142:CYS:SG	2.58	0.43
1:A:446:ARG:HB2	1:A:487:MET:HE2	1.99	0.43
1:A:497:THR:HG21	2:B:1149:GLU:OE1	2.19	0.43
1:A:598:LEU:O	1:A:599:SER:C	2.62	0.43
1:A:711:ARG:NE	7:I:95:THR:HG22	2.25	0.43
1:A:973:ILE:CG2	1:A:973:ILE:CA	2.84	0.43
2:B:418:LYS:CD	2:B:418:LYS:NZ	2.66	0.43
3:C:55:THR:O	3:C:151:GLN:HG2	2.19	0.43
3:C:102:GLN:CG	3:C:102:GLN:N	2.81	0.43
5:F:81:THR:HB	5:F:144:GLU:OE1	2.19	0.43
6:H:63:LEU:H	6:H:63:LEU:HD12	1.81	0.43
6:H:138:GLU:C	6:H:140:ALA:N	2.71	0.43
7:I:45:ARG:CD	7:I:45:ARG:CB	2.86	0.43
9:K:65:HIS:CD2	9:K:67:PHE:H	2.28	0.43
10:L:44:ASP:O	10:L:45:ALA:HB3	2.18	0.43
2:B:324:ILE:N	2:B:324:ILE:HD12	2.34	0.43
2:B:1189:ILE:HG22	2:B:1190:ASP:N	2.33	0.43
4:E:30:ILE:HD12	4:E:30:ILE:HG23	1.64	0.43
1:A:110:CYS:SG	1:A:167:CYS:HB3	2.59	0.43
1:A:566:ILE:CG2	1:A:566:ILE:C	2.91	0.43
1:A:1203:ASN:O	1:A:1204:ASP:C	2.62	0.43
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.54	0.43
2:B:296:GLU:O	2:B:300:HIS:CD2	2.72	0.43
2:B:365:THR:HG21	2:B:370:PHE:CG	2.54	0.43
2:B:642:ASP:HA	2:B:643:ASP:HA	1.12	0.43
2:B:773:MET:C	2:B:775:LYS:N	2.76	0.43
5:F:120:ILE:HG23	5:F:120:ILE:HD12	1.71	0.43
8:J:7:CYS:SG	8:J:46:CYS:N	2.92	0.43
1:A:53:LEU:HD23	1:A:54:ASN:N	2.34	0.43
1:A:567:LYS:CD	6:H:95:TYR:CD2	3.00	0.43
2:B:292:ILE:HD12	2:B:292:ILE:N	2.33	0.43
2:B:323:VAL:C	2:B:324:ILE:HD12	2.44	0.43
3:C:216:GLY:O	3:C:217:ASP:C	2.62	0.43
6:H:47:PHE:CG	6:H:95:TYR:CD1	3.07	0.43
8:J:6:ARG:HD2	8:J:6:ARG:HH11	1.62	0.43
1:A:74:MET:H	1:A:74:MET:HG3	1.83	0.42
1:A:359:LEU:HA	1:A:359:LEU:HD23	1.69	0.42
1:A:369:SER:CA	9:K:2:ASN:HD21	2.32	0.42
1:A:768:GLN:HE21	1:A:816:HIS:HA	1.84	0.42
1:A:1074:GLU:O	1:A:1077:THR:HB	2.18	0.42
2:B:293:PRO:HA	7:I:12:ASN:ND2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:712:PRO:HA	2:B:733:HIS:NE2	2.34	0.42
3:C:69:LEU:O	8:J:6:ARG:NH2	2.49	0.42
8:J:20:SER:O	8:J:24:LEU:HG	2.18	0.42
1:A:164:ARG:C	1:A:166:GLY:N	2.76	0.42
1:A:587:HIS:CD2	1:A:966:ASN:OD1	2.62	0.42
2:B:259:TYR:OH	2:B:279:ASP:OD2	2.35	0.42
2:B:297:ILE:HD12	2:B:297:ILE:HG23	1.83	0.42
4:E:5:ASN:O	4:E:9:ILE:HG13	2.18	0.42
4:E:37:LEU:HA	4:E:38:PRO:HD2	1.80	0.42
1:A:35:ILE:N	1:A:35:ILE:CD1	2.79	0.42
1:A:203:SER:OG	1:A:206:GLU:HG2	2.18	0.42
1:A:216:VAL:HA	1:A:219:PHE:CZ	2.53	0.42
1:A:875:ALA:HB2	1:A:1366:ARG:HD3	2.00	0.42
1:A:1287:TYR:O	1:A:1302:PRO:HA	2.19	0.42
1:A:1446:ASP:OD1	1:A:1448:GLU:HG3	2.19	0.42
2:B:1162:ILE:HA	2:B:1162:ILE:HD13	1.77	0.42
2:B:1166:CYS:SG	2:B:1182:CYS:SG	3.17	0.42
3:C:73:GLN:HA	3:C:133:ILE:HD11	2.01	0.42
3:C:239:PRO:O	3:C:240:VAL:C	2.60	0.42
1:A:391:LEU:HD23	1:A:391:LEU:HA	1.71	0.42
1:A:412:ARG:C	1:A:413:ILE:HD13	2.44	0.42
1:A:446:ARG:HG2	1:A:478:TYR:O	2.19	0.42
1:A:807:GLY:CA	2:B:761:HIS:CE1	3.01	0.42
1:A:1203:ASN:C	1:A:1205:LYS:N	2.78	0.42
1:A:1263:ILE:HG23	1:A:1263:ILE:HD12	2.01	0.42
1:A:1438:THR:HB	2:B:1142:GLY:O	2.18	0.42
2:B:104:GLU:HB2	2:B:108:VAL:HA	2.02	0.42
2:B:118:ARG:NH2	2:B:194:GLU:CG	2.82	0.42
2:B:658:ILE:O	2:B:658:ILE:CG2	2.66	0.42
2:B:1010:LEU:HA	2:B:1010:LEU:HD12	1.52	0.42
1:A:61:ILE:CA	1:A:61:ILE:CG2	2.91	0.42
1:A:507:VAL:HB	1:A:508:PRO:HD3	2.02	0.42
1:A:1004:ASN:OD1	4:E:167:ARG:HG3	2.18	0.42
1:A:1264:GLU:OE2	7:I:46:HIS:HD2	2.02	0.42
2:B:648:HIS:HB2	2:B:649:LYS:H	1.64	0.42
3:C:15:LYS:O	3:C:240:VAL:HG23	2.19	0.42
3:C:80:LEU:HD12	3:C:80:LEU:HA	1.49	0.42
6:H:105:GLU:O	6:H:107:VAL:N	2.52	0.42
1:A:219:PHE:CD1	1:A:219:PHE:C	2.97	0.42
1:A:1438:THR:HG22	2:B:1144:ALA:HB3	2.02	0.42
2:B:65:GLU:HG2	2:B:66:ASP:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:705:MET:HB3	2:B:706:GLN:HE21	1.84	0.42
3:C:100:THR:HG22	3:C:101:LEU:N	2.34	0.42
1:A:1259:MET:O	1:A:1260:LEU:C	2.60	0.42
2:B:555:ILE:HG23	2:B:555:ILE:HD12	1.84	0.42
2:B:706:GLN:CG	2:B:706:GLN:OE1	2.50	0.42
2:B:770:GLN:HE22	2:B:1093:GLN:HE22	1.68	0.42
2:B:830:TYR:O	2:B:831:SER:OG	2.33	0.42
2:B:969:ARG:HH11	2:B:969:ARG:HD3	1.44	0.42
2:B:1022:THR:HG23	2:B:1022:THR:O	2.20	0.42
3:C:148:ARG:NH1	8:J:64:ASN:HA	2.34	0.42
4:E:2:ASP:O	4:E:3:GLN:C	2.63	0.42
4:E:37:LEU:HD23	4:E:42:PHE:HB2	2.01	0.42
6:H:18:GLY:O	6:H:19:ARG:HB2	2.20	0.42
10:L:38:LEU:HG	10:L:39:SER:N	2.35	0.42
1:A:908:LEU:HA	1:A:908:LEU:HD23	1.73	0.42
1:A:1006:ILE:HG23	1:A:1006:ILE:HD12	1.53	0.42
1:A:1120:LEU:HD21	1:A:1131:ALA:HB2	2.02	0.42
1:A:1267:MET:HB3	1:A:1267:MET:HE3	1.34	0.42
2:B:961:LEU:CD1	2:B:961:LEU:HG	2.21	0.42
2:B:1182:CYS:CB	2:B:1185:CYS:HB2	2.49	0.42
3:C:242:GLN:NE2	3:C:246:ARG:HE	2.18	0.42
4:E:179:GLN:H	4:E:179:GLN:HG2	1.44	0.42
10:L:31:CYS:SG	10:L:51:CYS:SG	3.10	0.42
1:A:567:LYS:HB2	1:A:568:PRO:CD	2.40	0.42
1:A:606:LEU:HD23	1:A:613:ILE:HG21	2.01	0.42
1:A:1239:ARG:CD	1:A:1239:ARG:CB	2.78	0.42
2:B:65:GLU:O	2:B:67:SER:N	2.53	0.42
2:B:269:ILE:HB	2:B:282:ILE:CD1	2.49	0.42
2:B:408:LEU:O	2:B:409:ALA:C	2.63	0.42
2:B:806:THR:HG23	2:B:808:ALA:N	2.33	0.42
2:B:1163:CYS:HB3	2:B:1166:CYS:SG	2.60	0.42
3:C:55:THR:O	3:C:55:THR:HG22	2.19	0.42
3:C:148:ARG:O	3:C:149:LYS:C	2.63	0.42
4:E:28:TYR:CE1	4:E:75:MET:CE	3.03	0.42
4:E:161:LYS:NZ	4:E:172:GLU:OE2	2.49	0.42
6:H:103:LYS:CE	6:H:135:LEU:O	2.67	0.42
1:A:533:LYS:HZ3	1:A:745:GLN:HE22	1.66	0.42
1:A:1003:LYS:CG	1:A:1003:LYS:CE	2.94	0.42
2:B:915:THR:CA	2:B:915:THR:CG2	2.84	0.42
6:H:50:ALA:HB3	6:H:53:ASP:OD2	2.20	0.42
1:A:49:LYS:CE	1:A:49:LYS:CG	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:LEU:O	1:A:164:ARG:NH2	2.51	0.41
1:A:571:LEU:HA	1:A:571:LEU:HD12	1.76	0.41
1:A:1134:ILE:HG22	1:A:1306:LEU:HD11	2.02	0.41
2:B:189:LEU:HD23	2:B:189:LEU:HA	1.88	0.41
2:B:384:ARG:NH2	2:B:396:ASP:OD2	2.53	0.41
2:B:953:LEU:HD23	2:B:953:LEU:C	2.45	0.41
9:K:10:PHE:HD1	9:K:11:LEU:HD13	1.84	0.41
10:L:64:LEU:HD23	10:L:64:LEU:HA	1.87	0.41
1:A:71:GLN:O	1:A:72:GLU:O	2.37	0.41
1:A:587:HIS:HE2	1:A:969:GLN:HG2	1.81	0.41
1:A:913:LEU:HD12	1:A:914:GLU:N	2.34	0.41
1:A:1263:ILE:HA	1:A:1263:ILE:HD13	2.01	0.41
2:B:235:SER:OG	2:B:236:HIS:HD2	2.03	0.41
2:B:744:HIS:CD2	2:B:745:PRO:HD2	2.55	0.41
2:B:896:ASP:OD2	10:L:29:TYR:OH	2.24	0.41
3:C:46:ILE:HD12	3:C:72:LEU:HD11	2.02	0.41
1:A:560:ILE:O	1:A:561:PRO:C	2.59	0.41
2:B:113:TYR:CD2	2:B:192:LEU:CD2	3.03	0.41
2:B:758:PHE:N	2:B:759:PRO:CD	2.82	0.41
2:B:955:THR:HG21	10:L:55:ILE:HD13	2.02	0.41
2:B:1221:SER:OG	5:F:72:LYS:HD2	2.20	0.41
