



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:55 PM UTC

PDB ID : 2CXE / pdb_00002cxe
Title : Crystal structure of octameric ribulose-1,5-bisphosphate carboxylase/oxygenase (Rubisco) from *Pyrococcus horikoshii* OT3 (form-2 crystal)
Authors : Mizohata, E.; Mishima, C.; Akasaka, R.; Uda, H.; Terada, T.; Shirouzu, M.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2005-06-28
Resolution : 3.00 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
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

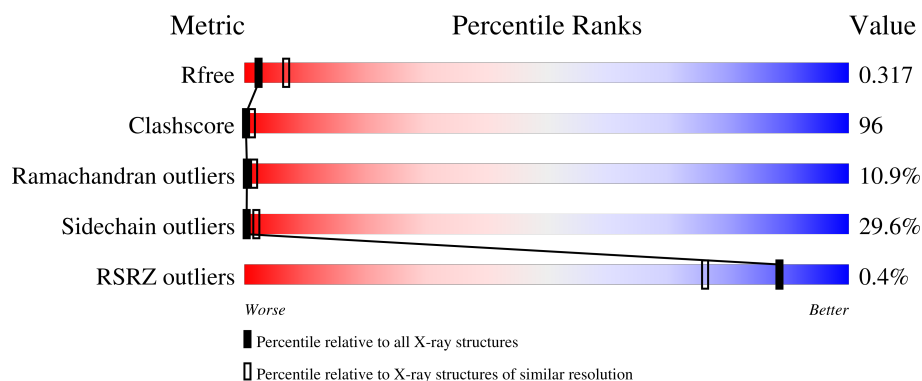
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	430	 • 22% 46% 27% •
1	B	430	 • 21% 46% 27% •
1	C	430	 • 21% 46% 27% •
1	D	430	 • 21% 46% 27% •

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13348 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 Ribulose biphosphate carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	416	Total	C	N	O	S	0	0	0
			3286	2107	565	599	15			
1	B	416	Total	C	N	O	S	0	0	0
			3286	2107	565	599	15			
1	C	416	Total	C	N	O	S	0	0	0
			3286	2107	565	599	15			
1	D	416	Total	C	N	O	S	0	0	0
			3286	2107	565	599	15			

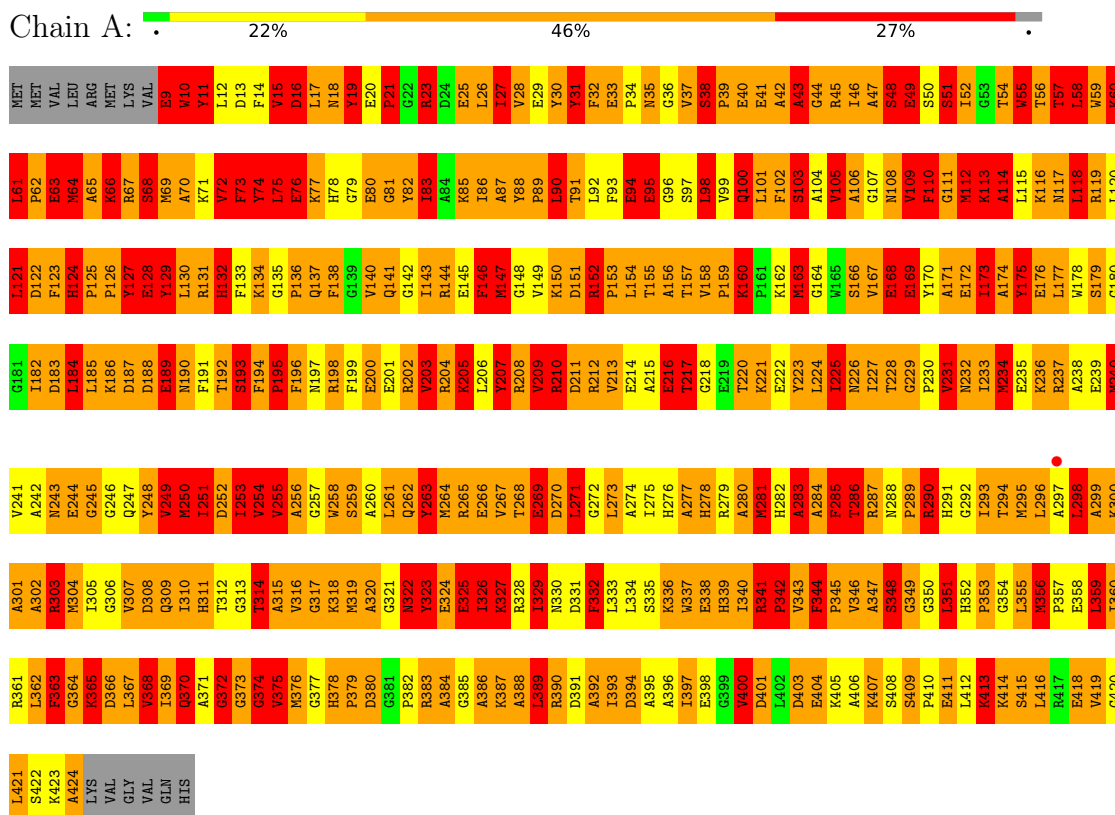
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	52	Total	O	0	0
			52	52		
2	B	51	Total	O	0	0
			51	51		
2	C	52	Total	O	0	0
			52	52		
2	D	49	Total	O	0	0
			49	49		

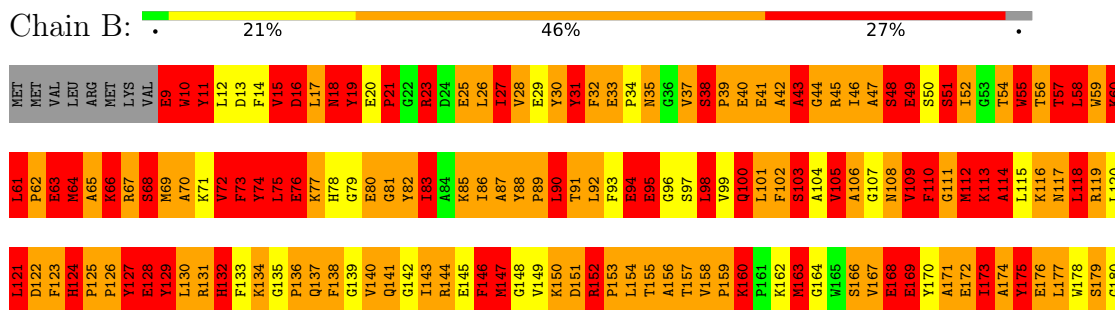
3 Residue-property plots

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: Ribulose biphosphate carboxylase



• Molecule 1: Ribulose biphosphate carboxylase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	171.48Å 149.21Å 107.46Å 90.00° 127.37° 90.00°	Depositor
Resolution (Å)	46.72 – 3.00 46.72 – 3.00	Depositor EDS
% Data completeness (in resolution range)	85.7 (46.72-3.00) 85.7 (46.72-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 2.91Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.295 , 0.328 0.286 , 0.317	Depositor DCC
R_{free} test set	1838 reflections (4.25%)	wwPDB-VP
Wilson B-factor (Å ²)	63.7	Xtriage
Anisotropy	0.760	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 60.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.002 for -h-2*1,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13348	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	3.95	548/3365 (16.3%)	3.22	527/4546 (11.6%)
1	B	3.95	547/3365 (16.3%)	3.22	524/4546 (11.5%)
1	C	3.95	550/3365 (16.3%)	3.22	527/4546 (11.6%)
1	D	3.95	547/3365 (16.3%)	3.22	524/4546 (11.5%)
All	All	3.95	2192/13460 (16.3%)	3.22	2102/18184 (11.6%)

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	16
1	B	0	16
1	C	0	16
1	D	0	16
All	All	0	64