3:C:145:CYS:SG	3:C:146:LYS:N	2.94	0.41
7:I:15:TYR:CD1	7:I:30:ARG:HG3	2.55	0.41
1:A:84:ILE:CG2	1:A:241:VAL:CG2	2.98	0.41
1:A:187:LYS:HD2	1:A:194:ALA:HB2	2.02	0.41
1:A:476:SER:N	1:A:477:PRO:CD	2.83	0.41
1:A:487:MET:HE3	1:A:487:MET:HG3	1.96	0.41
1:A:557:ASP:OD1	1:A:557:ASP:C	2.62	0.41
2:B:121:ASN:N	2:B:121:ASN:HD22	2.17	0.41
2:B:778:MET:HE2	2:B:794:ASN:OD1	2.20	0.41
2:B:788:ARG:HD3	2:B:788:ARG:HH11	1.65	0.41
10:L:34:CYS:SG	10:L:51:CYS:HB3	2.60	0.41
2:B:393:LYS:NZ	2:B:621:GLU:CD	2.77	0.41
2:B:1194:ILE:O	2:B:1194:ILE:HG13	2.20	0.41
4:E:112:TYR:CD1	4:E:112:TYR:C	2.96	0.41
6:H:32:THR:HB	6:H:33:GLN:OE1	2.20	0.41
7:I:40:SER:HB2	7:I:41:PRO:CD	2.50	0.41
7:I:111:THR:HG21	7:I:113:ASP:HB2	2.02	0.41
10:L:48:CYS:SG	10:L:51:CYS:SG	3.13	0.41
1:A:176:LYS:NZ	1:A:178:GLY:O	2.32	0.41
1:A:867:ILE:HD13	1:A:867:ILE:HG21	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:914:GLU:C	1:A:916:GLY:H	2.28	0.41
1:A:1150:SER:OG	7:I:46:HIS:HB3	2.20	0.41
1:A:1435:PRO:HA	1:A:1439:GLY:O	2.21	0.41
2:B:25:ILE:HD13	2:B:25:ILE:N	2.35	0.41
2:B:1050:ILE:H	2:B:1050:ILE:HD12	1.86	0.41
3:C:265:MET:CE	3:C:265:MET:CG	2.96	0.41
4:E:78:LEU:HG	4:E:79:TRP:N	2.34	0.41
7:I:98:VAL:HG21	7:I:113:ASP:HB2	2.02	0.41
1:A:523:ILE:CB	1:A:622:VAL:HG13	2.47	0.41
1:A:868:TYR:CE1	1:A:1064:VAL:CG1	3.03	0.41
1:A:1204:ASP:O	1:A:1204:ASP:CG	2.64	0.41
2:B:99:LYS:NZ	2:B:183:GLU:OE1	2.53	0.41
3:C:193:TYR:CD1	3:C:193:TYR:C	2.98	0.41
3:C:266:ASP:OD1	3:C:266:ASP:N	2.52	0.41
6:H:59:ILE:CG2	6:H:60:ALA:N	2.82	0.41
9:K:59:ALA:HA	9:K:74:ARG:O	2.20	0.41
1:A:366:VAL:O	1:A:367:PRO:C	2.57	0.41
1:A:1364:ASN:HD22	1:A:1366:ARG:N	2.04	0.41
2:B:1064:TYR:O	2:B:1065:GLN:C	2.57	0.41
4:E:52:ARG:CG	4:E:53:PRO:HD3	2.51	0.41
6:H:136:LYS:CA	6:H:137:GLN:N	2.66	0.41
10:L:34:CYS:HB3	10:L:51:CYS:SG	2.61	0.41
1:A:19:PHE:HB2	1:A:1417:GLU:O	2.21	0.41
1:A:325:ILE:O	1:A:325:ILE:HG22	2.21	0.41
1:A:516:SER:O	1:A:517:ASN:C	2.61	0.41
1:A:595:THR:HG22	1:A:596:THR:N	2.35	0.41
1:A:676:MET:SD	1:A:676:MET:CB	3.01	0.41
1:A:689:LYS:O	1:A:693:VAL:HG23	2.20	0.41
1:A:722:LEU:HD23	1:A:722:LEU:HA	1.93	0.41
1:A:899:VAL:CG1	1:A:929:LEU:HD13	2.51	0.41
1:A:962:ARG:O	1:A:963:ILE:C	2.56	0.41
1:A:964:ILE:HD13	1:A:964:ILE:HA	1.66	0.41
1:A:1035:TYR:O	1:A:1036:ARG:HB2	2.21	0.41
1:A:1094:VAL:O	1:A:1095:THR:C	2.62	0.41
1:A:1127:ASP:OD2	1:A:1130:GLN:HB2	2.20	0.41
1:A:1356:ILE:HD13	1:A:1356:ILE:HG21	1.74	0.41
2:B:749:LEU:HD23	2:B:749:LEU:HA	1.82	0.41
2:B:904:ARG:C	2:B:905:VAL:HG13	2.46	0.41
2:B:1165:ILE:CD1	2:B:1165:ILE:CB	2.84	0.41
3:C:43:THR:HG23	3:C:44:LEU:H	1.85	0.41
3:C:112:ASN:ND2	3:C:146:LYS:HG2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:109:VAL:HG13	5:F:110:ASP:N	2.31	0.41
6:H:130:ARG:HB2	6:H:133:ASN:HD22	1.85	0.41
7:I:14:LEU:HB3	7:I:27:PHE:HB3	2.03	0.41
8:J:49:MET:HE2	8:J:49:MET:HB2	1.65	0.41
1:A:55:ASP:H	1:A:56:PRO:HD3	1.85	0.41
1:A:325:ILE:HG21	1:A:325:ILE:HD13	1.60	0.41
1:A:1098:VAL:N	1:A:1099:PRO:CD	2.84	0.41
1:A:1264:GLU:O	1:A:1264:GLU:HG2	2.19	0.41
2:B:564:GLU:OE2	2:B:591:ARG:HD2	2.21	0.41
2:B:885:MET:CE	2:B:885:MET:HB3	2.50	0.41
2:B:952:VAL:HG22	2:B:966:VAL:HG22	2.03	0.41
2:B:1077:THR:HG22	2:B:1079:LYS:N	2.24	0.41
3:C:33:LEU:HG	3:C:37:MET:HE2	2.03	0.41
3:C:55:THR:HB	3:C:152:GLU:H	1.86	0.41
3:C:240:VAL:HG23	3:C:240:VAL:H	1.48	0.41
6:H:47:PHE:CD2	6:H:47:PHE:O	2.74	0.41
6:H:95:TYR:C	6:H:96:VAL:HG23	2.44	0.41
1:A:265:LYS:CE	1:A:302:THR:CG2	2.99	0.40
1:A:457:ALA:HB3	1:A:506:ALA:HA	2.02	0.40
2:B:28:GLU:CD	2:B:807:ARG:HH22	2.29	0.40
2:B:100:PRO:CD	2:B:180:TYR:CZ	2.94	0.40
2:B:259:TYR:HB2	2:B:268:THR:HG22	2.03	0.40
2:B:435:THR:O	2:B:435:THR:CG2	2.69	0.40
3:C:11:ARG:O	3:C:12:GLU:HG3	2.21	0.40
3:C:32:SER:O	3:C:36:VAL:HG23	2.21	0.40
3:C:208:GLU:C	3:C:210:GLU:H	2.28	0.40
4:E:120:ALA:C	4:E:122:LYS:N	2.79	0.40
4:E:168:TYR:O	4:E:169:ARG:HB2	2.21	0.40
5:F:128:LYS:HA	5:F:128:LYS:HD3	1.83	0.40
6:H:48:PRO:C	6:H:49:VAL:HG23	2.46	0.40
6:H:105:GLU:O	6:H:106:GLU:C	2.64	0.40
1:A:42:ASP:OD2	1:A:47:ARG:HG2	2.21	0.40
1:A:92:HIS:HD2	1:A:94:GLY:N	2.19	0.40
1:A:541:ILE:HG22	1:A:546:VAL:HG23	2.03	0.40
1:A:672:ASP:HB3	1:A:674:PRO:HD2	2.03	0.40
1:A:871:ASP:CB	4:E:204:THR:HG23	2.42	0.40
1:A:1111:MET:HE3	1:A:1111:MET:HB2	2.03	0.40
1:A:1319:VAL:HA	1:A:1320:PRO:HD3	1.88	0.40
2:B:324:ILE:HG13	2:B:329:THR:HG22	2.03	0.40
9:K:100:ALA:O	9:K:103:THR:HB	2.20	0.40
1:A:601:LYS:NZ	1:A:601:LYS:CD	2.81	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:121:ASN:HD22	2:B:121:ASN:H	1.68	0.40
2:B:384:ARG:O	2:B:385:LEU:C	2.62	0.40
2:B:423:LYS:O	2:B:426:LYS:N	2.53	0.40
3:C:33:LEU:O	3:C:37:MET:HG3	2.21	0.40
3:C:66:ARG:O	3:C:67:LEU:C	2.63	0.40
3:C:77:ILE:HD12	3:C:77:ILE:HA	1.82	0.40
5:F:93:ILE:HD13	5:F:93:ILE:HG21	1.78	0.40
1:A:241:VAL:HA	1:A:242:PRO:HD2	1.90	0.40
1:A:543:LEU:O	1:A:547:LEU:HG	2.20	0.40
1:A:696:GLU:O	1:A:697:ALA:C	2.63	0.40
1:A:699:ALA:HA	7:I:112:SER:O	2.21	0.40
1:A:731:ARG:O	1:A:732:LEU:C	2.60	0.40
1:A:971:PHE:O	1:A:972:HIS:C	2.63	0.40
1:A:993:LEU:HD22	1:A:1046:LEU:HD22	2.04	0.40
1:A:1284:MET:HE2	1:A:1284:MET:HB2	1.77	0.40
2:B:25:ILE:HD13	2:B:25:ILE:H	1.85	0.40
2:B:35:SER:HA	2:B:811:TYR:CE2	2.56	0.40
2:B:639:ILE:HG23	2:B:639:ILE:HD12	1.70	0.40
3:C:167:HIS:CD2	3:C:169:LYS:HG2	2.57	0.40
7:I:16:PRO:HG3	7:I:27:PHE:HE2	1.86	0.40
1:A:145:LYS:HE2	1:A:149:GLU:CD	2.46	0.40
1:A:1151:GLU:HA	7:I:44:TYR:O	2.21	0.40
2:B:296:GLU:O	2:B:300:HIS:HD2	2.05	0.40
2:B:1197:PRO:O	2:B:1200:ALA:HB3	2.22	0.40
3:C:9:LYS:CD	3:C:9:LYS:CB	2.83	0.40
3:C:84:ARG:HD2	9:K:11:LEU:HD21	2.03	0.40
3:C:99:LEU:N	3:C:99:LEU:CD1	2.71	0.40
3:C:114:TYR:HB3	3:C:140:ASN:O	2.21	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	1335/1733 (77%)	1187 (89%)	91 (7%)	57 (4%)	2	16
2	B	1071/1224 (88%)	924 (86%)	104 (10%)	43 (4%)	2	17
3	C	264/318 (83%)	231 (88%)	23 (9%)	10 (4%)	2	18
4	E	213/215 (99%)	183 (86%)	16 (8%)	14 (7%)	1	7
5	F	81/155 (52%)	73 (90%)	6 (7%)	2 (2%)	4	27
6	H	129/146 (88%)	89 (69%)	19 (15%)	21 (16%)	0	0
7	I	119/122 (98%)	110 (92%)	8 (7%)	1 (1%)	16	50
8	J	62/70 (89%)	58 (94%)	4 (6%)	0	100	100
9	K	112/120 (93%)	98 (88%)	12 (11%)	2 (2%)	6	34
10	L	44/70 (63%)	24 (54%)	13 (30%)	7 (16%)	0	0
All	All	3430/4173 (82%)	2977 (87%)	296 (9%)	157 (5%)	2	15