All (2192) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	64	MET	SD-CE	46.26	2.95	1.79
1	A	64	MET	SD-CE	46.22	2.95	1.79
1	B	64	MET	SD-CE	46.21	2.95	1.79
1	D	64	MET	SD-CE	46.21	2.95	1.79
1	C	281	MET	SD-CE	35.43	2.68	1.79
1	D	281	MET	SD-CE	35.41	2.68	1.79
1	A	281	MET	SD-CE	35.40	2.68	1.79
1	B	281	MET	SD-CE	35.39	2.68	1.79
1	D	319	MET	SD-CE	27.62	2.48	1.79
1	A	319	MET	SD-CE	27.61	2.48	1.79
1	B	319	MET	SD-CE	27.60	2.48	1.79
1	C	319	MET	SD-CE	27.60	2.48	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	182	ILE	CA-CB	-19.34	1.33	1.54
1	B	182	ILE	CA-CB	-19.33	1.33	1.54
1	C	182	ILE	CA-CB	-19.30	1.33	1.54
1	D	182	ILE	CA-CB	-19.28	1.33	1.54
1	B	57	THR	CA-CB	18.85	1.85	1.53
1	D	57	THR	CA-CB	18.83	1.85	1.53
1	A	57	THR	CA-CB	18.83	1.85	1.53
1	C	57	THR	CA-CB	18.81	1.85	1.53
1	C	216	GLU	CA-C	18.34	1.77	1.52
1	D	216	GLU	CA-C	18.34	1.77	1.52
1	A	216	GLU	CA-C	18.33	1.77	1.52
1	B	216	GLU	CA-C	18.32	1.77	1.52
1	C	216	GLU	CG-CD	18.08	1.97	1.52
1	A	216	GLU	CG-CD	18.08	1.97	1.52
1	B	216	GLU	CG-CD	18.08	1.97	1.52
1	D	216	GLU	CG-CD	18.08	1.97	1.52
1	B	347	ALA	CA-CB	-18.06	1.28	1.52
1	C	347	ALA	CA-CB	-18.04	1.28	1.52
1	A	347	ALA	CA-CB	-18.04	1.28	1.52
1	D	347	ALA	CA-CB	-18.00	1.28	1.52
1	D	226	ASN	C-O	17.80	1.44	1.23
1	C	226	ASN	C-O	17.79	1.44	1.23
1	B	226	ASN	C-O	17.77	1.44	1.23
1	A	226	ASN	C-O	17.77	1.44	1.23
1	A	233	ILE	CA-CB	-17.34	1.30	1.54
1	C	233	ILE	CA-CB	-17.33	1.30	1.54
1	B	233	ILE	CA-CB	-17.32	1.30	1.54
1	D	233	ILE	CA-CB	-17.32	1.30	1.54
1	B	69	MET	SD-CE	16.75	2.21	1.79
1	C	69	MET	SD-CE	16.72	2.21	1.79
1	A	69	MET	SD-CE	16.71	2.21	1.79
1	D	69	MET	SD-CE	16.69	2.21	1.79
1	D	104	ALA	CA-CB	-16.55	1.29	1.53
1	C	56	THR	CA-CB	16.52	1.75	1.53
1	D	56	THR	CA-CB	16.51	1.75	1.53
1	B	56	THR	CA-CB	16.50	1.75	1.53
1	B	104	ALA	CA-CB	-16.50	1.29	1.53
1	A	56	THR	CA-CB	16.49	1.75	1.53
1	A	104	ALA	CA-CB	-16.49	1.29	1.53
1	C	104	ALA	CA-CB	-16.48	1.29	1.53
1	B	56	THR	CA-C	15.85	1.73	1.53
1	D	56	THR	CA-C	15.83	1.73	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	56	THR	CA-C	15.83	1.73	1.53
1	C	56	THR	CA-C	15.78	1.73	1.53
1	D	234	MET	SD-CE	15.22	2.17	1.79
1	A	234	MET	SD-CE	15.20	2.17	1.79
1	B	234	MET	SD-CE	15.20	2.17	1.79
1	C	234	MET	SD-CE	15.17	2.17	1.79
1	B	341	ARG	CZ-NH1	14.99	1.53	1.32
1	D	341	ARG	CZ-NH1	14.98	1.53	1.32
1	C	341	ARG	CZ-NH1	14.96	1.53	1.32
1	A	341	ARG	CZ-NH1	14.95	1.53	1.32
1	D	20	GLU	C-O	14.46	1.38	1.25
1	B	20	GLU	C-O	14.43	1.38	1.25
1	A	20	GLU	C-O	14.40	1.38	1.25
1	C	20	GLU	C-O	14.34	1.38	1.25
1	D	338	GLU	C-O	14.23	1.38	1.24
1	B	338	GLU	C-O	14.22	1.38	1.24
1	A	338	GLU	C-O	14.16	1.38	1.24
1	C	338	GLU	C-O	14.15	1.38	1.24
1	B	266	GLU	CA-CB	-14.13	1.31	1.53
1	C	266	GLU	CA-CB	-14.12	1.31	1.53
1	A	266	GLU	CA-CB	-14.11	1.31	1.53
1	D	266	GLU	CA-CB	-14.11	1.31	1.53
1	D	91	THR	C-O	13.99	1.43	1.24
1	B	91	THR	C-O	13.97	1.43	1.24
1	C	91	THR	C-O	13.97	1.43	1.24
1	A	91	THR	C-O	13.94	1.43	1.24
1	C	61	LEU	CA-C	13.80	1.70	1.52
1	D	61	LEU	CA-C	13.80	1.70	1.52
1	A	61	LEU	CA-C	13.76	1.70	1.52
1	B	61	LEU	CA-C	13.76	1.70	1.52
1	A	304	MET	SD-CE	13.43	2.13	1.79
1	D	304	MET	SD-CE	13.43	2.13	1.79
1	B	304	MET	SD-CE	13.42	2.13	1.79
1	C	304	MET	SD-CE	13.42	2.13	1.79
1	C	216	GLU	CD-OE2	13.38	1.50	1.25
1	B	216	GLU	CD-OE2	13.37	1.50	1.25
1	D	216	GLU	CD-OE2	13.37	1.50	1.25
1	A	216	GLU	CD-OE2	13.36	1.50	1.25
1	B	302	ALA	CA-CB	-13.15	1.31	1.53
1	C	302	ALA	CA-CB	-13.13	1.31	1.53
1	D	366	ASP	CA-C	-13.11	1.37	1.53
1	A	302	ALA	CA-CB	-13.10	1.31	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	346	VAL	CA-CB	-13.10	1.37	1.53
1	D	302	ALA	CA-CB	-13.07	1.31	1.53
1	A	346	VAL	CA-CB	-13.06	1.37	1.53
1	C	346	VAL	CA-CB	-13.06	1.37	1.53
1	A	366	ASP	CA-C	-13.04	1.37	1.53
1	B	366	ASP	CA-C	-13.02	1.37	1.53
1	C	366	ASP	CA-C	-13.02	1.37	1.53
1	B	346	VAL	CA-CB	-13.01	1.37	1.53
1	C	289	PRO	C-O	12.75	1.36	1.23
1	A	289	PRO	C-O	12.75	1.36	1.23
1	A	346	VAL	C-O	12.73	1.38	1.24
1	B	289	PRO	C-O	12.72	1.36	1.23
1	D	289	PRO	C-O	12.71	1.36	1.23
1	D	346	VAL	C-O	12.71	1.38	1.24
1	B	346	VAL	C-O	12.69	1.37	1.24
1	C	346	VAL	C-O	12.68	1.37	1.24
1	D	375	VAL	CA-CB	-12.44	1.42	1.55
1	A	375	VAL	CA-CB	-12.43	1.42	1.55
1	B	375	VAL	CA-CB	-12.41	1.42	1.55
1	C	375	VAL	CA-CB	-12.40	1.42	1.55
1	D	198	ARG	NE-CZ	12.22	1.46	1.33
1	B	198	ARG	NE-CZ	12.18	1.46	1.33
1	A	198	ARG	NE-CZ	12.16	1.46	1.33
1	C	198	ARG	NE-CZ	12.12	1.46	1.33
1	C	329	ILE	C-O	-12.06	1.09	1.24
1	A	329	ILE	C-O	-12.01	1.09	1.24
1	D	320	ALA	C-O	11.99	1.39	1.24
1	C	320	ALA	C-O	11.99	1.39	1.24
1	D	329	ILE	C-O	-11.98	1.09	1.24
1	D	419	VAL	CA-CB	11.98	1.72	1.54
1	A	141	GLN	CG-CD	11.98	1.82	1.52
1	B	141	GLN	CG-CD	11.98	1.81	1.52
1	B	329	ILE	C-O	-11.98	1.09	1.24
1	D	141	GLN	CG-CD	11.97	1.81	1.52
1	B	419	VAL	CA-CB	11.97	1.72	1.54
1	C	141	GLN	CG-CD	11.96	1.81	1.52
1	A	320	ALA	C-O	11.95	1.39	1.24
1	A	419	VAL	CA-CB	11.95	1.72	1.54
1	B	320	ALA	C-O	11.95	1.39	1.24
1	C	419	VAL	CA-CB	11.94	1.72	1.54
1	D	230	PRO	C-O	11.81	1.38	1.23
1	B	230	PRO	C-O	11.80	1.38	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	230	PRO	C-O	11.78	1.38	1.23
1	B	320	ALA	CA-C	11.75	1.68	1.52
1	D	320	ALA	CA-C	11.75	1.68	1.52
1	C	230	PRO	C-O	11.72	1.38	1.23
1	A	320	ALA	CA-C	11.72	1.68	1.52
1	C	320	ALA	CA-C	11.66	1.68	1.52
1	C	47	ALA	C-O	-11.54	1.08	1.24
1	A	47	ALA	C-O	-11.54	1.08	1.24
1	D	47	ALA	C-O	-11.53	1.08	1.24
1	B	47	ALA	C-O	-11.52	1.08	1.24
1	C	60	LYS	CA-C	11.37	1.68	1.52
1	B	60	LYS	CA-C	11.37	1.68	1.52
1	A	60	LYS	CA-C	11.36	1.68	1.52
1	D	60	LYS	CA-C	11.35	1.68	1.52
1	C	261	LEU	N-CA	11.30	1.60	1.46
1	A	261	LEU	N-CA	11.27	1.60	1.46
1	D	261	LEU	N-CA	11.26	1.60	1.46
1	D	235	GLU	CA-C	-11.22	1.38	1.52
1	B	220	THR	C-O	11.21	1.38	1.23
1	B	261	LEU	N-CA	11.20	1.60	1.46
1	A	220	THR	C-O	11.20	1.38	1.23
1	C	278	HIS	CA-C	-11.19	1.39	1.52
1	B	147	MET	SD-CE	11.19	2.07	1.79
1	C	147	MET	SD-CE	11.19	2.07	1.79
1	A	147	MET	SD-CE	11.19	2.07	1.79
1	A	235	GLU	CA-C	-11.18	1.38	1.52
1	B	235	GLU	CA-C	-11.18	1.38	1.52
1	D	147	MET	SD-CE	11.18	2.07	1.79
1	D	220	THR	C-O	11.18	1.38	1.23
1	C	220	THR	C-O	11.17	1.38	1.23
1	C	57	THR	CA-C	11.16	1.67	1.52
1	C	235	GLU	CA-C	-11.15	1.38	1.52
1	D	57	THR	CA-C	11.15	1.67	1.52
1	B	57	THR	CA-C	11.15	1.67	1.52
1	A	57	THR	CA-C	11.14	1.67	1.52
1	D	278	HIS	CA-C	-11.12	1.40	1.52
1	A	278	HIS	CA-C	-11.11	1.40	1.52
1	B	278	HIS	CA-C	-11.09	1.40	1.52
1	C	250	MET	SD-CE	10.99	2.07	1.79
1	B	250	MET	SD-CE	10.97	2.06	1.79
1	A	250	MET	SD-CE	10.97	2.06	1.79
1	D	250	MET	SD-CE	10.97	2.06	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	306	GLY	C-O	10.96	1.38	1.23
1	A	306	GLY	C-O	10.93	1.38	1.23
1	C	306	GLY	C-O	10.92	1.38	1.23
1	B	328	ARG	N-CA	10.92	1.60	1.46
1	D	328	ARG	N-CA	10.92	1.60	1.46
1	D	306	GLY	C-O	10.91	1.38	1.23
1	A	328	ARG	N-CA	10.91	1.60	1.46
1	C	328	ARG	N-CA	10.86	1.60	1.46
1	C	171	ALA	CA-CB	10.85	1.70	1.53
1	D	65	ALA	CA-C	-10.84	1.39	1.52
1	B	65	ALA	CA-C	-10.81	1.39	1.52
1	A	171	ALA	CA-CB	10.80	1.70	1.53
1	D	171	ALA	CA-CB	10.79	1.70	1.53
1	C	65	ALA	CA-C	-10.79	1.39	1.52
1	A	65	ALA	CA-C	-10.78	1.39	1.52
1	B	171	ALA	CA-CB	10.75	1.70	1.53
1	C	113	LYS	CA-C	10.63	1.66	1.52
1	A	113	LYS	CA-C	10.57	1.66	1.52
1	B	113	LYS	CA-C	10.57	1.66	1.52
1	D	113	LYS	CA-C	10.53	1.66	1.52
1	B	186	LYS	C-O	-10.53	1.11	1.24
1	C	186	LYS	C-O	-10.51	1.11	1.24
1	A	35	ASN	C-O	10.50	1.37	1.24
1	D	95	GLU	N-CA	10.50	1.59	1.45
1	A	186	LYS	C-O	-10.50	1.11	1.24
1	C	95	GLU	N-CA	10.50	1.59	1.45
1	D	35	ASN	C-O	10.50	1.37	1.24
1	D	186	LYS	CE-NZ	10.49	1.80	1.49
1	A	95	GLU	N-CA	10.49	1.59	1.45
1	D	186	LYS	C-O	-10.48	1.11	1.24
1	A	186	LYS	CE-NZ	10.48	1.80	1.49
1	B	35	ASN	C-O	10.48	1.37	1.24
1	B	95	GLU	N-CA	10.48	1.59	1.45
1	C	186	LYS	CE-NZ	10.48	1.80	1.49
1	C	35	ASN	C-O	10.47	1.37	1.24
1	B	186	LYS	CE-NZ	10.46	1.80	1.49
1	D	136	PRO	CA-C	-10.46	1.40	1.52
1	A	136	PRO	CA-C	-10.42	1.40	1.52
1	C	136	PRO	CA-C	-10.39	1.40	1.52
1	B	136	PRO	CA-C	-10.38	1.40	1.52
1	C	360	ILE	CA-CB	-10.36	1.42	1.54
1	B	360	ILE	CA-CB	-10.36	1.42	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	360	ILE	CA-CB	-10.36	1.42	1.54
1	D	249	VAL	CB-CG1	-10.35	1.18	1.52
1	A	360	ILE	CA-CB	-10.34	1.42	1.54
1	B	249	VAL	CB-CG1	-10.34	1.18	1.52
1	A	249	VAL	CB-CG1	-10.34	1.18	1.52
1	C	249	VAL	CB-CG1	-10.31	1.18	1.52
1	D	266	GLU	CD-OE1	10.31	1.45	1.25
1	A	266	GLU	CD-OE1	10.29	1.45	1.25
1	B	266	GLU	CD-OE1	10.29	1.45	1.25
1	A	95	GLU	CA-CB	10.28	1.68	1.53
1	D	95	GLU	CA-CB	10.28	1.68	1.53
1	B	95	GLU	CA-CB	10.27	1.68	1.53
1	C	266	GLU	CD-OE1	10.25	1.44	1.25
1	C	95	GLU	CA-CB	10.24	1.67	1.53
1	D	239	GLU	CD-OE2	10.15	1.44	1.25
1	C	239	GLU	CD-OE2	10.13	1.44	1.25
1	A	239	GLU	CD-OE2	10.12	1.44	1.25
1	B	239	GLU	CD-OE2	10.11	1.44	1.25
1	D	320	ALA	CA-CB	10.01	1.70	1.53
1	C	320	ALA	CA-CB	9.97	1.70	1.53
1	C	105	VAL	CA-CB	-9.97	1.41	1.54
1	A	320	ALA	CA-CB	9.96	1.70	1.53
1	B	273	LEU	C-O	9.95	1.36	1.24
1	B	320	ALA	CA-CB	9.95	1.70	1.53
1	A	66	LYS	CG-CD	9.94	1.82	1.52
1	D	66	LYS	CG-CD	9.93	1.82	1.52
1	A	273	LEU	C-O	9.93	1.36	1.24
1	B	66	LYS	CG-CD	9.92	1.82	1.52
1	C	66	LYS	CG-CD	9.92	1.82	1.52
1	B	105	VAL	CA-CB	-9.91	1.41	1.54
1	A	105	VAL	CA-CB	-9.90	1.41	1.54
1	D	273	LEU	C-O	9.90	1.36	1.24
1	D	151	ASP	C-O	9.90	1.35	1.23
1	C	151	ASP	C-O	9.89	1.35	1.23
1	D	105	VAL	CA-CB	-9.89	1.41	1.54
1	D	151	ASP	CB-CG	9.89	1.76	1.52
1	C	273	LEU	C-O	9.89	1.36	1.24
1	C	151	ASP	CB-CG	9.89	1.76	1.52
1	B	151	ASP	CB-CG	9.88	1.76	1.52
1	A	151	ASP	CB-CG	9.88	1.76	1.52
1	A	151	ASP	C-O	9.87	1.35	1.23
1	B	151	ASP	C-O	9.86	1.35	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	188	ASP	C-O	-9.85	1.11	1.24
1	B	188	ASP	C-O	-9.84	1.11	1.24
1	D	188	ASP	C-O	-9.82	1.11	1.24
1	B	68	SER	CA-C	9.82	1.66	1.52
1	B	260	ALA	N-CA	-9.81	1.33	1.46
1	B	250	MET	N-CA	9.81	1.58	1.46
1	C	188	ASP	C-O	-9.81	1.12	1.24
1	A	68	SER	CA-C	9.80	1.66	1.52
1	A	260	ALA	N-CA	-9.79	1.33	1.46
1	D	68	SER	CA-C	9.78	1.65	1.52
1	C	68	SER	CA-C	9.78	1.65	1.52
1	A	250	MET	N-CA	9.75	1.58	1.46
1	D	260	ALA	N-CA	-9.74	1.33	1.46
1	C	260	ALA	N-CA	-9.73	1.33	1.46
1	C	250	MET	N-CA	9.72	1.58	1.46
1	D	250	MET	N-CA	9.72	1.58	1.46
1	B	132	HIS	C-O	-9.70	1.11	1.23
1	A	132	HIS	C-O	-9.69	1.11	1.23
1	D	132	HIS	C-O	-9.68	1.11	1.23
1	B	252	ASP	CA-C	-9.66	1.39	1.52
1	C	89	PRO	C-O	9.64	1.34	1.23
1	B	89	PRO	C-O	9.64	1.34	1.23
1	D	252	ASP	CA-C	-9.63	1.39	1.52
1	C	132	HIS	C-O	-9.62	1.11	1.23
1	A	252	ASP	CA-C	-9.61	1.39	1.52
1	A	89	PRO	C-O	9.61	1.34	1.23
1	B	275	ILE	CA-CB	-9.60	1.42	1.54
1	C	252	ASP	CA-C	-9.59	1.39	1.52
1	B	94	GLU	CA-C	-9.58	1.41	1.52
1	C	21	PRO	CA-CB	9.57	1.65	1.53
1	D	94	GLU	CA-C	-9.57	1.41	1.52
1	A	56	THR	C-O	9.56	1.36	1.23
1	C	275	ILE	CA-CB	-9.56	1.42	1.54
1	C	56	THR	C-O	9.56	1.36	1.23
1	D	275	ILE	CA-CB	-9.56	1.42	1.54
1	A	94	GLU	CA-C	-9.56	1.41	1.52
1	C	94	GLU	CA-C	-9.56	1.41	1.52
1	D	56	THR	C-O	9.55	1.36	1.23
1	A	275	ILE	CA-CB	-9.55	1.42	1.54
1	D	89	PRO	C-O	9.55	1.34	1.23
1	A	21	PRO	CA-CB	9.54	1.65	1.53
1	B	56	THR	C-O	9.54	1.36	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	21	PRO	CA-CB	9.53	1.65	1.53
1	D	21	PRO	CA-CB	9.51	1.65	1.53
1	B	172	GLU	CG-CD	9.51	1.75	1.52
1	D	172	GLU	CG-CD	9.51	1.75	1.52
1	A	172	GLU	CG-CD	9.50	1.75	1.52
1	C	172	GLU	CG-CD	9.50	1.75	1.52
1	B	151	ASP	CG-OD1	9.49	1.43	1.25
1	B	328	ARG	NE-CZ	9.49	1.43	1.33
1	C	151	ASP	CG-OD1	9.48	1.43	1.25
1	A	151	ASP	CG-OD1	9.48	1.43	1.25
1	A	328	ARG	NE-CZ	9.48	1.43	1.33
1	D	151	ASP	CG-OD1	9.47	1.43	1.25
1	D	240	MET	CA-C	-9.45	1.39	1.52
1	C	328	ARG	NE-CZ	9.45	1.43	1.33
1	C	240	MET	CA-C	-9.44	1.39	1.52
1	D	328	ARG	NE-CZ	9.44	1.43	1.33
1	A	240	MET	CA-C	-9.43	1.39	1.52
1	B	240	MET	CA-C	-9.43	1.39	1.52
1	A	361	ARG	CZ-NH2	9.42	1.45	1.33
1	C	361	ARG	CZ-NH2	9.42	1.45	1.33
1	C	356	MET	SD-CE	9.42	2.03	1.79
1	A	356	MET	SD-CE	9.41	2.03	1.79
1	B	361	ARG	CZ-NH2	9.41	1.45	1.33
1	C	301	ALA	CA-CB	-9.40	1.38	1.53
1	D	361	ARG	CZ-NH2	9.40	1.45	1.33
1	A	301	ALA	CA-CB	-9.40	1.38	1.53
1	B	356	MET	SD-CE	9.40	2.03	1.79
1	D	356	MET	SD-CE	9.39	2.03	1.79
1	B	301	ALA	CA-CB	-9.38	1.38	1.53
1	D	301	ALA	CA-CB	-9.38	1.38	1.53
1	C	283	ALA	CA-C	9.38	1.65	1.52
1	D	110	PHE	CA-C	9.38	1.65	1.52
1	B	200	GLU	CG-CD	9.38	1.75	1.52
1	B	283	ALA	CA-C	9.37	1.65	1.52
1	A	117	ASN	CA-C	9.36	1.64	1.52
1	C	200	GLU	CG-CD	9.37	1.75	1.52
1	D	117	ASN	CA-C	9.36	1.64	1.52
1	C	117	ASN	CA-C	9.36	1.64	1.52
1	A	200	GLU	CG-CD	9.36	1.75	1.52
1	B	117	ASN	CA-C	9.36	1.64	1.52
1	D	200	GLU	CG-CD	9.34	1.75	1.52
1	A	283	ALA	CA-C	9.34	1.65	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	110	PHE	CA-C	9.33	1.65	1.52
1	D	319	MET	CA-C	9.33	1.64	1.53
1	B	110	PHE	CA-C	9.32	1.65	1.52
1	B	319	MET	CA-C	9.32	1.64	1.53
1	C	110	PHE	CA-C	9.31	1.65	1.52
1	A	319	MET	CA-C	9.31	1.64	1.53
1	B	76	GLU	CD-OE2	9.30	1.43	1.25
1	D	76	GLU	CD-OE2	9.29	1.43	1.25
1	D	283	ALA	CA-C	9.29	1.65	1.52
1	C	319	MET	CA-C	9.27	1.64	1.53
1	D	280	ALA	C-O	9.27	1.35	1.24
1	A	76	GLU	CD-OE2	9.27	1.43	1.25
1	C	66	LYS	CD-CE	9.27	1.80	1.52
1	D	66	LYS	CD-CE	9.26	1.80	1.52
1	B	132	HIS	CA-C	-9.26	1.41	1.53
1	C	193	SER	CA-C	9.26	1.63	1.52
1	C	339	HIS	CA-C	-9.26	1.40	1.52
1	B	339	HIS	CA-C	-9.25	1.40	1.52
1	B	145	GLU	CA-C	-9.25	1.41	1.52
1	B	66	LYS	CD-CE	9.25	1.80	1.52
1	A	66	LYS	CD-CE	9.24	1.80	1.52
1	A	280	ALA	C-O	9.23	1.35	1.24
1	C	76	GLU	CD-OE2	9.23	1.42	1.25
1	D	132	HIS	CA-C	-9.23	1.41	1.53
1	C	280	ALA	C-O	9.23	1.35	1.24
1	A	212	ARG	C-O	9.23	1.35	1.24
1	A	339	HIS	CA-C	-9.22	1.40	1.52
1	C	132	HIS	CA-C	-9.22	1.41	1.53
1	C	212	ARG	C-O	9.22	1.35	1.24
1	D	339	HIS	CA-C	-9.22	1.41	1.52
1	B	280	ALA	CA-C	9.22	1.64	1.52
1	A	132	HIS	CA-C	-9.21	1.41	1.53
1	A	145	GLU	CA-C	-9.21	1.41	1.52
1	A	193	SER	CA-C	9.21	1.63	1.52
1	D	193	SER	CA-C	9.21	1.63	1.52
1	D	212	ARG	C-O	9.21	1.35	1.24
1	C	145	GLU	CA-C	-9.21	1.41	1.52
1	D	280	ALA	CA-C	9.21	1.64	1.52
1	B	193	SER	CA-C	9.20	1.63	1.52
1	A	280	ALA	CA-C	9.20	1.64	1.52
1	B	280	ALA	C-O	9.20	1.35	1.24
1	D	145	GLU	CA-C	-9.20	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	212	ARG	C-O	9.19	1.35	1.24
1	C	280	ALA	CA-C	9.18	1.64	1.52
1	A	240	MET	CG-SD	9.18	2.03	1.80
1	B	240	MET	CG-SD	9.18	2.03	1.80
1	D	240	MET	CG-SD	9.17	2.03	1.80
1	C	240	MET	CG-SD	9.16	2.03	1.80
1	C	329	ILE	CA-CB	-9.12	1.42	1.54
1	B	329	ILE	CA-CB	-9.10	1.42	1.54
1	D	271	LEU	CG-CD2	-9.10	1.22	1.52
1	B	258	TRP	N-CA	9.09	1.57	1.46
1	D	258	TRP	N-CA	9.09	1.57	1.46
1	A	271	LEU	CG-CD2	-9.09	1.22	1.52
1	C	201	GLU	CD-OE2	9.09	1.42	1.25
1	A	217	THR	CA-CB	9.09	1.67	1.53
1	B	271	LEU	CG-CD2	-9.09	1.22	1.52
1	A	258	TRP	N-CA	9.08	1.57	1.46
1	A	329	ILE	CA-CB	-9.08	1.42	1.54
1	D	201	GLU	CD-OE2	9.08	1.42	1.25
1	C	271	LEU	CG-CD2	-9.08	1.22	1.52
1	D	329	ILE	CA-CB	-9.07	1.42	1.54
1	A	201	GLU	CD-OE2	9.07	1.42	1.25
1	B	38	SER	CA-C	-9.07	1.43	1.53
1	B	266	GLU	CD-OE2	9.07	1.42	1.25
1	C	217	THR	CA-CB	9.07	1.67	1.53
1	C	266	GLU	CD-OE2	9.06	1.42	1.25
1	A	266	GLU	CD-OE2	9.06	1.42	1.25
1	C	38	SER	CA-C	-9.05	1.43	1.53
1	D	217	THR	CA-CB	9.05	1.67	1.53
1	B	201	GLU	CD-OE2	9.05	1.42	1.25
1	B	217	THR	CA-CB	9.05	1.67	1.53
1	A	38	SER	CA-C	-9.04	1.43	1.53
1	C	258	TRP	N-CA	9.04	1.57	1.46
1	D	224	LEU	C-O	-9.04	1.13	1.23
1	D	38	SER	CA-C	-9.02	1.43	1.53
1	D	266	GLU	CD-OE2	9.02	1.42	1.25
1	B	224	LEU	C-O	-9.02	1.13	1.23
1	C	224	LEU	C-O	-9.02	1.13	1.23
1	A	224	LEU	C-O	-9.00	1.13	1.23
1	B	266	GLU	CA-C	-8.99	1.41	1.52
1	D	369	ILE	CA-C	-8.97	1.41	1.52
1	A	266	GLU	CA-C	-8.97	1.41	1.52
1	D	266	GLU	CA-C	-8.96	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	369	ILE	CA-C	-8.96	1.41	1.52
1	C	27	ILE	CG1-CD1	8.95	1.86	1.51
1	C	266	GLU	CA-C	-8.95	1.41	1.52
1	D	27	ILE	CG1-CD1	8.94	1.86	1.51
1	A	27	ILE	CG1-CD1	8.94	1.86	1.51
1	A	369	ILE	CA-C	-8.94	1.41	1.52
1	C	208	ARG	NE-CZ	8.94	1.42	1.33
1	B	27	ILE	CG1-CD1	8.94	1.86	1.51
1	A	143	ILE	CA-C	-8.92	1.41	1.52
1	B	208	ARG	NE-CZ	8.91	1.42	1.33
1	A	208	ARG	NE-CZ	8.91	1.42	1.33
1	B	369	ILE	CA-C	-8.90	1.41	1.52
1	C	143	ILE	CA-C	-8.89	1.41	1.52
1	D	143	ILE	CA-C	-8.88	1.41	1.52
1	D	208	ARG	NE-CZ	8.88	1.42	1.33
1	C	310	ILE	CA-CB	-8.88	1.40	1.55
1	D	157	THR	CA-CB	-8.88	1.40	1.53
1	B	157	THR	CA-CB	-8.88	1.40	1.53
1	B	310	ILE	CA-CB	-8.88	1.40	1.55
1	A	310	ILE	CA-CB	-8.87	1.40	1.55
1	B	143	ILE	CA-C	-8.87	1.41	1.52
1	D	310	ILE	CA-CB	-8.87	1.40	1.55
1	A	157	THR	CA-CB	-8.86	1.40	1.53
1	C	157	THR	CA-CB	-8.86	1.40	1.53
1	B	68	SER	CA-CB	8.85	1.68	1.53
1	A	68	SER	CA-CB	8.82	1.68	1.53
1	D	68	SER	CA-CB	8.81	1.68	1.53
1	C	68	SER	CA-CB	8.80	1.68	1.53
1	C	230	PRO	CA-C	8.75	1.62	1.52
1	B	93	PHE	CA-C	-8.74	1.41	1.53
1	A	93	PHE	CA-C	-8.73	1.41	1.53
1	C	93	PHE	CA-C	-8.73	1.41	1.53
1	D	284	ALA	CA-CB	-8.71	1.38	1.53
1	D	93	PHE	CA-C	-8.70	1.41	1.53
1	B	66	LYS	CA-C	8.70	1.64	1.52
1	A	284	ALA	CA-CB	-8.70	1.38	1.53
1	A	230	PRO	CA-C	8.70	1.62	1.52
1	B	284	ALA	CA-CB	-8.69	1.38	1.53
1	C	284	ALA	CA-CB	-8.69	1.38	1.53
1	D	230	PRO	CA-C	8.69	1.62	1.52
1	C	66	LYS	CA-C	8.68	1.64	1.52
1	D	66	LYS	CA-C	8.68	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66	LYS	CA-C	8.68	1.64	1.52
1	C	216	GLU	CD-OE1	8.67	1.41	1.25
1	B	216	GLU	CD-OE1	8.66	1.41	1.25
1	B	230	PRO	CA-C	8.66	1.62	1.52
1	C	378	HIS	CA-C	8.66	1.61	1.53
1	D	378	HIS	CA-C	8.65	1.61	1.53
1	A	216	GLU	CD-OE1	8.64	1.41	1.25
1	B	216	GLU	CA-CB	8.64	1.68	1.53
1	A	378	HIS	CA-C	8.63	1.61	1.53
1	D	216	GLU	CD-OE1	8.62	1.41	1.25
1	A	163	MET	CA-C	-8.61	1.42	1.53
1	A	216	GLU	CA-CB	8.61	1.68	1.53
1	B	163	MET	CA-C	-8.60	1.42	1.53
1	B	378	HIS	CA-C	8.59	1.61	1.53
1	D	216	GLU	CA-CB	8.59	1.68	1.53
1	C	163	MET	CA-C	-8.58	1.42	1.53
1	B	211	ASP	CA-C	-8.56	1.42	1.52
1	C	216	GLU	CA-CB	8.56	1.68	1.53
1	A	211	ASP	CA-C	-8.53	1.42	1.52
1	D	211	ASP	CA-C	-8.53	1.42	1.52
1	D	300	LYS	CD-CE	8.53	1.78	1.52
1	D	163	MET	CA-C	-8.52	1.42	1.53
1	C	300	LYS	CD-CE	8.52	1.78	1.52
1	A	300	LYS	CD-CE	8.52	1.77	1.52
1	B	300	LYS	CD-CE	8.51	1.77	1.52
1	C	211	ASP	CA-C	-8.49	1.42	1.52
1	B	262	GLN	CA-C	-8.43	1.41	1.52
1	A	262	GLN	CA-C	-8.43	1.41	1.52
1	C	368	VAL	C-O	8.43	1.33	1.24
1	A	368	VAL	C-O	8.41	1.33	1.24
1	B	198	ARG	CD-NE	8.41	1.58	1.46
1	C	262	GLN	CA-C	-8.41	1.41	1.52
1	C	198	ARG	CD-NE	8.39	1.58	1.46
1	D	262	GLN	CA-C	-8.39	1.41	1.52
1	A	198	ARG	CD-NE	8.38	1.57	1.46
1	D	368	VAL	C-O	8.37	1.33	1.24
1	D	198	ARG	CD-NE	8.35	1.57	1.46
1	D	266	GLU	N-CA	-8.35	1.36	1.46
1	B	368	VAL	C-O	8.34	1.33	1.24
1	A	266	GLU	N-CA	-8.34	1.36	1.46
1	B	228	THR	C-O	-8.33	1.13	1.23
1	C	266	GLU	N-CA	-8.32	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	136	PRO	CG-CD	8.32	1.79	1.50
1	C	189	GLU	CD-OE1	8.32	1.41	1.25
1	A	368	VAL	CA-CB	-8.32	1.43	1.53
1	A	189	GLU	CD-OE1	8.31	1.41	1.25
1	D	228	THR	C-O	-8.31	1.13	1.23
1	B	189	GLU	CD-OE1	8.31	1.41	1.25
1	C	136	PRO	CG-CD	8.31	1.79	1.50
1	B	266	GLU	N-CA	-8.31	1.36	1.46
1	D	189	GLU	CD-OE1	8.31	1.41	1.25
1	C	368	VAL	CA-CB	-8.30	1.43	1.53
1	A	136	PRO	CG-CD	8.30	1.78	1.50
1	B	368	VAL	CA-CB	-8.30	1.43	1.53
1	A	228	THR	C-O	-8.30	1.13	1.23
1	D	368	VAL	CA-CB	-8.29	1.43	1.53
1	B	136	PRO	CG-CD	8.28	1.78	1.50
1	B	261	LEU	CA-C	-8.24	1.42	1.52
1	C	228	THR	C-O	-8.23	1.13	1.23
1	C	261	LEU	CA-C	-8.18	1.42	1.52
1	A	261	LEU	CA-C	-8.17	1.42	1.52
1	D	129	TYR	C-O	8.16	1.36	1.23
1	B	270	ASP	CG-OD2	8.15	1.40	1.25
1	C	269	GLU	CG-CD	8.15	1.72	1.52
1	B	269	GLU	CG-CD	8.14	1.72	1.52
1	D	318	LYS	N-CA	8.14	1.55	1.46
1	C	90	LEU	C-O	-8.14	1.13	1.24
1	A	269	GLU	CG-CD	8.13	1.72	1.52
1	A	318	LYS	N-CA	8.13	1.55	1.46
1	D	269	GLU	CG-CD	8.13	1.72	1.52
1	A	90	LEU	C-O	-8.13	1.13	1.24
1	D	261	LEU	CA-C	-8.13	1.42	1.52
1	C	354	GLY	C-O	8.13	1.33	1.23
1	B	129	TYR	C-O	8.12	1.36	1.23
1	C	270	ASP	CG-OD2	8.12	1.40	1.25
1	D	90	LEU	C-O	-8.13	1.13	1.24
1	A	270	ASP	CG-OD2	8.12	1.40	1.25
1	B	76	GLU	CG-CD	8.12	1.72	1.52
1	C	318	LYS	N-CA	8.12	1.55	1.46
1	B	90	LEU	C-O	-8.12	1.13	1.24
1	C	76	GLU	CG-CD	8.12	1.72	1.52
1	D	154	LEU	C-O	8.12	1.33	1.23
1	B	89	PRO	CA-C	8.11	1.62	1.52
1	D	76	GLU	CG-CD	8.12	1.72	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	270	ASP	CG-OD2	8.12	1.40	1.25
1	A	76	GLU	CG-CD	8.11	1.72	1.52
1	C	291	HIS	CA-C	8.11	1.62	1.52
1	A	129	TYR	C-O	8.11	1.36	1.23
1	D	88	TYR	N-CA	8.11	1.56	1.46
1	D	354	GLY	C-O	8.10	1.33	1.23
1	B	220	THR	CA-CB	-8.10	1.40	1.53
1	C	129	TYR	C-O	8.10	1.36	1.23
1	D	75	LEU	C-O	-8.10	1.15	1.23
1	B	75	LEU	C-O	-8.10	1.15	1.23
1	B	154	LEU	C-O	8.10	1.33	1.23
1	D	291	HIS	CA-C	8.10	1.62	1.52
1	D	376	MET	C-O	8.10	1.34	1.24
1	B	88	TYR	N-CA	8.09	1.56	1.46
1	A	154	LEU	C-O	8.09	1.33	1.23
1	B	318	LYS	N-CA	8.09	1.55	1.46
1	A	88	TYR	N-CA	8.09	1.56	1.46
1	D	220	THR	CA-CB	-8.09	1.40	1.53
1	A	354	GLY	C-O	8.08	1.33	1.23
1	A	220	THR	CA-CB	-8.08	1.40	1.53
1	A	291	HIS	CA-C	8.08	1.62	1.52
1	A	89	PRO	CA-C	8.07	1.61	1.52
1	B	354	GLY	C-O	8.07	1.33	1.23
1	B	376	MET	C-O	8.07	1.34	1.24
1	C	163	MET	SD-CE	8.07	1.99	1.79
1	A	57	THR	N-CA	8.06	1.56	1.46
1	A	376	MET	C-O	8.06	1.34	1.24
1	D	89	PRO	CA-C	8.06	1.61	1.52
1	C	154	LEU	C-O	8.06	1.33	1.23
1	D	163	MET	SD-CE	8.06	1.99	1.79
1	A	75	LEU	C-O	-8.06	1.15	1.23
1	A	163	MET	SD-CE	8.06	1.99	1.79
1	C	57	THR	N-CA	8.05	1.56	1.46
1	C	220	THR	CA-CB	-8.05	1.40	1.53
1	A	87	ALA	CA-C	8.05	1.62	1.52
1	B	57	THR	N-CA	8.04	1.56	1.46
1	B	87	ALA	CA-C	8.04	1.62	1.52
1	B	163	MET	SD-CE	8.04	1.99	1.79
1	C	87	ALA	CA-C	8.04	1.62	1.52
1	B	291	HIS	CA-C	8.04	1.62	1.52
1	D	57	THR	N-CA	8.03	1.56	1.46
1	B	260	ALA	C-O	-8.03	1.13	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	88	TYR	N-CA	8.03	1.56	1.46
1	C	89	PRO	CA-C	8.03	1.61	1.52
1	C	348	SER	CA-CB	8.02	1.67	1.53
1	D	269	GLU	CA-C	-8.02	1.43	1.52
1	D	325	GLU	CD-OE2	8.01	1.40	1.25
1	D	87	ALA	CA-C	8.00	1.62	1.52
1	C	376	MET	C-O	7.99	1.34	1.24
1	A	260	ALA	C-O	-7.98	1.13	1.24
1	B	80	GLU	CD-OE1	7.98	1.40	1.25
1	C	75	LEU	C-O	-7.98	1.16	1.23
1	A	80	GLU	CD-OE1	7.98	1.40	1.25
1	B	348	SER	CA-CB	7.98	1.67	1.53
1	C	269	GLU	CA-C	-7.97	1.43	1.52
1	A	325	GLU	CD-OE2	7.97	1.40	1.25
1	B	80	GLU	CG-CD	7.97	1.72	1.52
1	A	348	SER	CA-CB	7.96	1.67	1.53
1	D	80	GLU	CG-CD	7.96	1.72	1.52
1	D	260	ALA	C-O	-7.96	1.13	1.24
1	B	366	ASP	CG-OD1	7.96	1.40	1.25
1	B	325	GLU	CD-OE2	7.96	1.40	1.25
1	A	269	GLU	CA-C	-7.96	1.43	1.52
1	D	348	SER	CA-CB	7.95	1.67	1.53
1	C	325	GLU	CD-OE2	7.95	1.40	1.25
1	C	80	GLU	CD-OE1	7.95	1.40	1.25
1	A	80	GLU	CG-CD	7.95	1.72	1.52
1	C	260	ALA	C-O	-7.94	1.13	1.24
1	A	73	PHE	CA-C	-7.94	1.41	1.52
1	D	80	GLU	CD-OE1	7.93	1.40	1.25
1	C	80	GLU	CG-CD	7.93	1.71	1.52
1	C	275	ILE	C-O	-7.93	1.13	1.24
1	C	320	ALA	C-N	7.93	1.45	1.33
1	C	380	ASP	C-O	7.93	1.34	1.24
1	A	275	ILE	C-O	-7.93	1.13	1.24
1	B	73	PHE	CA-C	-7.93	1.41	1.52
1	D	275	ILE	C-O	-7.93	1.13	1.24
1	B	275	ILE	C-O	-7.92	1.13	1.24
1	C	366	ASP	CG-OD1	7.92	1.40	1.25
1	D	73	PHE	CA-C	-7.92	1.41	1.52
1	B	320	ALA	C-N	7.91	1.45	1.33
1	B	172	GLU	CD-OE1	7.91	1.40	1.25
1	B	380	ASP	C-O	7.91	1.34	1.24
1	A	366	ASP	CG-OD1	7.91	1.40	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	380	ASP	C-O	7.91	1.34	1.24
1	A	320	ALA	C-N	7.91	1.45	1.33
1	C	73	PHE	CA-C	-7.90	1.41	1.52
1	B	269	GLU	CA-C	-7.90	1.43	1.52
1	C	172	GLU	CD-OE1	7.89	1.40	1.25
1	D	380	ASP	C-O	7.89	1.34	1.24
1	D	366	ASP	CG-OD1	7.89	1.40	1.25
1	B	63	GLU	CD-OE1	7.88	1.40	1.25
1	A	172	GLU	CD-OE1	7.88	1.40	1.25
1	B	322	ASN	C-O	-7.88	1.14	1.24
1	D	322	ASN	C-O	-7.88	1.14	1.24
1	D	320	ALA	C-N	7.87	1.45	1.33
1	A	322	ASN	C-O	-7.87	1.14	1.24
1	C	18	ASN	CG-ND2	7.87	1.49	1.33
1	D	390	ARG	CA-C	-7.86	1.42	1.52
1	D	63	GLU	CD-OE1	7.85	1.40	1.25
1	D	18	ASN	CG-ND2	7.85	1.49	1.33
1	C	63	GLU	CD-OE1	7.85	1.40	1.25
1	C	203	VAL	CA-C	-7.85	1.42	1.52
1	D	203	VAL	CA-C	-7.85	1.42	1.52
1	D	172	GLU	CD-OE1	7.84	1.40	1.25
1	A	18	ASN	CG-ND2	7.84	1.49	1.33
1	A	63	GLU	CD-OE1	7.84	1.40	1.25
1	A	203	VAL	CA-C	-7.84	1.42	1.52
1	B	203	VAL	CA-C	-7.84	1.42	1.52
1	C	322	ASN	C-O	-7.84	1.14	1.24
1	B	18	ASN	CG-ND2	7.83	1.49	1.33
1	B	390	ARG	CA-C	-7.82	1.42	1.52
1	A	221	LYS	CA-C	-7.81	1.43	1.52
1	B	250	MET	CA-C	7.81	1.63	1.52
1	B	160	LYS	CD-CE	7.81	1.75	1.52
1	A	390	ARG	CA-C	-7.81	1.42	1.52
1	B	260	ALA	CA-CB	-7.80	1.41	1.53
1	C	160	LYS	CD-CE	7.80	1.75	1.52
1	A	260	ALA	CA-CB	-7.80	1.41	1.53
1	C	390	ARG	CA-C	-7.80	1.42	1.52
1	A	56	THR	N-CA	7.79	1.60	1.46
1	A	160	LYS	CD-CE	7.79	1.75	1.52
1	C	260	ALA	CA-CB	-7.79	1.41	1.53
1	C	392	ALA	CA-CB	7.79	1.65	1.53
1	C	56	THR	N-CA	7.79	1.60	1.46
1	D	260	ALA	CA-CB	-7.79	1.41	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	221	LYS	CA-C	-7.78	1.43	1.52
1	B	122	ASP	CG-OD2	7.78	1.40	1.25
1	D	122	ASP	CG-OD2	7.78	1.40	1.25
1	C	221	LYS	CA-C	-7.78	1.43	1.52
1	A	250	MET	CA-C	7.78	1.63	1.52
1	D	160	LYS	CD-CE	7.78	1.75	1.52
1	B	392	ALA	CA-CB	7.78	1.65	1.53
1	B	56	THR	N-CA	7.77	1.59	1.46
1	A	392	ALA	CA-CB	7.77	1.65	1.53
1	C	250	MET	CA-C	7.77	1.63	1.52
1	D	250	MET	CA-C	7.76	1.63	1.52
1	A	122	ASP	CG-OD2	7.76	1.40	1.25
1	D	56	THR	N-CA	7.75	1.59	1.46
1	B	124	HIS	C-O	7.75	1.33	1.24
1	A	124	HIS	C-O	7.75	1.33	1.24
1	B	221	LYS	CA-C	-7.74	1.43	1.52
1	D	168	GLU	CD-OE2	7.73	1.40	1.25
1	D	392	ALA	CA-CB	7.73	1.65	1.53
1	C	122	ASP	CG-OD2	7.72	1.40	1.25
1	C	386	ALA	C-O	-7.72	1.14	1.24
1	C	124	HIS	C-O	7.71	1.33	1.24
1	D	124	HIS	C-O	7.71	1.33	1.24
1	C	258	TRP	C-O	-7.71	1.14	1.24
1	D	386	ALA	C-O	-7.71	1.14	1.24
1	B	101	LEU	N-CA	7.70	1.56	1.46
1	A	168	GLU	CD-OE2	7.70	1.40	1.25
1	D	258	TRP	C-O	-7.70	1.14	1.24
1	D	354	GLY	CA-C	7.69	1.61	1.51
1	B	168	GLU	CD-OE2	7.69	1.40	1.25
1	B	212	ARG	CZ-NH1	7.69	1.43	1.32
1	B	354	GLY	CA-C	7.69	1.61	1.51
1	B	147	MET	CA-CB	-7.69	1.41	1.53
1	C	168	GLU	CD-OE2	7.69	1.40	1.25
1	D	101	LEU	N-CA	7.67	1.56	1.46
1	A	386	ALA	C-O	-7.67	1.14	1.24
1	B	258	TRP	C-O	-7.67	1.15	1.24
1	B	386	ALA	C-O	-7.66	1.14	1.24
1	A	258	TRP	C-O	-7.66	1.15	1.24
1	A	354	GLY	CA-C	7.66	1.61	1.51
1	C	61	LEU	CG-CD2	7.65	1.77	1.52
1	C	212	ARG	CZ-NH1	7.65	1.43	1.32
1	C	354	GLY	CA-C	7.65	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	212	ARG	CZ-NH1	7.64	1.43	1.32
1	C	101	LEU	N-CA	7.64	1.56	1.46
1	D	61	LEU	CG-CD2	7.64	1.77	1.52
1	A	61	LEU	CG-CD2	7.64	1.77	1.52
1	B	61	LEU	CG-CD2	7.63	1.77	1.52
1	A	101	LEU	N-CA	7.63	1.56	1.46
1	C	261	LEU	C-O	-7.63	1.15	1.24
1	D	126	PRO	CA-C	7.62	1.61	1.52
1	D	212	ARG	CZ-NH1	7.62	1.43	1.32
1	A	261	LEU	C-O	-7.62	1.15	1.24
1	C	312	THR	C-O	7.60	1.33	1.24
1	C	137	GLN	CA-C	-7.60	1.42	1.52
1	A	312	THR	C-O	7.59	1.33	1.24
1	C	307	VAL	CB-CG2	-7.59	1.27	1.52
1	A	307	VAL	CB-CG2	-7.58	1.27	1.52
1	D	261	LEU	C-O	-7.58	1.15	1.24
1	D	137	GLN	CA-C	-7.58	1.42	1.52
1	B	261	LEU	C-O	-7.58	1.15	1.24
1	B	307	VAL	CB-CG2	-7.58	1.27	1.52
1	C	18	ASN	CB-CG	7.58	1.71	1.52
1	D	307	VAL	CB-CG2	-7.57	1.27	1.52
1	B	18	ASN	CB-CG	7.57	1.71	1.52
1	A	126	PRO	CA-C	7.57	1.61	1.52
1	A	137	GLN	CA-C	-7.57	1.42	1.52
1	A	18	ASN	CB-CG	7.57	1.71	1.52
1	B	151	ASP	CA-C	7.57	1.60	1.53
1	C	151	ASP	CA-C	7.57	1.60	1.53
1	D	312	THR	C-O	7.56	1.33	1.24
1	D	18	ASN	CB-CG	7.56	1.71	1.52
1	B	137	GLN	CA-C	-7.54	1.42	1.52
1	B	312	THR	C-O	7.54	1.33	1.24
1	B	126	PRO	CA-C	7.54	1.61	1.52
1	C	126	PRO	CA-C	7.53	1.61	1.52
1	A	151	ASP	CA-C	7.52	1.60	1.53
1	B	324	GLU	C-O	-7.52	1.14	1.24
1	C	198	ARG	CZ-NH1	7.52	1.43	1.32
1	B	310	ILE	CA-C	7.52	1.61	1.52
1	D	127	TYR	N-CA	7.51	1.55	1.46
1	D	129	TYR	CA-C	7.51	1.61	1.52
1	D	151	ASP	CA-C	7.51	1.60	1.53
1	A	198	ARG	CZ-NH1	7.50	1.43	1.32
1	D	172	GLU	CD-OE2	7.50	1.39	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	129	TYR	CA-C	7.49	1.61	1.52
1	A	129	TYR	CA-C	7.49	1.61	1.52
1	B	198	ARG	CZ-NH1	7.49	1.43	1.32
1	A	310	ILE	CA-C	7.48	1.61	1.52
1	B	129	TYR	CA-C	7.47	1.61	1.52
1	D	324	GLU	C-O	-7.47	1.14	1.24
1	C	172	GLU	CD-OE2	7.47	1.39	1.25
1	A	172	GLU	CD-OE2	7.46	1.39	1.25
1	B	172	GLU	CD-OE2	7.46	1.39	1.25
1	C	127	TYR	N-CA	7.46	1.55	1.46
1	B	127	TYR	N-CA	7.46	1.55	1.46
1	D	175	TYR	CZ-OH	7.46	1.53	1.38
1	A	127	TYR	N-CA	7.45	1.55	1.46
1	C	310	ILE	CA-C	7.45	1.61	1.52
1	C	59	TRP	CA-C	-7.45	1.43	1.52
1	D	198	ARG	CZ-NH1	7.45	1.43	1.32
1	A	324	GLU	C-O	-7.45	1.14	1.24
1	C	324	GLU	C-O	-7.45	1.14	1.24
1	D	262	GLN	N-CA	-7.45	1.36	1.46
1	B	59	TRP	CA-C	-7.44	1.43	1.52
1	B	175	TYR	CZ-OH	7.44	1.53	1.38
1	C	406	ALA	C-O	7.43	1.33	1.24
1	B	336	LYS	CD-CE	7.43	1.74	1.52
1	C	262	GLN	N-CA	-7.43	1.36	1.46
1	C	174	ALA	CA-CB	-7.43	1.41	1.53
1	A	175	TYR	CZ-OH	7.43	1.53	1.38
1	A	336	LYS	CD-CE	7.43	1.74	1.52
1	C	336	LYS	CD-CE	7.43	1.74	1.52
1	D	310	ILE	CA-C	7.43	1.61	1.52
1	A	262	GLN	N-CA	-7.42	1.36	1.46
1	B	152	ARG	CA-C	-7.42	1.43	1.52
1	B	262	GLN	N-CA	-7.42	1.36	1.46
1	D	174	ALA	CA-CB	-7.42	1.41	1.53
1	D	336	LYS	CD-CE	7.42	1.74	1.52
1	A	174	ALA	CA-CB	-7.42	1.41	1.53
1	B	406	ALA	C-O	7.41	1.33	1.24
1	D	246	GLY	C-O	7.41	1.33	1.23
1	A	246	GLY	C-O	7.41	1.33	1.23
1	A	59	TRP	CA-C	-7.41	1.43	1.52
1	D	59	TRP	CA-C	-7.41	1.43	1.52
1	B	174	ALA	CA-CB	-7.41	1.41	1.53
1	C	175	TYR	CZ-OH	7.41	1.53	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	26	LEU	CA-C	-7.39	1.43	1.52
1	A	175	TYR	CD1-CE1	7.39	1.60	1.38
1	C	175	TYR	CD1-CE1	7.39	1.60	1.38
1	B	175	TYR	CD1-CE1	7.39	1.60	1.38
1	C	246	GLY	C-O	7.39	1.33	1.23
1	D	175	TYR	CD1-CE1	7.39	1.60	1.38
1	C	26	LEU	CA-C	-7.38	1.43	1.52
1	B	246	GLY	C-O	7.38	1.33	1.23
1	D	152	ARG	CA-C	-7.37	1.43	1.52
1	D	26	LEU	CA-C	-7.37	1.43	1.52
1	A	26	LEU	CA-C	-7.37	1.43	1.52
1	A	406	ALA	C-O	7.37	1.33	1.24
1	A	152	ARG	CA-C	-7.36	1.43	1.52
1	D	208	ARG	CD-NE	7.36	1.56	1.46
1	B	208	ARG	CD-NE	7.35	1.56	1.46
1	D	406	ALA	C-O	7.35	1.33	1.24
1	A	208	ARG	CD-NE	7.34	1.56	1.46
1	C	152	ARG	CA-C	-7.33	1.43	1.52
1	C	208	ARG	CD-NE	7.33	1.56	1.46
1	C	270	ASP	CA-C	-7.33	1.43	1.52
1	A	147	MET	CA-CB	-7.32	1.41	1.53
1	C	147	MET	CA-CB	-7.31	1.41	1.53
1	D	300	LYS	CA-C	-7.31	1.45	1.53
1	B	300	LYS	CA-C	-7.31	1.45	1.53
1	D	231	VAL	CA-CB	-7.31	1.46	1.54
1	D	221	LYS	C-O	-7.31	1.15	1.23
1	A	231	VAL	CA-CB	-7.30	1.46	1.54
1	B	325	GLU	C-O	-7.30	1.16	1.23
1	D	325	GLU	C-O	-7.30	1.16	1.23
1	C	325	GLU	C-O	-7.30	1.16	1.23
1	D	147	MET	CA-CB	-7.30	1.41	1.53
1	C	243	ASN	CG-OD1	7.30	1.37	1.23
1	A	243	ASN	CG-OD1	7.29	1.37	1.23
1	A	270	ASP	CA-C	-7.29	1.43	1.52
1	B	243	ASN	CG-OD1	7.29	1.37	1.23
1	A	300	LYS	CA-C	-7.29	1.45	1.53
1	D	270	ASP	CA-C	-7.29	1.43	1.52
1	C	221	LYS	C-O	-7.28	1.15	1.23
1	A	221	LYS	C-O	-7.28	1.15	1.23
1	D	243	ASN	CG-OD1	7.28	1.37	1.23
1	A	325	GLU	C-O	-7.28	1.16	1.23
1	B	270	ASP	CA-C	-7.27	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	411	GLU	CA-C	7.27	1.62	1.52
1	C	231	VAL	CA-CB	-7.26	1.46	1.54
1	D	326	ILE	CA-CB	-7.26	1.44	1.54
1	D	400	VAL	CA-CB	-7.26	1.44	1.54
1	C	209	VAL	C-O	7.25	1.32	1.24
1	B	326	ILE	CA-CB	-7.25	1.44	1.54
1	C	300	LYS	CA-C	-7.25	1.45	1.53
1	B	221	LYS	C-O	-7.25	1.15	1.23
1	D	209	VAL	C-O	7.24	1.32	1.24
1	B	231	VAL	CA-CB	-7.24	1.46	1.54
1	D	411	GLU	CA-C	7.24	1.62	1.52
1	A	411	GLU	CA-C	7.24	1.62	1.52
1	B	209	VAL	C-O	7.24	1.32	1.24
1	A	400	VAL	CA-CB	-7.23	1.44	1.54
1	C	143	ILE	C-O	-7.23	1.15	1.24
1	B	143	ILE	C-O	-7.23	1.15	1.24
1	C	326	ILE	CA-CB	-7.23	1.44	1.54
1	A	326	ILE	CA-CB	-7.22	1.44	1.54
1	A	209	VAL	C-O	7.22	1.32	1.24
1	C	411	GLU	CA-C	7.21	1.62	1.52
1	C	400	VAL	CA-CB	-7.21	1.44	1.54
1	D	143	ILE	C-O	-7.21	1.15	1.24
1	D	217	THR	C-O	7.20	1.32	1.24
1	B	168	GLU	CG-CD	7.19	1.70	1.52
1	A	143	ILE	C-O	-7.19	1.15	1.24
1	B	400	VAL	CA-CB	-7.18	1.44	1.54
1	A	168	GLU	CG-CD	7.18	1.70	1.52
1	C	168	GLU	CG-CD	7.18	1.70	1.52
1	C	225	ILE	C-O	-7.17	1.14	1.24
1	C	249	VAL	C-O	-7.17	1.15	1.24
1	D	168	GLU	CG-CD	7.17	1.70	1.52
1	A	225	ILE	C-O	-7.16	1.14	1.24
1	A	249	VAL	C-O	-7.16	1.15	1.24
1	A	103	SER	C-O	7.15	1.32	1.24
1	C	55	TRP	CA-CB	-7.15	1.41	1.53
1	D	249	VAL	C-O	-7.15	1.15	1.24
1	B	225	ILE	C-O	-7.15	1.14	1.24
1	A	217	THR	C-O	7.14	1.32	1.24
1	A	55	TRP	CA-CB	-7.14	1.41	1.53
1	B	103	SER	C-O	7.14	1.32	1.24
1	B	55	TRP	CA-CB	-7.14	1.41	1.53
1	D	55	TRP	CA-CB	-7.14	1.41	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	274	ALA	N-CA	7.13	1.55	1.46
1	D	103	SER	C-O	7.13	1.32	1.24
1	C	217	THR	C-O	7.12	1.32	1.24
1	B	249	VAL	C-O	-7.12	1.15	1.24
1	A	274	ALA	N-CA	7.11	1.55	1.46
1	B	217	THR	C-O	7.11	1.32	1.24
1	D	225	ILE	C-O	-7.11	1.14	1.24
1	D	419	VAL	CB-CG2	7.11	1.76	1.52
1	A	419	VAL	CB-CG2	7.11	1.76	1.52
1	C	274	ALA	N-CA	7.11	1.55	1.46
1	B	419	VAL	CB-CG2	7.10	1.75	1.52
1	D	241	VAL	C-O	7.10	1.33	1.24
1	B	241	VAL	C-O	7.10	1.33	1.24
1	C	159	PRO	CA-C	7.09	1.61	1.52
1	C	419	VAL	CB-CG2	7.09	1.75	1.52
1	C	103	SER	C-O	7.08	1.32	1.24
1	B	172	GLU	CA-C	7.07	1.62	1.52
1	A	172	GLU	CA-C	7.07	1.62	1.52
1	C	241	VAL	C-O	7.07	1.33	1.24
1	D	172	GLU	CA-C	7.07	1.62	1.52
1	D	274	ALA	N-CA	7.06	1.54	1.46
1	D	302	ALA	N-CA	-7.06	1.36	1.46
1	C	77	LYS	CD-CE	7.06	1.73	1.52
1	A	241	VAL	C-O	7.06	1.33	1.24
1	C	172	GLU	CA-C	7.06	1.62	1.52
1	B	77	LYS	CD-CE	7.05	1.73	1.52
1	D	87	ALA	C-N	7.05	1.41	1.33
1	A	159	PRO	CA-C	7.05	1.61	1.52
1	B	328	ARG	CZ-NH1	7.05	1.42	1.32
1	A	302	ALA	N-CA	-7.05	1.36	1.46
1	A	77	LYS	CD-CE	7.04	1.73	1.52
1	B	302	ALA	N-CA	-7.04	1.36	1.46
1	A	87	ALA	C-N	7.03	1.41	1.33
1	C	302	ALA	N-CA	-7.03	1.36	1.46
1	D	18	ASN	CA-C	-7.03	1.43	1.52
1	D	77	LYS	CD-CE	7.03	1.73	1.52
1	B	159	PRO	CA-C	7.02	1.61	1.52
1	A	363	PHE	CA-C	7.02	1.61	1.52
1	B	341	ARG	CZ-NH2	7.02	1.42	1.33
1	C	10	TRP	CD2-CE3	7.01	1.51	1.40
1	B	87	ALA	C-N	7.01	1.41	1.33
1	D	159	PRO	CA-C	7.01	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	328	ARG	CZ-NH1	7.00	1.42	1.32
1	C	328	ARG	CZ-NH1	7.00	1.42	1.32
1	B	18	ASN	CA-C	-7.00	1.43	1.52
1	C	363	PHE	CA-C	7.00	1.61	1.52
1	C	87	ALA	C-N	7.00	1.41	1.33
1	D	65	ALA	N-CA	6.99	1.54	1.46
1	A	10	TRP	CD2-CE3	6.99	1.51	1.40
1	C	340	ILE	CA-CB	-6.99	1.43	1.53
1	D	75	LEU	CA-C	-6.99	1.47	1.53
1	A	341	ARG	CZ-NH2	6.99	1.42	1.33
1	B	389	LEU	CG-CD2	-6.99	1.29	1.52
1	B	363	PHE	CA-C	6.99	1.61	1.52
1	B	62	PRO	CA-C	-6.99	1.43	1.52
1	B	65	ALA	N-CA	6.98	1.54	1.46
1	D	328	ARG	CZ-NH1	6.98	1.42	1.32
1	D	389	LEU	CG-CD2	-6.98	1.29	1.52
1	B	10	TRP	CD2-CE3	6.98	1.51	1.40
1	D	10	TRP	CD2-CE3	6.97	1.51	1.40
1	D	363	PHE	CA-C	6.97	1.61	1.52
1	A	389	LEU	CG-CD2	-6.97	1.29	1.52
1	D	341	ARG	CZ-NH2	6.97	1.42	1.33
1	B	247	GLN	CG-CD	6.97	1.69	1.52
1	C	62	PRO	CA-C	-6.97	1.43	1.52
1	C	177	LEU	C-O	6.97	1.32	1.24
1	A	18	ASN	CA-C	-6.96	1.43	1.52
1	A	65	ALA	N-CA	6.96	1.54	1.46
1	C	389	LEU	CG-CD2	-6.96	1.29	1.52
1	D	212	ARG	NE-CZ	6.96	1.40	1.33
1	D	247	GLN	CG-CD	6.96	1.69	1.52
1	A	247	GLN	CG-CD	6.95	1.69	1.52
1	A	340	ILE	CA-CB	-6.95	1.43	1.53
1	C	212	ARG	NE-CZ	6.95	1.40	1.33
1	A	62	PRO	CA-C	-6.94	1.43	1.52
1	B	340	ILE	CA-CB	-6.93	1.43	1.53
1	D	177	LEU	C-O	6.93	1.32	1.24
1	C	18	ASN	CA-C	-6.93	1.43	1.52
1	A	177	LEU	C-O	6.92	1.32	1.24
1	C	341	ARG	CZ-NH2	6.92	1.42	1.33
1	D	62	PRO	CA-C	-6.92	1.43	1.52
1	C	247	GLN	CG-CD	6.92	1.69	1.52
1	D	340	ILE	CA-CB	-6.91	1.43	1.53
1	A	75	LEU	CA-C	-6.91	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	65	ALA	N-CA	6.91	1.54	1.46
1	C	75	LEU	CA-C	-6.90	1.47	1.53
1	A	212	ARG	NE-CZ	6.89	1.40	1.33
1	B	177	LEU	C-O	6.87	1.31	1.24
1	B	212	ARG	NE-CZ	6.85	1.40	1.33
1	B	75	LEU	CA-C	-6.84	1.47	1.53
1	D	57	THR	C-N	6.84	1.42	1.33
1	B	359	LEU	C-O	6.83	1.31	1.24
1	C	231	VAL	CA-C	-6.83	1.44	1.52
1	C	57	THR	C-N	6.83	1.42	1.33
1	A	62	PRO	CA-CB	-6.82	1.44	1.53
1	B	57	THR	C-N	6.82	1.42	1.33
1	A	359	LEU	C-O	6.82	1.31	1.24
1	B	192	THR	C-O	6.82	1.32	1.24
1	D	396	ALA	CA-CB	6.82	1.64	1.53
1	D	332	PHE	CA-C	-6.82	1.44	1.52
1	D	359	LEU	C-O	6.82	1.31	1.24
1	D	261	LEU	CG-CD2	-6.81	1.30	1.52
1	B	62	PRO	CA-CB	-6.81	1.44	1.53
1	A	57	THR	C-N	6.81	1.42	1.33
1	A	332	PHE	CA-C	-6.81	1.44	1.52
1	D	192	THR	C-O	6.81	1.32	1.24
1	A	261	LEU	CG-CD2	-6.80	1.30	1.52
1	B	261	LEU	CG-CD2	-6.80	1.30	1.52
1	C	62	PRO	CA-CB	-6.80	1.44	1.53
1	C	261	LEU	CG-CD2	-6.79	1.30	1.52
1	C	96	GLY	CA-C	6.79	1.61	1.51
1	C	192	THR	C-O	6.79	1.32	1.24
1	A	231	VAL	CA-C	-6.79	1.44	1.52
1	D	62	PRO	CA-CB	-6.79	1.44	1.53
1	A	396	ALA	CA-CB	6.79	1.64	1.53
1	B	231	VAL	CA-C	-6.79	1.44	1.52
1	C	332	PHE	CA-C	-6.79	1.44	1.52
1	B	332	PHE	CA-C	-6.78	1.44	1.52
1	C	396	ALA	CA-CB	6.78	1.64	1.53
1	B	396	ALA	CA-CB	6.78	1.64	1.53
1	A	308	ASP	CA-C	-6.78	1.42	1.52
1	B	387	LYS	CD-CE	6.78	1.72	1.52
1	C	359	LEU	C-O	6.78	1.31	1.24
1	D	231	VAL	CA-C	-6.78	1.44	1.52
1	C	308	ASP	CA-C	-6.77	1.42	1.52
1	B	340	ILE	CG1-CD1	-6.77	1.25	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	387	LYS	CD-CE	6.77	1.72	1.52
1	D	340	ILE	CG1-CD1	-6.77	1.25	1.51
1	A	192	THR	C-O	6.76	1.32	1.24
1	A	340	ILE	CG1-CD1	-6.76	1.25	1.51
1	C	145	GLU	CG-CD	6.76	1.69	1.52
1	D	96	GLY	CA-C	6.76	1.61	1.51
1	A	387	LYS	CD-CE	6.76	1.72	1.52
1	B	308	ASP	CA-C	-6.76	1.42	1.52
1	B	145	GLU	CG-CD	6.76	1.69	1.52
1	D	145	GLU	CG-CD	6.76	1.69	1.52
1	A	96	GLY	CA-C	6.75	1.61	1.51
1	C	340	ILE	CG1-CD1	-6.75	1.25	1.51
1	D	308	ASP	CA-C	-6.75	1.42	1.52
1	B	207	TYR	CA-C	-6.75	1.44	1.52
1	D	225	ILE	CA-CB	-6.75	1.46	1.54
1	A	145	GLU	CG-CD	6.75	1.69	1.52
1	A	207	TYR	CA-C	-6.75	1.44	1.52
1	C	340	ILE	N-CA	6.74	1.55	1.46
1	C	387	LYS	CD-CE	6.74	1.72	1.52
1	C	75	LEU	CG-CD1	-6.73	1.30	1.52
1	B	340	ILE	N-CA	6.73	1.55	1.46
1	B	96	GLY	CA-C	6.72	1.61	1.51
1	C	188	ASP	CA-CB	6.72	1.62	1.53
1	D	340	ILE	N-CA	6.72	1.55	1.46
1	C	423	LYS	CA-CB	6.72	1.63	1.53
1	C	59	TRP	CD2-CE3	6.71	1.50	1.40
1	D	188	ASP	CA-CB	6.71	1.62	1.53
1	D	11	TYR	CA-C	-6.71	1.43	1.52
1	A	75	LEU	CG-CD1	-6.71	1.30	1.52
1	B	59	TRP	CD2-CE3	6.71	1.50	1.40
1	B	72	VAL	C-O	-6.71	1.17	1.23
1	B	225	ILE	CA-CB	-6.71	1.46	1.54
1	D	75	LEU	CG-CD1	-6.71	1.30	1.52
1	D	72	VAL	C-O	-6.70	1.17	1.23
1	C	207	TYR	CA-C	-6.70	1.44	1.52
1	B	75	LEU	CG-CD1	-6.70	1.30	1.52
1	A	340	ILE	N-CA	6.70	1.54	1.46
1	D	207	TYR	CA-C	-6.70	1.44	1.52
1	A	11	TYR	CA-C	-6.70	1.43	1.52
1	B	423	LYS	CA-CB	6.70	1.63	1.53
1	B	213	VAL	C-O	-6.69	1.16	1.24
1	B	11	TYR	CA-C	-6.69	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	59	TRP	CD2-CE3	6.68	1.50	1.40
1	A	72	VAL	C-O	-6.68	1.17	1.23
1	C	225	ILE	CA-CB	-6.68	1.46	1.54
1	D	423	LYS	CA-CB	6.68	1.63	1.53
1	A	423	LYS	CA-CB	6.68	1.63	1.53
1	B	137	GLN	CD-NE2	6.68	1.47	1.33
1	A	225	ILE	CA-CB	-6.68	1.46	1.54
1	C	137	GLN	CD-NE2	6.67	1.47	1.33
1	D	137	GLN	CD-NE2	6.67	1.47	1.33
1	A	188	ASP	CA-CB	6.67	1.62	1.53
1	B	188	ASP	CA-CB	6.67	1.62	1.53
1	A	137	GLN	CD-NE2	6.66	1.47	1.33
1	A	213	VAL	C-O	-6.66	1.16	1.24
1	C	186	LYS	CA-C	-6.66	1.44	1.52
1	C	11	TYR	CA-C	-6.65	1.43	1.52
1	D	213	VAL	C-O	-6.65	1.16	1.24
1	C	72	VAL	C-O	-6.65	1.17	1.23
1	C	49	GLU	CA-C	-6.63	1.43	1.52
1	D	59	TRP	CD2-CE3	6.63	1.50	1.40
1	A	264	MET	C-O	6.63	1.32	1.24
1	D	56	THR	CB-CG2	6.63	1.74	1.52
1	D	192	THR	CB-CG2	-6.62	1.30	1.52
1	B	49	GLU	CA-C	-6.62	1.43	1.52
1	A	56	THR	CB-CG2	6.62	1.74	1.52
1	B	192	THR	CB-CG2	-6.62	1.30	1.52
1	B	186	LYS	CA-C	-6.62	1.44	1.52
1	D	43	ALA	CA-C	6.61	1.61	1.52
1	A	43	ALA	CA-C	6.61	1.61	1.52
1	C	19	TYR	C-O	6.61	1.31	1.23
1	C	56	THR	CB-CG2	6.61	1.74	1.52
1	C	264	MET	C-O	6.61	1.32	1.24