All (157) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	ILE
1	A	45	GLN
1	A	47	ARG
1	A	59	GLY
1	A	60	SER
1	A	62	ASP
1	A	65	LEU
1	A	69	THR
1	A	72	GLU
1	A	120	GLU
1	A	155	GLU
1	A	156	ASP
1	A	157	ASP
1	A	190	ALA
1	A	286	HIS
1	A	326	ARG
1	A	400	PRO
1	A	418	SER
1	A	465	TYR
1	A	567	LYS
1	A	672	ASP
1	A	707	GLY
1	A	1080	THR
1	A	1221	LYS

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Mol	Chain	Res	Type
1	A	1403	GLU
1	A	1448	GLU
2	B	66	ASP
2	B	105	SER
2	B	108	VAL
2	B	109	THR
2	B	165	VAL
2	B	230	ALA
2	B	645	SER
2	B	646	LEU
2	B	733	HIS
2	B	864	LYS
2	B	879	ARG
2	B	957	ASN
2	B	1108	ARG
2	B	1128	LEU
2	B	1167	GLY
3	C	4	GLU
3	C	9	LYS
3	C	206	ASN
4	E	48	ASP
4	E	64	PRO
5	F	73	ALA
6	H	32	THR
6	H	52	GLN
6	H	77	ARG
6	H	78	SER
6	H	90	ALA
6	H	104	PHE
6	H	105	GLU
6	H	107	VAL
6	H	136	LYS
6	H	139	ASN
7	I	4	PHE
9	K	111	LEU
10	L	28	LYS
10	L	39	SER
10	L	45	ALA
10	L	50	ASP
10	L	58	LYS
1	A	57	ARG
1	A	193	ASP