1	C	43	ALA	CA-C	6.61	1.61	1.52
1	A	186	LYS	CA-C	-6.61	1.44	1.52
1	A	192	THR	CB-CG2	-6.61	1.30	1.52
1	C	166	SER	C-O	6.61	1.32	1.23
1	B	56	THR	CB-CG2	6.60	1.74	1.52
1	B	19	TYR	C-O	6.60	1.31	1.23
1	A	19	TYR	C-O	6.60	1.31	1.23
1	B	264	MET	C-O	6.60	1.32	1.24
1	A	211	ASP	C-O	-6.59	1.16	1.24
1	C	10	TRP	CE2-CZ2	6.59	1.53	1.39
1	C	213	VAL	C-O	-6.59	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	192	THR	CB-CG2	-6.59	1.30	1.52
1	A	49	GLU	CA-C	-6.59	1.44	1.52
1	A	396	ALA	C-O	-6.59	1.16	1.24
1	B	211	ASP	C-O	-6.59	1.16	1.24
1	D	211	ASP	C-O	-6.59	1.16	1.24
1	D	343	VAL	CA-C	6.59	1.61	1.52
1	C	271	LEU	CG-CD1	-6.58	1.30	1.52
1	B	343	VAL	CA-C	6.58	1.61	1.52
1	C	211	ASP	C-O	-6.58	1.16	1.24
1	C	401	ASP	CG-OD2	6.58	1.37	1.25
1	A	343	VAL	CA-C	6.58	1.61	1.52
1	C	343	VAL	CA-C	6.58	1.61	1.52
1	D	19	TYR	C-O	6.58	1.31	1.23
1	D	264	MET	C-O	6.58	1.32	1.24
1	B	43	ALA	CA-C	6.57	1.61	1.52
1	D	49	GLU	CA-C	-6.57	1.44	1.52
1	A	10	TRP	CE2-CZ2	6.57	1.53	1.39
1	B	396	ALA	C-O	-6.57	1.16	1.24
1	C	396	ALA	N-CA	6.57	1.54	1.46
1	D	85	LYS	CE-NZ	6.57	1.69	1.49
1	A	85	LYS	CE-NZ	6.56	1.69	1.49
1	C	85	LYS	CE-NZ	6.56	1.69	1.49
1	A	271	LEU	CG-CD1	-6.56	1.30	1.52
1	D	324	GLU	CG-CD	6.56	1.68	1.52
1	D	186	LYS	CA-C	-6.56	1.44	1.52
1	D	271	LEU	CG-CD1	-6.55	1.30	1.52
1	D	396	ALA	C-O	-6.55	1.16	1.24
1	A	166	SER	C-O	6.55	1.32	1.23
1	C	324	GLU	CG-CD	6.55	1.68	1.52
1	A	324	GLU	CG-CD	6.55	1.68	1.52
1	B	333	LEU	CA-C	-6.55	1.44	1.52
1	A	401	ASP	CG-OD2	6.54	1.37	1.25
1	C	396	ALA	C-O	-6.54	1.16	1.24
1	D	173	ILE	CA-C	-6.54	1.43	1.52
1	B	401	ASP	CG-OD2	6.54	1.37	1.25
1	B	324	GLU	CG-CD	6.54	1.68	1.52
1	D	401	ASP	CG-OD2	6.53	1.37	1.25
1	B	271	LEU	CG-CD1	-6.53	1.30	1.52
1	B	85	LYS	CE-NZ	6.53	1.69	1.49
1	B	166	SER	C-O	6.53	1.32	1.23
1	D	10	TRP	CE2-CZ2	6.53	1.53	1.39
1	D	166	SER	C-O	6.53	1.32	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	29	GLU	C-O	-6.53	1.16	1.24
1	B	10	TRP	CE2-CZ2	6.52	1.53	1.39
1	A	396	ALA	N-CA	6.52	1.53	1.46
1	D	285	PHE	CB-CG	6.52	1.65	1.50
1	D	333	LEU	CA-C	-6.51	1.44	1.52
1	A	173	ILE	CA-C	-6.51	1.43	1.52
1	A	333	LEU	CA-C	-6.51	1.44	1.52
1	C	177	LEU	N-CA	-6.51	1.38	1.46
1	C	285	PHE	CB-CG	6.51	1.65	1.50
1	A	285	PHE	CB-CG	6.51	1.65	1.50
1	C	173	ILE	CA-C	-6.50	1.43	1.52
1	C	332	PHE	C-O	-6.50	1.16	1.24
1	D	177	LEU	N-CA	-6.50	1.38	1.46
1	B	177	LEU	N-CA	-6.50	1.38	1.46
1	A	29	GLU	C-O	-6.49	1.16	1.24
1	D	164	GLY	CA-C	6.49	1.61	1.51
1	C	333	LEU	CA-C	-6.49	1.44	1.52
1	D	404	GLU	CD-OE2	6.49	1.37	1.25
1	A	164	GLY	CA-C	6.48	1.61	1.51
1	D	396	ALA	N-CA	6.48	1.53	1.46
1	A	177	LEU	N-CA	-6.48	1.38	1.46
1	B	164	GLY	CA-C	6.48	1.61	1.51
1	B	396	ALA	N-CA	6.48	1.53	1.46
1	D	29	GLU	C-O	-6.48	1.16	1.24
1	C	29	GLU	C-O	-6.47	1.16	1.24
1	C	404	GLU	CD-OE2	6.47	1.37	1.25
1	D	251	ILE	CA-CB	-6.47	1.46	1.54
1	B	404	GLU	CD-OE2	6.47	1.37	1.25
1	A	332	PHE	C-O	-6.47	1.16	1.24
1	C	380	ASP	CA-C	6.47	1.61	1.52
1	B	332	PHE	C-O	-6.47	1.16	1.24
1	A	404	GLU	CD-OE2	6.46	1.37	1.25
1	B	173	ILE	CA-C	-6.46	1.43	1.52
1	B	285	PHE	CB-CG	6.46	1.65	1.50
1	A	251	ILE	CA-CB	-6.45	1.46	1.54
1	C	164	GLY	CA-C	6.45	1.60	1.51
1	B	82	TYR	CB-CG	-6.44	1.37	1.51
1	C	251	ILE	CA-CB	-6.44	1.46	1.54
1	D	332	PHE	C-O	-6.44	1.16	1.24
1	A	380	ASP	CA-C	6.43	1.61	1.52
1	A	82	TYR	CB-CG	-6.43	1.37	1.51
1	B	251	ILE	CA-CB	-6.43	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	423	LYS	CB-CG	6.43	1.71	1.52
1	C	423	LYS	CB-CG	6.42	1.71	1.52
1	D	366	ASP	CB-CG	6.42	1.68	1.52
1	A	423	LYS	CB-CG	6.41	1.71	1.52
1	B	423	LYS	CB-CG	6.41	1.71	1.52
1	A	222	GLU	CB-CG	-6.41	1.33	1.52
1	D	82	TYR	CB-CG	-6.41	1.37	1.51
1	C	82	TYR	CB-CG	-6.40	1.37	1.51
1	D	208	ARG	CZ-NH1	6.40	1.41	1.32
1	D	222	GLU	CB-CG	-6.40	1.33	1.52
1	B	222	GLU	CB-CG	-6.40	1.33	1.52
1	B	380	ASP	CA-C	6.40	1.61	1.52
1	C	222	GLU	CB-CG	-6.39	1.33	1.52
1	C	328	ARG	CD-NE	6.39	1.55	1.46
1	C	277	ALA	CA-CB	-6.38	1.43	1.53
1	D	328	ARG	CD-NE	6.38	1.55	1.46
1	A	208	ARG	CZ-NH1	6.38	1.41	1.32
1	D	46	ILE	CA-C	6.38	1.60	1.52
1	C	95	GLU	CD-OE1	6.38	1.37	1.25
1	D	95	GLU	CD-OE1	6.38	1.37	1.25
1	A	95	GLU	CD-OE1	6.38	1.37	1.25
1	A	366	ASP	CB-CG	6.38	1.68	1.52
1	B	46	ILE	CA-C	6.38	1.60	1.52
1	D	380	ASP	CA-C	6.38	1.61	1.52
1	B	419	VAL	CB-CG1	6.37	1.73	1.52
1	C	419	VAL	CB-CG1	6.37	1.73	1.52
1	C	366	ASP	CB-CG	6.37	1.68	1.52
1	D	179	SER	C-O	-6.37	1.16	1.24
1	B	95	GLU	CD-OE1	6.37	1.37	1.25
1	B	208	ARG	CZ-NH1	6.36	1.41	1.32
1	B	366	ASP	CB-CG	6.36	1.68	1.52
1	A	419	VAL	CB-CG1	6.36	1.73	1.52
1	B	277	ALA	CA-CB	-6.36	1.43	1.53
1	C	46	ILE	CA-C	6.36	1.60	1.52
1	D	419	VAL	CB-CG1	6.36	1.73	1.52
1	A	328	ARG	CD-NE	6.36	1.55	1.46
1	B	328	ARG	CD-NE	6.36	1.55	1.46
1	C	208	ARG	CZ-NH1	6.36	1.41	1.32
1	D	277	ALA	CA-CB	-6.36	1.43	1.53
1	A	277	ALA	CA-CB	-6.35	1.43	1.53
1	A	249	VAL	N-CA	-6.35	1.38	1.46
1	B	57	THR	C-O	6.35	1.31	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	243	ASN	CA-C	-6.35	1.45	1.52
1	A	179	SER	C-O	-6.34	1.16	1.24
1	A	46	ILE	CA-C	6.34	1.60	1.52
1	B	83	ILE	C-O	-6.34	1.17	1.24
1	C	407	LYS	CA-C	6.34	1.61	1.52
1	A	407	LYS	CA-C	6.34	1.61	1.52
1	C	179	SER	C-O	-6.33	1.16	1.24
1	A	243	ASN	CA-C	-6.33	1.45	1.52
1	B	249	VAL	N-CA	-6.33	1.38	1.46
1	A	57	THR	C-O	6.32	1.31	1.24
1	D	407	LYS	CA-C	6.32	1.61	1.52
1	B	179	SER	C-O	-6.32	1.16	1.24
1	D	57	THR	C-O	6.32	1.31	1.24
1	D	249	VAL	N-CA	-6.32	1.38	1.46
1	C	249	VAL	N-CA	-6.31	1.38	1.46
1	D	243	ASN	CA-C	-6.31	1.45	1.52
1	C	57	THR	C-O	6.31	1.31	1.24
1	C	243	ASN	CA-C	-6.31	1.45	1.52
1	A	83	ILE	C-O	-6.30	1.17	1.24
1	B	407	LYS	CA-C	6.29	1.61	1.52
1	C	83	ILE	C-O	-6.29	1.17	1.24
1	D	205	LYS	C-O	6.29	1.31	1.24
1	D	265	ARG	C-O	6.29	1.31	1.24
1	D	264	MET	SD-CE	-6.29	1.63	1.79
1	C	264	MET	SD-CE	-6.28	1.63	1.79
1	A	264	MET	SD-CE	-6.27	1.63	1.79
1	B	264	MET	SD-CE	-6.27	1.63	1.79
1	C	205	LYS	C-O	6.27	1.31	1.24
1	D	83	ILE	C-O	-6.27	1.17	1.24
1	A	355	LEU	CG-CD1	-6.26	1.31	1.52
1	A	205	LYS	C-O	6.26	1.31	1.24
1	D	307	VAL	CA-CB	-6.26	1.47	1.54
1	B	145	GLU	CD-OE1	6.26	1.37	1.25
1	C	355	LEU	CG-CD1	-6.25	1.31	1.52
1	B	355	LEU	CG-CD1	-6.25	1.31	1.52
1	A	369	ILE	CA-CB	-6.25	1.46	1.54
1	B	265	ARG	C-O	6.25	1.31	1.24
1	A	45	ARG	C-O	-6.25	1.16	1.24
1	C	265	ARG	C-O	6.25	1.31	1.24
1	C	424	ALA	N-CA	6.25	1.58	1.46
1	D	267	VAL	CB-CG1	-6.25	1.31	1.52
1	A	265	ARG	C-O	6.25	1.31	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	33	GLU	CA-C	-6.25	1.45	1.52
1	C	45	ARG	C-O	-6.25	1.16	1.24
1	C	369	ILE	CA-CB	-6.24	1.46	1.54
1	D	355	LEU	CG-CD1	-6.24	1.31	1.52
1	A	424	ALA	N-CA	6.24	1.58	1.46
1	B	45	ARG	C-O	-6.24	1.16	1.24
1	B	369	ILE	CA-CB	-6.24	1.46	1.54
1	A	145	GLU	CD-OE1	6.24	1.37	1.25
1	C	145	GLU	CD-OE1	6.24	1.37	1.25
1	B	205	LYS	C-O	6.23	1.31	1.24
1	D	33	GLU	CA-C	-6.23	1.45	1.52
1	A	341	ARG	NE-CZ	6.23	1.40	1.33
1	B	47	ALA	CA-CB	-6.23	1.42	1.53
1	B	267	VAL	CB-CG1	-6.23	1.31	1.52
1	B	424	ALA	N-CA	6.23	1.58	1.46
1	D	160	LYS	CE-NZ	6.23	1.68	1.49
1	A	267	VAL	CB-CG1	-6.23	1.31	1.52
1	D	145	GLU	CD-OE1	6.23	1.37	1.25
1	B	255	VAL	C-O	6.23	1.31	1.24
1	C	267	VAL	CB-CG1	-6.23	1.31	1.52
1	B	341	ARG	NE-CZ	6.23	1.39	1.33
1	C	160	LYS	CE-NZ	6.23	1.68	1.49
1	C	341	ARG	NE-CZ	6.23	1.39	1.33
1	A	160	LYS	CE-NZ	6.22	1.68	1.49
1	A	33	GLU	CA-C	-6.22	1.45	1.52
1	B	329	ILE	C-N	-6.22	1.26	1.33
1	D	266	GLU	CB-CG	-6.22	1.33	1.52
1	C	329	ILE	C-N	-6.22	1.26	1.33
1	D	369	ILE	CA-CB	-6.22	1.46	1.54
1	A	266	GLU	CB-CG	-6.21	1.33	1.52
1	B	160	LYS	CE-NZ	6.21	1.68	1.49
1	A	259	SER	N-CA	-6.21	1.38	1.46
1	B	266	GLU	CB-CG	-6.21	1.33	1.52
1	C	266	GLU	CB-CG	-6.21	1.33	1.52
1	D	424	ALA	N-CA	6.20	1.58	1.46
1	A	47	ALA	CA-CB	-6.20	1.42	1.53
1	D	45	ARG	C-O	-6.20	1.16	1.24
1	C	371	ALA	CA-CB	-6.19	1.44	1.53
1	A	371	ALA	CA-CB	-6.19	1.44	1.53
1	D	371	ALA	CA-CB	-6.19	1.44	1.53
1	A	307	VAL	CA-CB	-6.18	1.47	1.54
1	B	112	MET	N-CA	6.18	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	172	GLU	CA-CB	-6.18	1.43	1.53
1	C	112	MET	N-CA	6.18	1.54	1.46
1	D	259	SER	N-CA	-6.18	1.38	1.46
1	B	259	SER	N-CA	-6.18	1.38	1.46
1	C	47	ALA	CA-CB	-6.18	1.42	1.53
1	C	255	VAL	C-O	6.18	1.31	1.24
1	A	255	VAL	C-O	6.18	1.31	1.24
1	C	33	GLU	CA-C	-6.18	1.45	1.52
1	D	58	LEU	CA-C	-6.18	1.45	1.52
1	A	112	MET	N-CA	6.17	1.54	1.46
1	B	307	VAL	CA-CB	-6.17	1.47	1.54
1	C	58	LEU	CA-C	-6.17	1.45	1.52
1	D	329	ILE	C-N	-6.17	1.26	1.33
1	C	259	SER	N-CA	-6.17	1.38	1.46
1	B	332	PHE	CA-CB	-6.17	1.43	1.53
1	B	371	ALA	CA-CB	-6.16	1.44	1.53
1	C	45	ARG	CZ-NH2	6.16	1.41	1.33
1	D	47	ALA	CA-CB	-6.16	1.42	1.53
1	A	58	LEU	CA-C	-6.16	1.45	1.52
1	C	307	VAL	CA-CB	-6.16	1.47	1.54
1	A	329	ILE	C-N	-6.15	1.26	1.33
1	B	188	ASP	CB-CG	6.15	1.67	1.52
1	A	188	ASP	CB-CG	6.15	1.67	1.52
1	D	404	GLU	CD-OE1	6.15	1.37	1.25
1	D	188	ASP	CB-CG	6.14	1.67	1.52
1	A	172	GLU	CA-CB	-6.14	1.43	1.53
1	C	404	GLU	CD-OE1	6.14	1.37	1.25
1	D	112	MET	N-CA	6.14	1.54	1.46
1	A	404	GLU	CD-OE1	6.14	1.37	1.25
1	A	102	PHE	CA-CB	-6.14	1.43	1.53
1	D	102	PHE	CA-CB	-6.14	1.43	1.53
1	D	172	GLU	CA-CB	-6.14	1.43	1.53
1	A	45	ARG	CZ-NH2	6.14	1.41	1.33
1	C	188	ASP	CB-CG	6.13	1.67	1.52
1	C	332	PHE	CA-CB	-6.13	1.43	1.53
1	C	172	GLU	CA-CB	-6.13	1.43	1.53
1	B	404	GLU	CD-OE1	6.13	1.36	1.25
1	A	288	ASN	CB-CG	-6.13	1.36	1.52
1	B	102	PHE	CA-CB	-6.13	1.43	1.53
1	C	250	MET	C-O	6.13	1.31	1.23
1	D	45	ARG	CZ-NH2	6.13	1.41	1.33
1	C	102	PHE	CA-CB	-6.12	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	288	ASN	CB-CG	-6.12	1.36	1.52
1	C	286	THR	CA-C	-6.12	1.41	1.52
1	D	312	THR	CA-C	6.12	1.58	1.52
1	D	341	ARG	NE-CZ	6.12	1.39	1.33
1	D	255	VAL	C-O	6.12	1.31	1.24
1	B	167	VAL	CB-CG2	6.12	1.72	1.52
1	D	288	ASN	CB-CG	-6.12	1.36	1.52
1	A	419	VAL	C-O	6.11	1.33	1.23
1	B	288	ASN	CB-CG	-6.11	1.36	1.52
1	D	250	MET	C-O	6.11	1.31	1.23
1	C	167	VAL	CB-CG2	6.11	1.72	1.52
1	D	332	PHE	CA-CB	-6.11	1.43	1.53
1	A	167	VAL	CB-CG2	6.11	1.72	1.52
1	A	286	THR	CA-C	-6.11	1.41	1.52
1	B	286	THR	CA-C	-6.11	1.41	1.52
1	A	332	PHE	CA-CB	-6.11	1.43	1.53
1	C	101	LEU	CB-CG	-6.10	1.41	1.53
1	D	286	THR	CA-C	-6.10	1.41	1.52
1	D	167	VAL	CB-CG2	6.10	1.72	1.52
1	A	189	GLU	CD-OE2	6.10	1.36	1.25
1	A	250	MET	C-O	6.10	1.31	1.23
1	B	45	ARG	CZ-NH2	6.09	1.41	1.33
1	B	189	GLU	CD-OE2	6.09	1.36	1.25
1	C	189	GLU	CA-C	6.09	1.60	1.52
1	D	419	VAL	C-O	6.09	1.33	1.23
1	A	101	LEU	CB-CG	-6.09	1.41	1.53
1	B	58	LEU	CA-C	-6.09	1.45	1.52
1	C	189	GLU	CD-OE2	6.09	1.36	1.25
1	D	309	GLN	CA-CB	-6.09	1.43	1.53
1	B	312	THR	CA-C	6.08	1.58	1.52
1	B	419	VAL	C-O	6.08	1.33	1.23
1	C	419	VAL	C-O	6.08	1.33	1.23
1	D	189	GLU	CD-OE2	6.08	1.36	1.25
1	A	312	THR	CA-C	6.08	1.58	1.52
1	B	101	LEU	CB-CG	-6.08	1.41	1.53
1	A	309	GLN	CA-CB	-6.07	1.43	1.53
1	A	189	GLU	CA-C	6.07	1.60	1.52
1	C	309	GLN	CA-CB	-6.07	1.43	1.53
1	A	137	GLN	N-CA	-6.07	1.38	1.46
1	B	189	GLU	CA-C	6.07	1.60	1.52
1	C	137	GLN	N-CA	-6.06	1.38	1.46
1	D	424	ALA	CA-CB	6.06	1.72	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	424	ALA	CA-CB	6.06	1.72	1.52
1	B	137	GLN	N-CA	-6.06	1.38	1.46
1	C	349	GLY	C-O	6.06	1.32	1.23
1	D	101	LEU	CB-CG	-6.06	1.41	1.53
1	D	189	GLU	CA-C	6.06	1.60	1.52
1	B	250	MET	C-O	6.05	1.31	1.23
1	C	138	PHE	CA-CB	-6.05	1.41	1.54
1	D	293	ILE	CA-CB	-6.05	1.46	1.54
1	B	138	PHE	CA-CB	-6.05	1.41	1.54
1	C	424	ALA	CA-CB	6.05	1.72	1.52
1	D	137	GLN	N-CA	-6.05	1.38	1.46
1	B	424	ALA	CA-CB	6.05	1.72	1.52
1	A	138	PHE	CA-CB	-6.05	1.41	1.54
1	D	349	GLY	C-O	6.04	1.32	1.23
1	D	138	PHE	CA-CB	-6.04	1.41	1.54
1	D	222	GLU	CA-CB	-6.04	1.44	1.53
1	B	309	GLN	CA-CB	-6.04	1.43	1.53
1	A	67	ARG	CA-C	6.03	1.61	1.52
1	C	130	LEU	CG-CD1	-6.03	1.32	1.52
1	A	293	ILE	CA-CB	-6.03	1.46	1.54
1	B	349	GLY	C-O	6.03	1.32	1.23
1	D	67	ARG	CA-C	6.03	1.61	1.52
1	D	358	GLU	CD-OE2	6.03	1.36	1.25
1	C	67	ARG	CA-C	6.02	1.61	1.52
1	D	29	GLU	CA-C	-6.02	1.45	1.52
1	B	293	ILE	CA-CB	-6.02	1.46	1.54
1	C	339	HIS	CB-CG	-6.02	1.41	1.50
1	A	114	ALA	C-O	-6.02	1.16	1.24
1	B	67	ARG	CA-C	6.02	1.61	1.52
1	C	114	ALA	C-O	-6.02	1.16	1.24
1	A	130	LEU	CG-CD1	-6.02	1.32	1.52
1	A	349	GLY	C-O	6.02	1.32	1.23
1	A	358	GLU	CD-OE2	6.02	1.36	1.25
1	B	66	LYS	N-CA	-6.02	1.39	1.46
1	A	339	HIS	CB-CG	-6.01	1.41	1.50
1	B	358	GLU	CD-OE2	6.01	1.36	1.25
1	C	222	GLU	CA-CB	-6.01	1.45	1.53
1	C	312	THR	CA-C	6.01	1.58	1.52
1	D	130	LEU	CG-CD1	-6.01	1.32	1.52
1	C	293	ILE	CA-CB	-6.00	1.46	1.54
1	D	348	SER	CB-OG	6.00	1.54	1.42
1	A	222	GLU	CA-CB	-6.00	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	87	ALA	C-O	6.00	1.30	1.23
1	C	29	GLU	CA-C	-6.00	1.45	1.52
1	B	339	HIS	CB-CG	-6.00	1.41	1.50
1	C	370	GLN	C-O	6.00	1.30	1.24
1	C	394	ASP	CA-CB	6.00	1.62	1.53
1	D	336	LYS	N-CA	6.00	1.53	1.45
1	A	72	VAL	CA-CB	-5.99	1.46	1.53
1	A	394	ASP	CA-CB	5.99	1.62	1.53
1	D	234	MET	C-O	5.99	1.31	1.24
1	B	130	LEU	CG-CD1	-5.99	1.32	1.52
1	B	20	GLU	CA-C	5.99	1.60	1.52
1	C	87	ALA	C-O	5.98	1.30	1.23
1	A	348	SER	CB-OG	5.98	1.54	1.42
1	B	222	GLU	CA-CB	-5.98	1.45	1.53
1	B	158	VAL	CA-CB	-5.98	1.46	1.54
1	D	72	VAL	CA-CB	-5.97	1.46	1.53
1	A	29	GLU	CA-C	-5.97	1.45	1.52
1	C	336	LYS	N-CA	5.97	1.53	1.45
1	D	87	ALA	C-O	5.97	1.30	1.23
1	D	339	HIS	CB-CG	-5.97	1.41	1.50
1	B	114	ALA	C-O	-5.97	1.16	1.24
1	B	394	ASP	CA-CB	5.97	1.62	1.53
1	D	114	ALA	C-O	-5.97	1.16	1.24
1	A	234	MET	C-O	5.97	1.31	1.24
1	B	234	MET	C-O	5.97	1.31	1.24
1	B	29	GLU	CA-C	-5.96	1.45	1.52
1	B	72	VAL	CA-CB	-5.96	1.46	1.53
1	C	234	MET	C-O	5.96	1.31	1.24
1	D	158	VAL	CA-CB	-5.96	1.46	1.54
1	A	20	GLU	CA-C	5.96	1.60	1.52
1	B	348	SER	CB-OG	5.96	1.54	1.42
1	C	358	GLU	CD-OE2	5.96	1.36	1.25
1	A	87	ALA	C-O	5.96	1.30	1.23
1	A	327	LYS	CD-CE	5.95	1.70	1.52
1	D	394	ASP	CA-CB	5.95	1.62	1.53
1	A	336	LYS	N-CA	5.95	1.53	1.45
1	C	72	VAL	CA-CB	-5.95	1.46	1.53
1	C	327	LYS	CD-CE	5.95	1.70	1.52
1	D	253	ILE	CA-CB	-5.95	1.46	1.54
1	D	361	ARG	C-O	-5.95	1.17	1.24
1	D	184	LEU	C-O	-5.94	1.17	1.24
1	B	327	LYS	CD-CE	5.94	1.70	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	43	ALA	CA-CB	5.94	1.63	1.53
1	D	327	LYS	CD-CE	5.94	1.70	1.52
1	A	184	LEU	C-O	-5.94	1.17	1.24
1	C	355	LEU	CG-CD2	-5.94	1.32	1.52
1	B	336	LYS	N-CA	5.93	1.53	1.45
1	A	158	VAL	CA-CB	-5.93	1.46	1.54
1	A	66	LYS	N-CA	-5.93	1.39	1.46
1	C	348	SER	CB-OG	5.93	1.54	1.42
1	A	370	GLN	C-O	5.93	1.30	1.24
1	D	20	GLU	CA-C	5.93	1.60	1.52
1	B	184	LEU	C-O	-5.92	1.17	1.24
1	D	355	LEU	CG-CD2	-5.92	1.33	1.52
1	A	355	LEU	CG-CD2	-5.92	1.33	1.52
1	C	43	ALA	CA-CB	5.92	1.63	1.53
1	C	66	LYS	N-CA	-5.92	1.39	1.46
1	C	20	GLU	CA-C	5.92	1.60	1.52
1	B	361	ARG	C-O	-5.92	1.17	1.24
1	B	370	GLN	C-O	5.92	1.30	1.24
1	B	113	LYS	CG-CD	5.92	1.70	1.52
1	B	355	LEU	CG-CD2	-5.92	1.33	1.52
1	B	346	VAL	CA-C	5.91	1.60	1.52
1	A	113	LYS	CG-CD	5.91	1.70	1.52
1	A	253	ILE	CA-CB	-5.91	1.46	1.54
1	C	113	LYS	CG-CD	5.91	1.70	1.52
1	D	346	VAL	CA-C	5.91	1.60	1.52
1	A	43	ALA	CA-CB	5.91	1.63	1.53
1	A	346	VAL	CA-C	5.90	1.60	1.52
1	B	43	ALA	CA-CB	5.90	1.63	1.53
1	C	346	VAL	CA-C	5.90	1.60	1.52
1	D	113	LYS	CG-CD	5.90	1.70	1.52
1	D	134	LYS	CA-C	-5.90	1.44	1.52
1	D	66	LYS	N-CA	-5.90	1.39	1.46
1	A	361	ARG	C-O	-5.90	1.17	1.24
1	B	295	MET	SD-CE	-5.90	1.64	1.79
1	C	230	PRO	C-N	5.90	1.41	1.33
1	C	253	ILE	CA-CB	-5.90	1.46	1.54
1	C	295	MET	SD-CE	-5.89	1.64	1.79
1	B	59	TRP	C-O	-5.89	1.16	1.23
1	D	295	MET	SD-CE	-5.89	1.64	1.79
1	D	238	ALA	C-O	5.88	1.31	1.24
1	D	370	GLN	C-O	5.88	1.30	1.24
1	C	361	ARG	C-O	-5.88	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	419	VAL	N-CA	5.88	1.54	1.46
1	A	295	MET	SD-CE	-5.88	1.64	1.79
1	C	158	VAL	CA-CB	-5.88	1.46	1.54
1	B	253	ILE	CA-CB	-5.88	1.46	1.54
1	B	108	ASN	C-O	5.88	1.31	1.24
1	C	202	ARG	CA-C	-5.88	1.45	1.52
1	C	184	LEU	C-O	-5.88	1.17	1.24
1	B	419	VAL	N-CA	5.87	1.54	1.46
1	A	42	ALA	N-CA	5.87	1.53	1.46
1	D	59	TRP	C-O	-5.87	1.16	1.23
1	D	77	LYS	CG-CD	5.87	1.70	1.52
1	B	238	ALA	C-O	5.87	1.31	1.24
1	A	77	LYS	CG-CD	5.87	1.70	1.52
1	C	59	TRP	C-O	-5.87	1.16	1.23
1	C	77	LYS	CG-CD	5.87	1.70	1.52
1	D	90	LEU	CA-C	5.87	1.60	1.52
1	B	134	LYS	CA-C	-5.86	1.44	1.52
1	C	134	LYS	CA-C	-5.86	1.44	1.52
1	C	194	PHE	CE2-CZ	5.86	1.56	1.38
1	C	90	LEU	CA-C	5.86	1.60	1.52
1	A	230	PRO	C-N	5.86	1.41	1.33
1	B	77	LYS	CG-CD	5.86	1.70	1.52
1	D	251	ILE	CA-C	5.86	1.59	1.52
1	B	367	LEU	CG-CD1	-5.86	1.33	1.52
1	A	202	ARG	CA-C	-5.86	1.45	1.52
1	B	376	MET	SD-CE	-5.86	1.65	1.79
1	C	77	LYS	C-O	-5.86	1.17	1.23
1	C	376	MET	SD-CE	-5.86	1.65	1.79
1	A	367	LEU	CG-CD1	-5.85	1.33	1.52
1	B	202	ARG	CA-C	-5.85	1.45	1.52
1	A	59	TRP	C-O	-5.85	1.16	1.23
1	C	108	ASN	C-O	5.85	1.31	1.24
1	C	419	VAL	N-CA	5.85	1.54	1.46
1	D	299	ALA	CA-C	-5.85	1.44	1.52
1	B	251	ILE	CA-C	5.85	1.59	1.52
1	A	376	MET	SD-CE	-5.84	1.65	1.79
1	B	77	LYS	C-O	-5.84	1.17	1.23
1	C	42	ALA	N-CA	5.84	1.53	1.46
1	C	238	ALA	C-O	5.84	1.31	1.24
1	D	47	ALA	CA-C	-5.84	1.44	1.52
1	D	376	MET	SD-CE	-5.84	1.65	1.79
1	B	230	PRO	C-N	5.84	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	367	LEU	CG-CD1	-5.84	1.33	1.52
1	A	238	ALA	C-O	5.84	1.31	1.24
1	C	299	ALA	CA-C	-5.84	1.44	1.52
1	D	230	PRO	C-N	5.84	1.41	1.33
1	B	101	LEU	CG-CD2	-5.84	1.33	1.52
1	D	42	ALA	N-CA	5.84	1.53	1.46
1	B	194	PHE	C-O	-5.84	1.16	1.24
1	D	194	PHE	CE2-CZ	5.84	1.56	1.38
1	A	194	PHE	C-O	-5.83	1.16	1.24
1	D	202	ARG	CA-C	-5.83	1.45	1.52
1	D	367	LEU	CG-CD1	-5.83	1.33	1.52
1	A	134	LYS	CA-C	-5.83	1.44	1.52
1	A	194	PHE	CE2-CZ	5.83	1.56	1.38
1	D	101	LEU	CG-CD2	-5.83	1.33	1.52
1	D	419	VAL	N-CA	5.83	1.53	1.46
1	A	198	ARG	CA-C	5.83	1.60	1.52
1	D	194	PHE	C-O	-5.83	1.16	1.24
1	D	198	ARG	CA-C	5.83	1.60	1.52
1	D	108	ASN	C-O	5.83	1.31	1.24
1	A	101	LEU	CG-CD2	-5.82	1.33	1.52
1	B	42	ALA	N-CA	5.82	1.53	1.46
1	B	190	ASN	CG-OD1	5.82	1.34	1.23
1	C	47	ALA	CA-C	-5.82	1.44	1.52
1	C	198	ARG	CA-C	5.82	1.60	1.52
1	B	47	ALA	CA-C	-5.82	1.44	1.52
1	A	251	ILE	CA-C	5.82	1.59	1.52
1	A	90	LEU	CA-C	5.82	1.60	1.52
1	D	167	VAL	C-O	-5.82	1.17	1.24
1	C	101	LEU	CG-CD2	-5.82	1.33	1.52
1	A	190	ASN	CG-OD1	5.82	1.34	1.23
1	A	340	ILE	C-O	5.82	1.29	1.24
1	B	370	GLN	CG-CD	-5.82	1.37	1.52
1	A	108	ASN	C-O	5.81	1.31	1.24
1	D	190	ASN	CG-OD1	5.81	1.34	1.23
1	B	194	PHE	CE2-CZ	5.81	1.56	1.38
1	B	196	PHE	CA-CB	-5.81	1.43	1.53
1	B	198	ARG	CA-C	5.81	1.60	1.52
1	D	370	GLN	CG-CD	-5.81	1.37	1.52
1	A	167	VAL	C-O	-5.81	1.17	1.24
1	C	134	LYS	CD-CE	5.81	1.69	1.52
1	D	27	ILE	CB-CG1	5.81	1.65	1.53
1	D	263	TYR	CA-CB	-5.81	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	190	ASN	CG-OD1	5.81	1.34	1.23
1	D	196	PHE	CA-CB	-5.80	1.43	1.53
1	B	340	ILE	C-O	5.80	1.29	1.24
1	A	299	ALA	CA-C	-5.80	1.44	1.52
1	C	421	LEU	CA-C	5.80	1.60	1.52
1	B	167	VAL	C-O	-5.80	1.17	1.24
1	A	370	GLN	CG-CD	-5.80	1.37	1.52
1	D	134	LYS	CD-CE	5.80	1.69	1.52
1	C	167	VAL	C-O	-5.79	1.17	1.24
1	A	77	LYS	C-O	-5.79	1.17	1.23
1	C	340	ILE	C-O	5.79	1.29	1.24
1	A	47	ALA	CA-C	-5.79	1.44	1.52
1	A	134	LYS	CD-CE	5.79	1.69	1.52
1	C	194	PHE	C-O	-5.79	1.16	1.24
1	B	90	LEU	CA-C	5.78	1.60	1.52
1	A	196	PHE	CA-CB	-5.78	1.43	1.53
1	D	77	LYS	C-O	-5.78	1.17	1.23
1	A	27	ILE	CB-CG1	5.78	1.65	1.53
1	B	234	MET	CA-C	5.78	1.60	1.52
1	B	27	ILE	CB-CG1	5.77	1.65	1.53
1	C	370	GLN	CG-CD	-5.77	1.37	1.52
1	D	157	THR	C-O	-5.77	1.17	1.24
1	B	157	THR	C-O	-5.77	1.17	1.24
1	C	263	TYR	CA-CB	-5.77	1.44	1.53
1	A	421	LEU	CA-C	5.77	1.60	1.52
1	B	134	LYS	CD-CE	5.77	1.69	1.52
1	B	217	THR	N-CA	5.77	1.53	1.46
1	B	299	ALA	CA-C	-5.77	1.44	1.52
1	B	40	GLU	CD-OE2	5.77	1.36	1.25
1	C	40	GLU	CD-OE2	5.77	1.36	1.25
1	A	348	SER	C-O	5.76	1.31	1.24
1	C	27	ILE	CB-CG1	5.76	1.65	1.53
1	D	348	SER	C-O	5.76	1.31	1.24
1	A	40	GLU	CD-OE2	5.76	1.36	1.25
1	D	40	GLU	CD-OE2	5.76	1.36	1.25
1	D	340	ILE	C-O	5.75	1.29	1.24
1	B	82	TYR	CA-CB	-5.75	1.43	1.53
1	A	207	TYR	CG-CD1	5.75	1.51	1.39
1	B	367	LEU	CA-C	-5.75	1.45	1.52
1	C	251	ILE	CA-C	5.75	1.59	1.52
1	A	263	TYR	CA-CB	-5.75	1.44	1.53
1	C	348	SER	C-O	5.75	1.31	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	421	LEU	CA-C	5.74	1.60	1.52
1	C	196	PHE	CA-CB	-5.74	1.43	1.53
1	D	217	THR	N-CA	5.74	1.53	1.46
1	D	421	LEU	CA-C	5.74	1.60	1.52
1	A	217	THR	N-CA	5.74	1.53	1.46
1	C	157	THR	C-O	-5.74	1.17	1.24
1	A	257	GLY	N-CA	5.74	1.50	1.45
1	B	348	SER	C-O	5.74	1.31	1.24
1	C	217	THR	N-CA	5.74	1.53	1.46
1	D	234	MET	CA-C	5.73	1.60	1.52
1	B	257	GLY	N-CA	5.73	1.50	1.45
1	C	234	MET	CA-C	5.73	1.60	1.52
1	C	257	GLY	N-CA	5.73	1.50	1.45
1	D	82	TYR	CA-CB	-5.73	1.43	1.53
1	A	87	ALA	N-CA	5.73	1.52	1.46
1	A	367	LEU	CA-C	-5.73	1.45	1.52
1	B	263	TYR	CA-CB	-5.73	1.44	1.53
1	D	104	ALA	C-N	-5.73	1.25	1.33
1	C	207	TYR	CG-CD1	5.73	1.51	1.39
1	A	104	ALA	C-N	-5.72	1.25	1.33
1	B	108	ASN	CB-CG	-5.72	1.37	1.52
1	D	207	TYR	CG-CD1	5.72	1.51	1.39
1	A	234	MET	CA-C	5.72	1.60	1.52
1	B	277	ALA	CA-C	-5.72	1.46	1.52
1	A	82	TYR	CA-CB	-5.72	1.43	1.53
1	C	367	LEU	CA-C	-5.71	1.45	1.52
1	A	330	ASN	CA-CB	-5.71	1.44	1.53
1	B	87	ALA	N-CA	5.71	1.52	1.46
1	C	330	ASN	CA-CB	-5.71	1.44	1.53
1	D	134	LYS	CE-NZ	5.71	1.66	1.49
1	A	134	LYS	CE-NZ	5.71	1.66	1.49
1	B	104	ALA	C-N	-5.71	1.25	1.33
1	C	104	ALA	C-N	-5.71	1.25	1.33
1	D	108	ASN	CB-CG	-5.71	1.37	1.52
1	A	157	THR	C-O	-5.71	1.17	1.24
1	C	143	ILE	CA-CB	-5.71	1.46	1.54
1	D	257	GLY	N-CA	5.71	1.50	1.45
1	B	207	TYR	CG-CD1	5.70	1.51	1.39
1	B	330	ASN	CA-CB	-5.70	1.44	1.53
1	A	108	ASN	CB-CG	-5.70	1.37	1.52
1	C	87	ALA	N-CA	5.70	1.52	1.46
1	D	330	ASN	CA-CB	-5.70	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	134	LYS	CE-NZ	5.69	1.66	1.49
1	C	68	SER	CB-OG	5.69	1.53	1.42
1	D	87	ALA	N-CA	5.69	1.52	1.46
1	C	82	TYR	CA-CB	-5.69	1.43	1.53
1	D	367	LEU	CA-C	-5.69	1.45	1.52
1	B	143	ILE	CA-CB	-5.68	1.46	1.54
1	C	134	LYS	CE-NZ	5.68	1.66	1.49
1	A	277	ALA	CA-C	-5.68	1.46	1.52
1	A	95	GLU	CA-C	-5.67	1.45	1.53
1	C	108	ASN	CB-CG	-5.67	1.37	1.52
1	D	277	ALA	CA-C	-5.67	1.46	1.52
1	A	143	ILE	CA-CB	-5.66	1.46	1.54
1	B	95	GLU	CA-C	-5.66	1.45	1.53
1	D	196	PHE	N-CA	5.66	1.53	1.46
1	A	68	SER	CB-OG	5.66	1.53	1.42
1	B	233	ILE	CG1-CD1	-5.66	1.29	1.51
1	C	196	PHE	N-CA	5.66	1.53	1.46
1	D	143	ILE	CA-CB	-5.66	1.46	1.54
1	D	48	SER	CA-CB	5.66	1.63	1.53
1	D	68	SER	CB-OG	5.65	1.53	1.42
1	B	125	PRO	CA-C	5.65	1.57	1.52
1	C	233	ILE	CG1-CD1	-5.65	1.29	1.51
1	D	20	GLU	C-N	5.64	1.40	1.33
1	A	233	ILE	CG1-CD1	-5.64	1.29	1.51
1	C	277	ALA	CA-C	-5.64	1.46	1.52
1	B	48	SER	CA-CB	5.64	1.63	1.53
1	C	95	GLU	CA-C	-5.64	1.45	1.53
1	D	95	GLU	CA-C	-5.64	1.45	1.53
1	A	48	SER	CA-CB	5.64	1.62	1.53
1	B	68	SER	CB-OG	5.63	1.53	1.42
1	A	20	GLU	C-N	5.63	1.40	1.33
1	A	196	PHE	N-CA	5.63	1.53	1.46
1	B	346	VAL	CB-CG2	-5.63	1.33	1.52
1	C	20	GLU	C-N	5.63	1.40	1.33
1	D	233	ILE	CG1-CD1	-5.63	1.29	1.51
1	D	125	PRO	CA-C	5.62	1.57	1.52
1	C	48	SER	CA-CB	5.62	1.62	1.53
1	C	346	VAL	CB-CG2	-5.62	1.34	1.52
1	A	346	VAL	CB-CG2	-5.61	1.34	1.52
1	B	20	GLU	C-N	5.61	1.40	1.33
1	B	196	PHE	N-CA	5.61	1.53	1.46
1	A	125	PRO	CA-C	5.61	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	51	SER	CA-CB	-5.60	1.44	1.53
1	C	221	LYS	N-CA	-5.60	1.39	1.46
1	C	15	VAL	CA-CB	-5.60	1.45	1.55
1	D	346	VAL	CB-CG2	-5.59	1.34	1.52
1	B	351	LEU	CG-CD2	-5.59	1.34	1.52
1	C	125	PRO	CA-C	5.59	1.57	1.52
1	A	351	LEU	CG-CD2	-5.58	1.34	1.52
1	D	17	LEU	CA-C	-5.58	1.42	1.52
1	C	17	LEU	CA-C	-5.58	1.42	1.52
1	C	18	ASN	N-CA	-5.57	1.39	1.46
1	A	15	VAL	CA-CB	-5.57	1.45	1.55
1	B	18	ASN	N-CA	-5.57	1.39	1.46
1	B	221	LYS	N-CA	-5.57	1.39	1.46
1	A	203	VAL	CB-CG2	-5.57	1.34	1.52
1	B	17	LEU	CA-C	-5.57	1.42	1.52
1	A	51	SER	CA-CB	-5.56	1.44	1.53
1	B	371	ALA	C-N	5.56	1.41	1.33
1	C	203	VAL	CB-CG2	-5.56	1.34	1.52
1	A	17	LEU	CA-C	-5.56	1.42	1.52
1	C	336	LYS	CA-C	-5.56	1.45	1.53
1	D	351	LEU	CG-CD2	-5.56	1.34	1.52
1	B	203	VAL	CB-CG2	-5.55	1.34	1.52
1	C	351	LEU	CG-CD2	-5.55	1.34	1.52
1	C	371	ALA	C-N	5.55	1.41	1.33
1	C	71	LYS	C-O	5.55	1.30	1.23
1	A	221	LYS	N-CA	-5.55	1.39	1.46
1	C	51	SER	CA-CB	-5.55	1.44	1.53
1	D	203	VAL	CB-CG2	-5.55	1.34	1.52
1	B	15	VAL	CA-CB	-5.54	1.45	1.55
1	A	371	ALA	C-N	5.54	1.41	1.33
1	C	137	GLN	C-O	-5.54	1.17	1.24
1	D	15	VAL	CA-CB	-5.54	1.45	1.55
1	A	18	ASN	N-CA	-5.54	1.39	1.46
1	B	336	LYS	CA-C	-5.54	1.45	1.53
1	A	137	GLN	C-O	-5.54	1.17	1.24
1	A	336	LYS	CA-C	-5.54	1.45	1.53
1	B	296	LEU	N-CA	5.54	1.53	1.46
1	B	372	GLY	C-O	5.54	1.31	1.23
1	A	71	LYS	C-O	5.53	1.30	1.23
1	C	113	LYS	CB-CG	5.53	1.69	1.52
1	A	287	ARG	N-CA	5.53	1.53	1.46
1	B	51	SER	CA-CB	-5.53	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	253	ILE	CB-CG2	-5.53	1.34	1.52
1	B	387	LYS	N-CA	5.53	1.53	1.46
1	C	287	ARG	N-CA	5.53	1.53	1.46
1	D	137	GLN	C-O	-5.53	1.17	1.24
1	D	287	ARG	N-CA	5.53	1.53	1.46
1	D	336	LYS	CA-C	-5.52	1.45	1.53
1	B	113	LYS	CB-CG	5.52	1.69	1.52
1	A	296	LEU	N-CA	5.52	1.53	1.46
1	A	253	ILE	CB-CG2	-5.52	1.34	1.52
1	A	113	LYS	CB-CG	5.52	1.69	1.52
1	D	113	LYS	CB-CG	5.52	1.69	1.52
1	D	387	LYS	N-CA	5.52	1.53	1.46
1	B	253	ILE	CB-CG1	-5.52	1.42	1.53
1	B	71	LYS	C-O	5.51	1.30	1.23
1	C	253	ILE	CB-CG2	-5.51	1.34	1.52
1	D	296	LEU	N-CA	5.51	1.53	1.46
1	D	371	ALA	C-N	5.51	1.41	1.33
1	D	221	LYS	N-CA	-5.51	1.39	1.46
1	C	372	GLY	C-O	5.51	1.31	1.23
1	D	142	GLY	C-O	5.51	1.31	1.23
1	D	253	ILE	CB-CG2	-5.51	1.34	1.52
1	A	387	LYS	N-CA	5.50	1.53	1.46
1	B	287	ARG	N-CA	5.50	1.53	1.46
1	B	137	GLN	C-O	-5.50	1.17	1.24
1	C	142	GLY	C-O	5.50	1.31	1.23
1	D	372	GLY	C-O	5.50	1.31	1.23
1	B	142	GLY	C-O	5.49	1.31	1.23
1	B	147	MET	C-O	-5.49	1.17	1.24
1	D	18	ASN	N-CA	-5.49	1.39	1.46
1	C	296	LEU	N-CA	5.49	1.53	1.46
1	A	253	ILE	CB-CG1	-5.49	1.42	1.53
1	D	71	LYS	C-O	5.49	1.30	1.23
1	D	195	PRO	CA-CB	-5.48	1.46	1.53
1	D	328	ARG	CZ-NH2	5.48	1.40	1.33
1	C	253	ILE	CB-CG1	-5.48	1.42	1.53
1	A	372	GLY	C-O	5.48	1.31	1.23
1	C	387	LYS	N-CA	5.47	1.53	1.46
1	D	253	ILE	CB-CG1	-5.47	1.42	1.53
1	B	195	PRO	CA-CB	-5.47	1.46	1.53
1	D	123	PHE	CD1-CE1	5.47	1.55	1.38
1	A	56	THR	C-N	5.47	1.41	1.33
1	C	56	THR	C-N	5.47	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	328	ARG	CZ-NH2	5.46	1.40	1.33
1	A	195	PRO	CA-CB	-5.46	1.46	1.53
1	A	359	LEU	CA-C	-5.46	1.45	1.52
1	C	23	ARG	NE-CZ	5.46	1.39	1.33
1	C	244	GLU	C-O	-5.46	1.16	1.24
1	B	359	LEU	CA-C	-5.46	1.45	1.52
1	A	155	THR	CA-CB	-5.45	1.44	1.53
1	C	195	PRO	CA-CB	-5.45	1.46	1.53
1	C	123	PHE	CD1-CE1	5.45	1.55	1.38
1	A	123	PHE	CD1-CE1	5.45	1.55	1.38
1	D	155	THR	CA-CB	-5.45	1.44	1.53
1	B	71	LYS	CA-C	5.45	1.58	1.52
1	D	23	ARG	NE-CZ	5.45	1.39	1.33
1	A	328	ARG	CZ-NH2	5.45	1.40	1.33
1	A	142	GLY	C-O	5.44	1.31	1.23
1	D	359	LEU	CA-C	-5.44	1.45	1.52
1	A	244	GLU	C-O	-5.44	1.16	1.24
1	B	123	PHE	CD1-CE1	5.44	1.54	1.38
1	B	155	THR	CA-CB	-5.44	1.44	1.53
1	C	359	LEU	CA-C	-5.44	1.45	1.52
1	A	23	ARG	NE-CZ	5.43	1.39	1.33
1	D	56	THR	C-N	5.43	1.41	1.33
1	B	56	THR	C-N	5.42	1.41	1.33
1	B	23	ARG	NE-CZ	5.42	1.39	1.33
1	B	244	GLU	C-O	-5.42	1.16	1.24
1	C	155	THR	CA-CB	-5.42	1.44	1.53
1	C	235	GLU	CA-CB	-5.41	1.44	1.53
1	C	187	ASP	CA-C	-5.41	1.45	1.53
1	B	16	ASP	CB-CG	-5.41	1.38	1.52
1	D	71	LYS	CA-C	5.41	1.58	1.52
1	C	367	LEU	CG-CD2	5.40	1.70	1.52
1	D	270	ASP	CG-OD1	5.40	1.35	1.25
1	D	187	ASP	CA-C	-5.40	1.45	1.53
1	B	367	LEU	CG-CD2	5.40	1.70	1.52
1	A	16	ASP	CB-CG	-5.40	1.38	1.52
1	C	16	ASP	CB-CG	-5.40	1.38	1.52
1	D	235	GLU	CA-CB	-5.40	1.44	1.53
1	B	187	ASP	CA-C	-5.39	1.45	1.53
1	B	235	GLU	CA-CB	-5.39	1.44	1.53
1	D	360	ILE	CA-C	-5.39	1.46	1.52
1	A	367	LEU	CG-CD2	5.39	1.70	1.52
1	C	360	ILE	CA-C	-5.39	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	270	ASP	CG-OD1	5.38	1.35	1.25
1	D	367	LEU	CG-CD2	5.38	1.70	1.52
1	A	235	GLU	CA-CB	-5.38	1.44	1.53
1	A	71	LYS	CA-C	5.37	1.58	1.52
1	D	16	ASP	CB-CG	-5.37	1.38	1.52
1	A	187	ASP	CA-C	-5.37	1.45	1.53
1	A	244	GLU	CG-CD	-5.37	1.38	1.52
1	A	360	ILE	CA-C	-5.37	1.46	1.52
1	C	91	THR	CA-C	5.37	1.59	1.52
1	D	244	GLU	CG-CD	-5.37	1.38	1.52
1	A	116	LYS	CG-CD	5.37	1.68	1.52
1	B	151	ASP	N-CA	-5.37	1.39	1.46
1	B	328	ARG	CZ-NH2	5.37	1.40	1.33
1	C	270	ASP	CG-OD1	5.37	1.35	1.25
1	B	116	LYS	CG-CD	5.37	1.68	1.52
1	C	151	ASP	CG-OD2	5.37	1.35	1.25
1	B	360	ILE	CA-C	-5.36	1.46	1.52
1	C	151	ASP	N-CA	-5.36	1.39	1.46
1	B	244	GLU	CG-CD	-5.36	1.38	1.52
1	B	236	LYS	CG-CD	5.36	1.68	1.52
1	C	116	LYS	CG-CD	5.36	1.68	1.52
1	B	100	GLN	CD-NE2	5.36	1.44	1.33
1	B	270	ASP	CG-OD1	5.36	1.35	1.25
1	A	151	ASP	CG-OD2	5.36	1.35	1.25
1	D	116	LYS	CG-CD	5.36	1.68	1.52
1	D	9	GLU	N-CA	5.35	1.56	1.46
1	A	151	ASP	N-CA	-5.35	1.39	1.46
1	A	236	LYS	CG-CD	5.35	1.68	1.52
1	B	151	ASP	CG-OD2	5.35	1.35	1.25
1	C	244	GLU	CG-CD	-5.35	1.38	1.52
1	D	100	GLN	CD-NE2	5.35	1.44	1.33
1	D	253	ILE	CA-C	-5.35	1.45	1.52
1	A	100	GLN	CD-NE2	5.34	1.44	1.33
1	D	63	GLU	CD-OE2	5.34	1.35	1.25
1	D	236	LYS	CG-CD	5.34	1.68	1.52
1	C	71	LYS	CA-C	5.34	1.58	1.52
1	A	298	LEU	CG-CD1	5.34	1.70	1.52
1	A	63	GLU	CD-OE2	5.34	1.35	1.25
1	D	64	MET	CB-CG	-5.34	1.36	1.52
1	A	91	THR	CA-C	5.33	1.59	1.52
1	C	116	LYS	C-O	-5.33	1.16	1.23
1	C	100	GLN	CD-NE2	5.33	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	236	LYS	CG-CD	5.33	1.68	1.52
1	C	413	LYS	N-CA	5.33	1.53	1.46
1	D	413	LYS	N-CA	5.33	1.53	1.46
1	C	223	TYR	N-CA	5.33	1.52	1.46
1	B	116	LYS	CE-NZ	5.33	1.65	1.49
1	B	298	LEU	CG-CD1	5.33	1.70	1.52
1	C	9	GLU	N-CA	5.33	1.56	1.46
1	A	9	GLU	N-CA	5.32	1.56	1.46
1	A	64	MET	CB-CG	-5.32	1.36	1.52
1	A	116	LYS	CE-NZ	5.32	1.65	1.49
1	D	151	ASP	CG-OD2	5.32	1.35	1.25
1	B	9	GLU	N-CA	5.32	1.56	1.46
1	A	413	LYS	N-CA	5.32	1.53	1.46
1	C	298	LEU	CG-CD1	5.32	1.70	1.52
1	B	64	MET	CB-CG	-5.32	1.36	1.52
1	A	391	ASP	CA-C	-5.32	1.46	1.52
1	D	151	ASP	N-CA	-5.32	1.39	1.46
1	D	298	LEU	CG-CD1	5.32	1.70	1.52
1	C	64	MET	CB-CG	-5.31	1.36	1.52
1	B	253	ILE	CA-C	-5.31	1.45	1.52
1	D	116	LYS	C-O	-5.31	1.16	1.23
1	D	391	ASP	CA-C	-5.31	1.46	1.52
1	C	116	LYS	CE-NZ	5.31	1.65	1.49
1	C	63	GLU	CD-OE2	5.31	1.35	1.25
1	D	116	LYS	CE-NZ	5.31	1.65	1.49
1	B	223	TYR	N-CA	5.31	1.52	1.46
1	A	223	TYR	N-CA	5.30	1.52	1.46
1	B	413	LYS	N-CA	5.30	1.53	1.46
1	D	328	ARG	CG-CD	5.30	1.68	1.52
1	A	253	ILE	CA-C	-5.30	1.45	1.52
1	A	116	LYS	C-O	-5.30	1.16	1.23
1	D	92	LEU	N-CA	-5.30	1.38	1.45
1	B	70	ALA	CA-CB	-5.30	1.45	1.53
1	B	91	THR	CA-C	5.30	1.59	1.52
1	C	111	GLY	CA-C	-5.30	1.44	1.51
1	D	70	ALA	CA-CB	-5.30	1.45	1.53
1	D	336	LYS	CE-NZ	5.30	1.65	1.49
1	D	223	TYR	N-CA	5.29	1.52	1.46
1	B	116	LYS	C-O	-5.29	1.16	1.23
1	D	91	THR	CA-C	5.29	1.59	1.52
1	D	316	VAL	C-O	5.29	1.30	1.24
1	C	336	LYS	CE-NZ	5.29	1.65	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	31	TYR	CE2-CZ	5.29	1.50	1.38
1	A	336	LYS	CE-NZ	5.28	1.65	1.49
1	C	310	ILE	C-O	5.28	1.29	1.23
1	B	328	ARG	CG-CD	5.28	1.68	1.52
1	B	63	GLU	CD-OE2	5.28	1.35	1.25
1	A	328	ARG	CG-CD	5.28	1.68	1.52
1	B	31	TYR	CE2-CZ	5.28	1.50	1.38
1	C	92	LEU	N-CA	-5.28	1.38	1.45
1	C	328	ARG	CG-CD	5.28	1.68	1.52
1	B	391	ASP	CA-C	-5.27	1.46	1.52
1	A	92	LEU	N-CA	-5.27	1.38	1.45
1	A	401	ASP	CA-C	-5.27	1.45	1.52
1	C	290	ARG	CG-CD	5.27	1.68	1.52
1	A	310	ILE	C-O	5.27	1.29	1.23
1	B	290	ARG	CG-CD	5.27	1.68	1.52
1	C	391	ASP	CA-C	-5.27	1.46	1.52
1	C	253	ILE	CA-C	-5.27	1.45	1.52
1	B	316	VAL	C-O	5.26	1.30	1.24
1	C	41	GLU	C-O	-5.26	1.17	1.24
1	C	70	ALA	CA-CB	-5.26	1.45	1.53
1	A	31	TYR	CE2-CZ	5.26	1.50	1.38
1	B	290	ARG	CD-NE	5.26	1.53	1.46
1	C	57	THR	CB-OG1	5.26	1.52	1.43
1	D	290	ARG	CG-CD	5.26	1.68	1.52
1	B	336	LYS	CE-NZ	5.26	1.65	1.49
1	D	57	THR	CB-OG1	5.26	1.52	1.43
1	D	290	ARG	CD-NE	5.26	1.53	1.46
1	A	41	GLU	C-O	-5.26	1.17	1.24
1	A	290	ARG	CG-CD	5.26	1.68	1.52
1	A	316	VAL	C-O	5.25	1.30	1.24
1	B	309	GLN	CB-CG	-5.25	1.36	1.52
1	B	11	TYR	CG-CD1	5.25	1.50	1.39
1	B	92	LEU	N-CA	-5.25	1.38	1.45
1	D	401	ASP	CA-C	-5.25	1.45	1.52
1	A	70	ALA	CA-CB	-5.25	1.45	1.53
1	B	401	ASP	CA-C	-5.25	1.45	1.52
1	C	316	VAL	C-O	5.25	1.30	1.24
1	C	401	ASP	CA-C	-5.25	1.45	1.52
1	D	380	ASP	C-N	5.25	1.41	1.33
1	A	57	THR	CB-OG1	5.24	1.52	1.43
1	D	309	GLN	CB-CG	-5.24	1.36	1.52
1	A	268	THR	CA-C	5.24	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	41	GLU	C-O	-5.24	1.17	1.24
1	B	49	GLU	C-O	-5.24	1.17	1.24
1	C	31	TYR	CE2-CZ	5.24	1.50	1.38
1	C	290	ARG	CD-NE	5.24	1.53	1.46
1	D	268	THR	CA-C	5.24	1.60	1.52
1	A	11	TYR	CG-CD1	5.24	1.50	1.39
1	A	309	GLN	CB-CG	-5.24	1.36	1.52
1	D	41	GLU	C-O	-5.24	1.17	1.24
1	B	57	THR	CB-OG1	5.23	1.52	1.43
1	C	49	GLU	C-O	-5.23	1.17	1.24
1	B	268	THR	CA-C	5.23	1.60	1.52
1	D	310	ILE	C-O	5.23	1.29	1.23
1	C	11	TYR	CG-CD1	5.22	1.50	1.39
1	C	380	ASP	C-N	5.22	1.41	1.33
1	D	138	PHE	N-CA	5.22	1.53	1.46
1	A	290	ARG	CD-NE	5.22	1.53	1.46
1	C	309	GLN	CB-CG	-5.22	1.36	1.52
1	B	372	GLY	N-CA	5.22	1.52	1.45
1	A	111	GLY	CA-C	-5.22	1.44	1.51
1	A	383	ARG	C-O	5.22	1.30	1.24
1	C	327	LYS	C-O	-5.22	1.17	1.24
1	B	111	GLY	CA-C	-5.21	1.44	1.51
1	C	268	THR	CA-C	5.21	1.60	1.52
1	A	49	GLU	C-O	-5.20	1.17	1.24
1	B	383	ARG	C-O	5.20	1.30	1.24
1	D	11	TYR	CG-CD1	5.20	1.50	1.39
1	B	310	ILE	C-O	5.20	1.29	1.23
1	A	380	ASP	C-N	5.20	1.41	1.33
1	D	415	SER	N-CA	5.20	1.52	1.45
1	A	327	LYS	C-O	-5.19	1.17	1.24
1	B	380	ASP	C-N	5.19	1.41	1.33
1	B	415	SER	N-CA	5.19	1.52	1.45
1	D	327	LYS	C-O	-5.19	1.17	1.24
1	A	147	MET	C-O	-5.18	1.17	1.24
1	D	146	PHE	CA-C	-5.18	1.46	1.52
1	A	372	GLY	N-CA	5.18	1.52	1.45
1	C	383	ARG	C-O	5.18	1.30	1.24
1	C	278	HIS	C-O	5.18	1.30	1.23
1	A	415	SER	N-CA	5.17	1.52	1.45
1	B	138	PHE	N-CA	5.17	1.53	1.46
1	C	138	PHE	N-CA	5.17	1.53	1.46
1	C	168	GLU	N-CA	-5.17	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	147	MET	C-O	-5.17	1.17	1.24
1	D	372	GLY	N-CA	5.17	1.52	1.45
1	C	372	GLY	N-CA	5.17	1.52	1.45
1	D	49	GLU	C-O	-5.17	1.17	1.24
1	D	111	GLY	CA-C	-5.17	1.44	1.51
1	A	138	PHE	N-CA	5.16	1.53	1.46
1	B	278	HIS	C-O	5.16	1.30	1.23
1	C	49	GLU	CG-CD	5.16	1.65	1.52
1	C	147	MET	C-O	-5.15	1.17	1.24
1	A	278	HIS	C-O	5.14	1.29	1.23
1	B	168	GLU	N-CA	-5.14	1.39	1.46
1	D	124	HIS	CB-CG	-5.14	1.43	1.50
1	B	146	PHE	CA-C	-5.14	1.46	1.52
1	B	327	LYS	C-O	-5.14	1.17	1.24
1	C	244	GLU	CD-OE1	5.14	1.35	1.25
1	A	146	PHE	CA-C	-5.14	1.46	1.52
1	C	415	SER	N-CA	5.14	1.52	1.45
1	D	100	GLN	C-O	5.14	1.30	1.24
1	D	244	GLU	CD-OE1	5.14	1.35	1.25
1	D	383	ARG	C-O	5.14	1.30	1.24
1	A	100	GLN	C-O	5.14	1.30	1.24
1	C	204	ARG	CZ-NH1	5.13	1.40	1.32
1	A	49	GLU	CG-CD	5.13	1.64	1.52
1	A	168	GLU	N-CA	-5.13	1.39	1.46
1	B	244	GLU	CD-OE1	5.13	1.35	1.25
1	C	23	ARG	CA-C	5.13	1.59	1.52
1	A	160	LYS	C-N	5.13	1.44	1.34
1	A	244	GLU	CD-OE1	5.13	1.35	1.25
1	B	17	LEU	CG-CD1	-5.13	1.35	1.52
1	C	160	LYS	C-N	5.13	1.44	1.34
1	B	23	ARG	CD-NE	5.12	1.53	1.46
1	A	23	ARG	CD-NE	5.12	1.53	1.46
1	D	49	GLU	CG-CD	5.12	1.64	1.52
1	D	278	HIS	C-O	5.12	1.29	1.23
1	D	398	GLU	CD-OE1	5.12	1.35	1.25
1	A	204	ARG	CZ-NH1	5.12	1.40	1.32
1	D	23	ARG	CD-NE	5.12	1.53	1.46
1	B	204	ARG	CZ-NH1	5.12	1.40	1.32
1	B	100	GLN	C-O	5.11	1.30	1.24
1	A	17	LEU	CG-CD1	-5.11	1.35	1.52
1	B	49	GLU	CG-CD	5.11	1.64	1.52
1	B	118	LEU	CA-C	-5.11	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	23	ARG	CD-NE	5.11	1.53	1.46
1	C	146	PHE	CA-C	-5.11	1.46	1.52
1	D	17	LEU	CG-CD1	-5.11	1.35	1.52
1	D	204	ARG	CZ-NH1	5.11	1.40	1.32
1	C	100	GLN	C-O	5.11	1.30	1.24
1	C	17	LEU	CG-CD1	-5.10	1.35	1.52
1	D	423	LYS	N-CA	5.10	1.52	1.46
1	A	398	GLU	CD-OE1	5.10	1.35	1.25
1	C	398	GLU	CD-OE1	5.10	1.35	1.25
1	B	317	GLY	C-N	5.10	1.40	1.33
1	B	398	GLU	CD-OE1	5.10	1.35	1.25
1	D	241	VAL	CA-CB	-5.09	1.47	1.54
1	A	23	ARG	CA-C	5.09	1.59	1.52
1	A	111	GLY	C-O	-5.09	1.17	1.23
1	A	124	HIS	CB-CG	-5.09	1.43	1.50
1	D	118	LEU	CA-C	-5.09	1.46	1.52
1	D	168	GLU	N-CA	-5.09	1.39	1.46
1	B	160	LYS	C-N	5.09	1.44	1.34
1	B	374	GLY	C-O	5.09	1.30	1.23
1	B	423	LYS	N-CA	5.09	1.52	1.46
1	C	124	HIS	CB-CG	-5.09	1.43	1.50
1	C	317	GLY	C-N	5.09	1.40	1.33
1	C	20	GLU	CD-OE1	5.09	1.35	1.25
1	C	111	GLY	C-O	-5.09	1.17	1.23
1	A	423	LYS	N-CA	5.08	1.52	1.46
1	A	118	LEU	CA-C	-5.08	1.46	1.52
1	D	160	LYS	C-N	5.08	1.44	1.34
1	A	383	ARG	CZ-NH2	5.08	1.40	1.33
1	B	106	ALA	CA-CB	5.08	1.62	1.53
1	C	106	ALA	CA-CB	5.08	1.62	1.53
1	D	106	ALA	CA-CB	5.08	1.62	1.53
1	D	111	GLY	C-O	-5.08	1.17	1.23
1	B	124	HIS	CB-CG	-5.08	1.43	1.50
1	A	106	ALA	CA-CB	5.07	1.62	1.53
1	C	383	ARG	CZ-NH2	5.07	1.40	1.33
1	D	212	ARG	CB-CG	5.07	1.67	1.52
1	A	20	GLU	CD-OE1	5.07	1.34	1.25
1	D	20	GLU	CD-OE1	5.07	1.34	1.25
1	D	123	PHE	CD2-CE2	5.07	1.53	1.38
1	B	23	ARG	CA-C	5.07	1.59	1.52
1	C	423	LYS	N-CA	5.07	1.52	1.46
1	D	23	ARG	CA-C	5.07	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	383	ARG	CZ-NH2	5.07	1.40	1.33
1	B	415	SER	CA-CB	5.06	1.61	1.54
1	D	378	HIS	C-O	5.06	1.30	1.24
1	B	200	GLU	CD-OE2	5.06	1.34	1.25
1	A	415	SER	CA-CB	5.06	1.61	1.54
1	B	20	GLU	CD-OE1	5.06	1.34	1.25
1	D	374	GLY	C-O	5.06	1.30	1.23
1	A	374	GLY	C-O	5.06	1.30	1.23
1	A	317	GLY	C-N	5.06	1.40	1.33
1	A	241	VAL	CA-CB	-5.05	1.47	1.54
1	B	141	GLN	CD-NE2	5.05	1.43	1.33
1	B	312	THR	CB-CG2	-5.05	1.35	1.52
1	C	228	THR	CA-C	-5.05	1.46	1.52
1	B	123	PHE	CD2-CE2	5.05	1.53	1.38
1	B	383	ARG	CZ-NH2	5.05	1.40	1.33
1	A	212	ARG	CB-CG	5.05	1.67	1.52
1	B	241	VAL	CA-CB	-5.05	1.47	1.54
1	C	118	LEU	C-O	-5.05	1.17	1.24
1	A	123	PHE	CD2-CE2	5.05	1.53	1.38
1	A	200	GLU	CD-OE2	5.05	1.34	1.25
1	C	141	GLN	CD-NE2	5.05	1.43	1.33
1	D	200	GLU	CD-OE2	5.05	1.34	1.25
1	C	123	PHE	CD2-CE2	5.05	1.53	1.38
1	B	323	TYR	CA-CB	-5.04	1.45	1.53
1	B	212	ARG	CB-CG	5.04	1.67	1.52
1	C	415	SER	CA-CB	5.04	1.61	1.54
1	C	212	ARG	CB-CG	5.04	1.67	1.52
1	C	419	VAL	C-N	5.04	1.39	1.33
1	A	312	THR	CB-CG2	-5.04	1.35	1.52
1	B	111	GLY	C-O	-5.04	1.17	1.23
1	C	167	VAL	CA-CB	-5.04	1.48	1.54
1	C	312	THR	CB-CG2	-5.04	1.35	1.52
1	A	141	GLN	CD-NE2	5.04	1.43	1.33
1	C	118	LEU	CA-C	-5.04	1.46	1.52
1	D	141	GLN	CD-NE2	5.04	1.43	1.33
1	C	323	TYR	CA-CB	-5.04	1.45	1.53
1	A	228	THR	CA-C	-5.03	1.46	1.52
1	C	241	VAL	CA-CB	-5.03	1.47	1.54
1	B	228	THR	CA-C	-5.03	1.46	1.52
1	C	85	LYS	CD-CE	5.03	1.67	1.52
1	C	374	GLY	C-O	5.03	1.30	1.23
1	D	218	GLY	C-O	-5.03	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	228	THR	CA-C	-5.03	1.46	1.52
1	A	323	TYR	CA-CB	-5.03	1.45	1.53
1	B	196	PHE	CA-C	5.03	1.59	1.52
1	C	378	HIS	C-O	5.03	1.30	1.24
1	D	167	VAL	CA-CB	-5.03	1.48	1.54
1	C	218	GLY	C-O	-5.02	1.16	1.24
1	D	168	GLU	CB-CG	5.02	1.67	1.52
1	D	317	GLY	C-N	5.02	1.40	1.33
1	C	200	GLU	CD-OE2	5.02	1.34	1.25
1	B	167	VAL	CA-CB	-5.02	1.48	1.54
1	D	312	THR	CB-CG2	-5.02	1.35	1.52
1	A	319	MET	CB-CG	5.02	1.67	1.52
1	B	378	HIS	C-O	5.02	1.30	1.24
1	C	319	MET	CB-CG	5.02	1.67	1.52
1	A	378	HIS	C-O	5.01	1.30	1.24
1	C	196	PHE	CA-C	5.01	1.59	1.52
1	D	402	LEU	CA-C	5.01	1.59	1.52
1	A	196	PHE	CA-C	5.01	1.59	1.52
1	B	85	LYS	CD-CE	5.01	1.67	1.52
1	A	218	GLY	C-O	-5.01	1.17	1.24
1	D	306	GLY	C-N	5.01	1.40	1.33
1	D	415	SER	CA-CB	5.01	1.61	1.54
1	A	255	VAL	CB-CG2	5.01	1.69	1.52
1	C	309	GLN	C-O	5.01	1.29	1.23
1	D	319	MET	CB-CG	5.01	1.67	1.52
1	D	118	LEU	C-O	-5.01	1.17	1.24
1	A	167	VAL	CA-CB	-5.01	1.48	1.54
1	A	309	GLN	C-O	5.01	1.29	1.23
1	B	218	GLY	C-O	-5.01	1.17	1.24
1	C	63	GLU	CG-CD	5.01	1.64	1.52
1	A	168	GLU	CB-CG	5.00	1.67	1.52
1	C	255	VAL	CB-CG2	5.00	1.69	1.52
1	D	309	GLN	C-O	5.00	1.29	1.23
1	B	255	VAL	CB-CG2	5.00	1.69	1.52
1	B	319	MET	CB-CG	5.00	1.67	1.52
1	D	255	VAL	CB-CG2	5.00	1.69	1.52
1	A	85	LYS	CD-CE	5.00	1.67	1.52
1	B	168	GLU	CB-CG	5.00	1.67	1.52

All (2102) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	289	PRO	N-CA-C	17.45	132.83	114.68
1	C	289	PRO	N-CA-C	17.44	132.81	114.68
1	B	289	PRO	N-CA-C	17.43	132.81	114.68
1	A	289	PRO	N-CA-C	17.42	132.79	114.68
1	C	378	HIS	CA-C-N	17.16	138.15	119.28
1	C	378	HIS	C-N-CA	17.16	138.15	119.28
1	A	378	HIS	CA-C-N	17.14	138.13	119.28
1	A	378	HIS	C-N-CA	17.14	138.13	119.28
1	D	378	HIS	CA-C-N	17.14	138.13	119.28
1	D	378	HIS	C-N-CA	17.14	138.13	119.28
1	B	378	HIS	CA-C-N	17.12	138.12	119.28
1	B	378	HIS	C-N-CA	17.12	138.12	119.28
1	B	314	THR	N-CA-C	16.78	133.00	109.18
1	A	314	THR	N-CA-C	16.73	132.94	109.18
1	D	314	THR	N-CA-C	16.73	132.94	109.18
1	C	314	THR	N-CA-C	16.73	132.94	109.18
1	C	217	THR	N-CA-C	16.62	131.06	111.11
1	D	217	THR	N-CA-C	16.62	131.05	111.11
1	A	217	THR	N-CA-C	16.61	131.05	111.11
1	B	217	THR	N-CA-C	16.61	131.04	111.11
1	D	20	GLU	CA-C-N	16.57	138.85	120.13
1	D	20	GLU	C-N-CA	16.57	138.85	120.13
1	B	20	GLU	CA-C-N	16.55	138.83	120.13
1	B	20	GLU	C-N-CA	16.55	138.83	120.13
1	A	20	GLU	CA-C-N	16.53	138.81	120.13
1	A	20	GLU	C-N-CA	16.53	138.81	120.13
1	C	20	GLU	CA-C-N	16.53	138.80	120.13
1	C	20	GLU	C-N-CA	16.53	138.80	120.13
1	B	88	TYR	CA-C-N	15.05	135.71	119.90
1	B	88	TYR	C-N-CA	15.05	135.71	119.90
1	D	88	TYR	CA-C-N	15.03	135.68	119.90
1	D	88	TYR	C-N-CA	15.03	135.68	119.90
1	A	88	TYR	CA-C-N	15.03	135.68	119.90
1	A	88	TYR	C-N-CA	15.03	135.68	119.90
1	C	88	TYR	CA-C-N	14.99	135.64	119.90
1	C	88	TYR	C-N-CA	14.99	135.64	119.90
1	B	58	LEU	N-CA-C	14.52	129.97	111.24
1	A	58	LEU	N-CA-C	14.52	129.97	111.24
1	C	58	LEU	N-CA-C	14.51	129.96	111.24
1	D	58	LEU	N-CA-C	14.50	129.95	111.24
1	D	245	GLY	CA-C-N	-13.04	112.81	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	245	GLY	C-N-CA	-13.04	112.81	122.33
1	C	265	ARG	N-CA-C	-13.03	97.06	111.14
1	B	245	GLY	CA-C-N	-13.02	112.83	122.33
1	B	245	GLY	C-N-CA	-13.02	112.83	122.33
1	B	94	GLU	N-CA-C	-13.01	87.00	108.34
1	A	94	GLU	N-CA-C	-13.01	87.01	108.34
1	D	94	GLU	N-CA-C	-13.01	87.01	108.34
1	A	265	ARG	N-CA-C	-13.00	97.10	111.14
1	C	94	GLU	N-CA-C	-13.00	87.02	108.34
1	A	245	GLY	CA-C-N	-13.00	112.84	122.33
1	A	245	GLY	C-N-CA	-13.00	112.84	122.33
1	B	265	ARG	N-CA-C	-12.99	97.11	111.14
1	C	245	GLY	CA-C-N	-12.98	112.85	122.33
1	C	245	GLY	C-N-CA	-12.98	112.85	122.33
1	D	265	ARG	N-CA-C	-12.96	97.14	111.14
1	B	91	THR	CA-C-O	12.37	134.19	119.59
1	A	91	THR	CA-C-O	12.36	134.18	119.59
1	D	91	THR	CA-C-O	12.36	134.17	119.59
1	C	91	THR	CA-C-O	12.33	134.14	119.59
1	A	341	ARG	NE-CZ-NH2	-12.09	108.32	119.20
1	B	341	ARG	NE-CZ-NH2	-12.07	108.34	119.20
1	C	341	ARG	NE-CZ-NH2	-12.07	108.34	119.20
1	D	341	ARG	NE-CZ-NH2	-12.03	108.37	119.20
1	C	196	PHE	N-CA-C	11.87	127.54	113.18
1	A	196	PHE	N-CA-C	11.85	127.52	113.18
1	D	196	PHE	N-CA-C	11.85	127.51	113.18
1	B	196	PHE	N-CA-C	11.82	127.48	113.18
1	D	151	ASP	N-CA-C	11.79	128.58	111.96
1	A	151	ASP	N-CA-C	11.78	128.57	111.96
1	C	151	ASP	N-CA-C	11.76	128.55	111.96
1	B	151	ASP	N-CA-C	11.75	128.53	111.96
1	B	55	TRP	CA-C-N	11.72	139.90	122.67
1	B	55	TRP	C-N-CA	11.72	139.90	122.67
1	C	55	TRP	CA-C-N	11.72	139.90	122.67
1	C	55	TRP	C-N-CA	11.72	139.90	122.67
1	D	55	TRP	CA-C-N	11.71	139.88	122.67
1	D	55	TRP	C-N-CA	11.71	139.88	122.67
1	A	55	TRP	CA-C-N	11.71	139.88	122.67
1	A	55	TRP	C-N-CA	11.71	139.88	122.67
1	D	239	GLU	CG-CD-OE1	-11.43	92.11	118.40
1	A	239	GLU	CG-CD-OE1	-11.43	92.11	118.40
1	B	239	GLU	CG-CD-OE1	-11.42	92.12	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	27	ILE	N-CA-C	11.42	124.36	107.80
1	C	239	GLU	CG-CD-OE1	-11.42	92.14	118.40
1	A	27	ILE	N-CA-C	11.41	124.34	107.80
1	D	27	ILE	N-CA-C	11.40	124.33	107.80
1	B	27	ILE	N-CA-C	11.39	124.31	107.80
1	D	172	GLU	N-CA-C	11.35	125.06	111.33
1	A	172	GLU	N-CA-C	11.31	125.02	111.33
1	C	172	GLU	N-CA-C	11.31	125.02	111.33
1	B	172	GLU	N-CA-C	11.27	124.97	111.33
1	C	95	GLU	N-CA-CB	11.27	125.57	110.25
1	A	95	GLU	N-CA-CB	11.24	125.53	110.25
1	B	95	GLU	N-CA-CB	11.23	125.53	110.25
1	D	95	GLU	N-CA-CB	11.22	125.52	110.25
1	D	116	LYS	N-CA-C	-11.10	97.91	112.68
1	A	116	LYS	N-CA-C	-11.10	97.92	112.68
1	B	116	LYS	N-CA-C	-11.09	97.93	112.68
1	C	116	LYS	N-CA-C	-11.06	97.96	112.68
1	C	141	GLN	N-CA-CB	-10.72	94.31	110.07
1	D	339	HIS	CA-C-O	-10.72	109.06	120.42
1	A	339	HIS	CA-C-O	-10.70	109.08	120.42
1	A	141	GLN	N-CA-CB	-10.68	94.38	110.07
1	C	339	HIS	CA-C-O	-10.68	109.10	120.42
1	D	141	GLN	N-CA-CB	-10.68	94.38	110.07
1	B	141	GLN	N-CA-CB	-10.65	94.41	110.07
1	B	339	HIS	CA-C-O	-10.63	109.15	120.42
1	D	364	GLY	CA-C-O	-10.53	112.60	122.39
1	C	364	GLY	CA-C-O	-10.52	112.60	122.39
1	A	364	GLY	CA-C-O	-10.50	112.62	122.39
1	B	363	PHE	N-CA-C	10.49	126.57	112.30
1	D	363	PHE	N-CA-C	10.47	126.55	112.30
1	C	363	PHE	N-CA-C	10.47	126.54	112.30
1	B	216	GLU	CA-C-N	10.47	134.67	120.54
1	B	216	GLU	C-N-CA	10.47	134.67	120.54
1	B	364	GLY	CA-C-O	-10.47	112.65	122.39
1	A	363	PHE	N-CA-C	10.46	126.53	112.30
1	C	216	GLU	CA-C-N	10.46	134.66	120.54
1	C	216	GLU	C-N-CA	10.46	134.66	120.54
1	B	85	LYS	N-CA-C	-10.45	90.16	108.13
1	A	216	GLU	CA-C-N	10.45	134.64	120.54
1	A	216	GLU	C-N-CA	10.45	134.64	120.54
1	D	216	GLU	CA-C-N	10.43	134.63	120.54
1	D	216	GLU	C-N-CA	10.43	134.63	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	85	LYS	N-CA-C	-10.42	90.21	108.13
1	C	85	LYS	N-CA-C	-10.40	90.24	108.13
1	D	85	LYS	N-CA-C	-10.40	90.24	108.13
1	D	371	ALA	CA-C-O	-10.26	110.28	121.78
1	B	371	ALA	CA-C-O	-10.25	110.31	121.78
1	A	371	ALA	CA-C-O	-10.24	110.31	121.78
1	C	371	ALA	CA-C-O	-10.20	110.35	121.78
1	D	338	GLU	O-C-N	10.19	134.16	121.33
1	A	330	ASN	N-CA-C	10.18	128.07	111.37
1	B	330	ASN	N-CA-C	10.17	128.05	111.37
1	A	338	GLU	O-C-N	10.17	134.14	121.33
1	D	330	ASN	N-CA-C	10.17	128.04	111.37
1	C	330	ASN	N-CA-C	10.16	128.04	111.37
1	C	338	GLU	O-C-N	10.16	134.14	121.33
1	B	338	GLU	O-C-N	10.14	134.11	121.33
1	A	21	PRO	CA-C-N	9.94	131.98	121.45
1	A	21	PRO	C-N-CA	9.94	131.98	121.45
1	C	21	PRO	CA-C-N	9.93	131.98	121.45
1	C	21	PRO	C-N-CA	9.93	131.98	121.45
1	D	21	PRO	CA-C-N	9.93	131.98	121.45
1	D	21	PRO	C-N-CA	9.93	131.98	121.45
1	B	21	PRO	CA-C-N	9.93	131.97	121.45
1	B	21	PRO	C-N-CA	9.93	131.97	121.45
1	A	68	SER	CA-CB-OG	9.91	130.92	111.10
1	D	68	SER	CA-CB-OG	9.91	130.92	111.10
1	C	68	SER	CA-CB-OG	9.90	130.90	111.10
1	B	68	SER	CA-CB-OG	9.89	130.89	111.10
1	C	141	GLN	N-CA-C	9.86	123.96	111.24
1	A	141	GLN	N-CA-C	9.85	123.95	111.24
1	D	141	GLN	N-CA-C	9.84	123.94	111.24
1	B	141	GLN	N-CA-C	9.83	123.92	111.24
1	C	246	GLY	CA-C-O	-9.76	111.30	120.57
1	C	258	TRP	N-CA-C	9.76	123.30	111.40
1	A	246	GLY	CA-C-O	-9.75	111.31	120.57
1	D	258	TRP	N-CA-C	9.75	123.29	111.40
1	B	246	GLY	CA-C-O	-9.74	111.31	120.57
1	D	246	GLY	CA-C-O	-9.74	111.31	120.57
1	D	21	PRO	O-C-N	9.73	134.03	123.03
1	A	258	TRP	N-CA-C	9.73	123.27	111.40
1	A	21	PRO	O-C-N	9.72	134.01	123.03
1	B	258	TRP	N-CA-C	9.72	123.25	111.40
1	C	21	PRO	O-C-N	9.70	133.99	123.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	269	GLU	O-C-N	9.70	132.12	122.03
1	C	269	GLU	O-C-N	9.70	132.12	122.03
1	A	269	GLU	O-C-N	9.68	132.10	122.03
1	B	21	PRO	O-C-N	9.68	133.97	123.03
1	D	269	GLU	O-C-N	9.64	132.06	122.03
1	B	28	VAL	CA-C-O	-9.56	110.34	120.48
1	C	28	VAL	CA-C-O	-9.56	110.34	120.48
1	D	28	VAL	CA-C-O	-9.55	110.36	120.48
1	A	28	VAL	CA-C-O	-9.55	110.36	120.48
1	D	150	LYS	CA-C-N	-9.48	107.73	122.42
1	D	150	LYS	C-N-CA	-9.48	107.73	122.42
1	B	150	LYS	CA-C-N	-9.47	107.73	122.42
1	B	150	LYS	C-N-CA	-9.47	107.73	122.42
1	C	150	LYS	CA-C-N	-9.47	107.73	122.42
1	C	150	LYS	C-N-CA	-9.47	107.73	122.42
1	A	150	LYS	CA-C-N	-9.47	107.74	122.42
1	A	150	LYS	C-N-CA	-9.47	107.74	122.42
1	C	147	MET	CA-C-N	-9.46	108.85	122.29
1	C	147	MET	C-N-CA	-9.46	108.85	122.29
1	A	147	MET	CA-C-N	-9.44	108.88	122.29
1	A	147	MET	C-N-CA	-9.44	108.88	122.29
1	B	147	MET	CA-C-N	-9.44	108.89	122.29
1	B	147	MET	C-N-CA	-9.44	108.89	122.29
1	D	147	MET	CA-C-N	-9.44	108.89	122.29
1	D	147	MET	C-N-CA	-9.44	108.89	122.29
1	A	334	LEU	N-CA-C	9.42	124.58	113.18
1	C	334	LEU	N-CA-C	9.41	124.57	113.18
1	B	334	LEU	N-CA-C	9.41	124.56	113.18
1	D	334	LEU	N-CA-C	9.40	124.55	113.18
1	D	302	ALA	N-CA-C	9.37	124.34	113.19
1	D	184	LEU	N-CA-C	9.37	124.58	107.99
1	A	302	ALA	N-CA-C	9.35	124.32	113.19
1	A	184	LEU	N-CA-C	9.35	124.54	107.99
1	C	184	LEU	N-CA-C	9.35	124.54	107.99
1	B	302	ALA	N-CA-C	9.35	124.31	113.19
1	D	259	SER	CA-C-O	9.35	130.80	119.49
1	C	302	ALA	N-CA-C	9.34	124.31	113.19
1	B	184	LEU	N-CA-C	9.34	124.52	107.99
1	B	157	THR	N-CA-CB	-9.33	96.09	110.65
1	A	259	SER	CA-C-O	9.33	130.78	119.49
1	C	259	SER	CA-C-O	9.33	130.78	119.49
1	B	259	SER	CA-C-O	9.33	130.77	119.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	157	THR	N-CA-CB	-9.31	96.12	110.65
1	C	157	THR	N-CA-CB	-9.31	96.12	110.65
1	D	157	THR	N-CA-CB	-9.30	96.15	110.65
1	B	196	PHE	CA-C-N	9.21	134.98	121.26
1	B	196	PHE	C-N-CA	9.21	134.98	121.26
1	C	196	PHE	CA-C-N	9.19	134.96	121.26
1	C	196	PHE	C-N-CA	9.19	134.96	121.26
1	A	196	PHE	CA-C-N	9.19	134.95	121.26
1	A	196	PHE	C-N-CA	9.19	134.95	121.26
1	D	196	PHE	CA-C-N	9.19	134.95	121.26
1	D	196	PHE	C-N-CA	9.19	134.95	121.26
1	C	384	ALA	N-CA-C	-9.16	102.10	113.28
1	C	261	LEU	CB-CA-C	-9.14	95.31	110.85
1	A	261	LEU	CB-CA-C	-9.14	95.32	110.85
1	A	384	ALA	N-CA-C	-9.14	102.13	113.28
1	B	261	LEU	CB-CA-C	-9.13	95.33	110.85
1	D	384	ALA	N-CA-C	-9.13	102.14	113.28
1	C	248	TYR	N-CA-C	9.13	123.92	109.50
1	D	248	TYR	N-CA-C	9.13	123.92	109.50
1	D	261	LEU	CB-CA-C	-9.13	95.33	110.85
1	B	248	TYR	N-CA-C	9.12	123.92	109.50
1	A	248	TYR	N-CA-C	9.12	123.91	109.50
1	B	384	ALA	N-CA-C	-9.12	102.16	113.28
1	A	160	LYS	N-CA-C	-9.11	96.57	110.32
1	C	160	LYS	N-CA-C	-9.10	96.58	110.32
1	B	160	LYS	N-CA-C	-9.10	96.58	110.32
1	D	160	LYS	N-CA-C	-9.10	96.59	110.32
1	C	366	ASP	O-C-N	9.06	133.69	122.63
1	B	366	ASP	O-C-N	9.04	133.66	122.63
1	A	366	ASP	O-C-N	9.03	133.64	122.63
1	C	274	ALA	CA-C-O	-8.99	110.06	120.49
1	D	274	ALA	CA-C-O	-8.99	110.06	120.49
1	A	274	ALA	CA-C-O	-8.98	110.07	120.49
1	D	366	ASP	O-C-N	8.98	133.58	122.63
1	B	274	ALA	CA-C-O	-8.96	110.10	120.49
1	C	216	GLU	CB-CA-C	8.96	128.25	110.42
1	D	216	GLU	CB-CA-C	8.95	128.23	110.42
1	A	216	GLU	CB-CA-C	8.95	128.22	110.42
1	B	216	GLU	CB-CA-C	8.94	128.21	110.42
1	B	255	VAL	CA-C-N	8.93	135.38	121.19
1	B	255	VAL	C-N-CA	8.93	135.38	121.19
1	C	255	VAL	CA-C-N	8.90	135.35	121.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	255	VAL	C-N-CA	8.90	135.35	121.19
1	A	255	VAL	CA-C-N	8.89	135.33	121.19
1	A	255	VAL	C-N-CA	8.89	135.33	121.19
1	D	255	VAL	CA-C-N	8.89	135.32	121.19
1	D	255	VAL	C-N-CA	8.89	135.32	121.19
1	B	201	GLU	CG-CD-OE1	-8.86	98.02	118.40
1	A	201	GLU	CG-CD-OE1	-8.84	98.08	118.40
1	D	201	GLU	CG-CD-OE1	-8.82	98.10	118.40
1	C	201	GLU	CG-CD-OE1	-8.82	98.11	118.40
1	B	386	ALA	N-CA-C	-8.80	100.87	111.69
1	C	386	ALA	N-CA-C	-8.79	100.87	111.69
1	A	386	ALA	N-CA-C	-8.79	100.87	111.69
1	C	172	GLU	N-CA-CB	-8.79	96.87	110.06
1	D	386	ALA	N-CA-C	-8.79	100.88	111.69
1	B	172	GLU	N-CA-CB	-8.79	96.88	110.06
1	A	172	GLU	N-CA-CB	-8.76	96.92	110.06
1	D	172	GLU	N-CA-CB	-8.76	96.92	110.06
1	C	266	GLU	CB-CG-CD	-8.68	97.84	112.60
1	A	266	GLU	CB-CG-CD	-8.68	97.85	112.60
1	B	411	GLU	N-CA-C	-8.68	101.79	112.38
1	A	411	GLU	N-CA-C	-8.68	101.79	112.38
1	B	266	GLU	CB-CG-CD	-8.67	97.86	112.60
1	D	266	GLU	CB-CG-CD	-8.67	97.86	112.60
1	D	411	GLU	N-CA-C	-8.67	101.80	112.38
1	C	411	GLU	N-CA-C	-8.66	101.82	112.38
1	C	75	LEU	CA-C-O	-8.64	111.56	120.63
1	B	75	LEU	CA-C-O	-8.63	111.57	120.63
1	A	75	LEU	CA-C-O	-8.62	111.58	120.63
1	D	75	LEU	CA-C-O	-8.62	111.58	120.63
1	D	65	ALA	N-CA-C	-8.55	101.54	111.03
1	D	222	GLU	CG-CD-OE2	-8.54	98.77	118.40
1	A	65	ALA	N-CA-C	-8.53	101.56	111.03
1	A	222	GLU	CG-CD-OE2	-8.53	98.78	118.40
1	B	105	VAL	N-CA-C	8.53	127.08	109.34
1	C	222	GLU	CG-CD-OE2	-8.53	98.78	118.40
1	C	105	VAL	N-CA-C	8.53	127.08	109.34
1	A	105	VAL	N-CA-C	8.53	127.08	109.34
1	B	222	GLU	CG-CD-OE2	-8.53	98.79	118.40
1	D	105	VAL	N-CA-C	8.52	127.06	109.34
1	B	65	ALA	N-CA-C	-8.51	101.58	111.03
1	C	65	ALA	N-CA-C	-8.51	101.58	111.03
1	B	415	SER	CA-C-N	8.47	133.49	121.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	415	SER	C-N-CA	8.47	133.49	121.71
1	B	394	ASP	N-CA-C	-8.47	100.69	111.02
1	A	415	SER	CA-C-N	8.45	133.45	121.71
1	A	415	SER	C-N-CA	8.45	133.45	121.71
1	A	394	ASP	N-CA-C	-8.44	100.72	111.02
1	C	394	ASP	N-CA-C	-8.44	100.72	111.02
1	C	270	ASP	CA-CB-CG	-8.44	104.16	112.60
1	D	376	MET	CG-SD-CE	-8.44	82.33	100.90
1	C	376	MET	CG-SD-CE	-8.44	82.34	100.90
1	D	270	ASP	CA-CB-CG	-8.44	104.17	112.60
1	A	270	ASP	CA-CB-CG	-8.43	104.17	112.60
1	C	415	SER	CA-C-N	8.43	133.43	121.71
1	C	415	SER	C-N-CA	8.43	133.43	121.71
1	A	376	MET	CG-SD-CE	-8.43	82.35	100.90
1	D	394	ASP	N-CA-C	-8.43	100.74	111.02
1	D	415	SER	CA-C-N	8.43	133.42	121.71
1	D	415	SER	C-N-CA	8.43	133.42	121.71
1	B	270	ASP	CA-CB-CG	-8.42	104.18	112.60
1	B	376	MET	CG-SD-CE	-8.42	82.37	100.90
1	D	244	GLU	CA-CB-CG	-8.42	97.27	114.10
1	A	238	ALA	N-CA-C	-8.41	102.19	111.36
1	A	244	GLU	CA-CB-CG	-8.41	97.28	114.10
1	B	238	ALA	N-CA-C	-8.41	102.19	111.36
1	B	300	LYS	CG-CD-CE	8.41	130.64	111.30
1	C	244	GLU	CA-CB-CG	-8.41	97.28	114.10
1	D	238	ALA	N-CA-C	-8.40	102.20	111.36
1	D	146	PHE	N-CA-C	8.40	120.43	111.28
1	B	146	PHE	N-CA-C	8.40	120.43	111.28
1	D	300	LYS	CG-CD-CE	8.39	130.61	111.30
1	B	244	GLU	CA-CB-CG	-8.39	97.32	114.10
1	A	300	LYS	CG-CD-CE	8.39	130.59	111.30
1	C	300	LYS	CG-CD-CE	8.38	130.58	111.30
1	C	238	ALA	N-CA-C	-8.37	102.23	111.36
1	A	146	PHE	N-CA-C	8.37	120.40	111.28
1	D	239	GLU	CG-CD-OE2	8.37	137.65	118.40
1	A	239	GLU	CG-CD-OE2	8.36	137.62	118.40
1	C	146	PHE	N-CA-C	8.35	120.39	111.28
1	B	239	GLU	CG-CD-OE2	8.34	137.59	118.40
1	C	239	GLU	CG-CD-OE2	8.34	137.57	118.40
1	A	242	ALA	N-CA-C	-8.31	101.76	112.23
1	B	242	ALA	N-CA-C	-8.31	101.76	112.23
1	C	242	ALA	N-CA-C	-8.30	101.77	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	242	ALA	N-CA-C	-8.29	101.78	112.23
1	A	370	GLN	CA-CB-CG	-8.28	97.54	114.10
1	C	370	GLN	CA-CB-CG	-8.27	97.56	114.10
1	B	370	GLN	CA-CB-CG	-8.27	97.57	114.10
1	D	370	GLN	CA-CB-CG	-8.27	97.57	114.10
1	D	299	ALA	N-CA-C	-8.26	102.96	112.87
1	A	299	ALA	N-CA-C	-8.26	102.96	112.87
1	C	299	ALA	N-CA-C	-8.24	102.98	112.87
1	A	336	LYS	CG-CD-CE	8.24	130.25	111.30
1	D	94	GLU	CA-C-O	-8.24	111.51	120.24
1	D	336	LYS	CG-CD-CE	8.24	130.25	111.30
1	B	336	LYS	CG-CD-CE	8.23	130.24	111.30
1	C	336	LYS	CG-CD-CE	8.23	130.22	111.30
1	D	98	LEU	N-CA-C	-8.23	102.39	111.36
1	A	94	GLU	CA-C-O	-8.22	111.52	120.24
1	B	299	ALA	N-CA-C	-8.22	103.00	112.87
1	B	360	ILE	CB-CA-C	-8.22	101.53	111.81
1	A	98	LEU	N-CA-C	-8.21	102.41	111.36
1	A	360	ILE	CB-CA-C	-8.21	101.55	111.81
1	C	94	GLU	CA-C-O	-8.21	111.54	120.24
1	C	98	LEU	N-CA-C	-8.20	102.42	111.36
1	C	360	ILE	CB-CA-C	-8.20	101.56	111.81
1	D	360	ILE	CB-CA-C	-8.20	101.56	111.81
1	B	94	GLU	CA-C-O	-8.19	111.56	120.24
1	B	98	LEU	N-CA-C	-8.19	102.44	111.36
1	A	246	GLY	CA-C-N	-8.18	109.56	122.65
1	A	246	GLY	C-N-CA	-8.18	109.56	122.65
1	D	246	GLY	CA-C-N	-8.18	109.56	122.65
1	D	246	GLY	C-N-CA	-8.18	109.56	122.65
1	B	246	GLY	CA-C-N	-8.16	109.59	122.65
1	B	246	GLY	C-N-CA	-8.16	109.59	122.65
1	C	246	GLY	CA-C-N	-8.16	109.59	122.65
1	C	246	GLY	C-N-CA	-8.16	109.59	122.65
1	A	122	ASP	N-CA-C	-8.12	96.74	108.60
1	D	122	ASP	N-CA-C	-8.12	96.74	108.60
1	D	237	ARG	NE-CZ-NH2	-8.11	111.90	119.20
1	B	122	ASP	N-CA-C	-8.11	96.76	108.60
1	C	122	ASP	N-CA-C	-8.11	96.76	108.60
1	D	174	ALA	N-CA-C	-8.10	102.04	111.03
1	C	174	ALA	N-CA-C	-8.10	102.04	111.03
1	A	237	ARG	NE-CZ-NH2	-8.08	111.93	119.20
1	A	174	ALA	N-CA-C	-8.08	102.06	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	237	ARG	NE-CZ-NH2	-8.08	111.93	119.20
1	B	174	ALA	N-CA-C	-8.07	102.07	111.03
1	C	237	ARG	NE-CZ-NH2	-8.05	111.95	119.20
1	C	75	LEU	N-CA-C	-8.00	93.28	107.28
1	A	75	LEU	N-CA-C	-8.00	93.28	107.28
1	D	75	LEU	N-CA-C	-8.00	93.28	107.28
1	B	75	LEU	N-CA-C	-7.99	93.31	107.28
1	C	254	VAL	N-CA-C	7.97	122.12	111.44
1	A	254	VAL	N-CA-C	7.97	122.12	111.44
1	B	254	VAL	N-CA-C	7.96	122.11	111.44
1	A	194	PHE	CA-C-N	-7.96	109.89	119.84
1	A	194	PHE	C-N-CA	-7.96	109.89	119.84
1	B	194	PHE	CA-C-N	-7.96	109.89	119.84
1	B	194	PHE	C-N-CA	-7.96	109.89	119.84
1	A	61	LEU	CA-C-N	7.96	127.95	119.76
1	A	61	LEU	C-N-CA	7.96	127.95	119.76
1	D	254	VAL	N-CA-C	7.95	122.09	111.44
1	B	309	GLN	CA-C-N	-7.94	111.42	122.69
1	B	309	GLN	C-N-CA	-7.94	111.42	122.69
1	C	61	LEU	CA-C-N	7.93	127.93	119.76
1	C	61	LEU	C-N-CA	7.93	127.93	119.76
1	D	194	PHE	CA-C-N	-7.93	109.92	119.84
1	D	194	PHE	C-N-CA	-7.93	109.92	119.84
1	D	130	LEU	O-C-N	-7.93	111.52	122.46
1	A	309	GLN	CA-C-N	-7.93	111.43	122.69
1	A	309	GLN	C-N-CA	-7.93	111.43	122.69
1	C	194	PHE	CA-C-N	-7.93	109.93	119.84
1	C	194	PHE	C-N-CA	-7.93	109.93	119.84
1	D	309	GLN	CA-C-N	-7.93	111.43	122.69
1	D	309	GLN	C-N-CA	-7.93	111.43	122.69
1	B	61	LEU	CA-C-N	7.92	127.92	119.76
1	B	61	LEU	C-N-CA	7.92	127.92	119.76
1	B	356	MET	CG-SD-CE	7.92	118.33	100.90
1	C	356	MET	CG-SD-CE	7.92	118.33	100.90
1	B	311	HIS	N-CA-C	-7.92	97.69	110.20
1	A	356	MET	CG-SD-CE	7.92	118.32	100.90
1	D	356	MET	CG-SD-CE	7.92	118.32	100.90
1	C	309	GLN	CA-C-N	-7.92	111.45	122.69
1	C	309	GLN	C-N-CA	-7.92	111.45	122.69
1	C	292	GLY	CA-C-N	-7.91	111.28	122.75
1	C	292	GLY	C-N-CA	-7.91	111.28	122.75
1	C	382	PRO	CA-C-N	-7.91	107.51	120.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	382	PRO	C-N-CA	-7.91	107.51	120.72
1	D	61	LEU	CA-C-N	7.91	127.91	119.76
1	D	61	LEU	C-N-CA	7.91	127.91	119.76
1	A	292	GLY	CA-C-N	-7.91	111.28	122.75
1	A	292	GLY	C-N-CA	-7.91	111.28	122.75
1	A	311	HIS	N-CA-C	-7.91	97.70	110.20
1	B	292	GLY	CA-C-N	-7.91	111.28	122.75
1	B	292	GLY	C-N-CA	-7.91	111.28	122.75
1	D	311	HIS	N-CA-C	-7.91	97.71	110.20
1	A	382	PRO	CA-C-N	-7.90	107.52	120.72
1	A	382	PRO	C-N-CA	-7.90	107.52	120.72
1	B	93	PHE	CA-C-O	-7.90	112.04	121.60
1	B	382	PRO	CA-C-N	-7.90	107.53	120.72
1	B	382	PRO	C-N-CA	-7.90	107.53	120.72
1	D	382	PRO	CA-C-N	-7.90	107.53	120.72
1	D	382	PRO	C-N-CA	-7.90	107.53	120.72
1	B	130	LEU	O-C-N	-7.89	111.58	122.46
1	C	311	HIS	N-CA-C	-7.88	97.74	110.20
1	D	292	GLY	CA-C-N	-7.88	111.32	122.75
1	D	292	GLY	C-N-CA	-7.88	111.32	122.75
1	C	130	LEU	O-C-N	-7.88	111.58	122.46
1	A	130	LEU	O-C-N	-7.88	111.59	122.46
1	D	93	PHE	CA-C-O	-7.88	112.07	121.60
1	A	93	PHE	CA-C-O	-7.87	112.07	121.60
1	C	156	ALA	CA-C-N	7.87	134.09	123.00
1	C	156	ALA	C-N-CA	7.87	134.09	123.00
1	C	93	PHE	CA-C-O	-7.84	112.11	121.60
1	A	156	ALA	CA-C-N	7.84	134.05	123.00
1	A	156	ALA	C-N-CA	7.84	134.05	123.00
1	D	156	ALA	CA-C-N	7.84	134.05	123.00
1	D	156	ALA	C-N-CA	7.84	134.05	123.00
1	B	156	ALA	CA-C-N	7.83	134.04	123.00
1	B	156	ALA	C-N-CA	7.83	134.04	123.00
1	D	275	ILE	CG1-CB-CG2	-7.83	87.21	110.70
1	B	275	ILE	CG1-CB-CG2	-7.83	87.22	110.70
1	B	269	GLU	N-CA-C	-7.83	102.44	110.97
1	C	275	ILE	CG1-CB-CG2	-7.83	87.22	110.70
1	A	275	ILE	CG1-CB-CG2	-7.82	87.23	110.70
1	C	234	MET	N-CA-C	-7.82	101.87	111.33
1	A	269	GLU	N-CA-C	-7.82	102.45	110.97
1	A	234	MET	N-CA-C	-7.81	101.88	111.33
1	C	160	LYS	CB-CA-C	7.81	119.45	108.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	234	MET	N-CA-C	-7.80	101.89	111.33
1	C	269	GLU	N-CA-C	-7.80	102.46	110.97
1	B	160	LYS	CB-CA-C	7.80	119.44	108.76
1	D	269	GLU	N-CA-C	-7.79	102.48	110.97
1	A	160	LYS	CB-CA-C	7.79	119.42	108.76
1	D	234	MET	N-CA-C	-7.78	101.91	111.33
1	D	160	LYS	CB-CA-C	7.78	119.42	108.76
1	B	359	LEU	O-C-N	7.78	130.18	122.09
1	D	208	ARG	NE-CZ-NH1	7.77	129.27	121.50
1	B	32	PHE	N-CA-C	7.76	120.52	108.96
1	B	119	ARG	CG-CD-NE	-7.76	94.93	112.00
1	A	119	ARG	CG-CD-NE	-7.75	94.94	112.00
1	C	119	ARG	CG-CD-NE	-7.75	94.94	112.00
1	D	119	ARG	CG-CD-NE	-7.75	94.95	112.00
1	A	32	PHE	N-CA-C	7.75	120.51	108.96
1	C	32	PHE	N-CA-C	7.75	120.50	108.96
1	D	275	ILE	CB-CA-C	-7.75	100.94	111.63
1	A	359	LEU	O-C-N	7.74	130.14	122.09
1	C	359	LEU	O-C-N	7.73	130.13	122.09
1	A	208	ARG	NE-CZ-NH1	7.73	129.23	121.50
1	D	359	LEU	O-C-N	7.73	130.13	122.09
1	C	208	ARG	NE-CZ-NH1	7.72	129.22	121.50
1	B	275	ILE	CB-CA-C	-7.72	100.98	111.63
1	A	275	ILE	CB-CA-C	-7.72	100.98	111.63
1	C	198	ARG	CD-NE-CZ	7.71	135.20	124.40
1	D	32	PHE	N-CA-C	7.71	120.44	108.96
1	C	275	ILE	CB-CA-C	-7.70	101.00	111.63
1	A	160	LYS	CD-CE-NZ	7.70	136.54	111.90
1	B	208	ARG	NE-CZ-NH1	7.70	129.20	121.50
1	D	160	LYS	CD-CE-NZ	7.70	136.52	111.90
1	D	83	ILE	CA-C-O	-7.69	111.66	120.66
1	B	160	LYS	CD-CE-NZ	7.69	136.52	111.90
1	C	160	LYS	CD-CE-NZ	7.69	136.51	111.90
1	A	83	ILE	CA-C-O	-7.68	111.67	120.66
1	D	70	ALA	N-CA-C	-7.68	98.23	110.14
1	B	70	ALA	N-CA-C	-7.68	98.24	110.14
1	D	198	ARG	CD-NE-CZ	7.68	135.15	124.40
1	A	70	ALA	N-CA-C	-7.68	98.24	110.14
1	A	198	ARG	CD-NE-CZ	7.68	135.15	124.40
1	B	83	ILE	CA-C-O	-7.67	111.69	120.66
1	C	83	ILE	CA-C-O	-7.66	111.69	120.66
1	C	70	ALA	N-CA-C	-7.66	98.27	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	66	LYS	CB-CG-CD	7.65	128.91	111.30
1	B	198	ARG	CD-NE-CZ	7.65	135.12	124.40
1	A	66	LYS	CB-CG-CD	7.64	128.87	111.30
1	D	66	LYS	CB-CG-CD	7.64	128.88	111.30
1	C	66	LYS	CB-CG-CD	7.64	128.86	111.30
1	D	28	VAL	N-CA-CB	-7.64	100.86	111.25
1	A	28	VAL	N-CA-CB	-7.63	100.88	111.25
1	B	28	VAL	N-CA-CB	-7.62	100.89	111.25
1	C	28	VAL	N-CA-CB	-7.62	100.89	111.25
1	C	280	ALA	CA-C-N	7.61	136.07	121.54
1	C	280	ALA	C-N-CA	7.61	136.07	121.54
1	D	280	ALA	CA-C-N	7.59	136.03	121.54
1	D	280	ALA	C-N-CA	7.59	136.03	121.54
1	D	56	THR	CA-C-N	7.58	136.03	121.54
1	D	56	THR	C-N-CA	7.58	136.03	121.54
1	A	280	ALA	CA-C-N	7.58	136.03	121.54
1	A	280	ALA	C-N-CA	7.58	136.03	121.54
1	B	280	ALA	CA-C-N	7.58	136.03	121.54
1	B	280	ALA	C-N-CA	7.58	136.03	121.54
1	B	157	THR	N-CA-C	7.58	120.77	108.41
1	C	157	THR	N-CA-C	7.58	120.76	108.41
1	D	157	THR	N-CA-C	7.57	120.75	108.41
1	A	157	THR	N-CA-C	7.57	120.75	108.41
1	B	56	THR	CA-C-N	7.57	135.99	121.54
1	B	56	THR	C-N-CA	7.57	135.99	121.54
1	A	56	THR	CA-C-N	7.56	135.99	121.54
1	A	56	THR	C-N-CA	7.56	135.99	121.54
1	B	392	ALA	N-CA-C	-7.56	103.03	111.28
1	D	366	ASP	CB-CG-OD2	-7.56	101.02	118.40
1	C	56	THR	CA-C-N	7.55	135.97	121.54
1	C	56	THR	C-N-CA	7.55	135.97	121.54
1	D	392	ALA	N-CA-C	-7.55	103.05	111.28
1	A	366	ASP	CB-CG-OD2	-7.55	101.04	118.40
1	A	392	ALA	N-CA-C	-7.54	103.06	111.28
1	C	366	ASP	CB-CG-OD2	-7.54	101.07	118.40
1	B	366	ASP	CB-CG-OD2	-7.54	101.07	118.40
1	B	257	GLY	CA-C-N	-7.53	108.14	120.71
1	B	257	GLY	C-N-CA	-7.53	108.14	120.71
1	D	259	SER	N-CA-CB	-7.53	97.53	110.32
1	A	257	GLY	CA-C-N	-7.52	108.15	120.71
1	A	257	GLY	C-N-CA	-7.52	108.15	120.71
1	D	257	GLY	CA-C-N	-7.52	108.15	120.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	257	GLY	C-N-CA	-7.52	108.15	120.71
1	C	257	GLY	CA-C-N	-7.52	108.16	120.71
1	C	257	GLY	C-N-CA	-7.52	108.16	120.71
1	C	259	SER	N-CA-CB	-7.52	97.54	110.32
1	C	392	ALA	N-CA-C	-7.51	103.09	111.28
1	A	259	SER	N-CA-CB	-7.51	97.55	110.32
1	B	259	SER	N-CA-CB	-7.51	97.55	110.32
1	C	309	GLN	CA-CB-CG	-7.50	99.10	114.10
1	D	310	ILE	CG1-CB-CG2	7.50	133.21	110.70
1	D	309	GLN	CA-CB-CG	-7.50	99.11	114.10
1	A	310	ILE	CG1-CB-CG2	7.49	133.18	110.70
1	B	310	ILE	CG1-CB-CG2	7.49	133.15	110.70
1	A	309	GLN	CA-CB-CG	-7.48	99.13	114.10
1	C	310	ILE	CG1-CB-CG2	7.48	133.15	110.70
1	C	109	VAL	CB-CA-C	7.48	121.45	111.88
1	B	109	VAL	CB-CA-C	7.48	121.45	111.88
1	B	309	GLN	CA-CB-CG	-7.47	99.15	114.10
1	A	109	VAL	CB-CA-C	7.45	121.42	111.88
1	D	64	MET	CG-SD-CE	7.44	117.27	100.90
1	A	64	MET	CG-SD-CE	7.44	117.27	100.90
1	B	64	MET	CG-SD-CE	7.44	117.26	100.90
1	C	64	MET	CG-SD-CE	7.44	117.26	100.90
1	D	90	LEU	CD1-CG-CD2	-7.41	94.49	110.80
1	D	109	VAL	CB-CA-C	7.41	121.37	111.88
1	A	90	LEU	CD1-CG-CD2	-7.39	94.53	110.80
1	B	90	LEU	CD1-CG-CD2	-7.39	94.55	110.80
1	C	90	LEU	CD1-CG-CD2	-7.38	94.55	110.80
1	B	218	GLY	N-CA-C	-7.37	105.08	114.37
1	C	218	GLY	N-CA-C	-7.37	105.08	114.37
1	D	175	TYR	CE1-CZ-OH	7.37	142.00	119.90
1	A	218	GLY	N-CA-C	-7.36	105.09	114.37
1	C	175	TYR	CE1-CZ-OH	7.36	141.98	119.90
1	A	175	TYR	CE1-CZ-OH	7.35	141.96	119.90
1	D	218	GLY	N-CA-C	-7.35	105.10	114.37
1	B	175	TYR	CE1-CZ-OH	7.35	141.95	119.90
1	D	80	GLU	CG-CD-OE1	7.35	135.30	118.40
1	B	233	ILE	CB-CA-C	-7.34	102.41	112.24
1	C	344	PHE	N-CA-C	-7.34	99.24	110.32
1	B	80	GLU	CG-CD-OE1	7.33	135.27	118.40
1	C	80	GLU	CG-CD-OE1	7.33	135.26	118.40
1	A	80	GLU	CG-CD-OE1	7.33	135.26	118.40
1	D	233	ILE	CB-CA-C	-7.33	102.42	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	233	ILE	CB-CA-C	-7.32	102.44	112.24
1	C	95	GLU	CB-CG-CD	7.31	125.03	112.60
1	C	330	ASN	CB-CA-C	-7.31	98.70	110.84
1	A	233	ILE	CB-CA-C	-7.31	102.44	112.24
1	D	95	GLU	CB-CG-CD	7.31	125.03	112.60
1	B	330	ASN	CB-CA-C	-7.31	98.71	110.84
1	A	344	PHE	N-CA-C	-7.31	99.29	110.32
1	D	330	ASN	CB-CA-C	-7.31	98.71	110.84
1	B	344	PHE	N-CA-C	-7.30	99.29	110.32
1	A	330	ASN	CB-CA-C	-7.30	98.72	110.84
1	B	95	GLU	CB-CG-CD	7.29	124.99	112.60
1	D	344	PHE	N-CA-C	-7.29	99.32	110.32
1	A	95	GLU	CB-CG-CD	7.28	124.98	112.60
1	B	131	ARG	NE-CZ-NH2	-7.28	112.65	119.20
1	C	231	VAL	N-CA-C	7.28	118.00	110.36
1	B	247	GLN	N-CA-C	-7.26	103.99	112.92
1	B	231	VAL	N-CA-C	7.26	117.98	110.36
1	C	360	ILE	O-C-N	7.26	129.41	121.94
1	A	247	GLN	N-CA-C	-7.26	103.99	112.92
1	A	360	ILE	O-C-N	7.25	129.41	121.94
1	D	247	GLN	N-CA-C	-7.25	104.00	112.92
1	A	231	VAL	N-CA-C	7.25	117.97	110.36
1	B	160	LYS	CA-C-O	-7.24	111.72	120.05
1	C	247	GLN	N-CA-C	-7.24	104.01	112.92
1	D	231	VAL	N-CA-C	7.24	117.96	110.36
1	D	360	ILE	O-C-N	7.24	129.39	121.94
1	C	244	GLU	OE1-CD-OE2	7.23	140.26	122.90
1	A	131	ARG	NE-CZ-NH2	-7.23	112.69	119.20
1	C	30	TYR	N-CA-C	7.23	121.34	110.14
1	B	244	GLU	OE1-CD-OE2	7.22	140.24	122.90
1	D	160	LYS	CA-C-O	-7.22	111.75	120.05
1	A	244	GLU	OE1-CD-OE2	7.22	140.22	122.90
1	C	160	LYS	CA-C-O	-7.22	111.75	120.05
1	B	360	ILE	O-C-N	7.21	129.37	121.94
1	D	244	GLU	OE1-CD-OE2	7.21	140.21	122.90
1	C	131	ARG	NE-CZ-NH2	-7.21	112.71	119.20
1	A	160	LYS	CA-C-O	-7.21	111.77	120.05
1	B	49	GLU	CA-CB-CG	-7.20	99.71	114.10
1	A	30	TYR	N-CA-C	7.19	121.29	110.14
1	A	49	GLU	CA-CB-CG	-7.19	99.72	114.10
1	D	49	GLU	CA-CB-CG	-7.19	99.72	114.10
1	C	21	PRO	CA-N-CD	-7.18	101.94	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	131	ARG	NE-CZ-NH2	-7.18	112.74	119.20
1	D	383	ARG	N-CA-C	7.18	121.30	112.54
1	B	30	TYR	N-CA-C	7.17	121.26	110.14
1	C	49	GLU	CA-CB-CG	-7.17	99.75	114.10
1	D	30	TYR	N-CA-C	7.17	121.25	110.14
1	D	332	PHE	CA-C-N	7.17	129.76	120.44
1	D	332	PHE	C-N-CA	7.17	129.76	120.44
1	A	21	PRO	CA-N-CD	-7.17	101.97	112.00
1	A	332	PHE	CA-C-N	7.17	129.76	120.44
1	A	332	PHE	C-N-CA	7.17	129.76	120.44
1	B	332	PHE	CA-C-N	7.17	129.76	120.44
1	B	332	PHE	C-N-CA	7.17	129.76	120.44
1	C	332	PHE	CA-C-N	7.17	129.76	120.44
1	C	332	PHE	C-N-CA	7.17	129.76	120.44
1	D	21	PRO	CA-N-CD	-7.16	101.98	112.00
1	B	21	PRO	CA-N-CD	-7.16	101.98	112.00
1	A	383	ARG	N-CA-C	7.15	121.27	112.54
1	C	147	MET	CA-CB-CG	-7.15	99.80	114.10
1	A	147	MET	CA-CB-CG	-7.15	99.81	114.10
1	C	383	ARG	N-CA-C	7.14	121.26	112.54
1	D	147	MET	CA-CB-CG	-7.14	99.81	114.10
1	B	147	MET	CA-CB-CG	-7.14	99.82	114.10
1	B	383	ARG	N-CA-C	7.14	121.25	112.54
1	A	189	GLU	N-CA-C	7.13	125.99	110.80
1	D	189	GLU	N-CA-C	7.12	125.97	110.80
1	B	189	GLU	N-CA-C	7.12	125.96	110.80
1	C	189	GLU	N-CA-C	7.11	125.93	110.80
1	B	92	LEU	CA-C-N	-7.09	109.99	123.32
1	B	92	LEU	C-N-CA	-7.09	109.99	123.32
1	D	92	LEU	CA-C-N	-7.08	110.01	123.32
1	D	92	LEU	C-N-CA	-7.08	110.01	123.32
1	C	92	LEU	CA-C-N	-7.08	110.02	123.32
1	C	92	LEU	C-N-CA	-7.08	110.02	123.32
1	A	366	ASP	CB-CG-OD1	7.07	134.66	118.40
1	D	269	GLU	CA-C-N	7.07	130.62	120.79
1	D	269	GLU	C-N-CA	7.07	130.62	120.79
1	A	92	LEU	CA-C-N	-7.07	110.03	123.32
1	A	92	LEU	C-N-CA	-7.07	110.03	123.32
1	C	366	ASP	CB-CG-OD1	7.07	134.66	118.40
1	B	366	ASP	CB-CG-OD1	7.07	134.65	118.40
1	D	366	ASP	CB-CG-OD1	7.06	134.65	118.40
1	C	20	GLU	CA-C-O	7.06	126.25	119.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	400	VAL	N-CA-C	7.06	124.02	109.34
1	D	314	THR	CA-C-N	7.05	134.94	123.37
1	D	314	THR	C-N-CA	7.05	134.94	123.37
1	B	419	VAL	CA-C-N	7.05	127.63	119.94
1	B	419	VAL	C-N-CA	7.05	127.63	119.94
1	A	20	GLU	CA-C-O	7.05	126.25	119.62
1	A	419	VAL	CA-C-N	7.04	127.62	119.94
1	A	419	VAL	C-N-CA	7.04	127.62	119.94
1	C	419	VAL	CA-C-N	7.04	127.62	119.94
1	C	419	VAL	C-N-CA	7.04	127.62	119.94
1	D	158	VAL	N-CA-C	-7.04	93.67	108.88
1	D	400	VAL	N-CA-C	7.04	123.99	109.34
1	B	400	VAL	N-CA-C	7.04	123.99	109.34
1	C	269	GLU	CA-C-N	7.04	130.58	120.79
1	C	269	GLU	C-N-CA	7.04	130.58	120.79
1	A	400	VAL	N-CA-C	7.04	123.98	109.34
1	B	20	GLU	CA-C-O	7.04	126.24	119.62
1	B	198	ARG	NE-CZ-NH1	7.04	128.54	121.50
1	D	126	PRO	CA-C-O	-7.04	113.65	121.32
1	A	126	PRO	CA-C-O	-7.03	113.66	121.32
1	A	314	THR	CA-C-N	7.03	134.90	123.37
1	A	314	THR	C-N-CA	7.03	134.90	123.37
1	B	314	THR	CA-C-N	7.03	134.90	123.37
1	B	314	THR	C-N-CA	7.03	134.90	123.37
1	A	269	GLU	CA-C-N	7.03	130.56	120.79
1	A	269	GLU	C-N-CA	7.03	130.56	120.79
1	B	126	PRO	CA-C-O	-7.03	113.66	121.32
1	A	158	VAL	N-CA-C	-7.03	93.70	108.88
1	A	198	ARG	NE-CZ-NH1	7.03	128.53	121.50
1	C	314	THR	CA-C-N	7.03	134.90	123.37