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Mol	Chain	Res	Type
1	A	464	PRO
1	A	885	THR
1	A	1405	THR
2	B	432	MET
2	B	436	VAL
2	B	451	LYS
2	B	643	ASP
2	B	869	SER
2	B	887	HIS
2	B	940	PRO
2	B	1078	GLY
2	B	1097	HIS
2	B	1105	ALA
2	B	1158	PHE
3	C	56	THR
3	C	126	GLY
3	C	267	GLN
4	E	45	LYS
4	E	50	MET
4	E	56	LYS
4	E	118	PRO
4	E	126	SER
6	H	81	PRO
6	H	82	PRO
6	H	86	ASP
6	H	116	TYR
9	K	99	GLY
1	A	56	PRO
1	A	74	MET
1	A	75	ASN
1	A	278	THR
1	A	279	LEU
1	A	1204	ASP
1	A	1223	ASP
1	A	1234	GLU
1	A	1255	GLU
1	A	1280	GLU
1	A	1359	ASP
2	B	266	ALA
2	B	466	TRP
2	B	831	SER
2	B	1155	SER

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Mol	Chain	Res	Type
3	C	209	TYR
3	C	231	ASN
4	E	59	SER
6	H	18	GLY
6	H	53	ASP
6	H	128	ASN
6	H	135	LEU
1	A	32	VAL
1	A	38	PRO
1	A	196	GLU
1	A	408	ASP
1	A	915	SER
2	B	865	LYS
2	B	1189	ILE
2	B	1190	ASP
2	B	1221	SER
2	B	1222	ARG
4	E	2	ASP
4	E	74	ASP
10	L	41	SER
1	A	599	SER
1	A	706	HIS
1	A	958	VAL
1	A	1123	GLY
1	A	1263	ILE
2	B	90	ILE
2	B	106	ASP
2	B	424	LEU
3	C	18	VAL
4	E	127	ILE
6	H	19	ARG
6	H	89	LEU
6	H	119	GLY
10	L	46	VAL
1	A	52	GLY
2	B	56	ASP
3	C	217	ASP
4	E	44	ALA
5	F	76	LYS
2	B	1017	ILE
1	A	55	ASP
1	A	78	PRO

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Mol	Chain	Res	Type
1	A	1122	PRO
2	B	364	ILE
4	E	37	LEU
1	A	158	PRO
4	E	128	PRO
2	B	1099	VAL
2	B	1214	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	1184/1520 (78%)	969 (82%)	215 (18%)	2	9
2	B	947/1061 (89%)	772 (82%)	175 (18%)	1	9
3	C	234/274 (85%)	193 (82%)	41 (18%)	2	10
4	E	197/197 (100%)	149 (76%)	48 (24%)	1	4
5	F	73/137 (53%)	61 (84%)	12 (16%)	2	12
6	H	117/128 (91%)	70 (60%)	47 (40%)	0	0
7	I	115/116 (99%)	92 (80%)	23 (20%)	1	7
8	J	59/65 (91%)	45 (76%)	14 (24%)	1	4
9	K	99/102 (97%)	78 (79%)	21 (21%)	1	6
10	L	40/57 (70%)	20 (50%)	20 (50%)	0	0
All	All	3065/3657 (84%)	2449 (80%)	616 (20%)	1	7

All (616) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	11	LEU
1	A	15	LYS
1	A	22	PHE
1	A	34	LYS
1	A	36	ARG

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Mol	Chain	Res	Type
1	A	39	GLU
1	A	41	MET
1	A	44	THR
1	A	46	THR
1	A	49	LYS
1	A	58	LEU
1	A	60	SER
1	A	62	ASP
1	A	65	LEU
1	A	68	GLN
1	A	70	CYS
1	A	74	MET
1	A	84	ILE
1	A	90	VAL
1	A	93	VAL
1	A	96	ILE
1	A	106	VAL
1	A	107	CYS
1	A	110	CYS
1	A	112	LYS
1	A	114	LEU
1	A	120	GLU
1	A	123	ARG
1	A	129	LYS
1	A	132	LYS
1	A	133	LYS
1	A	138	ILE
1	A	141	LEU
1	A	143	LYS
1	A	144	THR
1	A	145	LYS
1	A	147	VAL
1	A	156	ASP
1	A	159	THR
1	A	160	GLN
1	A	162	VAL
1	A	163	SER
1	A	167	CYS
1	A	170	THR
1	A	174	ILE
1	A	176	LYS
1	A	182	VAL