1	C	314	THR	C-N-CA	7.03	134.90	123.37
1	B	158	VAL	N-CA-C	-7.03	93.70	108.88
1	B	269	GLU	CA-C-N	7.02	130.55	120.79
1	B	269	GLU	C-N-CA	7.02	130.55	120.79
1	D	419	VAL	CA-C-N	7.02	127.59	119.94
1	D	419	VAL	C-N-CA	7.02	127.59	119.94
1	C	158	VAL	N-CA-C	-7.02	93.72	108.88
1	B	306	GLY	N-CA-C	7.02	129.81	113.18
1	C	306	GLY	N-CA-C	7.02	129.81	113.18
1	C	126	PRO	CA-C-O	-7.02	113.67	121.32
1	A	306	GLY	N-CA-C	7.01	129.80	113.18
1	D	198	ARG	NE-CZ-NH1	7.01	128.51	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	306	GLY	N-CA-C	7.01	129.79	113.18
1	D	20	GLU	CA-C-O	7.01	126.21	119.62
1	C	272	GLY	CA-C-O	7.00	128.08	119.88
1	B	19	TYR	N-CA-C	7.00	120.11	110.24
1	D	19	TYR	N-CA-C	7.00	120.11	110.24
1	C	198	ARG	NE-CZ-NH1	7.00	128.50	121.50
1	B	104	ALA	CA-C-N	-7.00	109.38	121.97
1	B	104	ALA	C-N-CA	-7.00	109.38	121.97
1	D	272	GLY	CA-C-O	6.99	128.06	119.88
1	D	104	ALA	CA-C-N	-6.99	109.39	121.97
1	D	104	ALA	C-N-CA	-6.99	109.39	121.97
1	A	272	GLY	CA-C-O	6.99	128.05	119.88
1	A	19	TYR	N-CA-C	6.98	120.08	110.24
1	C	19	TYR	N-CA-C	6.98	120.09	110.24
1	A	104	ALA	CA-C-N	-6.97	109.42	121.97
1	A	104	ALA	C-N-CA	-6.97	109.42	121.97
1	D	397	ILE	N-CA-C	6.96	117.67	110.36
1	B	272	GLY	CA-C-O	6.96	128.02	119.88
1	C	104	ALA	CA-C-N	-6.95	109.46	121.97
1	C	104	ALA	C-N-CA	-6.95	109.46	121.97
1	C	397	ILE	N-CA-C	6.94	117.65	110.36
1	B	243	ASN	CA-C-O	-6.94	113.75	120.90
1	B	397	ILE	N-CA-C	6.94	117.64	110.36
1	A	313	GLY	N-CA-C	6.94	120.23	110.38
1	A	397	ILE	N-CA-C	6.93	117.64	110.36
1	C	243	ASN	CA-C-O	-6.93	113.76	120.90
1	D	313	GLY	N-CA-C	6.93	120.22	110.38
1	D	145	GLU	O-C-N	6.93	130.14	122.11
1	A	145	GLU	O-C-N	6.92	130.14	122.11
1	A	243	ASN	CA-C-O	-6.92	113.77	120.90
1	C	247	GLN	N-CA-CB	6.92	120.66	110.56
1	C	145	GLU	O-C-N	6.92	130.13	122.11
1	B	145	GLU	O-C-N	6.92	130.13	122.11
1	C	313	GLY	N-CA-C	6.90	120.18	110.38
1	A	220	THR	OG1-CB-CG2	6.90	123.10	109.30
1	B	313	GLY	N-CA-C	6.90	120.18	110.38
1	C	220	THR	OG1-CB-CG2	6.90	123.10	109.30
1	B	247	GLN	N-CA-CB	6.90	120.63	110.56
1	A	247	GLN	N-CA-CB	6.89	120.62	110.56
1	D	247	GLN	N-CA-CB	6.89	120.62	110.56
1	B	220	THR	OG1-CB-CG2	6.89	123.08	109.30
1	D	220	THR	OG1-CB-CG2	6.88	123.06	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	243	ASN	CA-C-O	-6.87	113.83	120.90
1	B	226	ASN	CA-C-O	6.86	132.31	120.85
1	C	226	ASN	CA-C-O	6.85	132.29	120.85
1	A	226	ASN	CA-C-O	6.84	132.28	120.85
1	B	183	ASP	N-CA-C	-6.83	101.11	111.56
1	B	193	SER	N-CA-C	6.83	120.78	108.69
1	D	193	SER	N-CA-C	6.83	120.78	108.69
1	A	193	SER	N-CA-C	6.83	120.77	108.69
1	B	167	VAL	CG1-CB-CG2	6.83	125.82	110.80
1	C	193	SER	N-CA-C	6.83	120.77	108.69
1	D	83	ILE	N-CA-CB	-6.82	103.07	111.67
1	D	183	ASP	N-CA-C	-6.82	101.12	111.56
1	A	83	ILE	N-CA-CB	-6.82	103.07	111.67
1	D	226	ASN	CA-C-O	6.82	132.24	120.85
1	A	167	VAL	CG1-CB-CG2	6.81	125.78	110.80
1	D	167	VAL	CG1-CB-CG2	6.80	125.77	110.80
1	B	83	ILE	N-CA-CB	-6.80	103.10	111.67
1	C	183	ASP	N-CA-C	-6.80	101.15	111.56
1	C	167	VAL	CG1-CB-CG2	6.80	125.75	110.80
1	A	183	ASP	N-CA-C	-6.80	101.16	111.56
1	D	290	ARG	NE-CZ-NH2	6.80	125.32	119.20
1	A	214	GLU	CA-CB-CG	-6.79	100.52	114.10
1	A	290	ARG	NE-CZ-NH2	6.79	125.31	119.20
1	B	81	GLY	N-CA-C	-6.79	97.09	113.18
1	C	214	GLU	CA-CB-CG	-6.79	100.52	114.10
1	B	44	GLY	N-CA-C	-6.79	97.10	113.18
1	B	74	TYR	N-CA-C	-6.79	96.35	110.80
1	D	390	ARG	CA-C-N	6.79	129.93	120.29
1	D	390	ARG	C-N-CA	6.79	129.93	120.29
1	D	214	GLU	CA-CB-CG	-6.78	100.53	114.10
1	B	214	GLU	CA-CB-CG	-6.78	100.54	114.10
1	C	83	ILE	N-CA-CB	-6.78	103.13	111.67
1	D	81	GLY	N-CA-C	-6.78	97.11	113.18
1	D	44	GLY	N-CA-C	-6.78	97.12	113.18
1	A	44	GLY	N-CA-C	-6.77	97.12	113.18
1	A	81	GLY	N-CA-C	-6.77	97.12	113.18
1	C	81	GLY	N-CA-C	-6.77	97.13	113.18
1	B	51	SER	CA-CB-OG	-6.77	97.56	111.10
1	A	51	SER	CA-CB-OG	-6.77	97.56	111.10
1	C	51	SER	CA-CB-OG	-6.77	97.56	111.10
1	D	74	TYR	N-CA-C	-6.77	96.38	110.80
1	A	74	TYR	N-CA-C	-6.76	96.39	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	44	GLY	N-CA-C	-6.76	97.15	113.18
1	C	74	TYR	N-CA-C	-6.76	96.40	110.80
1	A	390	ARG	O-C-N	6.76	131.01	122.23
1	C	390	ARG	CA-C-N	6.76	129.88	120.29
1	C	390	ARG	C-N-CA	6.76	129.88	120.29
1	B	390	ARG	O-C-N	6.75	131.01	122.23
1	C	135	GLY	CA-C-N	-6.75	113.73	120.21
1	C	135	GLY	C-N-CA	-6.75	113.73	120.21
1	D	51	SER	CA-CB-OG	-6.75	97.61	111.10
1	A	390	ARG	CA-C-N	6.74	129.87	120.29
1	A	390	ARG	C-N-CA	6.74	129.87	120.29
1	D	390	ARG	O-C-N	6.74	131.00	122.23
1	B	290	ARG	NE-CZ-NH2	6.74	125.27	119.20
1	C	390	ARG	O-C-N	6.74	130.99	122.23
1	A	141	GLN	O-C-N	6.73	129.92	122.11
1	B	390	ARG	CA-C-N	6.73	129.84	120.29
1	B	390	ARG	C-N-CA	6.73	129.84	120.29
1	D	141	GLN	CA-CB-CG	-6.73	100.64	114.10
1	C	141	GLN	CA-CB-CG	-6.72	100.65	114.10
1	A	141	GLN	CA-CB-CG	-6.72	100.66	114.10
1	C	141	GLN	O-C-N	6.72	129.91	122.11
1	D	141	GLN	O-C-N	6.72	129.90	122.11
1	D	135	GLY	CA-C-N	-6.72	113.76	120.21
1	D	135	GLY	C-N-CA	-6.72	113.76	120.21
1	A	135	GLY	CA-C-N	-6.71	113.77	120.21
1	A	135	GLY	C-N-CA	-6.71	113.77	120.21
1	B	135	GLY	CA-C-N	-6.71	113.77	120.21
1	B	135	GLY	C-N-CA	-6.71	113.77	120.21
1	B	141	GLN	O-C-N	6.71	129.89	122.11
1	B	141	GLN	CA-CB-CG	-6.71	100.69	114.10
1	B	208	ARG	CD-NE-CZ	6.71	133.79	124.40
1	C	290	ARG	NE-CZ-NH2	6.71	125.23	119.20
1	D	48	SER	N-CA-C	-6.71	96.52	110.80
1	A	208	ARG	CD-NE-CZ	6.70	133.78	124.40
1	C	208	ARG	CD-NE-CZ	6.70	133.78	124.40
1	B	136	PRO	O-C-N	6.70	131.16	122.86
1	D	214	GLU	CB-CG-CD	6.70	123.98	112.60
1	D	86	ILE	N-CA-C	-6.69	98.83	108.53
1	A	48	SER	N-CA-C	-6.69	96.55	110.80
1	A	86	ILE	N-CA-C	-6.69	98.83	108.53
1	C	48	SER	N-CA-C	-6.69	96.55	110.80
1	A	214	GLU	CB-CG-CD	6.68	123.96	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	214	GLU	CB-CG-CD	6.68	123.96	112.60
1	B	214	GLU	CB-CG-CD	6.68	123.96	112.60
1	B	48	SER	N-CA-C	-6.68	96.57	110.80
1	C	86	ILE	N-CA-C	-6.68	98.85	108.53
1	B	86	ILE	N-CA-C	-6.68	98.85	108.53
1	B	55	TRP	N-CA-C	6.67	125.01	110.80
1	C	136	PRO	O-C-N	6.67	131.13	122.86
1	D	208	ARG	CD-NE-CZ	6.66	133.73	124.40
1	C	202	ARG	CG-CD-NE	6.66	126.65	112.00
1	D	55	TRP	N-CA-C	6.66	124.99	110.80
1	A	136	PRO	O-C-N	6.66	131.12	122.86
1	A	202	ARG	CG-CD-NE	6.66	126.65	112.00
1	A	55	TRP	N-CA-C	6.66	124.98	110.80
1	B	202	ARG	CG-CD-NE	6.65	126.63	112.00
1	C	55	TRP	N-CA-C	6.65	124.97	110.80
1	D	85	LYS	CD-CE-NZ	6.65	133.18	111.90
1	B	85	LYS	CD-CE-NZ	6.64	133.16	111.90
1	D	202	ARG	CG-CD-NE	6.64	126.62	112.00
1	D	225	ILE	N-CA-C	6.64	117.72	110.21
1	A	85	LYS	CD-CE-NZ	6.64	133.14	111.90
1	B	227	ILE	CA-C-O	-6.64	112.48	120.78
1	B	225	ILE	N-CA-C	6.64	117.71	110.21
1	C	85	LYS	CD-CE-NZ	6.63	133.13	111.90
1	D	136	PRO	O-C-N	6.63	131.09	122.86
1	B	295	MET	N-CA-C	-6.63	103.27	111.75
1	C	295	MET	N-CA-C	-6.62	103.28	111.75
1	A	225	ILE	N-CA-C	6.61	117.68	110.21
1	C	310	ILE	CB-CA-C	6.61	121.47	110.30
1	B	310	ILE	CB-CA-C	6.61	121.46	110.30
1	D	310	ILE	CB-CA-C	6.60	121.45	110.30
1	A	310	ILE	CB-CA-C	6.60	121.45	110.30
1	C	225	ILE	N-CA-C	6.60	117.66	110.21
1	A	295	MET	N-CA-C	-6.60	103.31	111.75
1	D	227	ILE	CA-C-O	-6.59	112.54	120.78
1	A	227	ILE	CA-C-O	-6.58	112.55	120.78
1	B	416	LEU	N-CA-C	-6.58	97.79	110.56
1	D	72	VAL	CA-C-N	-6.58	112.13	123.25
1	D	72	VAL	C-N-CA	-6.58	112.13	123.25
1	C	214	GLU	CA-C-N	6.57	129.93	120.79
1	C	214	GLU	C-N-CA	6.57	129.93	120.79
1	D	295	MET	N-CA-C	-6.57	103.34	111.75
1	B	72	VAL	CA-C-N	-6.56	112.16	123.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	72	VAL	C-N-CA	-6.56	112.16	123.25
1	A	214	GLU	CA-C-N	6.56	129.90	120.79
1	A	214	GLU	C-N-CA	6.56	129.90	120.79
1	C	227	ILE	CA-C-O	-6.56	112.58	120.78
1	B	214	GLU	CA-C-N	6.55	129.90	120.79
1	B	214	GLU	C-N-CA	6.55	129.90	120.79
1	D	270	ASP	CB-CG-OD2	6.55	133.47	118.40
1	A	72	VAL	CA-C-N	-6.55	112.18	123.25
1	A	72	VAL	C-N-CA	-6.55	112.18	123.25
1	C	416	LEU	N-CA-C	-6.55	97.85	110.56
1	C	72	VAL	CA-C-N	-6.55	112.18	123.25
1	C	72	VAL	C-N-CA	-6.55	112.18	123.25
1	A	270	ASP	CB-CG-OD2	6.55	133.46	118.40
1	A	416	LEU	N-CA-C	-6.55	97.86	110.56
1	C	25	GLU	CA-C-N	6.55	131.13	122.42
1	C	25	GLU	C-N-CA	6.55	131.13	122.42
1	D	214	GLU	CA-C-N	6.55	129.89	120.79
1	D	214	GLU	C-N-CA	6.55	129.89	120.79
1	B	25	GLU	CA-C-N	6.54	131.12	122.42
1	B	25	GLU	C-N-CA	6.54	131.12	122.42
1	B	270	ASP	CB-CG-OD2	6.54	133.45	118.40
1	D	416	LEU	N-CA-C	-6.54	97.86	110.56
1	C	270	ASP	CB-CG-OD2	6.54	133.44	118.40
1	A	25	GLU	CA-C-N	6.54	131.11	122.42
1	A	25	GLU	C-N-CA	6.54	131.11	122.42
1	C	187	ASP	CB-CA-C	-6.53	96.88	110.40
1	B	187	ASP	CB-CA-C	-6.53	96.88	110.40
1	D	25	GLU	CA-C-N	6.53	131.11	122.42
1	D	25	GLU	C-N-CA	6.53	131.11	122.42
1	D	187	ASP	CB-CA-C	-6.53	96.89	110.40
1	A	187	ASP	CB-CA-C	-6.52	96.89	110.40
1	C	336	LYS	CA-C-N	-6.52	109.09	121.54
1	C	336	LYS	C-N-CA	-6.52	109.09	121.54
1	D	336	LYS	CA-C-N	-6.52	109.09	121.54
1	D	336	LYS	C-N-CA	-6.52	109.09	121.54
1	D	92	LEU	CB-CG-CD1	-6.51	91.17	110.70
1	B	76	GLU	N-CA-C	-6.51	100.34	110.17
1	A	76	GLU	N-CA-C	-6.51	100.34	110.17
1	A	336	LYS	CA-C-N	-6.51	109.11	121.54
1	A	336	LYS	C-N-CA	-6.51	109.11	121.54
1	A	92	LEU	CB-CG-CD1	-6.50	91.20	110.70
1	A	126	PRO	O-C-N	-6.50	114.92	122.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	126	PRO	O-C-N	-6.50	114.92	122.85
1	B	92	LEU	CB-CG-CD1	-6.50	91.20	110.70
1	D	222	GLU	CG-CD-OE1	6.50	133.35	118.40
1	D	405	LYS	CA-C-N	6.50	129.64	120.28
1	D	405	LYS	C-N-CA	6.50	129.64	120.28
1	B	126	PRO	O-C-N	-6.50	114.93	122.85
1	A	222	GLU	CG-CD-OE1	6.49	133.33	118.40
1	D	126	PRO	O-C-N	-6.49	114.93	122.85
1	B	222	GLU	CG-CD-OE1	6.49	133.33	118.40
1	C	92	LEU	CB-CG-CD1	-6.49	91.22	110.70
1	A	405	LYS	CA-C-N	6.49	129.62	120.28
1	A	405	LYS	C-N-CA	6.49	129.62	120.28
1	B	336	LYS	CA-C-N	-6.49	109.15	121.54
1	B	336	LYS	C-N-CA	-6.49	109.15	121.54
1	C	76	GLU	N-CA-C	-6.49	100.37	110.17
1	B	405	LYS	CA-C-N	6.49	129.62	120.28
1	B	405	LYS	C-N-CA	6.49	129.62	120.28
1	C	222	GLU	CG-CD-OE1	6.49	133.32	118.40
1	C	261	LEU	N-CA-CB	6.48	119.75	110.16
1	C	405	LYS	CA-C-N	6.48	129.61	120.28
1	C	405	LYS	C-N-CA	6.48	129.61	120.28
1	D	76	GLU	N-CA-C	-6.47	100.39	110.17
1	D	45	ARG	CA-C-O	-6.47	113.45	121.02
1	A	261	LEU	N-CA-CB	6.47	119.74	110.16
1	D	190	ASN	N-CA-CB	-6.47	101.23	110.81
1	A	190	ASN	N-CA-CB	-6.46	101.24	110.81
1	C	264	MET	CG-SD-CE	6.46	115.12	100.90
1	D	264	MET	CG-SD-CE	6.46	115.12	100.90
1	B	190	ASN	N-CA-CB	-6.46	101.25	110.81
1	A	264	MET	CG-SD-CE	6.46	115.11	100.90
1	B	264	MET	CG-SD-CE	6.46	115.11	100.90
1	B	261	LEU	N-CA-CB	6.46	119.72	110.16
1	D	261	LEU	N-CA-CB	6.45	119.71	110.16
1	C	190	ASN	N-CA-CB	-6.45	101.27	110.81
1	C	202	ARG	NE-CZ-NH2	6.44	125.00	119.20
1	A	45	ARG	CA-C-O	-6.43	113.49	121.02
1	C	233	ILE	CG1-CB-CG2	6.43	130.00	110.70
1	D	201	GLU	CG-CD-OE2	6.43	133.19	118.40
1	C	45	ARG	CA-C-O	-6.43	113.50	121.02
1	A	201	GLU	CG-CD-OE2	6.43	133.18	118.40
1	B	201	GLU	CG-CD-OE2	6.42	133.18	118.40
1	C	201	GLU	CG-CD-OE2	6.42	133.18	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	270	ASP	CA-C-O	-6.42	114.00	121.07
1	A	233	ILE	CG1-CB-CG2	6.42	129.95	110.70
1	B	45	ARG	CA-C-O	-6.41	113.52	121.02
1	B	233	ILE	CG1-CB-CG2	6.41	129.93	110.70
1	D	233	ILE	CG1-CB-CG2	6.41	129.93	110.70
1	B	86	ILE	CA-C-O	-6.41	113.42	120.72
1	C	86	ILE	CA-C-O	-6.41	113.42	120.72
1	A	270	ASP	CA-C-O	-6.40	114.03	121.07
1	C	223	TYR	CA-CB-CG	6.40	125.42	113.90
1	D	270	ASP	CA-C-O	-6.40	114.03	121.07
1	A	202	ARG	NE-CZ-NH2	6.40	124.96	119.20
1	C	270	ASP	CA-C-O	-6.40	114.03	121.07
1	A	223	TYR	CA-CB-CG	6.40	125.42	113.90
1	A	255	VAL	O-C-N	6.40	130.57	122.57
1	B	57	THR	N-CA-C	6.40	124.42	110.80
1	D	255	VAL	O-C-N	6.39	130.56	122.57
1	B	223	TYR	CA-CB-CG	6.39	125.41	113.90
1	C	255	VAL	O-C-N	6.39	130.55	122.57
1	A	86	ILE	CA-C-O	-6.38	113.44	120.72
1	C	57	THR	N-CA-C	6.38	124.40	110.80
1	D	223	TYR	CA-CB-CG	6.38	125.39	113.90
1	D	202	ARG	NE-CZ-NH2	6.38	124.94	119.20
1	B	202	ARG	NE-CZ-NH2	6.38	124.94	119.20
1	D	86	ILE	CA-C-O	-6.38	113.45	120.72
1	A	57	THR	N-CA-C	6.37	124.38	110.80
1	B	255	VAL	O-C-N	6.37	130.54	122.57
1	D	57	THR	N-CA-C	6.37	124.37	110.80
1	B	119	ARG	NE-CZ-NH1	-6.37	115.13	121.50
1	C	361	ARG	NE-CZ-NH1	-6.36	115.14	121.50
1	B	361	ARG	NE-CZ-NH1	-6.36	115.14	121.50
1	A	341	ARG	NE-CZ-NH1	6.36	127.86	121.50
1	A	361	ARG	NE-CZ-NH1	-6.36	115.14	121.50
1	D	341	ARG	NE-CZ-NH1	6.36	127.86	121.50
1	D	280	ALA	N-CA-C	-6.35	101.24	110.64
1	A	119	ARG	NE-CZ-NH1	-6.35	115.15	121.50
1	D	361	ARG	NE-CZ-NH1	-6.35	115.15	121.50
1	C	341	ARG	NE-CZ-NH1	6.34	127.84	121.50
1	D	92	LEU	N-CA-C	-6.34	105.47	113.72
1	C	119	ARG	NE-CZ-NH1	-6.34	115.16	121.50
1	C	92	LEU	N-CA-C	-6.34	105.48	113.72
1	B	341	ARG	NE-CZ-NH1	6.34	127.84	121.50
1	C	311	HIS	CA-C-O	-6.34	113.82	121.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	280	ALA	N-CA-C	-6.34	101.26	110.64
1	A	92	LEU	N-CA-C	-6.33	105.49	113.72
1	A	280	ALA	N-CA-C	-6.33	101.27	110.64
1	D	89	PRO	N-CA-C	-6.33	101.24	110.80
1	D	422	SER	CB-CA-C	-6.33	97.88	109.15
1	C	280	ALA	N-CA-C	-6.33	101.28	110.64
1	A	422	SER	CB-CA-C	-6.33	97.89	109.15
1	B	89	PRO	N-CA-C	-6.33	101.25	110.80
1	B	339	HIS	N-CA-CB	6.33	119.52	110.16
1	A	168	GLU	CG-CD-OE2	6.32	132.94	118.40
1	D	119	ARG	NE-CZ-NH1	-6.32	115.18	121.50
1	D	190	ASN	O-C-N	6.32	129.83	122.25
1	B	168	GLU	CG-CD-OE2	6.32	132.92	118.40
1	C	168	GLU	CG-CD-OE2	6.31	132.92	118.40
1	B	92	LEU	N-CA-C	-6.31	105.51	113.72
1	B	422	SER	CB-CA-C	-6.31	97.91	109.15
1	D	168	GLU	CG-CD-OE2	6.31	132.92	118.40
1	C	422	SER	CB-CA-C	-6.31	97.92	109.15
1	A	339	HIS	N-CA-CB	6.31	119.49	110.16
1	A	89	PRO	N-CA-C	-6.30	101.28	110.80
1	B	130	LEU	CB-CG-CD2	6.30	129.61	110.70
1	B	173	ILE	N-CA-C	-6.30	103.74	112.50
1	A	130	LEU	CB-CG-CD2	6.30	129.61	110.70
1	B	351	LEU	N-CA-C	-6.30	100.88	110.14
1	C	351	LEU	N-CA-C	-6.30	100.88	110.14
1	D	339	HIS	N-CA-CB	6.30	119.48	110.16
1	C	339	HIS	N-CA-CB	6.30	119.48	110.16
1	D	130	LEU	CB-CG-CD2	6.29	129.59	110.70
1	B	423	LYS	CA-CB-CG	6.29	126.69	114.10
1	A	190	ASN	O-C-N	6.29	129.80	122.25
1	A	351	LEU	N-CA-C	-6.29	100.89	110.14
1	A	423	LYS	CA-CB-CG	6.29	126.68	114.10
1	D	148	GLY	CA-C-O	6.29	125.24	118.95
1	A	254	VAL	CA-C-N	6.29	133.29	121.97
1	A	254	VAL	C-N-CA	6.29	133.29	121.97
1	D	423	LYS	CA-CB-CG	6.29	126.68	114.10
1	D	351	LEU	N-CA-C	-6.29	100.89	110.14
1	A	311	HIS	CA-C-O	-6.29	113.88	121.05
1	B	254	VAL	CA-C-N	6.29	133.28	121.97
1	B	254	VAL	C-N-CA	6.29	133.28	121.97
1	C	130	LEU	CB-CG-CD2	6.28	129.55	110.70
1	C	423	LYS	CA-CB-CG	6.28	126.67	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	173	ILE	N-CA-C	-6.28	103.77	112.50
1	C	89	PRO	N-CA-C	-6.28	101.32	110.80
1	C	190	ASN	O-C-N	6.28	129.78	122.25
1	B	190	ASN	O-C-N	6.28	129.78	122.25
1	C	113	LYS	CB-CG-CD	6.28	125.74	111.30
1	D	254	VAL	CA-C-N	6.28	133.26	121.97
1	D	254	VAL	C-N-CA	6.28	133.26	121.97
1	A	113	LYS	CB-CG-CD	6.27	125.73	111.30
1	B	311	HIS	CA-C-O	-6.27	113.90	121.05
1	A	369	ILE	N-CA-C	-6.27	99.55	108.58
1	C	254	VAL	CA-C-N	6.27	133.26	121.97
1	C	254	VAL	C-N-CA	6.27	133.26	121.97
1	D	113	LYS	CB-CG-CD	6.27	125.72	111.30
1	B	148	GLY	CA-C-O	6.27	125.22	118.95
1	A	148	GLY	CA-C-O	6.27	125.22	118.95
1	D	185	LEU	CA-C-N	-6.26	114.16	122.99
1	D	185	LEU	C-N-CA	-6.26	114.16	122.99
1	D	311	HIS	CA-C-O	-6.26	113.91	121.05
1	B	369	ILE	N-CA-C	-6.26	99.57	108.58
1	D	173	ILE	N-CA-C	-6.26	103.80	112.50
1	B	185	LEU	CA-C-N	-6.26	114.17	122.99
1	B	185	LEU	C-N-CA	-6.26	114.17	122.99
1	C	369	ILE	N-CA-C	-6.26	99.57	108.58
1	B	113	LYS	CB-CG-CD	6.25	125.69	111.30
1	C	173	ILE	N-CA-C	-6.25	103.82	112.50
1	A	185	LEU	CA-C-N	-6.25	114.18	122.99
1	A	185	LEU	C-N-CA	-6.25	114.18	122.99
1	C	187	ASP	CA-C-N	-6.25	113.38	122.19
1	C	187	ASP	C-N-CA	-6.25	113.38	122.19
1	D	187	ASP	CA-C-N	-6.25	113.38	122.19
1	D	187	ASP	C-N-CA	-6.25	113.38	122.19
1	A	60	LYS	N-CA-C	6.24	124.10	110.80
1	A	244	GLU	CG-CD-OE2	-6.24	104.05	118.40
1	C	244	GLU	CG-CD-OE2	-6.24	104.05	118.40
1	D	163	MET	N-CA-CB	6.24	120.71	110.97
1	B	60	LYS	N-CA-C	6.24	124.08	110.80
1	D	244	GLU	CG-CD-OE2	-6.24	104.06	118.40
1	B	38	SER	CB-CA-C	-6.23	99.24	109.46
1	B	244	GLU	CG-CD-OE2	-6.23	104.07	118.40
1	C	60	LYS	N-CA-C	6.23	124.07	110.80
1	A	187	ASP	CA-C-N	-6.23	113.41	122.19
1	A	187	ASP	C-N-CA	-6.23	113.41	122.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	369	ILE	N-CA-C	-6.23	99.61	108.58
1	C	237	ARG	NE-CZ-NH1	6.23	127.73	121.50
1	D	60	LYS	N-CA-C	6.23	124.06	110.80
1	C	185	LEU	CA-C-N	-6.22	114.21	122.99
1	C	185	LEU	C-N-CA	-6.22	114.21	122.99
1	D	339	HIS	O-C-N	6.22	129.25	122.15
1	C	38	SER	CB-CA-C	-6.22	99.26	109.46
1	A	339	HIS	O-C-N	6.22	129.24	122.15
1	A	38	SER	CB-CA-C	-6.21	99.27	109.46
1	C	148	GLY	CA-C-O	6.21	125.16	118.95
1	C	339	HIS	O-C-N	6.21	129.23	122.15
1	C	163	MET	N-CA-CB	6.21	120.65	110.97
1	D	38	SER	CB-CA-C	-6.21	99.28	109.46
1	A	163	MET	N-CA-CB	6.21	120.65	110.97
1	B	187	ASP	CA-C-N	-6.20	113.44	122.19
1	B	187	ASP	C-N-CA	-6.20	113.44	122.19
1	A	237	ARG	NE-CZ-NH1	6.19	127.69	121.50
1	B	17	LEU	N-CA-C	6.19	120.52	113.15
1	C	17	LEU	N-CA-C	6.19	120.52	113.15
1	B	339	HIS	O-C-N	6.19	129.21	122.15
1	B	163	MET	N-CA-CB	6.19	120.63	110.97
1	A	59	TRP	CB-CA-C	-6.19	99.59	109.80
1	B	304	MET	CA-C-O	-6.19	114.32	120.82
1	B	237	ARG	NE-CZ-NH1	6.18	127.68	121.50
1	D	59	TRP	CB-CA-C	-6.18	99.60	109.80
1	A	265	ARG	NE-CZ-NH1	-6.18	115.32	121.50
1	B	59	TRP	CB-CA-C	-6.18	99.61	109.80
1	C	59	TRP	CB-CA-C	-6.18	99.61	109.80
1	D	237	ARG	NE-CZ-NH1	6.18	127.68	121.50
1	D	265	ARG	NE-CZ-NH1	-6.18	115.32	121.50
1	A	17	LEU	N-CA-C	6.17	120.50	113.15
1	B	265	ARG	NE-CZ-NH1	-6.17	115.33	121.50
1	D	17	LEU	N-CA-C	6.17	120.50	113.15
1	C	265	ARG	NE-CZ-NH1	-6.17	115.33	121.50
1	D	251	ILE	CB-CG1-CD1	-6.16	100.87	113.80
1	B	127	TYR	CB-CA-C	-6.16	98.17	110.42
1	C	127	TYR	CB-CA-C	-6.15	98.17	110.42
1	D	177	LEU	N-CA-CB	-6.15	101.09	110.01
1	C	375	VAL	CA-C-O	-6.15	114.23	120.69
1	A	127	TYR	CB-CA-C	-6.15	98.19	110.42
1	B	375	VAL	CA-C-O	-6.15	114.23	120.69
1	C	177	LEU	N-CA-CB	-6.15	101.10	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	177	LEU	N-CA-CB	-6.15	101.10	110.01
1	D	127	TYR	CB-CA-C	-6.15	98.19	110.42
1	A	304	MET	CA-C-O	-6.14	114.37	120.82
1	B	251	ILE	CB-CG1-CD1	-6.14	100.90	113.80
1	A	375	VAL	CA-C-O	-6.14	114.24	120.69
1	B	177	LEU	N-CA-CB	-6.14	101.11	110.01
1	A	251	ILE	CB-CG1-CD1	-6.13	100.92	113.80
1	C	251	ILE	CB-CG1-CD1	-6.13	100.93	113.80
1	D	20	GLU	N-CA-CB	6.13	121.57	110.17
1	C	304	MET	CA-C-O	-6.13	114.39	120.82
1	A	20	GLU	N-CA-CB	6.12	121.55	110.17
1	B	20	GLU	N-CA-CB	6.12	121.54	110.17
1	C	271	LEU	CD1-CG-CD2	-6.11	97.36	110.80
1	C	20	GLU	N-CA-CB	6.10	121.52	110.17
1	D	304	MET	CA-C-O	-6.10	114.41	120.82
1	B	271	LEU	CD1-CG-CD2	-6.09	97.39	110.80
1	B	27	ILE	CA-CB-CG2	-6.09	100.14	110.50
1	D	242	ALA	CA-C-O	6.09	126.98	119.79
1	A	271	LEU	CD1-CG-CD2	-6.09	97.40	110.80
1	D	375	VAL	CA-C-O	-6.09	114.30	120.69
1	B	217	THR	CA-C-O	6.09	127.41	120.90
1	D	27	ILE	CA-CB-CG2	-6.08	100.16	110.50
1	A	27	ILE	CA-CB-CG2	-6.08	100.16	110.50
1	C	27	ILE	CA-CB-CG2	-6.08	100.17	110.50
1	C	242	ALA	CA-C-O	6.08	126.96	119.79
1	D	271	LEU	CD1-CG-CD2	-6.07	97.44	110.80
1	C	217	THR	CA-C-O	6.07	127.40	120.90
1	B	242	ALA	CA-C-O	6.07	126.95	119.79
1	C	141	GLN	CB-CA-C	6.06	120.86	110.86
1	D	80	GLU	CG-CD-OE2	-6.06	104.45	118.40
1	A	242	ALA	CA-C-O	6.06	126.94	119.79
1	D	141	GLN	CB-CA-C	6.06	120.86	110.86
1	A	141	GLN	CB-CA-C	6.05	120.85	110.86
1	C	80	GLU	CG-CD-OE2	-6.05	104.48	118.40
1	D	217	THR	CA-C-O	6.05	127.38	120.90
1	D	367	LEU	CA-CB-CG	-6.05	95.12	116.30
1	C	367	LEU	CA-CB-CG	-6.05	95.13	116.30
1	A	217	THR	CA-C-O	6.05	127.37	120.90
1	A	367	LEU	CA-CB-CG	-6.04	95.14	116.30
1	A	80	GLU	CG-CD-OE2	-6.04	104.50	118.40
1	B	80	GLU	CG-CD-OE2	-6.04	104.50	118.40
1	B	106	ALA	N-CA-C	-6.04	97.93	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	367	LEU	CA-CB-CG	-6.04	95.16	116.30
1	C	393	ILE	CB-CA-C	-6.04	104.15	112.24
1	B	141	GLN	CB-CA-C	6.03	120.81	110.86
1	B	298	LEU	CB-CA-C	6.03	121.11	110.85
1	B	393	ILE	CB-CA-C	-6.03	104.16	112.24
1	A	106	ALA	N-CA-C	-6.03	97.95	110.80
1	C	106	ALA	N-CA-C	-6.02	97.97	110.80
1	D	298	LEU	CB-CA-C	6.02	121.09	110.85
1	A	393	ILE	CB-CA-C	-6.02	104.17	112.24
1	C	362	LEU	N-CA-C	6.02	120.35	112.89
1	D	393	ILE	CB-CA-C	-6.02	104.17	112.24
1	A	298	LEU	CB-CA-C	6.01	121.07	110.85
1	D	106	ALA	N-CA-C	-6.01	97.99	110.80
1	A	362	LEU	N-CA-C	6.01	120.34	112.89
1	C	298	LEU	CB-CA-C	6.00	121.06	110.85
1	B	38	SER	CA-C-N	6.00	125.70	119.82
1	B	38	SER	C-N-CA	6.00	125.70	119.82
1	C	236	LYS	CB-CG-CD	6.00	125.11	111.30
1	A	310	ILE	CA-C-N	-6.00	112.84	121.42
1	A	310	ILE	C-N-CA	-6.00	112.84	121.42
1	B	310	ILE	CA-C-N	-6.00	112.84	121.42
1	B	310	ILE	C-N-CA	-6.00	112.84	121.42
1	C	38	SER	CA-C-N	6.00	125.70	119.82
1	C	38	SER	C-N-CA	6.00	125.70	119.82
1	C	332	PHE	CB-CA-C	-6.00	101.42	110.90
1	B	207	TYR	CB-CA-C	6.00	120.74	110.79
1	A	207	TYR	CB-CA-C	6.00	120.74	110.79
1	D	310	ILE	CA-C-N	-6.00	112.85	121.42
1	D	310	ILE	C-N-CA	-6.00	112.85	121.42
1	D	332	PHE	CB-CA-C	-6.00	101.43	110.90
1	A	332	PHE	CB-CA-C	-5.99	101.43	110.90
1	D	207	TYR	CB-CA-C	5.99	120.73	110.79
1	B	332	PHE	CB-CA-C	-5.99	101.44	110.90
1	B	362	LEU	N-CA-C	5.99	120.31	112.89
1	D	158	VAL	CB-CA-C	-5.99	100.46	111.36
1	B	144	ARG	N-CA-C	5.99	118.76	111.82
1	D	305	ILE	N-CA-C	-5.99	103.57	111.05
1	C	158	VAL	CB-CA-C	-5.98	100.47	111.36
1	B	236	LYS	CB-CG-CD	5.98	125.06	111.30
1	C	310	ILE	CA-C-N	-5.98	112.87	121.42
1	C	310	ILE	C-N-CA	-5.98	112.87	121.42
1	C	405	LYS	O-C-N	5.98	128.46	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	236	LYS	CB-CG-CD	5.98	125.05	111.30
1	A	158	VAL	CB-CA-C	-5.97	100.49	111.36
1	B	335	SER	CA-C-O	-5.97	114.77	121.81
1	B	305	ILE	N-CA-C	-5.97	103.59	111.05
1	C	207	TYR	CB-CA-C	5.97	120.70	110.79
1	D	335	SER	CA-C-O	-5.97	114.77	121.81
1	A	38	SER	CA-C-N	5.97	125.67	119.82
1	A	38	SER	C-N-CA	5.97	125.67	119.82
1	D	236	LYS	CB-CG-CD	5.97	125.03	111.30
1	C	144	ARG	N-CA-C	5.97	118.74	111.82
1	A	305	ILE	N-CA-C	-5.96	103.59	111.05
1	D	33	GLU	CA-CB-CG	-5.96	102.18	114.10
1	D	362	LEU	N-CA-C	5.96	120.28	112.89
1	D	144	ARG	N-CA-C	5.96	118.73	111.82
1	A	405	LYS	O-C-N	5.96	128.44	122.12
1	A	144	ARG	N-CA-C	5.96	118.73	111.82
1	B	405	LYS	O-C-N	5.96	128.43	122.12
1	A	335	SER	CA-C-O	-5.95	114.79	121.81
1	D	405	LYS	O-C-N	5.95	128.43	122.12
1	C	33	GLU	CA-CB-CG	-5.95	102.21	114.10
1	C	305	ILE	N-CA-C	-5.95	103.62	111.05
1	B	278	HIS	N-CA-C	-5.95	97.90	108.13
1	A	136	PRO	N-CA-C	-5.94	102.90	111.22
1	B	158	VAL	CB-CA-C	-5.94	100.54	111.36
1	D	38	SER	CA-C-N	5.94	125.64	119.82
1	D	38	SER	C-N-CA	5.94	125.64	119.82
1	A	33	GLU	CA-CB-CG	-5.94	102.22	114.10
1	B	33	GLU	CA-CB-CG	-5.94	102.22	114.10
1	B	101	LEU	CB-CG-CD2	-5.94	92.89	110.70
1	C	101	LEU	CB-CG-CD2	-5.94	92.89	110.70
1	C	218	GLY	CA-C-O	-5.94	113.28	119.27
1	B	128	GLU	N-CA-C	5.93	123.44	110.80
1	C	136	PRO	N-CA-C	-5.93	102.91	111.22
1	D	101	LEU	CB-CG-CD2	-5.93	92.90	110.70
1	A	128	GLU	N-CA-C	5.93	123.43	110.80
1	B	346	VAL	CA-C-O	5.93	127.60	120.66
1	C	289	PRO	CA-N-CD	-5.93	103.70	112.00
1	A	101	LEU	CB-CG-CD2	-5.93	92.92	110.70
1	A	278	HIS	N-CA-C	-5.93	97.94	108.13
1	B	58	LEU	CB-CA-C	-5.92	101.09	110.86
1	A	218	GLY	CA-C-O	-5.92	113.29	119.27
1	C	128	GLU	N-CA-C	5.92	123.41	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	218	GLY	CA-C-O	-5.92	113.29	119.27
1	C	278	HIS	N-CA-C	-5.92	97.95	108.13
1	B	136	PRO	N-CA-C	-5.92	102.94	111.22
1	D	136	PRO	N-CA-C	-5.92	102.94	111.22
1	A	289	PRO	CA-N-CD	-5.92	103.72	112.00
1	C	335	SER	CA-C-O	-5.92	114.83	121.81
1	B	289	PRO	CA-N-CD	-5.91	103.72	112.00
1	D	95	GLU	CA-C-O	-5.91	115.81	122.01
1	D	218	GLY	CA-C-O	-5.91	113.30	119.27
1	D	128	GLU	N-CA-C	5.91	123.38	110.80
1	D	58	LEU	CB-CA-C	-5.90	101.12	110.86
1	D	289	PRO	CA-N-CD	-5.90	103.74	112.00
1	C	346	VAL	CA-C-O	5.90	127.56	120.66
1	A	202	ARG	O-C-N	5.90	128.87	122.15
1	A	58	LEU	CB-CA-C	-5.90	101.13	110.86
1	D	278	HIS	N-CA-C	-5.89	97.99	108.13
1	D	407	LYS	CD-CE-NZ	5.89	130.76	111.90
1	B	407	LYS	CD-CE-NZ	5.89	130.75	111.90
1	C	365	LYS	N-CA-C	-5.89	106.18	113.19
1	A	95	GLU	CA-C-O	-5.89	115.83	122.01
1	A	407	LYS	CD-CE-NZ	5.89	130.74	111.90
1	D	365	LYS	N-CA-C	-5.89	106.19	113.19
1	A	346	VAL	CA-C-O	5.88	127.55	120.66
1	B	365	LYS	N-CA-C	-5.88	106.19	113.19
1	D	346	VAL	CA-C-O	5.88	127.54	120.66
1	C	407	LYS	CD-CE-NZ	5.88	130.71	111.90
1	B	202	ARG	O-C-N	5.88	128.85	122.15
1	C	58	LEU	CB-CA-C	-5.88	101.17	110.86
1	D	202	ARG	O-C-N	5.87	128.84	122.15
1	B	370	GLN	CB-CA-C	-5.87	101.29	110.74
1	C	21	PRO	N-CD-CG	5.87	112.00	103.20
1	D	249	VAL	CA-C-O	-5.86	113.45	120.78
1	C	370	GLN	CB-CA-C	-5.86	101.31	110.74
1	A	365	LYS	N-CA-C	-5.86	106.22	113.19
1	B	95	GLU	CA-C-O	-5.86	115.86	122.01
1	C	379	PRO	CA-N-CD	-5.86	103.80	112.00
1	D	370	GLN	CB-CA-C	-5.86	101.31	110.74
1	A	370	GLN	CB-CA-C	-5.85	101.32	110.74
1	B	226	ASN	CA-C-N	-5.85	111.44	121.97
1	B	226	ASN	C-N-CA	-5.85	111.44	121.97
1	A	249	VAL	CA-C-O	-5.85	113.47	120.78
1	C	202	ARG	O-C-N	5.85	128.82	122.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	21	PRO	N-CD-CG	5.84	111.97	103.20
1	A	226	ASN	CA-C-N	-5.84	111.45	121.97
1	A	226	ASN	C-N-CA	-5.84	111.45	121.97
1	C	249	VAL	CA-C-O	-5.84	113.47	120.78
1	A	231	VAL	CA-CB-CG1	-5.84	100.47	110.40
1	B	231	VAL	CA-CB-CG1	-5.84	100.47	110.40
1	C	95	GLU	CA-C-O	-5.84	115.88	122.01
1	C	231	VAL	CA-CB-CG1	-5.84	100.47	110.40
1	D	231	VAL	CA-CB-CG1	-5.84	100.47	110.40
1	B	249	VAL	CA-C-O	-5.84	113.48	120.78
1	A	46	ILE	O-C-N	-5.84	115.27	122.57
1	A	379	PRO	CA-N-CD	-5.84	103.83	112.00
1	C	46	ILE	O-C-N	-5.84	115.28	122.57
1	D	310	ILE	CA-C-O	-5.83	115.85	121.63
1	D	379	PRO	CA-N-CD	-5.83	103.83	112.00
1	D	226	ASN	CA-C-N	-5.83	111.47	121.97
1	D	226	ASN	C-N-CA	-5.83	111.47	121.97
1	B	46	ILE	O-C-N	-5.83	115.29	122.57
1	B	379	PRO	CA-N-CD	-5.83	103.84	112.00
1	C	415	SER	CA-C-O	5.83	125.20	118.97
1	A	310	ILE	CA-C-O	-5.82	115.86	121.63
1	C	244	GLU	N-CA-C	-5.82	106.26	113.19
1	D	21	PRO	N-CD-CG	5.82	111.93	103.20
1	D	204	ARG	N-CA-C	5.82	118.38	111.33
1	B	344	PHE	CA-C-N	-5.82	112.56	119.84
1	B	344	PHE	C-N-CA	-5.82	112.56	119.84
1	B	415	SER	CA-C-O	5.82	125.20	118.97
1	A	415	SER	CA-C-O	5.82	125.19	118.97
1	A	244	GLU	N-CA-C	-5.81	106.27	113.19
1	D	46	ILE	O-C-N	-5.81	115.30	122.57
1	B	21	PRO	N-CD-CG	5.81	111.92	103.20
1	C	76	GLU	CG-CD-OE2	5.81	131.77	118.40
1	B	310	ILE	CA-C-O	-5.81	115.88	121.63
1	A	204	ARG	N-CA-C	5.81	118.36	111.33
1	C	226	ASN	CA-C-N	-5.81	111.52	121.97
1	C	226	ASN	C-N-CA	-5.81	111.52	121.97
1	C	310	ILE	CA-C-O	-5.80	115.88	121.63
1	C	204	ARG	N-CA-C	5.80	118.35	111.33
1	D	415	SER	CA-C-O	5.80	125.18	118.97
1	D	254	VAL	O-C-N	5.80	129.76	121.82
1	A	344	PHE	CA-C-N	-5.79	112.60	119.84
1	A	344	PHE	C-N-CA	-5.79	112.60	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	146	PHE	CA-C-O	-5.79	114.41	120.55
1	A	76	GLU	CG-CD-OE2	5.79	131.72	118.40
1	D	344	PHE	CA-C-N	-5.79	112.61	119.84
1	D	344	PHE	C-N-CA	-5.79	112.61	119.84
1	D	146	PHE	CA-C-O	-5.78	114.42	120.55
1	A	146	PHE	CA-C-O	-5.78	114.42	120.55
1	A	254	VAL	O-C-N	5.78	129.74	121.82
1	B	76	GLU	CG-CD-OE2	5.78	131.69	118.40
1	C	216	GLU	N-CA-C	-5.78	98.49	110.80
1	C	379	PRO	N-CA-C	-5.78	105.85	113.65
1	D	76	GLU	CG-CD-OE2	5.78	131.70	118.40
1	B	146	PHE	CA-C-O	-5.78	114.43	120.55
1	B	244	GLU	N-CA-C	-5.78	106.32	113.19
1	C	254	VAL	O-C-N	5.78	129.73	121.82
1	D	216	GLU	N-CA-C	-5.78	98.50	110.80
1	A	216	GLU	N-CA-C	-5.77	98.51	110.80
1	B	216	GLU	N-CA-C	-5.76	98.52	110.80
1	B	254	VAL	O-C-N	5.76	129.72	121.82
1	B	330	ASN	CA-C-O	5.76	127.76	121.02
1	C	344	PHE	CA-C-N	-5.76	112.64	119.84
1	C	344	PHE	C-N-CA	-5.76	112.64	119.84
1	D	379	PRO	N-CA-C	-5.76	105.87	113.65
1	A	379	PRO	N-CA-C	-5.76	105.88	113.65
1	A	20	GLU	O-C-N	5.75	128.77	121.12
1	A	293	ILE	CA-CB-CG2	-5.75	100.72	110.50
1	B	95	GLU	CG-CD-OE2	-5.75	105.16	118.40
1	B	20	GLU	O-C-N	5.75	128.77	121.12
1	C	20	GLU	O-C-N	5.75	128.77	121.12
1	C	293	ILE	CG1-CB-CG2	5.75	127.96	110.70
1	B	368	VAL	N-CA-C	-5.75	98.86	107.37
1	C	87	ALA	CA-C-N	5.75	130.26	122.56
1	C	87	ALA	C-N-CA	5.75	130.26	122.56
1	B	293	ILE	CG1-CB-CG2	5.75	127.94	110.70
1	A	293	ILE	CG1-CB-CG2	5.75	127.94	110.70
1	C	293	ILE	CA-CB-CG2	-5.75	100.73	110.50
1	D	20	GLU	O-C-N	5.75	128.76	121.12
1	A	330	ASN	CA-C-O	5.74	127.74	121.02
1	B	379	PRO	N-CA-C	-5.74	105.90	113.65
1	D	196	PHE	CA-C-O	5.74	126.46	119.11
1	D	307	VAL	CG1-CB-CG2	-5.74	98.17	110.80
1	A	95	GLU	CG-CD-OE2	-5.74	105.20	118.40
1	A	413	LYS	CD-CE-NZ	5.74	130.27	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	413	LYS	CD-CE-NZ	5.74	130.27	111.90
1	C	54	THR	CA-C-N	5.74	132.50	121.54
1	C	54	THR	C-N-CA	5.74	132.50	121.54
1	D	330	ASN	CA-C-O	5.74	127.73	121.02
1	D	413	LYS	CD-CE-NZ	5.74	130.27	111.90
1	D	54	THR	CA-C-N	5.74	132.50	121.54
1	D	54	THR	C-N-CA	5.74	132.50	121.54
1	B	40	GLU	CA-CB-CG	-5.74	102.63	114.10
1	B	307	VAL	CG1-CB-CG2	-5.74	98.18	110.80
1	C	40	GLU	CA-CB-CG	-5.74	102.63	114.10
1	C	330	ASN	CA-C-O	5.74	127.73	121.02
1	D	87	ALA	CA-C-N	5.74	130.25	122.56
1	D	87	ALA	C-N-CA	5.74	130.25	122.56
1	C	413	LYS	CD-CE-NZ	5.73	130.25	111.90
1	A	54	THR	CA-C-N	5.73	132.49	121.54
1	A	54	THR	C-N-CA	5.73	132.49	121.54