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Mol	Chain	Res	Type
1	A	184	SER
1	A	186	LYS
1	A	191	THR
1	A	195	ASP
1	A	198	GLU
1	A	205	GLU
1	A	206	GLU
1	A	225	ASN
1	A	226	GLU
1	A	237	THR
1	A	239	LEU
1	A	246	VAL
1	A	247	ARG
1	A	261	ASP
1	A	263	THR
1	A	265	LYS
1	A	270	LEU
1	A	274	ILE
1	A	275	SER
1	A	286	HIS
1	A	289	ILE
1	A	326	ARG
1	A	346	ASP
1	A	351	THR
1	A	354	SER
1	A	412	ARG
1	A	413	ILE
1	A	416	ARG
1	A	419	LYS
1	A	436	ILE
1	A	451	HIS
1	A	461	LYS
1	A	466	SER
1	A	472	LEU
1	A	474	VAL
1	A	475	THR
1	A	493	GLN
1	A	495	GLU
1	A	497	THR
1	A	504	LEU
1	A	513	SER
1	A	535	THR

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Mol	Chain	Res	Type
1	A	537	ARG
1	A	543	LEU
1	A	566	ILE
1	A	571	LEU
1	A	586	ILE
1	A	588	LEU
1	A	590	ARG
1	A	597	LEU
1	A	599	SER
1	A	613	ILE
1	A	618	GLU
1	A	622	VAL
1	A	630	ILE
1	A	636	GLU
1	A	651	LYS
1	A	666	ILE
1	A	681	GLU
1	A	688	LYS
1	A	695	LYS
1	A	702	LEU
1	A	703	THR
1	A	705	LYS
1	A	708	MET
1	A	709	THR
1	A	710	LEU
1	A	720	ARG
1	A	728	LYS
1	A	735	VAL
1	A	737	LEU
1	A	741	ASN
1	A	744	LYS
1	A	752	LYS
1	A	794	PRO
1	A	795	GLU
1	A	810	PRO
1	A	821	ARG
1	A	830	LYS
1	A	840	ARG
1	A	843	LYS
1	A	858	ASN
1	A	895	LYS
1	A	903	ASN

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Mol	Chain	Res	Type
1	A	907	THR
1	A	909	ASP
1	A	918	GLU
1	A	919	ILE
1	A	920	LEU
1	A	960	ILE
1	A	973	ILE
1	A	974	ASP
1	A	979	SER
1	A	982	THR
1	A	1001	ARG
1	A	1003	LYS
1	A	1006	ILE
1	A	1015	VAL
1	A	1030	ARG
1	A	1039	LYS
1	A	1055	ARG
1	A	1064	VAL
1	A	1078	GLN
1	A	1081	LEU
1	A	1092	LYS
1	A	1096	SER
1	A	1101	LEU
1	A	1102	LYS
1	A	1109	LYS
1	A	1116	LEU
1	A	1118	VAL
1	A	1120	LEU
1	A	1129	GLU
1	A	1133	LEU
1	A	1134	ILE
1	A	1141	THR
1	A	1146	VAL
1	A	1161	THR
1	A	1165	GLU
1	A	1171	GLN
1	A	1172	LEU
1	A	1176	LEU
1	A	1187	GLN
1	A	1204	ASP
1	A	1208	THR
1	A	1217	LYS

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Mol	Chain	Res	Type
1	A	1219	THR
1	A	1222	ASN
1	A	1225	PHE
1	A	1230	GLU
1	A	1235	LYS
1	A	1236	LEU
1	A	1237	ILE
1	A	1243	VAL
1	A	1255	GLU
1	A	1258	HIS
1	A	1259	MET
1	A	1260	LEU
1	A	1267	MET
1	A	1269	GLU
1	A	1277	GLU
1	A	1279	ILE
1	A	1281	ARG
1	A	1290	LYS
1	A	1291	VAL
1	A	1293	SER
1	A	1299	VAL
1	A	1309	ASP
1	A	1318	THR
1	A	1322	ILE
1	A	1325	THR
1	A	1350	LYS
1	A	1359	ASP
1	A	1366	ARG
1	A	1372	VAL
1	A	1376	THR
1	A	1377	THR
1	A	1382	THR
1	A	1384	VAL
1	A	1404	GLU
1	A	1405	THR
1	A	1407	GLU
1	A	1426	GLU
1	A	1438	THR
1	A	1445	ILE
1	A	1448	GLU
1	A	1449	SER
2	B	18	PHE

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Mol	Chain	Res	Type
2	B	20	ASP
2	B	25	ILE
2	B	46	GLN
2	B	63	ILE
2	B	65	GLU
2	B	68	THR
2	B	69	LEU
2	B	89	GLU
2	B	90	ILE
2	B	92	PHE
2	B	98	THR
2	B	102	VAL
2	B	128	LEU
2	B	130	VAL
2	B	133	LYS
2	B	134	LYS
2	B	136	THR
2	B	138	GLU
2	B	164	LYS
2	B	167	ILE
2	B	172	ILE
2	B	178	ASN
2	B	179	CYS
2	B	183	GLU
2	B	194	GLU
2	B	199	MET
2	B	204	ILE
2	B	205	ILE
2	B	228	LYS
2	B	240	ILE
2	B	242	SER
2	B	244	LEU
2	B	248	SER
2	B	252	SER
2	B	261	ARG
2	B	264	SER
2	B	276	ILE
2	B	282	ILE
2	B	283	VAL
2	B	284	ILE
2	B	305	VAL
2	B	324	ILE

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Mol	Chain	Res	Type
2	B	328	GLU
2	B	347	LYS
2	B	358	LYS
2	B	367	LEU
2	B	371	GLU
2	B	373	ARG
2	B	387	LEU
2	B	417	PHE
2	B	422	LYS
2	B	423	LYS
2	B	425	THR
2	B	426	LYS
2	B	434	ARG
2	B	435	THR
2	B	436	VAL
2	B	448	ILE
2	B	453	ILE
2	B	463	THR
2	B	466	TRP
2	B	485	ARG
2	B	487	THR
2	B	498	THR
2	B	513	GLN
2	B	516	ASN
2	B	522	VAL
2	B	531	GLN
2	B	541	LEU
2	B	547	VAL
2	B	549	THR
2	B	550	ASP
2	B	552	MET
2	B	566	LEU
2	B	567	GLU
2	B	589	VAL
2	B	591	ARG
2	B	595	ARG
2	B	598	GLU
2	B	606	LYS
2	B	612	GLU
2	B	624	LEU
2	B	640	VAL
2	B	641	GLU

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Mol	Chain	Res	Type
2	B	645	SER
2	B	648	HIS
2	B	650	GLU
2	B	653	VAL
2	B	680	THR
2	B	690	VAL
2	B	691	GLU
2	B	693	ILE
2	B	706	GLN
2	B	710	LEU
2	B	722	ASP
2	B	723	VAL
2	B	733	HIS
2	B	736	THR
2	B	775	LYS
2	B	780	VAL
2	B	787	VAL
2	B	806	THR
2	B	838	SER
2	B	839	MET
2	B	860	MET
2	B	863	GLU
2	B	864	LYS
2	B	868	MET
2	B	870	ILE
2	B	871	THR
2	B	875	GLU
2	B	878	GLN
2	B	879	ARG
2	B	880	THR
2	B	881	ASN
2	B	882	THR
2	B	883	LEU
2	B	884	ARG
2	B	885	MET
2	B	889	THR
2	B	891	ASP
2	B	893	LEU
2	B	895	ASP
2	B	896	ASP
2	B	908	GLU
2	B	911	ILE