1	B	293	ILE	CA-CB-CG2	-5.73	100.75	110.50
1	D	261	LEU	CD1-CG-CD2	5.73	123.41	110.80
1	D	293	ILE	CG1-CB-CG2	5.73	127.90	110.70
1	A	40	GLU	CA-CB-CG	-5.73	102.64	114.10
1	D	293	ILE	CA-CB-CG2	-5.73	100.76	110.50
1	B	261	LEU	CD1-CG-CD2	5.73	123.40	110.80
1	C	307	VAL	CG1-CB-CG2	-5.73	98.20	110.80
1	B	54	THR	CA-C-N	5.73	132.48	121.54
1	B	54	THR	C-N-CA	5.73	132.48	121.54
1	A	307	VAL	CG1-CB-CG2	-5.72	98.20	110.80
1	D	95	GLU	CG-CD-OE2	-5.72	105.23	118.40
1	A	87	ALA	CA-C-N	5.72	130.23	122.56
1	A	87	ALA	C-N-CA	5.72	130.23	122.56
1	B	87	ALA	CA-C-N	5.72	130.23	122.56
1	B	87	ALA	C-N-CA	5.72	130.23	122.56
1	C	95	GLU	CG-CD-OE2	-5.72	105.24	118.40
1	A	368	VAL	N-CA-C	-5.72	98.90	107.37
1	D	210	ARG	CB-CG-CD	5.72	124.46	111.30
1	C	194	PHE	N-CA-C	5.72	119.49	109.48
1	D	40	GLU	CA-CB-CG	-5.72	102.66	114.10
1	D	368	VAL	N-CA-C	-5.72	98.91	107.37
1	B	210	ARG	CB-CG-CD	5.72	124.45	111.30
1	A	196	PHE	CA-C-O	5.71	126.42	119.11
1	B	194	PHE	N-CA-C	5.71	119.48	109.48
1	C	108	ASN	N-CA-C	-5.71	105.80	112.89
1	D	266	GLU	CA-C-N	-5.71	113.36	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	266	GLU	C-N-CA	-5.71	113.36	120.56
1	A	194	PHE	N-CA-C	5.71	119.47	109.48
1	A	210	ARG	CB-CG-CD	5.71	124.43	111.30
1	C	210	ARG	CB-CG-CD	5.71	124.43	111.30
1	D	194	PHE	N-CA-C	5.71	119.47	109.48
1	A	261	LEU	CD1-CG-CD2	5.71	123.35	110.80
1	C	368	VAL	N-CA-C	-5.70	98.93	107.37
1	B	266	GLU	CA-C-N	-5.70	113.38	120.56
1	B	266	GLU	C-N-CA	-5.70	113.38	120.56
1	D	46	ILE	CA-CB-CG1	-5.70	100.71	110.40
1	C	196	PHE	CA-C-O	5.70	126.40	119.11
1	A	266	GLU	CA-C-N	-5.69	113.39	120.56
1	A	266	GLU	C-N-CA	-5.69	113.39	120.56
1	D	108	ASN	N-CA-C	-5.69	105.83	112.89
1	B	46	ILE	CA-CB-CG1	-5.69	100.72	110.40
1	D	225	ILE	O-C-N	-5.69	116.68	122.54
1	A	65	ALA	O-C-N	5.69	128.17	122.03
1	A	46	ILE	CA-CB-CG1	-5.69	100.73	110.40
1	A	108	ASN	N-CA-C	-5.69	105.84	112.89
1	B	196	PHE	CA-C-O	5.69	126.39	119.11
1	C	266	GLU	CA-C-N	-5.69	113.39	120.56
1	C	266	GLU	C-N-CA	-5.69	113.39	120.56
1	D	17	LEU	CA-CB-CG	-5.69	96.40	116.30
1	A	17	LEU	CA-CB-CG	-5.68	96.40	116.30
1	C	261	LEU	CD1-CG-CD2	5.68	123.30	110.80
1	B	108	ASN	N-CA-C	-5.68	105.85	112.89
1	B	17	LEU	CA-CB-CG	-5.68	96.43	116.30
1	C	17	LEU	CA-CB-CG	-5.68	96.43	116.30
1	C	46	ILE	CA-CB-CG1	-5.68	100.75	110.40
1	C	65	ALA	O-C-N	5.68	128.16	122.03
1	C	423	LYS	CA-C-O	-5.67	114.50	120.80
1	D	260	ALA	N-CA-CB	-5.67	101.83	110.33
1	C	140	VAL	CA-C-O	5.67	126.88	119.85
1	D	140	VAL	CA-C-O	5.67	126.88	119.85
1	D	65	ALA	O-C-N	5.67	128.15	122.03
1	B	140	VAL	CA-C-O	5.66	126.87	119.85
1	B	272	GLY	CA-C-N	5.66	130.29	122.77
1	B	272	GLY	C-N-CA	5.66	130.29	122.77
1	C	225	ILE	O-C-N	-5.66	116.72	122.54
1	A	337	TRP	N-CA-C	-5.65	98.77	110.80
1	B	65	ALA	O-C-N	5.65	128.13	122.03
1	B	260	ALA	N-CA-CB	-5.65	101.86	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	337	TRP	N-CA-C	-5.65	98.77	110.80
1	B	337	TRP	N-CA-C	-5.65	98.77	110.80
1	C	260	ALA	N-CA-CB	-5.65	101.86	110.33
1	D	337	TRP	N-CA-C	-5.64	98.78	110.80
1	A	423	LYS	CA-C-O	-5.64	114.54	120.80
1	A	140	VAL	CA-C-O	5.64	126.84	119.85
1	C	124	HIS	CA-C-O	5.64	125.44	119.69
1	D	423	LYS	CA-C-O	-5.64	114.54	120.80
1	C	146	PHE	N-CA-CB	5.63	118.40	110.12
1	A	260	ALA	N-CA-CB	-5.63	101.88	110.33
1	B	225	ILE	CA-C-N	-5.63	114.09	123.33
1	B	225	ILE	C-N-CA	-5.63	114.09	123.33
1	A	225	ILE	O-C-N	-5.62	116.75	122.54
1	A	272	GLY	CA-C-N	5.62	130.25	122.77
1	A	272	GLY	C-N-CA	5.62	130.25	122.77
1	C	272	GLY	CA-C-N	5.62	130.25	122.77
1	C	272	GLY	C-N-CA	5.62	130.25	122.77
1	D	124	HIS	CA-C-O	5.62	125.43	119.69
1	A	146	PHE	N-CA-CB	5.62	118.38	110.12
1	A	124	HIS	CA-C-O	5.62	125.42	119.69
1	A	225	ILE	CA-C-N	-5.62	114.12	123.33
1	A	225	ILE	C-N-CA	-5.62	114.12	123.33
1	B	124	HIS	CA-C-O	5.62	125.42	119.69
1	C	102	PHE	N-CA-C	5.62	117.85	111.11
1	A	42	ALA	N-CA-C	-5.61	98.84	110.80
1	D	25	GLU	O-C-N	5.61	129.67	123.33
1	D	272	GLY	CA-C-N	5.61	130.24	122.77
1	D	272	GLY	C-N-CA	5.61	130.24	122.77
1	C	104	ALA	O-C-N	-5.61	115.87	122.32
1	A	102	PHE	N-CA-C	5.61	117.84	111.11
1	B	102	PHE	N-CA-C	5.61	117.84	111.11
1	C	80	GLU	CB-CG-CD	5.61	122.14	112.60
1	B	303	ARG	CA-C-N	5.61	127.73	120.44
1	B	303	ARG	C-N-CA	5.61	127.73	120.44
1	C	42	ALA	N-CA-C	-5.61	98.86	110.80
1	C	277	ALA	CA-C-O	-5.61	114.78	121.56
1	D	100	GLN	N-CA-C	-5.61	104.81	111.03
1	D	121	LEU	N-CA-C	5.61	120.11	112.04
1	B	42	ALA	N-CA-C	-5.61	98.86	110.80
1	B	423	LYS	CA-C-O	-5.61	114.58	120.80
1	D	146	PHE	N-CA-CB	5.60	118.35	110.12
1	C	225	ILE	CA-C-N	-5.60	114.15	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	225	ILE	C-N-CA	-5.60	114.15	123.33
1	C	303	ARG	CA-C-N	5.60	127.72	120.44
1	C	303	ARG	C-N-CA	5.60	127.72	120.44
1	D	102	PHE	N-CA-C	5.60	117.83	111.11
1	A	80	GLU	CB-CG-CD	5.59	122.11	112.60
1	A	303	ARG	CA-C-N	5.59	127.71	120.44
1	A	303	ARG	C-N-CA	5.59	127.71	120.44
1	B	80	GLU	CB-CG-CD	5.59	122.11	112.60
1	B	121	LEU	N-CA-C	5.59	120.09	112.04
1	B	146	PHE	N-CA-CB	5.59	118.34	110.12
1	C	121	LEU	N-CA-C	5.59	120.09	112.04
1	D	225	ILE	CA-C-N	-5.59	114.16	123.33
1	D	225	ILE	C-N-CA	-5.59	114.16	123.33
1	D	42	ALA	N-CA-C	-5.59	98.90	110.80
1	B	225	ILE	O-C-N	-5.59	116.78	122.54
1	A	256	ALA	CA-C-N	-5.58	115.15	122.63
1	A	256	ALA	C-N-CA	-5.58	115.15	122.63
1	B	256	ALA	CA-C-N	-5.58	115.15	122.63
1	B	256	ALA	C-N-CA	-5.58	115.15	122.63
1	B	346	VAL	N-CA-CB	-5.58	104.64	111.67
1	A	121	LEU	N-CA-C	5.58	120.07	112.04
1	C	100	GLN	N-CA-C	-5.58	104.84	111.03
1	D	80	GLU	CB-CG-CD	5.58	122.08	112.60
1	A	25	GLU	O-C-N	5.58	129.63	123.33
1	A	104	ALA	O-C-N	-5.58	115.91	122.32
1	A	277	ALA	CA-C-O	-5.57	114.82	121.56
1	D	303	ARG	CA-C-N	5.57	127.69	120.44
1	D	303	ARG	C-N-CA	5.57	127.69	120.44
1	D	366	ASP	CA-C-N	5.57	131.72	121.85
1	D	366	ASP	C-N-CA	5.57	131.72	121.85
1	A	100	GLN	N-CA-C	-5.57	104.85	111.03
1	B	209	VAL	CB-CA-C	-5.57	104.54	112.22
1	D	245	GLY	N-CA-C	5.57	126.37	113.18
1	A	101	LEU	CA-C-N	-5.56	113.03	120.54
1	A	101	LEU	C-N-CA	-5.56	113.03	120.54
1	C	256	ALA	CA-C-N	-5.56	115.18	122.63
1	C	256	ALA	C-N-CA	-5.56	115.18	122.63
1	C	25	GLU	O-C-N	5.56	129.61	123.33
1	B	277	ALA	CA-C-O	-5.56	114.83	121.56
1	A	209	VAL	CB-CA-C	-5.56	104.55	112.22
1	A	366	ASP	CA-C-N	5.56	131.69	121.85
1	A	366	ASP	C-N-CA	5.56	131.69	121.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	101	LEU	CA-C-N	-5.56	113.04	120.54
1	C	101	LEU	C-N-CA	-5.56	113.04	120.54
1	D	104	ALA	O-C-N	-5.56	115.93	122.32
1	D	187	ASP	N-CA-CB	5.56	118.39	110.44
1	B	25	GLU	O-C-N	5.56	129.61	123.33
1	C	209	VAL	CB-CA-C	-5.56	104.55	112.22
1	C	64	MET	CA-C-N	5.55	128.18	120.63
1	C	64	MET	C-N-CA	5.55	128.18	120.63
1	B	180	GLY	N-CA-C	-5.55	107.00	115.66
1	B	366	ASP	CA-C-N	5.55	131.68	121.85
1	B	366	ASP	C-N-CA	5.55	131.68	121.85
1	A	346	VAL	N-CA-CB	-5.55	104.67	111.67
1	A	64	MET	CA-C-N	5.55	128.18	120.63
1	A	64	MET	C-N-CA	5.55	128.18	120.63
1	B	187	ASP	N-CA-CB	5.55	118.37	110.44
1	C	180	GLY	N-CA-C	-5.55	107.00	115.66
1	A	180	GLY	N-CA-C	-5.55	107.01	115.66
1	B	101	LEU	CA-C-N	-5.55	113.05	120.54
1	B	101	LEU	C-N-CA	-5.55	113.05	120.54
1	C	187	ASP	N-CA-CB	5.55	118.37	110.44
1	C	366	ASP	CA-C-N	5.55	131.67	121.85
1	C	366	ASP	C-N-CA	5.55	131.67	121.85
1	A	187	ASP	N-CA-CB	5.54	118.37	110.44
1	D	277	ALA	CA-C-O	-5.54	114.85	121.56
1	C	245	GLY	N-CA-C	5.54	126.32	113.18
1	D	180	GLY	N-CA-C	-5.54	107.01	115.66
1	B	104	ALA	O-C-N	-5.54	115.95	122.32
1	D	209	VAL	CB-CA-C	-5.54	104.57	112.22
1	B	100	GLN	N-CA-C	-5.54	104.88	111.03
1	B	270	ASP	CB-CG-OD1	-5.54	105.67	118.40
1	D	77	LYS	CB-CG-CD	5.54	124.03	111.30
1	D	107	GLY	CA-C-O	5.54	130.20	120.57
1	D	256	ALA	CA-C-N	-5.54	115.21	122.63
1	D	256	ALA	C-N-CA	-5.54	115.21	122.63
1	D	270	ASP	CB-CG-OD1	-5.54	105.67	118.40
1	A	245	GLY	N-CA-C	5.53	126.30	113.18
1	C	107	GLY	N-CA-C	5.53	126.30	113.18
1	A	270	ASP	CB-CG-OD1	-5.53	105.68	118.40
1	B	328	ARG	CD-NE-CZ	5.53	132.14	124.40
1	C	107	GLY	CA-C-O	5.53	130.19	120.57
1	D	107	GLY	N-CA-C	5.53	126.28	113.18
1	D	346	VAL	N-CA-CB	-5.53	104.70	111.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	270	ASP	CB-CG-OD1	-5.53	105.69	118.40
1	C	346	VAL	N-CA-CB	-5.53	104.71	111.67
1	B	64	MET	CA-C-N	5.53	128.14	120.63
1	B	64	MET	C-N-CA	5.53	128.14	120.63
1	D	64	MET	CA-C-N	5.53	128.15	120.63
1	D	64	MET	C-N-CA	5.53	128.15	120.63
1	A	77	LYS	CB-CG-CD	5.52	124.00	111.30
1	A	107	GLY	N-CA-C	5.52	126.27	113.18
1	A	107	GLY	CA-C-O	5.52	130.18	120.57
1	D	101	LEU	CA-C-N	-5.52	113.09	120.54
1	D	101	LEU	C-N-CA	-5.52	113.09	120.54
1	B	77	LYS	CB-CG-CD	5.52	123.99	111.30
1	C	77	LYS	CB-CG-CD	5.51	123.98	111.30
1	D	328	ARG	CD-NE-CZ	5.51	132.12	124.40
1	A	328	ARG	CD-NE-CZ	5.51	132.11	124.40
1	B	107	GLY	N-CA-C	5.51	126.24	113.18
1	B	245	GLY	N-CA-C	5.51	126.24	113.18
1	B	107	GLY	CA-C-O	5.51	130.15	120.57
1	B	286	THR	CB-CA-C	-5.51	100.17	110.36
1	D	286	THR	CB-CA-C	-5.51	100.17	110.36
1	A	90	LEU	N-CA-C	5.50	122.52	110.80
1	B	90	LEU	N-CA-C	5.50	122.50	110.80
1	C	286	THR	CB-CA-C	-5.50	100.19	110.36
1	D	94	GLU	CB-CA-C	5.50	118.93	110.14
1	A	286	THR	CB-CA-C	-5.49	100.20	110.36
1	C	198	ARG	N-CA-C	-5.49	101.59	110.32
1	A	94	GLU	CB-CA-C	5.49	118.92	110.14
1	C	328	ARG	CD-NE-CZ	5.49	132.09	124.40
1	B	94	GLU	CB-CA-C	5.49	118.92	110.14
1	C	253	ILE	CA-C-O	-5.49	114.70	120.57
1	C	90	LEU	N-CA-C	5.48	122.48	110.80
1	D	198	ARG	N-CA-C	-5.48	101.61	110.32
1	B	368	VAL	CB-CA-C	-5.48	103.58	111.19
1	D	90	LEU	N-CA-C	5.47	122.46	110.80
1	A	198	ARG	N-CA-C	-5.47	101.62	110.32
1	A	253	ILE	CA-C-O	-5.47	114.72	120.57
1	D	368	VAL	CB-CA-C	-5.47	103.59	111.19
1	D	406	ALA	O-C-N	5.47	128.62	122.22
1	C	94	GLU	CB-CA-C	5.46	118.88	110.14
1	A	368	VAL	CB-CA-C	-5.46	103.60	111.19
1	B	198	ARG	N-CA-C	-5.46	101.64	110.32
1	B	253	ILE	CA-C-O	-5.46	114.73	120.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	109	VAL	N-CA-C	-5.46	104.63	110.36
1	C	368	VAL	CB-CA-C	-5.46	103.60	111.19
1	C	118	LEU	CA-C-N	-5.46	114.75	122.94
1	C	118	LEU	C-N-CA	-5.46	114.75	122.94
1	D	261	LEU	N-CA-C	-5.45	105.42	111.36
1	D	409	SER	CA-C-N	5.45	124.63	118.97
1	D	409	SER	C-N-CA	5.45	124.63	118.97
1	C	124	HIS	CA-C-N	5.44	125.99	120.38
1	C	124	HIS	C-N-CA	5.44	125.99	120.38
1	D	420	GLY	O-C-N	5.44	127.41	122.19
1	C	109	VAL	N-CA-C	-5.44	104.65	110.36
1	C	420	GLY	O-C-N	5.44	127.41	122.19
1	B	124	HIS	CA-C-N	5.44	125.98	120.38
1	B	124	HIS	C-N-CA	5.44	125.98	120.38
1	B	409	SER	CA-C-N	5.44	124.62	118.97
1	B	409	SER	C-N-CA	5.44	124.62	118.97
1	D	253	ILE	CA-C-O	-5.44	114.75	120.57
1	A	118	LEU	CA-C-N	-5.43	114.79	122.94
1	A	118	LEU	C-N-CA	-5.43	114.79	122.94
1	B	118	LEU	CA-C-N	-5.43	114.79	122.94
1	B	118	LEU	C-N-CA	-5.43	114.79	122.94
1	C	229	GLY	CA-C-N	5.43	125.43	119.89
1	C	229	GLY	C-N-CA	5.43	125.43	119.89
1	A	109	VAL	N-CA-C	-5.43	104.66	110.36
1	A	406	ALA	O-C-N	5.43	128.57	122.22
1	A	124	HIS	CA-C-N	5.42	125.97	120.38
1	A	124	HIS	C-N-CA	5.42	125.97	120.38
1	D	118	LEU	CA-C-N	-5.42	114.81	122.94
1	D	118	LEU	C-N-CA	-5.42	114.81	122.94
1	A	261	LEU	N-CA-C	-5.42	105.45	111.36
1	D	217	THR	CA-CB-CG2	5.42	119.71	110.50
1	D	124	HIS	CA-C-N	5.42	125.96	120.38
1	D	124	HIS	C-N-CA	5.42	125.96	120.38
1	D	147	MET	N-CA-C	-5.42	105.54	111.82
1	B	249	VAL	CA-C-N	5.42	129.87	121.26
1	B	249	VAL	C-N-CA	5.42	129.87	121.26
1	A	409	SER	CA-C-N	5.41	124.60	118.97
1	A	409	SER	C-N-CA	5.41	124.60	118.97
1	A	217	THR	CA-CB-CG2	5.41	119.70	110.50
1	B	217	THR	CA-CB-CG2	5.41	119.70	110.50
1	C	147	MET	N-CA-C	-5.41	105.54	111.82
1	D	109	VAL	N-CA-C	-5.41	104.68	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	41	GLU	CB-CG-CD	-5.41	103.40	112.60
1	A	420	GLY	O-C-N	5.41	127.38	122.19
1	C	357	PRO	CA-C-N	-5.41	113.03	120.28
1	C	357	PRO	C-N-CA	-5.41	113.03	120.28
1	C	406	ALA	O-C-N	5.41	128.55	122.22
1	C	261	LEU	N-CA-C	-5.41	105.47	111.36
1	C	217	THR	CA-CB-CG2	5.40	119.68	110.50
1	A	229	GLY	CA-C-N	5.40	125.40	119.89
1	A	229	GLY	C-N-CA	5.40	125.40	119.89
1	B	308	ASP	CA-C-N	5.40	131.45	121.94
1	B	308	ASP	C-N-CA	5.40	131.45	121.94
1	C	150	LYS	CA-C-O	-5.40	114.77	120.55
1	D	308	ASP	CA-C-N	5.40	131.45	121.94
1	D	308	ASP	C-N-CA	5.40	131.45	121.94
1	A	249	VAL	CA-C-N	5.40	129.84	121.26
1	A	249	VAL	C-N-CA	5.40	129.84	121.26
1	C	41	GLU	CB-CG-CD	-5.40	103.42	112.60
1	D	41	GLU	CB-CG-CD	-5.40	103.42	112.60
1	A	147	MET	N-CA-C	-5.40	105.56	111.82
1	B	41	GLU	CB-CG-CD	-5.40	103.42	112.60
1	B	261	LEU	N-CA-C	-5.39	105.48	111.36
1	B	229	GLY	CA-C-N	5.39	125.39	119.89
1	B	229	GLY	C-N-CA	5.39	125.39	119.89
1	B	406	ALA	O-C-N	5.39	128.53	122.22
1	A	308	ASP	CA-C-N	5.39	131.43	121.94
1	A	308	ASP	C-N-CA	5.39	131.43	121.94
1	C	249	VAL	CA-C-N	5.39	129.83	121.26
1	C	249	VAL	C-N-CA	5.39	129.83	121.26
1	C	28	VAL	CB-CA-C	-5.39	102.80	110.83
1	A	150	LYS	CA-C-O	-5.38	114.79	120.55
1	B	308	ASP	CA-C-O	-5.38	113.26	119.56
1	A	357	PRO	CA-C-N	-5.38	113.07	120.28
1	A	357	PRO	C-N-CA	-5.38	113.07	120.28
1	B	150	LYS	CA-C-O	-5.38	114.79	120.55
1	A	368	VAL	N-CA-CB	5.38	118.45	111.67
1	C	153	PRO	N-CA-C	-5.38	101.45	111.03
1	C	409	SER	CA-C-N	5.38	124.57	118.97
1	C	409	SER	C-N-CA	5.38	124.57	118.97
1	D	28	VAL	CB-CA-C	-5.38	102.81	110.83
1	A	28	VAL	CB-CA-C	-5.38	102.81	110.83
1	B	28	VAL	CB-CA-C	-5.38	102.81	110.83
1	B	153	PRO	N-CA-C	-5.38	101.45	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	17	LEU	O-C-N	5.38	131.08	122.42
1	D	17	LEU	O-C-N	5.38	131.08	122.42
1	A	275	ILE	CA-C-O	-5.38	114.98	121.54
1	B	368	VAL	N-CA-CB	5.38	118.44	111.67
1	B	420	GLY	O-C-N	5.38	127.35	122.19
1	C	308	ASP	CA-C-N	5.38	131.40	121.94
1	C	308	ASP	C-N-CA	5.38	131.40	121.94
1	B	409	SER	CB-CA-C	-5.37	105.06	110.65
1	D	249	VAL	CA-C-N	5.37	129.81	121.26
1	D	249	VAL	C-N-CA	5.37	129.81	121.26
1	A	153	PRO	N-CA-C	-5.37	101.47	111.03
1	C	368	VAL	N-CA-CB	5.37	118.44	111.67
1	D	275	ILE	CA-C-O	-5.37	114.99	121.54
1	D	153	PRO	N-CA-C	-5.37	101.47	111.03
1	A	17	LEU	O-C-N	5.37	131.06	122.42
1	A	409	SER	CB-CA-C	-5.37	105.07	110.65
1	C	275	ILE	CA-C-O	-5.37	114.99	121.54
1	A	195	PRO	N-CA-C	5.37	123.53	112.47
1	B	195	PRO	N-CA-C	5.37	123.53	112.47
1	B	308	ASP	O-C-N	5.37	128.78	122.34
1	D	229	GLY	CA-C-N	5.37	125.36	119.89
1	D	229	GLY	C-N-CA	5.37	125.36	119.89
1	B	408	SER	N-CA-C	-5.37	107.39	114.04
1	C	17	LEU	O-C-N	5.37	131.06	122.42
1	C	408	SER	N-CA-C	-5.37	107.39	114.04
1	D	117	ASN	CA-C-O	-5.37	115.34	121.40
1	D	368	VAL	N-CA-CB	5.37	118.43	111.67
1	B	243	ASN	O-C-N	5.36	127.82	122.03
1	C	409	SER	CB-CA-C	-5.36	105.07	110.65
1	D	357	PRO	CA-C-N	-5.36	113.10	120.28
1	D	357	PRO	C-N-CA	-5.36	113.10	120.28
1	D	409	SER	CB-CA-C	-5.36	105.08	110.65
1	B	231	VAL	N-CA-CB	5.36	116.46	110.51
1	D	408	SER	N-CA-C	-5.36	107.40	114.04
1	A	308	ASP	CA-C-O	-5.35	113.30	119.56
1	D	70	ALA	CA-C-O	-5.35	115.08	121.56
1	C	70	ALA	CA-C-O	-5.35	115.08	121.56
1	C	195	PRO	N-CA-C	5.35	123.50	112.47
1	D	195	PRO	N-CA-C	5.35	123.50	112.47
1	B	217	THR	CA-C-N	-5.35	115.86	123.08
1	B	217	THR	C-N-CA	-5.35	115.86	123.08
1	B	357	PRO	CA-C-N	-5.35	113.11	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	357	PRO	C-N-CA	-5.35	113.11	120.28
1	A	231	VAL	N-CA-CB	5.35	116.44	110.51
1	A	408	SER	N-CA-C	-5.35	107.41	114.04
1	B	147	MET	N-CA-C	-5.35	105.53	111.36
1	C	367	LEU	CB-CA-C	-5.35	98.55	109.94
1	D	150	LYS	CA-C-O	-5.35	114.83	120.55
1	D	231	VAL	N-CA-CB	5.35	116.44	110.51
1	D	367	LEU	CB-CA-C	-5.35	98.55	109.94
1	A	117	ASN	CA-C-O	-5.34	115.36	121.40
1	A	367	LEU	CB-CA-C	-5.34	98.56	109.94
1	C	231	VAL	N-CA-CB	5.34	116.44	110.51
1	C	243	ASN	O-C-N	5.34	127.80	122.03
1	B	275	ILE	CA-C-O	-5.34	115.03	121.54
1	C	281	MET	CB-CG-SD	5.34	128.72	112.70
1	C	365	LYS	CG-CD-CE	5.34	123.58	111.30
1	D	308	ASP	CA-C-O	-5.34	113.32	119.56
1	B	69	MET	CA-C-O	-5.33	115.42	121.72
1	A	70	ALA	CA-C-O	-5.33	115.11	121.56
1	B	281	MET	CB-CG-SD	5.33	128.70	112.70
1	B	365	LYS	CG-CD-CE	5.33	123.57	111.30
1	C	169	GLU	O-C-N	5.33	129.68	122.59
1	A	281	MET	CB-CG-SD	5.33	128.69	112.70
1	A	308	ASP	O-C-N	5.33	128.74	122.34
1	D	281	MET	CB-CG-SD	5.33	128.70	112.70
1	C	308	ASP	CA-C-O	-5.33	113.33	119.56
1	A	243	ASN	O-C-N	5.32	127.78	122.03
1	C	69	MET	CA-C-O	-5.32	115.44	121.72
1	C	308	ASP	O-C-N	5.32	128.73	122.34
1	D	169	GLU	O-C-N	5.32	129.67	122.59
1	D	365	LYS	CG-CD-CE	5.32	123.55	111.30
1	B	90	LEU	O-C-N	-5.32	115.51	122.59
1	B	117	ASN	CA-C-O	-5.32	115.39	121.40
1	A	169	GLU	O-C-N	5.32	129.66	122.59
1	A	365	LYS	CG-CD-CE	5.32	123.54	111.30
1	B	169	GLU	O-C-N	5.32	129.67	122.59
1	B	367	LEU	CB-CA-C	-5.32	98.61	109.94
1	D	308	ASP	O-C-N	5.32	128.72	122.34
1	C	117	ASN	CA-C-O	-5.32	115.39	121.40
1	D	217	THR	CA-C-N	-5.32	115.90	123.08
1	D	217	THR	C-N-CA	-5.32	115.90	123.08
1	A	11	TYR	CA-CB-CG	-5.32	104.33	113.90
1	A	90	LEU	O-C-N	-5.32	115.52	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	11	TYR	CA-CB-CG	-5.32	104.33	113.90
1	C	90	LEU	O-C-N	-5.32	115.52	122.59
1	D	367	LEU	CB-CG-CD1	-5.32	94.75	110.70
1	A	217	THR	CA-C-N	-5.31	115.91	123.08
1	A	217	THR	C-N-CA	-5.31	115.91	123.08
1	B	342	PRO	N-CA-C	5.31	119.42	111.14
1	A	367	LEU	CB-CG-CD1	-5.31	94.78	110.70
1	A	69	MET	CA-C-O	-5.30	115.46	121.72
1	B	70	ALA	CA-C-O	-5.30	115.14	121.56
1	D	119	ARG	CA-C-O	-5.30	114.97	120.70
1	A	119	ARG	CA-C-O	-5.30	114.97	120.70
1	B	119	ARG	CA-C-O	-5.30	114.97	120.70
1	A	360	ILE	N-CA-C	5.30	115.44	110.30
1	C	217	THR	CA-C-N	-5.30	115.92	123.08
1	C	217	THR	C-N-CA	-5.30	115.92	123.08
1	D	11	TYR	CA-CB-CG	-5.30	104.36	113.90
1	D	243	ASN	O-C-N	5.30	127.76	122.03
1	C	367	LEU	CB-CG-CD1	-5.30	94.80	110.70
1	A	250	MET	CG-SD-CE	-5.30	89.25	100.90
1	B	95	GLU	CA-C-N	-5.30	111.03	121.41
1	B	95	GLU	C-N-CA	-5.30	111.03	121.41
1	C	119	ARG	CA-C-O	-5.30	114.98	120.70
1	A	303	ARG	N-CA-C	-5.29	105.56	112.23
1	A	342	PRO	N-CA-C	5.29	119.40	111.14
1	B	11	TYR	CA-CB-CG	-5.29	104.37	113.90
1	D	90	LEU	O-C-N	-5.29	115.55	122.59
1	C	303	ARG	N-CA-C	-5.29	105.56	112.23
1	D	250	MET	CG-SD-CE	-5.29	89.26	100.90
1	D	69	MET	CA-C-O	-5.29	115.48	121.72
1	B	367	LEU	CB-CG-CD1	-5.29	94.83	110.70
1	C	27	ILE	CA-CB-CG1	5.29	119.39	110.40
1	B	250	MET	CG-SD-CE	-5.29	89.27	100.90
1	D	130	LEU	CA-C-O	5.29	125.87	119.31
1	C	250	MET	CG-SD-CE	-5.29	89.27	100.90
1	D	303	ARG	N-CA-C	-5.28	105.57	112.23
1	D	176	GLU	CG-CD-OE2	-5.28	106.25	118.40
1	D	95	GLU	CA-C-N	-5.28	111.06	121.41
1	D	95	GLU	C-N-CA	-5.28	111.06	121.41
1	B	303	ARG	N-CA-C	-5.28	105.58	112.23
1	C	360	ILE	N-CA-C	5.28	115.42	110.30
1	B	130	LEU	CA-C-O	5.28	125.85	119.31
1	C	66	LYS	CA-CB-CG	-5.28	103.55	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	176	GLU	CG-CD-OE2	-5.27	106.27	118.40
1	A	95	GLU	CA-C-N	-5.27	111.08	121.41
1	A	95	GLU	C-N-CA	-5.27	111.08	121.41
1	D	310	ILE	N-CA-C	5.27	117.65	108.90
1	B	360	ILE	N-CA-C	5.27	115.41	110.30
1	C	176	GLU	CG-CD-OE2	-5.27	106.28	118.40
1	D	342	PRO	N-CA-C	5.27	119.36	111.14
1	A	176	GLU	CG-CD-OE2	-5.27	106.28	118.40
1	C	235	GLU	O-C-N	5.27	127.78	122.09
1	A	27	ILE	CA-CB-CG1	5.27	119.35	110.40
1	C	342	PRO	N-CA-C	5.26	119.35	111.14
1	A	310	ILE	N-CA-C	5.26	117.63	108.90
1	B	66	LYS	CA-CB-CG	-5.26	103.58	114.10
1	A	130	LEU	CA-C-O	5.26	125.83	119.31
1	C	310	ILE	N-CA-C	5.26	117.63	108.90
1	D	66	LYS	CA-CB-CG	-5.26	103.58	114.10
1	A	66	LYS	CA-CB-CG	-5.26	103.58	114.10
1	B	310	ILE	N-CA-C	5.26	117.63	108.90
1	B	420	GLY	N-CA-C	-5.26	106.13	112.49
1	C	95	GLU	CA-C-N	-5.26	111.11	121.41
1	C	95	GLU	C-N-CA	-5.26	111.11	121.41
1	D	27	ILE	CA-CB-CG1	5.25	119.33	110.40
1	B	27	ILE	CA-CB-CG1	5.25	119.33	110.40
1	D	360	ILE	N-CA-C	5.25	115.39	110.30
1	D	187	ASP	CA-C-O	-5.25	115.91	121.94
1	B	237	ARG	CD-NE-CZ	-5.25	117.06	124.40
1	D	234	MET	CG-SD-CE	-5.24	89.36	100.90
1	B	235	GLU	O-C-N	5.24	127.75	122.09
1	A	234	MET	CG-SD-CE	-5.24	89.37	100.90
1	A	420	GLY	N-CA-C	-5.24	106.15	112.49
1	B	234	MET	CG-SD-CE	-5.24	89.38	100.90
1	C	234	MET	CG-SD-CE	-5.24	89.38	100.90
1	D	347	ALA	N-CA-CB	-5.23	103.03	110.46
1	D	420	GLY	N-CA-C	-5.23	106.16	112.49
1	B	333	LEU	N-CA-C	-5.23	105.47	111.07
1	B	347	ALA	N-CA-CB	-5.23	103.03	110.46
1	A	187	ASP	CA-C-O	-5.23	115.93	121.94
1	D	315	ALA	CB-CA-C	-5.23	104.08	111.76
1	A	237	ARG	CD-NE-CZ	-5.22	117.08	124.40
1	B	315	ALA	CB-CA-C	-5.22	104.08	111.76
1	C	130	LEU	CA-C-O	5.22	125.79	119.31
1	C	9	GLU	CG-CD-OE1	-5.22	106.39	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	420	GLY	N-CA-C	-5.22	106.17	112.49
1	A	235	GLU	O-C-N	5.22	127.73	122.09
1	B	187	ASP	CA-C-O	-5.22	115.94	121.94
1	C	187	ASP	CA-C-O	-5.22	115.94	121.94
1	D	237	ARG	CD-NE-CZ	-5.22	117.09	124.40
1	B	9	GLU	CG-CD-OE1	-5.22	106.39	118.40
1	C	315	ALA	CB-CA-C	-5.22	104.09	111.76
1	D	235	GLU	O-C-N	5.22	127.73	122.09
1	A	347	ALA	N-CA-CB	-5.22	103.05	110.46
1	C	347	ALA	N-CA-CB	-5.22	103.05	110.46
1	A	9	GLU	CG-CD-OE1	-5.21	106.41	118.40
1	A	345	PRO	N-CA-C	-5.21	101.73	112.47
1	B	336	LYS	N-CA-CB	5.21	117.82	110.36
1	B	345	PRO	N-CA-C	-5.21	101.73	112.47
1	C	237	ARG	CD-NE-CZ	-5.21	117.10	124.40
1	A	235	GLU	N-CA-C	-5.21	105.51	111.14
1	B	235	GLU	N-CA-C	-5.21	105.51	111.14
1	D	235	GLU	N-CA-C	-5.21	105.51	111.14
1	A	315	ALA	CB-CA-C	-5.21	104.11	111.76
1	C	345	PRO	N-CA-C	-5.21	101.75	112.47
1	C	293	ILE	CB-CG1-CD1	5.21	124.73	113.80
1	D	129	TYR	CE1-CZ-OH	-5.21	104.29	119.90
1	C	235	GLU	N-CA-C	-5.20	105.52	111.14
1	D	333	LEU	N-CA-C	-5.20	105.50	111.07
1	A	336	LYS	N-CA-CB	5.20	117.80	110.36
1	D	345	PRO	N-CA-C	-5.20	101.76	112.47
1	A	166	SER	N-CA-C	-5.20	102.77	110.46
1	A	293	ILE	CB-CG1-CD1	5.20	124.72	113.80
1	D	9	GLU	CG-CD-OE1	-5.20	106.44	118.40
1	B	167	VAL	CA-CB-CG1	-5.20	101.56	110.40
1	B	293	ILE	CB-CG1-CD1	5.20	124.71	113.80
1	C	26	LEU	CA-CB-CG	-5.20	98.11	116.30
1	C	36	GLY	O-C-N	5.20	128.24	122.47
1	B	129	TYR	CE1-CZ-OH	-5.19	104.32	119.90
1	D	293	ILE	CB-CG1-CD1	5.19	124.71	113.80
1	A	129	TYR	CE1-CZ-OH	-5.19	104.32	119.90
1	A	333	LEU	N-CA-C	-5.19	105.52	111.07
1	A	167	VAL	CA-CB-CG1	-5.19	101.58	110.40
1	A	26	LEU	CA-CB-CG	-5.19	98.14	116.30
1	B	26	LEU	CA-CB-CG	-5.19	98.15	116.30
1	B	166	SER	N-CA-C	-5.19	102.78	110.46
1	B	338	GLU	CA-C-N	5.19	127.66	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	338	GLU	C-N-CA	5.19	127.66	120.29
1	C	129	TYR	CE1-CZ-OH	-5.19	104.34	119.90
1	D	26	LEU	CA-CB-CG	-5.19	98.14	116.30
1	D	167	VAL	CA-CB-CG1	-5.19	101.58	110.40
1	C	336	LYS	N-CA-CB	5.19	117.78	110.36
1	C	166	SER	N-CA-C	-5.18	102.79	110.46
1	A	36	GLY	O-C-N	5.18	128.22	122.47
1	A	391	ASP	CB-CG-OD1	-5.18	106.48	118.40
1	C	333	LEU	N-CA-C	-5.18	105.53	111.07
1	D	166	SER	N-CA-C	-5.18	102.79	110.46
1	C	391	ASP	CB-CG-OD1	-5.18	106.49	118.40
1	B	26	LEU	N-CA-C	5.18	116.75	108.41
1	C	167	VAL	CA-CB-CG1	-5.18	101.60	110.40
1	B	204	ARG	N-CA-C	5.17	118.37	111.75
1	B	320	ALA	CA-C-N	5.17	131.55	121.41
1	B	320	ALA	C-N-CA	5.17	131.55	121.41
1	D	336	LYS	N-CA-CB	5.17	117.76	110.36
1	A	26	LEU	N-CA-C	5.17	116.74	108.41
1	B	360	ILE	N-CA-CB	5.17	116.26	110.62
1	B	391	ASP	CB-CG-OD1	-5.17	106.50	118.40
1	D	360	ILE	N-CA-CB	5.17	116.26	110.62
1	D	403	ASP	CB-CG-OD1	-5.17	106.50	118.40
1	A	338	GLU	CA-C-N	5.17	127.63	120.29
1	A	338	GLU	C-N-CA	5.17	127.63	120.29
1	C	338	GLU	CA-C-N	5.17	127.63	120.29
1	C	338	GLU	C-N-CA	5.17	127.63	120.29
1	D	391	ASP	CB-CG-OD1	-5.17	106.51	118.40
1	A	360	ILE	N-CA-CB	5.17	116.25	110.62
1	C	91	THR	CB-CA-C	-5.17	101.99	110.72
1	A	91	THR	CB-CA-C	-5.16	101.99	110.72
1	D	26	LEU	N-CA-C	5.16	116.72	108.41
1	C	26	LEU	N-CA-C	5.16	116.72	108.41
1	A	403	ASP	CB-CG-OD1	-5.16	106.54	118.40
1	D	91	THR	CB-CA-C	-5.16	102.00	110.72
1	D	289	PRO	O-C-N	5.16	131.82	122.33
1	A	320	ALA	CA-C-N	5.16	131.52	121.41
1	A	320	ALA	C-N-CA	5.16	131.52	121.41
1	B	403	ASP	CB-CG-OD1	-5.16	106.54	118.40
1	C	403	ASP	CB-CG-OD1	-5.16	106.54	118.40
1	D	338	GLU	CA-C-N	5.16	127.61	120.29
1	D	338	GLU	C-N-CA	5.16	127.61	120.29
1	C	360	ILE	N-CA-CB	5.15	116.24	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	289	PRO	O-C-N	5.15	131.80	122.33
1	C	320	ALA	CA-C-N	5.15	131.50	121.41
1	C	320	ALA	C-N-CA	5.15	131.50	121.41
1	D	320	ALA	CA-C-N	5.15	131.50	121.41
1	D	320	ALA	C-N-CA	5.15	131.50	121.41
1	B	91	THR	CB-CA-C	-5.14	102.03	110.72
1	C	26	LEU	CB-CA-C	-5.14	102.33	110.81
1	D	244	GLU	N-CA-C	-5.14	106.28	113.37
1	A	290	ARG	NE-CZ-NH1	-5.14	116.36	121.50
1	B	192	THR	O-C-N	5.14	129.42	122.59
1	B	290	ARG	NE-CZ-NH1	-5.13	116.36	121.50
1	B	195	PRO	N-CA-CB	-5.13	97.86	103.25
1	B	289	PRO	O-C-N	5.13	131.77	122.33
1	A	26	LEU	CB-CA-C	-5.13	102.35	110.81
1	C	192	THR	O-C-N	5.13	129.41	122.59
1	B	26	LEU	CB-CA-C	-5.12	102.36	110.81
1	C	289	PRO	O-C-N	5.12	131.76	122.33
1	D	26	LEU	CB-CA-C	-5.12	102.36	110.81
1	D	290	ARG	NE-CZ-NH1	-5.12	116.38	121.50
1	C	252	ASP	CA-C-O	-5.12	115.67	121.66
1	B	214	GLU	CG-CD-OE1	5.12	130.17	118.40
1	D	195	PRO	N-CA-CB	-5.11	97.88	103.25
1	A	192	THR	O-C-N	5.11	129.38	122.59
1	A	195	PRO	N-CA-CB	-5.11	97.89	103.25
1	C	195	PRO	N-CA-CB	-5.11	97.89	103.25
1	A	249	VAL	N-CA-C	5.10	119.96	109.34
1	C	249	VAL	N-CA-C	5.10	119.96	109.34
1	C	290	ARG	NE-CZ-NH1	-5.10	116.40	121.50
1	A	214	GLU	CG-CD-OE1	5.10	130.12	118.40
1	C	196	PHE	N-CA-CB	-5.10	101.85	110.41
1	C	214	GLU	CG-CD-OE1	5.10	130.13	118.40
1	D	249	VAL	N-CA-C	5.10	119.94	109.34
1	D	196	PHE	N-CA-CB	-5.10	101.85	110.41
1	A	196	PHE	N-CA-CB	-5.09	101.85	110.41
1	B	249	VAL	N-CA-C	5.09	119.94	109.34
1	D	252	ASP	CA-C-O	-5.09	115.70	121.66
1	A	252	ASP	CA-C-O	-5.09	115.70	121.66
1	B	196	PHE	N-CA-CB	-5.09	101.86	110.41
1	B	252	ASP	CA-C-O	-5.09	115.71	121.66
1	D	214	GLU	CG-CD-OE1	5.08	130.09	118.40
1	A	27	ILE	CA-C-O	5.08	125.97	120.53
1	C	285	PHE	CA-CB-CG	5.08	118.88	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	57	THR	CA-CB-OG1	5.08	117.22	109.60
1	B	9	GLU	CA-C-N	5.08	130.29	122.77
1	B	9	GLU	C-N-CA	5.08	130.29	122.77
1	C	27	ILE	CA-C-O	5.08	125.96	120.53
1	D	9	GLU	CA-C-N	5.08	130.28	122.77
1	D	9	GLU	C-N-CA	5.08	130.28	122.77
1	C	9	GLU	CA-C-N	5.08	130.28	122.77
1	C	9	GLU	C-N-CA	5.08	130.28	122.77
1	C	182	ILE	CA-CB-CG1	-5.07	101.78	110.40
1	D	285	PHE	CA-CB-CG	5.07	118.87	113.80
1	B	182	ILE	CA-CB-CG1	-5.07	101.78	110.40
1	A	66	LYS	CG-CD-CE	5.07	122.96	111.30
1	D	66	LYS	CG-CD-CE	5.07	122.96	111.30
1	D	192	THR	O-C-N	5.07	129.33	122.59
1	D	113	LYS	CB-CA-C	5.07	118.77	110.96
1	D	182	ILE	CA-CB-CG1	-5.07	101.78	110.40
1	D	276	HIS	N-CA-C	-5.07	101.14	109.40
1	A	9	GLU	CA-C-N	5.07	130.27	122.77
1	A	9	GLU	C-N-CA	5.07	130.27	122.77
1	A	182	ILE	CA-CB-CG1	-5.07	101.79	110.40
1	B	27	ILE	CA-C-O	5.07	125.95	120.53
1	B	66	LYS	CG-CD-CE	5.07	122.95	111.30
1	C	57	THR	CA-CB-OG1	5.06	117.20	109.60
1	C	66	LYS	CG-CD-CE	5.06	122.95	111.30
1	D	27	ILE	CA-C-O	5.06	125.95	120.53
1	C	376	MET	CA-C-O	5.05	125.81	120.10
1	A	57	THR	CA-CB-OG1	5.05	117.18	109.60
1	D	235	GLU	CB-CA-C	-5.05	102.92	110.90
1	B	155	THR	CA-C-O	-5.05	115.36	120.71
1	D	155	THR	CA-C-O	-5.05	115.36	120.71
1	B	57	THR	CA-CB-OG1	5.05	117.17	109.60
1	B	105	VAL	CB-CA-C	-5.05	103.01	111.29
1	A	113	LYS	CB-CA-C	5.05	118.73	110.96
1	A	235	GLU	CB-CA-C	-5.05	102.93	110.90
1	B	285	PHE	CA-CB-CG	5.04	118.84	113.80
1	A	105	VAL	CB-CA-C	-5.04	103.02	111.29
1	B	113	LYS	CB-CA-C	5.04	118.72	110.96
1	C	105	VAL	CB-CA-C	-5.04	103.02	111.29
1	A	155	THR	CA-C-O	-5.04	115.37	120.71
1	A	285	PHE	CA-CB-CG	5.04	118.84	113.80
1	B	235	GLU	CB-CA-C	-5.04	102.94	110.90
1	D	105	VAL	CB-CA-C	-5.04	103.03	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	249	VAL	CA-CB-CG2	5.04	118.96	110.40
1	B	253	ILE	CA-C-N	-5.03	111.63	120.29
1	B	253	ILE	C-N-CA	-5.03	111.63	120.29
1	C	235	GLU	CB-CA-C	-5.03	102.95	110.90
1	C	249	VAL	CA-CB-CG2	5.03	118.95	110.40
1	A	376	MET	CA-C-O	5.03	125.78	120.10
1	C	383	ARG	CG-CD-NE	5.03	123.07	112.00
1	A	383	ARG	CG-CD-NE	5.03	123.06	112.00
1	C	253	ILE	CA-C-N	-5.03	111.65	120.29
1	C	253	ILE	C-N-CA	-5.03	111.65	120.29
1	D	383	ARG	CG-CD-NE	5.02	123.05	112.00
1	A	23	ARG	CA-C-N	5.02	131.29	122.95
1	A	23	ARG	C-N-CA	5.02	131.29	122.95
1	C	113	LYS	CB-CA-C	5.02	118.69	110.96
1	B	383	ARG	CG-CD-NE	5.02	123.05	112.00
1	C	76	GLU	CG-CD-OE1	-5.02	106.85	118.40
1	D	23	ARG	CA-C-N	5.02	131.28	122.95
1	D	23	ARG	C-N-CA	5.02	131.28	122.95
1	A	76	GLU	CG-CD-OE1	-5.02	106.86	118.40
1	B	376	MET	CA-C-O	5.02	125.77	120.10
1	D	76	GLU	CG-CD-OE1	-5.02	106.86	118.40
1	A	249	VAL	CA-CB-CG2	5.02	118.93	110.40
1	D	365	LYS	CA-C-N	-5.02	115.35	122.77
1	D	365	LYS	C-N-CA	-5.02	115.35	122.77
1	A	253	ILE	CA-C-N	-5.01	111.66	120.29
1	A	253	ILE	C-N-CA	-5.01	111.66	120.29
1	D	376	MET	CA-C-O	5.01	125.77	120.10
1	B	76	GLU	CG-CD-OE1	-5.01	106.87	118.40
1	C	155	THR	CA-C-O	-5.01	115.40	120.71
1	A	102	PHE	CA-C-N	-5.01	111.97	121.54
1	A	102	PHE	C-N-CA	-5.01	111.97	121.54
1	B	424	ALA	N-CA-CB	5.01	117.92	110.40
1	C	348	SER	N-CA-C	-5.01	101.53	109.59
1	D	249	VAL	CA-CB-CG2	5.01	118.91	110.40
1	B	23	ARG	CA-C-N	5.01	131.26	122.95
1	B	23	ARG	C-N-CA	5.01	131.26	122.95
1	C	23	ARG	CA-C-N	5.01	131.26	122.95
1	C	23	ARG	C-N-CA	5.01	131.26	122.95
1	D	130	LEU	CD1-CG-CD2	-5.01	99.79	110.80
1	B	212	ARG	NE-CZ-NH1	5.00	126.50	121.50
1	C	365	LYS	CA-C-N	-5.00	115.36	122.77
1	C	365	LYS	C-N-CA	-5.00	115.36	122.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	365	LYS	CA-C-N	-5.00	115.37	122.77
1	A	365	LYS	C-N-CA	-5.00	115.37	122.77
1	C	424	ALA	N-CA-CB	5.00	117.90	110.40

There are no chirality outliers.

All (64) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	110	PHE	Sidechain
1	A	127	TYR	Sidechain
1	A	129	TYR	Sidechain
1	A	132	HIS	Sidechain
1	A	146	PHE	Sidechain
1	A	175	TYR	Sidechain
1	A	19	TYR	Sidechain
1	A	207	TYR	Sidechain
1	A	210	ARG	Sidechain
1	A	216	GLU	Mainchain
1	A	248	TYR	Sidechain
1	A	263	TYR	Sidechain
1	A	285	PHE	Sidechain
1	A	332	PHE	Sidechain
1	A	363	PHE	Sidechain
1	A	73	PHE	Sidechain
1	B	110	PHE	Sidechain
1	B	127	TYR	Sidechain
1	B	129	TYR	Sidechain
1	B	132	HIS	Sidechain
1	B	146	PHE	Sidechain
1	B	175	TYR	Sidechain
1	B	19	TYR	Sidechain
1	B	207	TYR	Sidechain
1	B	210	ARG	Sidechain
1	B	216	GLU	Mainchain
1	B	248	TYR	Sidechain
1	B	263	TYR	Sidechain
1	B	285	PHE	Sidechain
1	B	332	PHE	Sidechain
1	B	363	PHE	Sidechain
1	B	73	PHE	Sidechain
1	C	110	PHE	Sidechain
1	C	127	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	C	129	TYR	Sidechain
1	C	132	HIS	Sidechain
1	C	146	PHE	Sidechain
1	C	175	TYR	Sidechain
1	C	19	TYR	Sidechain
1	C	207	TYR	Sidechain
1	C	210	ARG	Sidechain
1	C	216	GLU	Mainchain
1	C	248	TYR	Sidechain
1	C	263	TYR	Sidechain
1	C	285	PHE	Sidechain
1	C	332	PHE	Sidechain
1	C	363	PHE	Sidechain
1	C	73	PHE	Sidechain
1	D	110	PHE	Sidechain
1	D	127	TYR	Sidechain
1	D	129	TYR	Sidechain
1	D	132	HIS	Sidechain
1	D	146	PHE	Sidechain
1	D	175	TYR	Sidechain
1	D	19	TYR	Sidechain
1	D	207	TYR	Sidechain
1	D	210	ARG	Sidechain
1	D	216	GLU	Mainchain
1	D	248	TYR	Sidechain
1	D	263	TYR	Sidechain
1	D	285	PHE	Sidechain
1	D	332	PHE	Sidechain
1	D	363	PHE	Sidechain
1	D	73	PHE	Sidechain