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Mol	Chain	Res	Type
2	B	933	SER
2	B	938	SER
2	B	942	ARG
2	B	948	ILE
2	B	955	THR
2	B	958	GLN
2	B	962	LYS
2	B	964	VAL
2	B	971	THR
2	B	973	ILE
2	B	974	PRO
2	B	975	GLN
2	B	983	ARG
2	B	996	ARG
2	B	997	GLU
2	B	999	MET
2	B	1007	VAL
2	B	1010	LEU
2	B	1051	THR
2	B	1056	SER
2	B	1060	ARG
2	B	1065	GLN
2	B	1077	THR
2	B	1085	ILE
2	B	1097	HIS
2	B	1099	VAL
2	B	1101	ASP
2	B	1103	ILE
2	B	1106	ARG
2	B	1150	ARG
2	B	1152	MET
2	B	1155	SER
2	B	1156	ASP
2	B	1159	ARG
2	B	1162	ILE
2	B	1163	CYS
2	B	1165	ILE
2	B	1174	LYS
2	B	1175	LEU
2	B	1178	ASN
2	B	1179	GLN
2	B	1183	LYS

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Mol	Chain	Res	Type
2	B	1185	CYS
2	B	1187	ASN
2	B	1211	ASN
2	B	1220	ARG
2	B	1222	ARG
2	B	1224	PHE
3	C	3	GLU
3	C	4	GLU
3	C	14	SER
3	C	23	SER
3	C	25	VAL
3	C	26	ASP
3	C	29	MET
3	C	33	LEU
3	C	43	THR
3	C	46	ILE
3	C	56	THR
3	C	57	VAL
3	C	86	CYS
3	C	93	ASP
3	C	102	GLN
3	C	110	THR
3	C	119	VAL
3	C	125	MET
3	C	127	ARG
3	C	129	ILE
3	C	137	LYS
3	C	154	LYS
3	C	163	ILE
3	C	178	PHE
3	C	184	ASN
3	C	185	LYS
3	C	186	LEU
3	C	197	SER
3	C	199	LYS
3	C	205	LYS
3	C	209	TYR
3	C	214	ASN
3	C	218	PRO
3	C	235	VAL
3	C	238	ILE
3	C	240	VAL

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Mol	Chain	Res	Type
3	C	245	VAL
3	C	251	LEU
3	C	265	MET
3	C	266	ASP
3	C	268	ASP
4	E	3	GLN
4	E	8	ASN
4	E	10	SER
4	E	14	ARG
4	E	33	GLU
4	E	34	GLU
4	E	36	GLU
4	E	37	LEU
4	E	49	SER
4	E	50	MET
4	E	57	MET
4	E	61	GLN
4	E	69	ILE
4	E	70	SER
4	E	74	ASP
4	E	78	LEU
4	E	81	GLU
4	E	82	PHE
4	E	84	ASP
4	E	90	VAL
4	E	91	LYS
4	E	92	THR
4	E	98	ILE
4	E	100	ILE
4	E	101	GLN
4	E	102	GLU
4	E	103	LYS
4	E	107	THR
4	E	116	ILE
4	E	118	PRO
4	E	119	SER
4	E	121	MET
4	E	123	LEU
4	E	129	PRO
4	E	134	THR
4	E	137	GLU
4	E	149	LEU

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Mol	Chain	Res	Type
4	E	158	SER
4	E	159	ASP
4	E	161	LYS
4	E	162	ARG
4	E	179	GLN
4	E	183	PRO
4	E	192	ARG
4	E	196	VAL
4	E	198	ILE
4	E	200	ARG
4	E	212	ARG
5	F	72	LYS
5	F	77	ASP
5	F	81	THR
5	F	82	THR
5	F	87	LYS
5	F	96	THR
5	F	97	ARG
5	F	103	MET
5	F	109	VAL
5	F	110	ASP
5	F	111	LEU
5	F	119	ARG
6	H	3	ASN
6	H	4	THR
6	H	5	LEU
6	H	6	PHE
6	H	7	ASP
6	H	13	SER
6	H	27	GLU
6	H	34	ASP
6	H	35	GLN
6	H	36	CYS
6	H	37	LYS
6	H	40	LEU
6	H	42	ILE
6	H	44	VAL
6	H	45	GLU
6	H	46	LEU
6	H	52	GLN
6	H	53	ASP
6	H	54	SER

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Mol	Chain	Res	Type
6	H	56	THR
6	H	63	LEU
6	H	77	ARG
6	H	78	SER
6	H	80	ARG
6	H	86	ASP
6	H	87	ARG
6	H	88	SER
6	H	89	LEU
6	H	91	ASP
6	H	92	ASP
6	H	93	TYR
6	H	105	GLU
6	H	106	GLU
6	H	108	SER
6	H	109	LYS
6	H	110	ASP
6	H	111	LEU
6	H	112	ILE
6	H	121	LEU
6	H	129	TYR
6	H	130	ARG
6	H	131	ASN
6	H	136	LYS
6	H	137	GLN
6	H	138	GLU
6	H	144	ILE
6	H	146	ARG
7	I	1	MET
7	I	2	THR
7	I	18	GLU
7	I	21	GLU
7	I	31	THR
7	I	32	CYS
7	I	40	SER
7	I	45	ARG
7	I	48	LEU
7	I	55	THR
7	I	59	VAL
7	I	75	CYS
7	I	76	PRO
7	I	77	LYS

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Mol	Chain	Res	Type
7	I	78	CYS
7	I	81	ARG
7	I	82	GLU
7	I	84	VAL
7	I	95	THR
7	I	116	ASN
7	I	117	LYS
7	I	119	THR
7	I	120	GLN
8	J	1	MET
8	J	3	VAL
8	J	7	CYS
8	J	9	SER
8	J	13	VAL
8	J	14	VAL
8	J	20	SER
8	J	28	ASP
8	J	38	ARG
8	J	42	LYS
8	J	48	ARG
8	J	50	ILE
8	J	62	ARG
8	J	64	ASN
9	K	1	MET
9	K	2	ASN
9	K	11	LEU
9	K	18	LYS
9	K	20	LYS
9	K	29	ASN
9	K	31	VAL
9	K	42	LEU
9	K	47	ARG
9	K	63	VAL
9	K	73	LEU
9	K	75	ILE
9	K	78	THR
9	K	79	GLU
9	K	93	SER
9	K	97	LYS
9	K	101	LEU
9	K	106	GLU
9	K	112	GLN

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Mol	Chain	Res	Type
9	K	113	THR
9	K	114	LEU
10	L	27	LEU
10	L	28	LYS
10	L	33	GLU
10	L	36	SER
10	L	38	LEU
10	L	42	ARG
10	L	44	ASP
10	L	46	VAL
10	L	49	LYS
10	L	50	ASP
10	L	51	CYS
10	L	54	ARG
10	L	58	LYS
10	L	60	ARG
10	L	61	THR
10	L	62	LYS
10	L	63	ARG
10	L	64	LEU
10	L	65	VAL
10	L	68	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (87) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	5	GLN
1	A	64	ASN
1	A	83	HIS
1	A	92	HIS
1	A	109	HIS
1	A	171	GLN
1	A	299	HIS
1	A	399	HIS
1	A	451	HIS
1	A	479	ASN
1	A	503	GLN
1	A	510	GLN
1	A	517	ASN
1	A	587	HIS
1	A	736	ASN

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Mol	Chain	Res	Type
1	A	741	ASN
1	A	742	ASN
1	A	745	GLN
1	A	768	GLN
1	A	786	HIS
1	A	858	ASN
1	A	903	ASN
1	A	926	GLN
1	A	994	GLN
1	A	1078	GLN
1	A	1140	HIS
1	A	1171	GLN
1	A	1173	HIS
1	A	1364	ASN
1	A	1432	GLN
2	B	121	ASN
2	B	215	GLN
2	B	236	HIS
2	B	300	HIS
2	B	383	ASN
2	B	395	GLN
2	B	433	GLN
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	531	GLN
2	B	538	ASN
2	B	590	HIS
2	B	657	HIS
2	B	706	GLN
2	B	744	HIS
2	B	862	GLN
2	B	951	GLN
2	B	958	GLN
2	B	984	HIS
2	B	1015	HIS
2	B	1025	HIS
2	B	1062	HIS
2	B	1065	GLN
2	B	1084	GLN
2	B	1093	GLN
2	B	1178	ASN

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Mol	Chain	Res	Type
2	B	1179	GLN
3	C	24	ASN
3	C	73	GLN
3	C	79	GLN
3	C	112	ASN
3	C	167	HIS
3	C	184	ASN
3	C	242	GLN
3	C	252	GLN
4	E	5	ASN
4	E	61	GLN
4	E	101	GLN
4	E	104	ASN
4	E	146	HIS
4	E	147	HIS
6	H	11	GLN
6	H	131	ASN
6	H	133	ASN
6	H	134	ASN
6	H	137	GLN
7	I	12	ASN
7	I	46	HIS
7	I	83	ASN
7	I	89	GLN
7	I	116	ASN
8	J	53	HIS
9	K	2	ASN
9	K	65	HIS
9	K	76	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 11 ligands modelled in this entry, 10 are monoatomic - leaving 1 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
13	ATP	A	3011	11	32,33,33	1.14	3 (9%)	48,52,52	1.73	8 (16%)

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
13	ATP	A	3011	11	-	2/22/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	3011	ATP	C2-N1	2.78	1.38	1.33
13	A	3011	ATP	C2-N3	2.72	1.38	1.33
13	A	3011	ATP	C8-N7	2.11	1.35	1.31

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	3011	ATP	N3-C2-N1	-5.59	120.11	128.58
13	A	3011	ATP	C5-C4-N3	-4.64	120.33	126.72
13	A	3011	ATP	N9-C8-N7	-3.78	108.57	113.94
13	A	3011	ATP	C2-N3-C4	3.49	120.34	111.83
13	A	3011	ATP	C5-N7-C8	3.44	108.86	103.45
13	A	3011	ATP	N3-C4-N9	3.05	132.35	127.17
13	A	3011	ATP	C4-C5-N7	-2.45	107.78	110.58
13	A	3011	ATP	C3'-C2'-C1'	2.04	105.32	101.46

There are no chirality outliers.

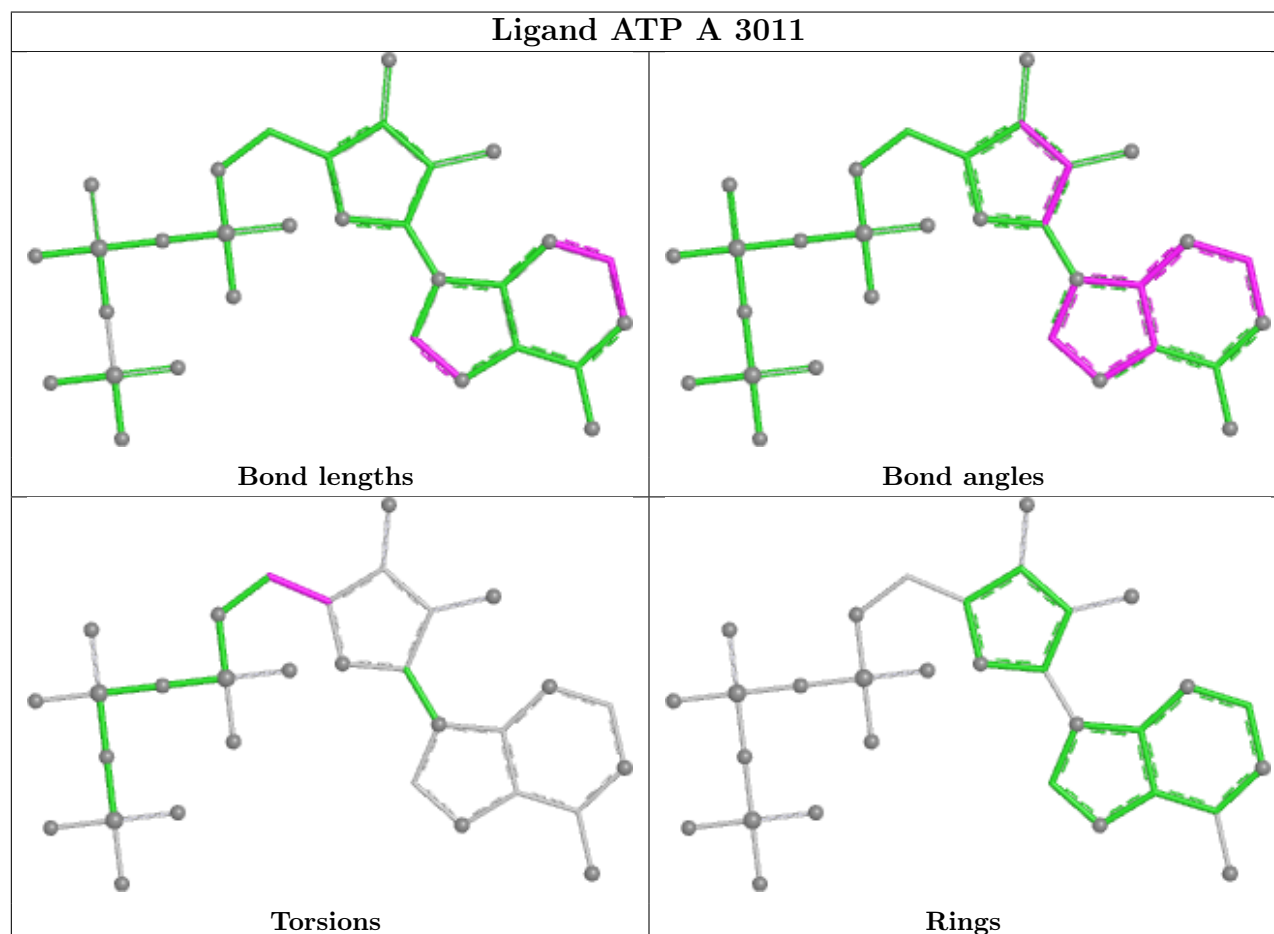
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	3011	ATP	O4'-C4'-C5'-O5'
13	A	3011	ATP	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	5
2	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	686:ALA	C	687:LYS	N	1.20
1	A	1064:VAL	C	1065:GLY	N	1.20
1	B	632:ARG	C	633:VAL	N	1.20
1	A	366:VAL	C	367:PRO	N	1.19
1	A	1195:LEU	C	1196:GLU	N	1.19
1	A	464:PRO	C	465:TYR	N	1.15

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	1352/1733 (78%)	-0.31	25 (1%) 67 48	9, 38, 105, 151	0
2	B	1091/1224 (89%)	-0.27	29 (2%) 56 36	10, 36, 111, 138	0
3	C	266/318 (83%)	-0.30	0 100 100	21, 42, 72, 123	0
4	E	215/215 (100%)	-0.07	1 (0%) 87 76	13, 51, 102, 134	0
5	F	83/155 (53%)	-0.49	0 100 100	18, 36, 64, 73	0
6	H	133/146 (91%)	0.62	8 (6%) 27 17	41, 79, 121, 132	0
7	I	121/122 (99%)	-0.16	2 (1%) 69 49	23, 44, 78, 108	0
8	J	64/70 (91%)	-0.57	0 100 100	21, 35, 61, 76	0
9	K	114/120 (95%)	-0.24	1 (0%) 81 64	21, 50, 72, 81	0
10	L	46/70 (65%)	0.62	3 (6%) 25 16	39, 89, 118, 121	0
All	All	3485/4173 (83%)	-0.24	69 (1%) 65 45	9, 41, 107, 151	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1176	LEU	5.4
2	B	883	LEU	4.5
1	A	248	PRO	4.3
2	B	882	THR	4.2
9	K	114	LEU	4.1
6	H	104	PHE	3.9
10	L	27	LEU	3.9
6	H	136	LYS	3.8
6	H	107	VAL	3.8
2	B	870	ILE	3.6
6	H	63	LEU	3.3
1	A	1450	LEU	3.3
2	B	866	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
6	H	132	LEU	3.2
2	B	733	HIS	3.2
2	B	1110	PRO	3.2
1	A	1080	THR	3.1
1	A	327	ALA	3.1
1	A	1254	ALA	3.1
1	A	191	THR	3.1
6	H	85	GLY	3.1
2	B	105	SER	3.1
1	A	37	PHE	3.1
1	A	53	LEU	3.0
1	A	194	ALA	3.0
2	B	106	ASP	2.9
7	I	121	PHE	2.8
2	B	1102	LYS	2.8
1	A	1232	ASN	2.8
2	B	436	VAL	2.8
2	B	245	GLU	2.7
2	B	869	SER	2.7
6	H	135	LEU	2.7
2	B	1100	ASP	2.7
1	A	56	PRO	2.6
6	H	139	ASN	2.6
2	B	1224	PHE	2.5
2	B	643	ASP	2.5
2	B	1101	ASP	2.5
10	L	46	VAL	2.5
1	A	1403	GLU	2.5
1	A	65	LEU	2.5
2	B	645	SER	2.5
4	E	102	GLU	2.5
1	A	188	ASP	2.4
1	A	1081	LEU	2.4
7	I	1	MET	2.4
1	A	190	ALA	2.3
2	B	1103	ILE	2.3
1	A	61	ILE	2.3
1	A	44	THR	2.2
1	A	262	LEU	2.2
1	A	324	SER	2.2
2	B	1107	ALA	2.2
1	A	1093	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	432	MET	2.2
2	B	18	PHE	2.2
2	B	247	GLY	2.1
2	B	723	VAL	2.1
2	B	435	THR	2.1
2	B	1106	ARG	2.1
2	B	1183	LYS	2.1
2	B	1105	ALA	2.1
10	L	25	ALA	2.1
1	A	187	LYS	2.1
2	B	1104	HIS	2.0
1	A	51	GLY	2.0
2	B	369	GLY	2.0
1	A	33	ALA	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.

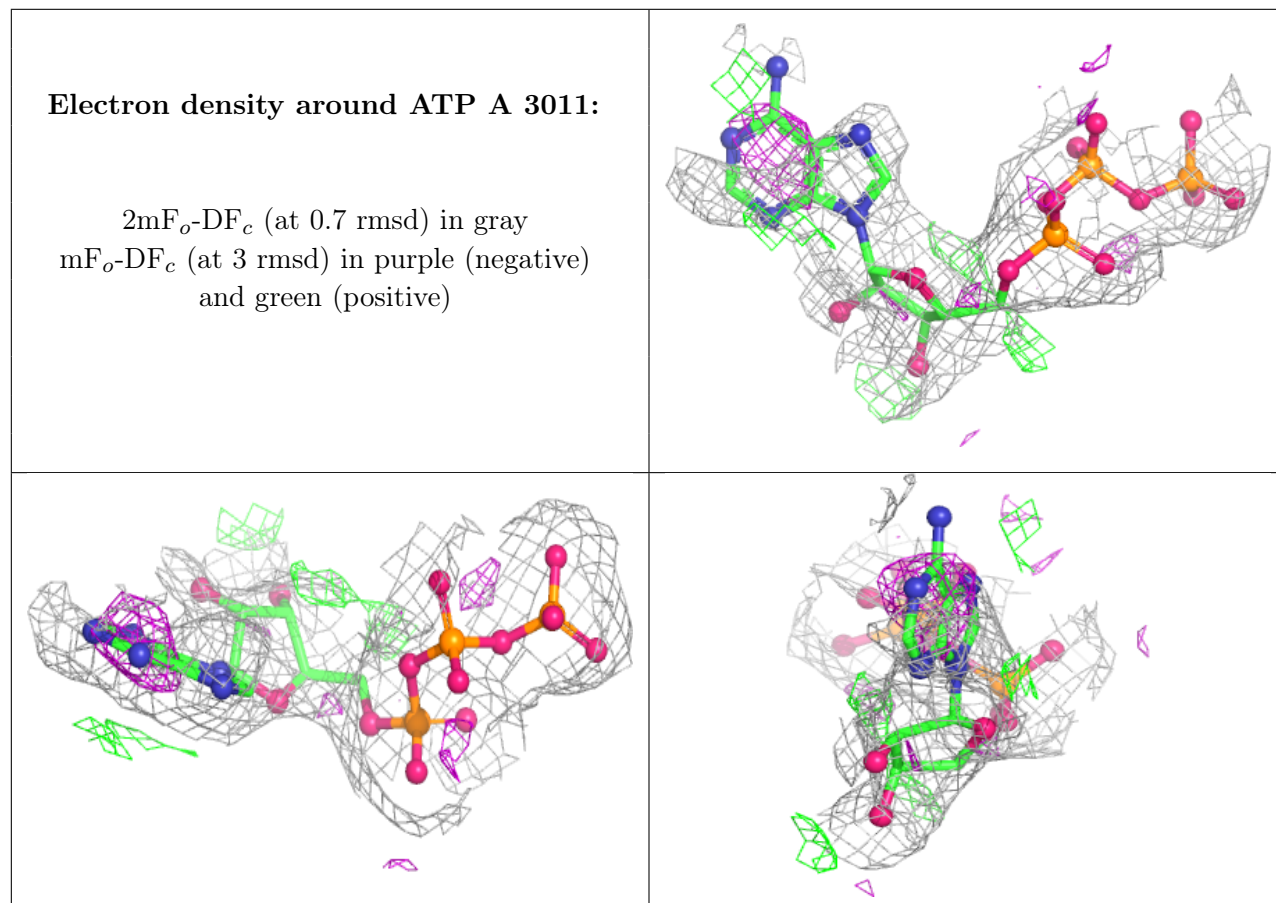
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
13	ATP	A	3011	31/31	0.86	0.13	69,74,83,83	0
12	ZN	I	3004	1/1	0.93	0.07	144,144,144,144	0
12	ZN	L	3005	1/1	0.93	0.07	139,139,139,139	0
12	ZN	I	3003	1/1	0.93	0.08	144,144,144,144	0
12	ZN	B	3007	1/1	0.96	0.06	108,108,108,108	0
12	ZN	A	3006	1/1	0.97	0.07	124,124,124,124	0
11	MN	A	3010	1/1	0.98	0.05	29,29,29,29	0
11	MN	A	3009	1/1	0.99	0.02	24,24,24,24	0
12	ZN	J	3001	1/1	0.99	0.06	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
12	ZN	C	3002	1/1	0.99	0.04	78,78,78,78	0
12	ZN	A	3008	1/1	0.99	0.04	96,96,96,96	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.