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	3286	0	3271	612	7
1	B	3286	0	3271	677	11
1	C	3286	0	3269	696	4

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3286	0	3269	628	10
2	A	52	0	0	1	1
2	B	51	0	0	2	0
2	C	52	0	0	6	0
2	D	49	0	0	2	1
All	All	13348	0	13080	2528	19

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 96.

All (2528) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:LYS:CD	1:A:336:LYS:CE	1.74	1.65
1:C:160:LYS:CD	1:C:160:LYS:CE	1.75	1.63
1:A:56:THR:CA	1:A:56:THR:CB	1.75	1.63
1:C:56:THR:CA	1:C:56:THR:CB	1.75	1.63
1:D:419:VAL:CB	1:D:419:VAL:CG2	1.76	1.63
1:D:56:THR:CA	1:D:56:THR:CB	1.75	1.63
1:B:336:LYS:CD	1:B:336:LYS:CE	1.74	1.63
1:D:300:LYS:CD	1:D:300:LYS:CE	1.78	1.62
1:B:419:VAL:CB	1:B:419:VAL:CG2	1.76	1.61
1:C:419:VAL:CB	1:C:419:VAL:CG2	1.75	1.61
1:B:300:LYS:CD	1:B:300:LYS:CE	1.78	1.60
1:C:336:LYS:CE	1:C:336:LYS:CD	1.74	1.60
1:A:300:LYS:CD	1:A:300:LYS:CE	1.78	1.60
1:D:200:GLU:CG	1:D:200:GLU:CD	1.75	1.59
1:D:336:LYS:CD	1:D:336:LYS:CE	1.74	1.59
1:A:66:LYS:CE	1:A:66:LYS:CD	1.80	1.59
1:B:56:THR:CB	1:B:56:THR:CA	1.75	1.59
1:D:61:LEU:CD2	1:D:61:LEU:CG	1.77	1.59
1:B:66:LYS:CD	1:B:66:LYS:CE	1.80	1.59
1:D:160:LYS:CE	1:D:160:LYS:CD	1.75	1.59
1:B:160:LYS:CD	1:B:160:LYS:CE	1.75	1.58
1:C:172:GLU:CG	1:C:172:GLU:CD	1.75	1.58
1:B:151:ASP:CG	1:B:151:ASP:CB	1.76	1.58
1:C:300:LYS:CD	1:C:300:LYS:CE	1.78	1.58
1:D:66:LYS:CE	1:D:66:LYS:CD	1.80	1.57
1:A:419:VAL:CB	1:A:419:VAL:CG2	1.76	1.57
1:D:160:LYS:CE	1:D:160:LYS:NZ	1.68	1.57
1:C:200:GLU:CG	1:C:200:GLU:CD	1.75	1.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:GLU:C	1:B:216:GLU:CA	1.77	1.56
1:C:61:LEU:CD2	1:C:61:LEU:CG	1.77	1.56
1:C:216:GLU:CA	1:C:216:GLU:C	1.77	1.56
1:B:172:GLU:CD	1:B:172:GLU:CG	1.75	1.56
1:D:172:GLU:CG	1:D:172:GLU:CD	1.75	1.56
1:C:151:ASP:CB	1:C:151:ASP:CG	1.76	1.56
1:C:85:LYS:NZ	1:C:85:LYS:CE	1.69	1.55
1:D:66:LYS:CD	1:D:66:LYS:CG	1.82	1.55
1:C:66:LYS:CG	1:C:66:LYS:CD	1.82	1.55
1:D:151:ASP:CB	1:D:151:ASP:CG	1.76	1.55
1:A:61:LEU:CD2	1:A:61:LEU:CG	1.77	1.55
1:A:66:LYS:CD	1:A:66:LYS:CG	1.82	1.55
1:A:151:ASP:CB	1:A:151:ASP:CG	1.76	1.55
1:A:160:LYS:CE	1:A:160:LYS:CD	1.75	1.55
1:D:136:PRO:CG	1:D:136:PRO:CD	1.79	1.55
1:A:85:LYS:NZ	1:A:85:LYS:CE	1.69	1.55
1:B:61:LEU:CD2	1:B:61:LEU:CG	1.77	1.55
1:A:172:GLU:CG	1:A:172:GLU:CD	1.75	1.54
1:D:85:LYS:NZ	1:D:85:LYS:CE	1.69	1.54
1:C:57:THR:CA	1:C:57:THR:CB	1.85	1.54
1:B:160:LYS:CE	1:B:160:LYS:NZ	1.68	1.54
1:C:66:LYS:CD	1:C:66:LYS:CE	1.80	1.54
1:A:200:GLU:CD	1:A:200:GLU:CG	1.75	1.54
1:A:216:GLU:CA	1:A:216:GLU:C	1.77	1.54
1:B:66:LYS:CD	1:B:66:LYS:CG	1.82	1.54
1:C:160:LYS:CE	1:C:160:LYS:NZ	1.68	1.54
1:D:216:GLU:CA	1:D:216:GLU:C	1.77	1.54
1:A:160:LYS:CE	1:A:160:LYS:NZ	1.68	1.53
1:D:57:THR:CA	1:D:57:THR:CB	1.85	1.53
1:B:57:THR:CA	1:B:57:THR:CB	1.85	1.52
1:B:200:GLU:CG	1:B:200:GLU:CD	1.75	1.52
1:B:85:LYS:NZ	1:B:85:LYS:CE	1.68	1.51
1:B:141:GLN:CD	1:B:141:GLN:CG	1.82	1.51
1:D:27:ILE:CG1	1:D:27:ILE:CD1	1.86	1.50
1:B:27:ILE:CG1	1:B:27:ILE:CD1	1.86	1.50
1:A:141:GLN:CG	1:A:141:GLN:CD	1.82	1.50
1:A:57:THR:CA	1:A:57:THR:CB	1.85	1.49
1:A:27:ILE:CG1	1:A:27:ILE:CD1	1.86	1.49
1:C:141:GLN:CG	1:C:141:GLN:CD	1.82	1.49
1:D:141:GLN:CG	1:D:141:GLN:CD	1.82	1.48
1:C:27:ILE:CG1	1:C:27:ILE:CD1	1.86	1.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:356:MET:SD	1:D:356:MET:CE	2.03	1.47
1:C:136:PRO:CG	1:C:136:PRO:CD	1.79	1.46
1:D:240:MET:SD	1:D:240:MET:CG	2.03	1.46
1:A:240:MET:SD	1:A:240:MET:CG	2.03	1.46
1:C:240:MET:SD	1:C:240:MET:CG	2.03	1.46
1:C:356:MET:CE	1:C:356:MET:SD	2.03	1.46
1:A:356:MET:CE	1:A:356:MET:SD	2.03	1.46
1:B:240:MET:CG	1:B:240:MET:SD	2.03	1.45
1:A:136:PRO:CG	1:A:136:PRO:CD	1.79	1.44
1:B:356:MET:CE	1:B:356:MET:SD	2.03	1.43
1:C:250:MET:SD	1:C:250:MET:CE	2.07	1.43
1:D:250:MET:CE	1:D:250:MET:SD	2.07	1.43
1:A:147:MET:CE	1:A:147:MET:SD	2.07	1.43
1:B:136:PRO:CG	1:B:136:PRO:CD	1.78	1.43
1:A:186:LYS:NZ	1:A:186:LYS:CE	1.80	1.42
1:A:250:MET:CE	1:A:250:MET:SD	2.07	1.42
1:B:250:MET:CE	1:B:250:MET:SD	2.07	1.42
1:B:147:MET:SD	1:B:147:MET:CE	2.07	1.42
1:D:186:LYS:NZ	1:D:186:LYS:CE	1.80	1.42
1:D:147:MET:CE	1:D:147:MET:SD	2.07	1.41
1:C:186:LYS:NZ	1:C:186:LYS:CE	1.80	1.41
1:B:186:LYS:NZ	1:B:186:LYS:CE	1.80	1.41
1:C:147:MET:CE	1:C:147:MET:SD	2.07	1.40
1:A:216:GLU:CG	1:A:216:GLU:CD	1.97	1.38
1:C:216:GLU:CG	1:C:216:GLU:CD	1.97	1.38
1:B:216:GLU:CD	1:B:216:GLU:CG	1.97	1.37
1:B:304:MET:CE	1:B:304:MET:SD	2.13	1.37
1:D:304:MET:CE	1:D:304:MET:SD	2.13	1.36
1:C:304:MET:CE	1:C:304:MET:SD	2.13	1.36
1:A:304:MET:CE	1:A:304:MET:SD	2.13	1.36
1:D:216:GLU:CG	1:D:216:GLU:CD	1.97	1.36
1:A:147:MET:CE	1:A:147:MET:HB3	1.56	1.34
1:D:147:MET:CE	1:D:147:MET:HB3	1.56	1.33
1:B:147:MET:CE	1:B:147:MET:HB3	1.56	1.33
1:D:234:MET:CE	1:D:234:MET:SD	2.17	1.32
1:A:234:MET:CE	1:A:234:MET:SD	2.17	1.32
1:C:234:MET:CE	1:C:234:MET:SD	2.17	1.32
1:C:147:MET:CE	1:C:147:MET:HB3	1.56	1.31
1:B:234:MET:CE	1:B:234:MET:SD	2.17	1.30
1:D:69:MET:CE	1:D:69:MET:SD	2.21	1.29
1:B:69:MET:CE	1:B:69:MET:SD	2.21	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:MET:CE	1:C:69:MET:SD	2.21	1.29
1:A:69:MET:SD	1:A:69:MET:CE	2.21	1.28
1:C:417:ARG:HD2	2:C:481:HOH:O	1.07	1.21
1:C:128:GLU:HG3	1:D:128:GLU:CG	1.69	1.19
1:D:55:TRP:CD2	1:D:57:THR:HG23	1.78	1.18
1:D:378:HIS:CE1	1:D:380:ASP:HB2	1.78	1.18
1:C:378:HIS:CE1	1:C:380:ASP:HB2	1.78	1.18
1:A:378:HIS:CE1	1:A:380:ASP:HB2	1.78	1.18
1:A:55:TRP:CD2	1:A:57:THR:HG23	1.78	1.18
1:C:55:TRP:CD2	1:C:57:THR:HG23	1.78	1.17
1:B:55:TRP:CD2	1:B:57:THR:HG23	1.78	1.17
1:C:417:ARG:CD	2:C:481:HOH:O	1.65	1.17
1:C:128:GLU:CG	1:D:128:GLU:HG3	1.74	1.17
1:B:378:HIS:CE1	1:B:380:ASP:HB2	1.78	1.16
1:A:253:ILE:HD13	1:A:277:ALA:HB1	1.17	1.16
1:B:253:ILE:HD13	1:B:277:ALA:HB1	1.17	1.15
1:B:303:ARG:NH2	1:B:342:PRO:HA	1.63	1.14
1:C:303:ARG:NH2	1:C:342:PRO:HA	1.63	1.13
1:A:303:ARG:NH2	1:A:342:PRO:HA	1.63	1.12
1:C:253:ILE:HD13	1:C:277:ALA:HB1	1.17	1.12
1:C:95:GLU:OE2	1:D:131:ARG:NH1	1.81	1.12
1:D:253:ILE:HD13	1:D:277:ALA:HB1	1.17	1.11
1:D:303:ARG:NH2	1:D:342:PRO:HA	1.63	1.10
1:D:147:MET:HB3	1:D:147:MET:HE3	1.32	1.09
1:A:147:MET:HB3	1:A:147:MET:HE3	1.32	1.09
1:C:147:MET:HB3	1:C:147:MET:HE3	1.32	1.08
1:B:264:MET:O	1:B:268:THR:HG23	1.55	1.07
1:B:123:PHE:CZ	1:B:300:LYS:HG2	1.89	1.06
1:B:147:MET:HB3	1:B:147:MET:HE3	1.32	1.06
1:A:123:PHE:CZ	1:A:300:LYS:HG2	1.89	1.06
1:C:123:PHE:CZ	1:C:300:LYS:HG2	1.89	1.06
1:A:415:SER:O	1:A:419:VAL:HG23	1.56	1.05
1:A:303:ARG:HH21	1:A:342:PRO:CA	1.70	1.05
1:C:131:ARG:NH1	1:D:95:GLU:OE2	1.90	1.05
1:D:123:PHE:CZ	1:D:300:LYS:HG2	1.89	1.05
1:A:120:LEU:O	1:A:294:THR:HG23	1.56	1.05
1:C:264:MET:O	1:C:268:THR:HG23	1.55	1.04
1:C:415:SER:O	1:C:419:VAL:HG23	1.55	1.04
1:D:264:MET:O	1:D:268:THR:HG23	1.55	1.04
1:A:160:LYS:H	1:A:376:MET:HE2	1.19	1.04
1:B:120:LEU:O	1:B:294:THR:HG23	1.56	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:303:ARG:HH21	1:C:342:PRO:CA	1.70	1.04
1:D:303:ARG:HH21	1:D:342:PRO:CA	1.70	1.04
1:A:264:MET:O	1:A:268:THR:HG23	1.55	1.04
1:B:160:LYS:H	1:B:376:MET:HE2	1.19	1.04
1:B:303:ARG:HH21	1:B:342:PRO:CA	1.70	1.04
1:B:415:SER:O	1:B:419:VAL:HG23	1.56	1.04
1:D:415:SER:O	1:D:419:VAL:HG23	1.56	1.04
1:C:303:ARG:HH21	1:C:342:PRO:HA	0.88	1.03
1:C:128:GLU:CG	1:D:128:GLU:CG	2.33	1.03
1:D:120:LEU:O	1:D:294:THR:HG23	1.56	1.03
1:A:303:ARG:HH21	1:A:342:PRO:HA	0.88	1.02
1:C:120:LEU:O	1:C:294:THR:HG23	1.56	1.02
1:D:160:LYS:H	1:D:376:MET:HE2	1.19	1.02
1:D:303:ARG:HH21	1:D:342:PRO:HA	0.88	1.02
1:B:303:ARG:HH21	1:B:342:PRO:HA	0.88	1.02
1:C:160:LYS:H	1:C:376:MET:HE2	1.19	1.01
1:C:319:MET:CE	1:C:319:MET:SD	2.48	1.01
1:D:319:MET:CE	1:D:319:MET:SD	2.48	1.01
1:A:319:MET:CE	1:A:319:MET:SD	2.48	1.01
1:A:365:LYS:HD3	1:A:365:LYS:H	1.26	1.01
1:B:110:PHE:O	1:C:283:ALA:HB1	1.61	1.01
1:A:113:LYS:H	1:A:113:LYS:HD2	1.26	1.01
1:B:319:MET:CE	1:B:319:MET:SD	2.48	1.01
1:B:283:ALA:HB1	1:C:110:PHE:O	1.61	1.00
1:C:213:VAL:O	1:C:217:THR:HG23	1.61	1.00
1:B:147:MET:CE	1:B:147:MET:CB	2.40	1.00
1:D:384:ALA:HB1	1:D:411:GLU:HG2	1.44	1.00
1:B:231:VAL:HG21	1:C:231:VAL:HG21	1.42	1.00
1:B:365:LYS:HD3	1:B:365:LYS:H	1.26	0.99
1:A:384:ALA:HB1	1:A:411:GLU:HG2	1.44	0.99
1:D:213:VAL:O	1:D:217:THR:HG23	1.61	0.99
1:A:147:MET:CE	1:A:147:MET:CB	2.40	0.99
1:A:117:ASN:ND2	1:A:290:ARG:HB2	1.78	0.98
1:D:147:MET:CE	1:D:147:MET:CB	2.40	0.98
1:A:213:VAL:O	1:A:217:THR:HG23	1.61	0.98
1:C:365:LYS:H	1:C:365:LYS:HD3	1.26	0.98
1:D:117:ASN:ND2	1:D:290:ARG:HB2	1.78	0.98
1:C:117:ASN:ND2	1:C:290:ARG:HB2	1.78	0.98
1:C:147:MET:CE	1:C:147:MET:CB	2.40	0.98
1:D:167:VAL:HG22	1:D:197:ASN:HA	1.46	0.98
1:A:167:VAL:HG22	1:A:197:ASN:HA	1.46	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:VAL:O	1:B:217:THR:HG23	1.61	0.97
1:C:253:ILE:CD1	1:C:277:ALA:HB1	1.94	0.97
1:B:117:ASN:ND2	1:B:290:ARG:HB2	1.78	0.97
1:C:167:VAL:HG22	1:C:197:ASN:HA	1.46	0.97
1:D:113:LYS:H	1:D:113:LYS:HD2	1.26	0.97
1:C:113:LYS:H	1:C:113:LYS:HD2	1.26	0.97
1:D:253:ILE:CD1	1:D:277:ALA:HB1	1.94	0.97
1:C:126:PRO:O	1:C:127:TYR:C	2.07	0.97
1:D:137:GLN:HB2	1:D:265:ARG:NH2	1.80	0.97
1:C:137:GLN:HB2	1:C:265:ARG:NH2	1.80	0.97
1:A:137:GLN:HB2	1:A:265:ARG:NH2	1.80	0.96
1:B:384:ALA:HB1	1:B:411:GLU:HG2	1.44	0.96
1:C:384:ALA:HB1	1:C:411:GLU:HG2	1.44	0.96
1:B:167:VAL:HG22	1:B:197:ASN:HA	1.46	0.96
1:B:378:HIS:HE1	1:B:380:ASP:HB2	1.29	0.96
1:D:55:TRP:CE2	1:D:57:THR:HG23	2.00	0.96
1:D:365:LYS:HD3	1:D:365:LYS:H	1.26	0.96
1:A:253:ILE:CD1	1:A:277:ALA:HB1	1.94	0.96
1:B:113:LYS:H	1:B:113:LYS:HD2	1.26	0.96
1:B:253:ILE:CD1	1:B:277:ALA:HB1	1.94	0.96
1:C:55:TRP:CE2	1:C:57:THR:HG23	2.00	0.96
1:C:55:TRP:HH2	1:C:58:LEU:HB2	1.31	0.96
1:A:28:VAL:HG21	1:A:88:TYR:CE2	2.02	0.95
1:B:137:GLN:HB2	1:B:265:ARG:NH2	1.80	0.95
1:A:55:TRP:HH2	1:A:58:LEU:HB2	1.31	0.95
1:D:28:VAL:HG21	1:D:88:TYR:CE2	2.02	0.95
1:B:55:TRP:CE2	1:B:57:THR:HG23	2.01	0.95
1:D:126:PRO:O	1:D:127:TYR:C	2.07	0.95
1:B:55:TRP:HH2	1:B:58:LEU:HB2	1.31	0.95
1:C:28:VAL:HG21	1:C:88:TYR:CE2	2.01	0.95
1:B:123:PHE:O	1:B:300:LYS:HE3	1.67	0.94
1:D:15:VAL:HG13	1:D:72:VAL:CG2	1.97	0.94
1:A:55:TRP:CE2	1:A:57:THR:HG23	2.00	0.94
1:A:15:VAL:HG13	1:A:72:VAL:CG2	1.97	0.94
1:B:28:VAL:HG21	1:B:88:TYR:CE2	2.02	0.94
1:D:55:TRP:HH2	1:D:58:LEU:HB2	1.31	0.94
1:A:123:PHE:O	1:A:300:LYS:HE3	1.67	0.94
1:A:378:HIS:HE1	1:A:380:ASP:HB2	1.29	0.94
1:C:123:PHE:O	1:C:300:LYS:HE3	1.67	0.94
1:B:352:HIS:HB2	1:B:353:PRO:HD2	1.50	0.94
1:B:15:VAL:HG13	1:B:72:VAL:CG2	1.97	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:352:HIS:HB2	1:C:353:PRO:HD2	1.50	0.94
1:B:401:ASP:HB3	1:B:404:GLU:HG2	1.50	0.93
1:B:117:ASN:HD22	1:B:290:ARG:HB2	1.33	0.93
1:A:352:HIS:HB2	1:A:353:PRO:HD2	1.50	0.93
1:B:260:ALA:HB2	1:C:260:ALA:HB2	1.50	0.93
1:D:156:ALA:HB2	1:D:184:LEU:HB2	1.49	0.93
1:C:15:VAL:HG13	1:C:72:VAL:CG2	1.97	0.93
1:C:378:HIS:HE1	1:C:380:ASP:HB2	1.29	0.93
1:A:117:ASN:HD22	1:A:290:ARG:HB2	1.33	0.93
1:B:126:PRO:O	1:B:127:TYR:C	2.07	0.92
1:A:105:VAL:HG23	1:A:105:VAL:O	1.69	0.92
1:A:156:ALA:HB2	1:A:184:LEU:HB2	1.49	0.92
1:D:123:PHE:O	1:D:300:LYS:HE3	1.67	0.92
1:B:112:MET:HE3	1:B:115:LEU:HD11	1.51	0.91
1:C:76:GLU:HG2	1:C:77:LYS:N	1.86	0.91
1:C:156:ALA:HB2	1:C:184:LEU:HB2	1.49	0.91
1:B:156:ALA:HB2	1:B:184:LEU:HB2	1.49	0.91
1:D:401:ASP:HB3	1:D:404:GLU:HG2	1.51	0.91
1:A:401:ASP:HB3	1:A:404:GLU:HG2	1.50	0.91
1:C:323:TYR:CD1	1:C:323:TYR:O	2.24	0.91
1:A:323:TYR:O	1:A:323:TYR:CD1	2.24	0.91
1:C:401:ASP:HB3	1:C:404:GLU:HG2	1.50	0.91
1:B:323:TYR:O	1:B:323:TYR:CD1	2.24	0.91
1:D:112:MET:HE3	1:D:115:LEU:HD11	1.51	0.91
1:D:353:PRO:HG3	1:D:415:SER:OG	1.71	0.90
1:A:353:PRO:HG3	1:A:415:SER:OG	1.71	0.90
1:D:352:HIS:HB2	1:D:353:PRO:HD2	1.50	0.90
1:A:112:MET:HE3	1:A:115:LEU:HD11	1.51	0.90
1:B:76:GLU:HG2	1:B:77:LYS:N	1.86	0.90
1:B:28:VAL:CG2	1:B:88:TYR:HE2	1.85	0.90
1:D:28:VAL:CG2	1:D:88:TYR:HE2	1.85	0.90
1:D:323:TYR:O	1:D:323:TYR:CD1	2.24	0.90
1:D:105:VAL:HG23	1:D:105:VAL:O	1.69	0.90
1:D:378:HIS:HE1	1:D:380:ASP:HB2	1.29	0.90
1:B:105:VAL:HG23	1:B:105:VAL:O	1.69	0.89
1:C:353:PRO:HG3	1:C:415:SER:OG	1.71	0.89
1:A:76:GLU:HG2	1:A:77:LYS:N	1.86	0.89
1:C:105:VAL:HG23	1:C:105:VAL:O	1.69	0.89
1:D:76:GLU:HG2	1:D:77:LYS:N	1.86	0.89
1:D:199:PHE:CZ	1:D:225:ILE:HD11	2.08	0.89
1:A:199:PHE:CZ	1:A:225:ILE:HD11	2.08	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:MET:HE3	1:C:115:LEU:HD11	1.51	0.89
1:C:137:GLN:HB2	1:C:265:ARG:HH22	1.36	0.89
1:D:137:GLN:HB2	1:D:265:ARG:HH22	1.36	0.89
1:B:39:PRO:O	1:B:75:LEU:HD21	1.73	0.89
1:D:253:ILE:HD13	1:D:277:ALA:CB	2.03	0.89
1:B:137:GLN:HB2	1:B:265:ARG:HH22	1.36	0.89
1:B:23:ARG:HE	1:B:23:ARG:H	1.21	0.89
1:B:199:PHE:CZ	1:B:225:ILE:HD11	2.08	0.89
1:A:39:PRO:O	1:A:75:LEU:HD21	1.73	0.89
1:C:28:VAL:CG2	1:C:88:TYR:HE2	1.85	0.89
1:A:28:VAL:CG2	1:A:88:TYR:HE2	1.85	0.89
1:D:113:LYS:H	1:D:113:LYS:CD	1.85	0.89
1:A:346:VAL:HG22	1:A:368:VAL:CG2	2.03	0.89
1:C:199:PHE:CZ	1:C:225:ILE:HD11	2.08	0.89
1:D:23:ARG:HE	1:D:23:ARG:H	1.21	0.89
1:D:147:MET:HB3	1:D:147:MET:HE2	1.55	0.89
1:B:323:TYR:CE2	1:B:362:LEU:HD22	2.08	0.88
1:A:126:PRO:O	1:A:127:TYR:C	2.07	0.88
1:C:323:TYR:CE2	1:C:362:LEU:HD22	2.08	0.88
1:A:253:ILE:HD13	1:A:277:ALA:CB	2.03	0.88
1:D:39:PRO:O	1:D:75:LEU:HD21	1.73	0.88
1:B:353:PRO:HG3	1:B:415:SER:OG	1.71	0.88
1:C:39:PRO:O	1:C:75:LEU:HD21	1.73	0.88
1:C:311:HIS:HD2	1:C:346:VAL:CG1	1.87	0.88
1:C:147:MET:HB3	1:C:147:MET:HE2	1.55	0.88
1:C:55:TRP:CH2	1:C:58:LEU:HB2	2.08	0.88
1:D:311:HIS:HD2	1:D:346:VAL:CG1	1.87	0.88
1:B:147:MET:HB3	1:B:147:MET:HE2	1.55	0.88
1:C:117:ASN:HD22	1:C:290:ARG:HB2	1.33	0.88
1:D:55:TRP:CH2	1:D:58:LEU:HB2	2.08	0.88
1:C:10:TRP:HB3	1:C:13:ASP:OD1	1.74	0.88
1:C:10:TRP:O	1:C:12:LEU:N	2.07	0.88
1:C:128:GLU:HG3	1:D:128:GLU:HG3	0.89	0.88
1:A:10:TRP:O	1:A:12:LEU:N	2.07	0.87
1:C:113:LYS:H	1:C:113:LYS:CD	1.85	0.87
1:D:10:TRP:O	1:D:12:LEU:N	2.08	0.87
1:D:346:VAL:HG22	1:D:368:VAL:CG2	2.03	0.87
1:B:10:TRP:HB3	1:B:13:ASP:OD1	1.74	0.87
1:B:311:HIS:HD2	1:B:346:VAL:CG1	1.87	0.87
1:C:11:TYR:CD2	1:C:45:ARG:HG2	2.09	0.87
1:D:323:TYR:CE2	1:D:362:LEU:HD22	2.08	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:TYR:CE2	1:A:362:LEU:HD22	2.08	0.87
1:C:346:VAL:HG22	1:C:368:VAL:CG2	2.03	0.87
1:A:10:TRP:HB3	1:A:13:ASP:OD1	1.74	0.87
1:A:311:HIS:HD2	1:A:346:VAL:CG1	1.87	0.87
1:B:55:TRP:CH2	1:B:58:LEU:HB2	2.08	0.87
1:D:10:TRP:HB3	1:D:13:ASP:OD1	1.74	0.87
1:C:61:LEU:CD2	1:C:61:LEU:HG	2.04	0.87
1:A:11:TYR:CD2	1:A:45:ARG:HG2	2.09	0.87
1:A:137:GLN:HB2	1:A:265:ARG:HH22	1.36	0.87
1:A:10:TRP:HA	1:A:10:TRP:CE3	2.10	0.87
1:C:28:VAL:HG21	1:C:88:TYR:HE2	1.38	0.87
1:A:55:TRP:CH2	1:A:58:LEU:HB2	2.08	0.86
1:D:204:ARG:O	1:D:208:ARG:HD3	1.75	0.86
1:D:351:LEU:HD23	1:D:359:LEU:CD2	2.05	0.86
1:D:117:ASN:HD22	1:D:290:ARG:HB2	1.33	0.86
1:C:204:ARG:O	1:C:208:ARG:HD3	1.76	0.86
1:D:11:TYR:CD2	1:D:45:ARG:HG2	2.09	0.86
1:B:10:TRP:O	1:B:12:LEU:N	2.07	0.86
1:B:11:TYR:CD2	1:B:45:ARG:HG2	2.09	0.86
1:B:204:ARG:O	1:B:208:ARG:HD3	1.75	0.86
1:B:346:VAL:HG22	1:B:368:VAL:CG2	2.03	0.86
1:A:204:ARG:O	1:A:208:ARG:HD3	1.75	0.86
1:B:46:ILE:HG12	1:B:112:MET:HE1	1.58	0.86
1:A:351:LEU:HD23	1:A:359:LEU:CD2	2.05	0.86
1:A:28:VAL:HG21	1:A:88:TYR:HE2	1.38	0.86
1:C:23:ARG:H	1:C:23:ARG:HE	1.21	0.86
1:A:46:ILE:HG12	1:A:112:MET:HE1	1.58	0.86
1:B:10:TRP:HA	1:B:10:TRP:CE3	2.10	0.86
1:B:113:LYS:H	1:B:113:LYS:CD	1.85	0.85
1:B:351:LEU:HD23	1:B:359:LEU:CD2	2.05	0.85
1:C:10:TRP:HA	1:C:10:TRP:CE3	2.10	0.85
1:A:233:ILE:O	1:A:237:ARG:HG3	1.77	0.85
1:B:233:ILE:O	1:B:237:ARG:HG3	1.77	0.85
1:B:61:LEU:CD2	1:B:61:LEU:HG	2.04	0.85
1:A:23:ARG:HE	1:A:23:ARG:H	1.21	0.85
1:A:61:LEU:CD2	1:A:61:LEU:HG	2.04	0.85
1:A:147:MET:HB3	1:A:147:MET:HE2	1.55	0.85
1:D:46:ILE:HG12	1:D:112:MET:HE1	1.58	0.84
1:C:351:LEU:HD23	1:C:359:LEU:CD2	2.05	0.84
1:A:113:LYS:H	1:A:113:LYS:CD	1.85	0.84
1:B:253:ILE:HD13	1:B:277:ALA:CB	2.03	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:160:LYS:HZ1	1:D:373:GLY:H	1.25	0.84
1:D:233:ILE:O	1:D:237:ARG:HG3	1.77	0.84
1:D:28:VAL:CG2	1:D:88:TYR:CE2	2.60	0.84
1:D:123:PHE:CE1	1:D:300:LYS:HG2	2.13	0.84
1:D:160:LYS:N	1:D:376:MET:HE2	1.93	0.84
1:C:46:ILE:HG12	1:C:112:MET:HE1	1.58	0.83
1:C:233:ILE:O	1:C:237:ARG:HG3	1.77	0.83
1:C:253:ILE:HD13	1:C:277:ALA:CB	2.03	0.83
1:C:252:ASP:HB3	1:C:255:VAL:CG2	2.08	0.83
1:C:311:HIS:HD2	1:C:346:VAL:HG11	1.43	0.83
1:C:123:PHE:CE1	1:C:300:LYS:HG2	2.13	0.83
1:D:252:ASP:HB3	1:D:255:VAL:CG2	2.08	0.83
1:B:98:LEU:HD11	1:B:301:ALA:HB1	1.60	0.83
1:B:160:LYS:HZ1	1:B:373:GLY:H	1.22	0.83
1:C:160:LYS:N	1:C:376:MET:HE2	1.93	0.83
1:D:10:TRP:HA	1:D:10:TRP:CE3	2.10	0.83
1:D:28:VAL:HG21	1:D:88:TYR:HE2	1.38	0.83
1:B:311:HIS:HD2	1:B:346:VAL:HG11	1.43	0.83
1:A:123:PHE:CE1	1:A:300:LYS:HG2	2.13	0.83
1:A:252:ASP:HB3	1:A:255:VAL:CG2	2.08	0.83
1:C:160:LYS:HZ1	1:C:373:GLY:H	1.27	0.83
1:A:160:LYS:N	1:A:376:MET:HE2	1.93	0.83
1:B:252:ASP:HB3	1:B:255:VAL:CG2	2.08	0.83
1:B:123:PHE:CE1	1:B:300:LYS:HG2	2.13	0.83
1:D:311:HIS:HD2	1:D:346:VAL:HG11	1.43	0.83
1:A:311:HIS:HD2	1:A:346:VAL:HG11	1.43	0.83
1:C:276:HIS:HD2	1:C:309:GLN:HE21	1.27	0.83
1:A:10:TRP:HA	1:A:10:TRP:HE3	1.44	0.82
1:B:10:TRP:HA	1:B:10:TRP:HE3	1.44	0.82
1:B:28:VAL:HG21	1:B:88:TYR:HE2	1.38	0.82
1:C:28:VAL:CG2	1:C:88:TYR:CE2	2.60	0.82
1:D:61:LEU:CD2	1:D:61:LEU:HG	2.04	0.82
1:D:281:MET:HG2	1:D:281:MET:O	1.79	0.82
1:D:10:TRP:HA	1:D:10:TRP:HE3	1.44	0.82
1:A:28:VAL:CG2	1:A:88:TYR:CE2	2.60	0.82
1:B:375:VAL:HG13	1:B:385:GLY:C	2.05	0.82
1:C:10:TRP:HA	1:C:10:TRP:HE3	1.44	0.82
1:C:375:VAL:HG13	1:C:385:GLY:C	2.05	0.82
1:A:160:LYS:HZ1	1:A:373:GLY:H	1.22	0.82
1:A:231:VAL:CG1	1:A:234:MET:HE3	2.10	0.82
1:B:160:LYS:N	1:B:376:MET:HE2	1.93	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:375:VAL:HG13	1:D:385:GLY:C	2.05	0.82
1:A:375:VAL:HG13	1:A:385:GLY:C	2.05	0.82
1:B:281:MET:CE	1:B:281:MET:SD	2.68	0.82
1:D:281:MET:CE	1:D:281:MET:SD	2.68	0.82
1:B:281:MET:O	1:B:281:MET:HG2	1.79	0.82
1:D:27:ILE:HG23	1:D:86:ILE:O	1.80	0.82
1:D:298:LEU:HD23	1:D:298:LEU:C	2.05	0.81
1:A:281:MET:CE	1:A:281:MET:SD	2.68	0.81
1:A:298:LEU:HD23	1:A:298:LEU:C	2.05	0.81
1:A:98:LEU:HD11	1:A:301:ALA:HB1	1.60	0.81
1:B:169:GLU:HG2	1:C:60:LYS:NZ	1.95	0.81
1:B:231:VAL:CG1	1:B:234:MET:HE3	2.10	0.81
1:C:281:MET:CE	1:C:281:MET:SD	2.68	0.81
1:D:231:VAL:CG1	1:D:234:MET:HE3	2.09	0.81
1:A:27:ILE:HG23	1:A:86:ILE:O	1.80	0.81
1:B:28:VAL:CG2	1:B:88:TYR:CE2	2.60	0.81
1:A:281:MET:HG2	1:A:281:MET:O	1.79	0.81
1:D:98:LEU:HD11	1:D:301:ALA:HB1	1.60	0.81
1:C:231:VAL:CG1	1:C:234:MET:HE3	2.10	0.81
1:D:276:HIS:HD2	1:D:309:GLN:HE21	1.27	0.81
1:C:98:LEU:HD11	1:C:301:ALA:HB1	1.60	0.81
1:C:281:MET:O	1:C:281:MET:HG2	1.79	0.81
1:B:27:ILE:HG23	1:B:86:ILE:O	1.80	0.81
1:B:169:GLU:OE2	1:C:60:LYS:HE2	1.81	0.81
1:D:188:ASP:O	1:D:190:ASN:N	2.14	0.81
1:C:188:ASP:O	1:C:190:ASN:N	2.14	0.80
1:C:94:GLU:HG2	1:C:97:SER:HB3	1.63	0.80
1:C:298:LEU:HD23	1:C:298:LEU:C	2.05	0.80
1:B:276:HIS:HD2	1:B:309:GLN:HE21	1.27	0.80
1:C:27:ILE:HG23	1:C:86:ILE:O	1.80	0.80
1:C:55:TRP:CE2	1:C:57:THR:CG2	2.65	0.80
1:A:188:ASP:O	1:A:190:ASN:N	2.14	0.80
1:B:55:TRP:HH2	1:B:58:LEU:CB	1.94	0.80
1:D:94:GLU:HG2	1:D:97:SER:HB3	1.63	0.80
1:B:188:ASP:O	1:B:190:ASN:N	2.14	0.80
1:C:55:TRP:HH2	1:C:58:LEU:CB	1.94	0.80
1:A:94:GLU:HG2	1:A:97:SER:HB3	1.63	0.80
1:D:55:TRP:HH2	1:D:58:LEU:CB	1.94	0.80
1:B:94:GLU:HG2	1:B:97:SER:HB3	1.63	0.80
1:C:140:VAL:O	1:C:144:ARG:HB2	1.83	0.79
1:A:55:TRP:HH2	1:A:58:LEU:CB	1.94	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:LEU:HA	1:A:294:THR:HG21	1.65	0.79
1:A:140:VAL:O	1:A:144:ARG:HB2	1.83	0.79
1:A:276:HIS:HD2	1:A:309:GLN:HE21	1.27	0.79
1:A:278:HIS:HD2	1:A:280:ALA:H	1.30	0.79
1:B:140:VAL:O	1:B:144:ARG:HB2	1.83	0.79
1:A:55:TRP:CE2	1:A:57:THR:CG2	2.65	0.79
1:C:147:MET:HA	1:C:220:THR:HG21	1.65	0.79
1:B:121:LEU:HA	1:B:294:THR:HG21	1.65	0.79
1:B:55:TRP:CE2	1:B:57:THR:CG2	2.65	0.79
1:B:298:LEU:C	1:B:298:LEU:HD23	2.05	0.79
1:C:346:VAL:HG22	1:C:368:VAL:HG23	1.65	0.79
1:D:140:VAL:O	1:D:144:ARG:HB2	1.83	0.79
1:A:131:ARG:HA	1:A:339:HIS:CE1	2.18	0.79
1:D:55:TRP:CE2	1:D:57:THR:CG2	2.65	0.79
1:A:346:VAL:HG22	1:A:368:VAL:HG23	1.65	0.78
1:B:15:VAL:HG13	1:B:72:VAL:HG21	1.65	0.78
1:C:31:TYR:HD1	1:C:31:TYR:C	1.91	0.78
1:C:121:LEU:HA	1:C:294:THR:HG21	1.65	0.78
1:B:31:TYR:C	1:B:31:TYR:HD1	1.91	0.78
1:B:131:ARG:HA	1:B:339:HIS:CE1	2.18	0.78
1:B:279:ARG:HD3	1:B:295:MET:HE2	1.66	0.78
1:C:131:ARG:HA	1:C:339:HIS:CE1	2.18	0.78
1:B:31:TYR:C	1:B:31:TYR:CD1	2.61	0.78
1:C:156:ALA:O	1:C:370:GLN:HG2	1.84	0.78
1:D:279:ARG:HD3	1:D:295:MET:HE2	1.66	0.78
1:A:127:TYR:O	1:A:129:TYR:N	2.17	0.77
1:A:384:ALA:HB1	1:A:411:GLU:CG	2.15	0.77
1:C:31:TYR:C	1:C:31:TYR:CD1	2.61	0.77
1:C:128:GLU:CG	1:D:128:GLU:HG2	2.12	0.77
1:D:121:LEU:HA	1:D:294:THR:HG21	1.65	0.77
1:A:31:TYR:HD1	1:A:31:TYR:C	1.91	0.77
1:A:156:ALA:O	1:A:370:GLN:HG2	1.84	0.77
1:C:127:TYR:O	1:C:129:TYR:N	2.17	0.77
1:C:263:TYR:C	1:C:263:TYR:CD2	2.63	0.77
1:B:147:MET:HA	1:B:220:THR:HG21	1.65	0.77
1:C:74:TYR:CD2	1:C:75:LEU:N	2.53	0.77
1:D:131:ARG:HA	1:D:339:HIS:CE1	2.18	0.77
1:D:384:ALA:HB1	1:D:411:GLU:CG	2.15	0.77
1:A:156:ALA:CB	1:A:184:LEU:HB2	2.15	0.77
1:C:121:LEU:HA	1:C:294:THR:CG2	2.15	0.77
1:C:147:MET:HE3	1:C:220:THR:HG22	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:31:TYR:CD1	1:D:31:TYR:C	2.61	0.77
1:D:147:MET:HE3	1:D:220:THR:HG22	1.67	0.77
1:B:127:TYR:O	1:B:129:TYR:N	2.18	0.77
1:B:169:GLU:OE2	1:C:60:LYS:CE	2.33	0.77
1:C:35:ASN:O	1:C:35:ASN:OD1	2.03	0.77
1:D:121:LEU:HA	1:D:294:THR:CG2	2.15	0.77
1:A:35:ASN:OD1	1:A:35:ASN:O	2.03	0.77
1:A:121:LEU:HA	1:A:294:THR:CG2	2.15	0.77
1:B:74:TYR:CD2	1:B:75:LEU:N	2.53	0.77
1:D:31:TYR:C	1:D:31:TYR:HD1	1.91	0.77
1:D:346:VAL:HG22	1:D:368:VAL:HG23	1.65	0.77
1:B:121:LEU:HA	1:B:294:THR:CG2	2.15	0.77
1:B:156:ALA:O	1:B:370:GLN:HG2	1.84	0.77
1:C:15:VAL:HG13	1:C:72:VAL:HG21	1.65	0.77
1:B:318:LYS:CE	1:C:113:LYS:HZ2	1.98	0.77
1:D:127:TYR:O	1:D:129:TYR:N	2.17	0.77
1:D:147:MET:HA	1:D:220:THR:HG21	1.65	0.77
1:D:156:ALA:O	1:D:370:GLN:HG2	1.84	0.77
1:A:74:TYR:CD2	1:A:75:LEU:N	2.53	0.76
1:D:74:TYR:CD2	1:D:75:LEU:N	2.53	0.76
1:A:147:MET:HA	1:A:220:THR:HG21	1.65	0.76
1:D:12:LEU:O	1:D:15:VAL:HG23	1.85	0.76
1:A:31:TYR:C	1:A:31:TYR:CD1	2.61	0.76
1:C:351:LEU:HD23	1:C:359:LEU:HD21	1.68	0.76
1:C:384:ALA:HB1	1:C:411:GLU:CG	2.15	0.76
1:D:15:VAL:HG13	1:D:72:VAL:HG21	1.65	0.76
1:A:231:VAL:HG13	1:A:234:MET:HE3	1.68	0.76
1:C:278:HIS:HD2	1:C:280:ALA:H	1.30	0.76
1:D:131:ARG:HA	1:D:339:HIS:HE1	1.49	0.76
1:D:263:TYR:CD2	1:D:263:TYR:C	2.62	0.76
1:A:131:ARG:HA	1:A:339:HIS:HE1	1.49	0.76
1:A:225:ILE:HG13	1:A:226:ASN:N	2.01	0.76
1:A:263:TYR:C	1:A:263:TYR:CD2	2.63	0.76
1:B:35:ASN:OD1	1:B:35:ASN:O	2.03	0.76
1:C:231:VAL:HG13	1:C:234:MET:HE3	1.68	0.76
1:B:147:MET:HE3	1:B:220:THR:HG22	1.67	0.76
1:B:263:TYR:C	1:B:263:TYR:CD2	2.63	0.76
1:B:278:HIS:HD2	1:B:280:ALA:H	1.30	0.76
1:B:351:LEU:HD23	1:B:359:LEU:HD21	1.68	0.76
1:B:384:ALA:HB1	1:B:411:GLU:CG	2.15	0.76
1:C:225:ILE:HG13	1:C:226:ASN:N	2.01	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:TYR:HD2	1:A:75:LEU:N	1.84	0.76
1:B:12:LEU:O	1:B:15:VAL:HG23	1.85	0.76
1:B:346:VAL:HG22	1:B:368:VAL:HG23	1.65	0.76
1:D:35:ASN:OD1	1:D:35:ASN:O	2.03	0.76
1:A:351:LEU:HD23	1:A:359:LEU:HD21	1.68	0.76
1:A:12:LEU:O	1:A:15:VAL:HG23	1.85	0.76
1:D:351:LEU:HD23	1:D:359:LEU:HD21	1.68	0.76
1:A:26:LEU:HB3	1:A:88:TYR:HB2	1.67	0.76
1:C:74:TYR:HD2	1:C:75:LEU:N	1.84	0.76
1:D:225:ILE:HG13	1:D:226:ASN:N	2.01	0.76
1:A:15:VAL:HG13	1:A:72:VAL:HG21	1.65	0.75
1:A:279:ARG:HD3	1:A:295:MET:HE2	1.66	0.75
1:B:26:LEU:HB3	1:B:88:TYR:HB2	1.67	0.75
1:A:74:TYR:CD2	1:A:74:TYR:C	2.64	0.75
1:C:76:GLU:CG	1:C:77:LYS:N	2.49	0.75
1:D:74:TYR:CD2	1:D:74:TYR:C	2.64	0.75
1:D:156:ALA:CB	1:D:184:LEU:HB2	2.15	0.75
1:D:278:HIS:HD2	1:D:280:ALA:H	1.30	0.75
1:C:156:ALA:CB	1:C:184:LEU:HB2	2.15	0.75
1:D:26:LEU:HB3	1:D:88:TYR:HB2	1.67	0.75
1:C:74:TYR:CD2	1:C:74:TYR:C	2.64	0.75
1:C:131:ARG:HA	1:C:339:HIS:HE1	1.49	0.75
1:C:279:ARG:HD3	1:C:295:MET:HE2	1.66	0.75
1:A:31:TYR:CD1	1:A:32:PHE:N	2.55	0.75
1:A:194:PHE:O	1:A:195:PRO:C	2.28	0.75
1:B:60:LYS:NZ	1:C:169:GLU:HG2	2.01	0.75
1:C:12:LEU:O	1:C:15:VAL:HG23	1.85	0.75
1:B:76:GLU:CG	1:B:77:LYS:N	2.49	0.75
1:A:147:MET:HE3	1:A:220:THR:HG22	1.67	0.75
1:B:31:TYR:CD1	1:B:32:PHE:N	2.55	0.75
1:B:74:TYR:HD2	1:B:75:LEU:N	1.84	0.75
1:B:231:VAL:HG13	1:B:234:MET:HE3	1.68	0.75
1:D:14:PHE:CE2	1:D:48:SER:HA	2.21	0.74
1:D:231:VAL:HG13	1:D:234:MET:HE3	1.68	0.74
1:B:156:ALA:CB	1:B:184:LEU:HB2	2.15	0.74
1:C:14:PHE:CE2	1:C:48:SER:HA	2.22	0.74
1:D:76:GLU:CG	1:D:77:LYS:N	2.49	0.74
1:B:74:TYR:CD2	1:B:74:TYR:C	2.64	0.74
1:C:26:LEU:HB3	1:C:88:TYR:HB2	1.67	0.74
1:C:31:TYR:CD1	1:C:32:PHE:N	2.55	0.74
1:A:76:GLU:CG	1:A:77:LYS:N	2.49	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:GLU:CD	1:C:216:GLU:HA	2.13	0.74
1:B:225:ILE:HG13	1:B:226:ASN:N	2.01	0.74
1:D:31:TYR:CD1	1:D:32:PHE:N	2.55	0.74
1:D:216:GLU:C	1:D:216:GLU:N	2.45	0.74
1:A:216:GLU:CD	1:A:216:GLU:HA	2.13	0.74
1:D:279:ARG:O	1:D:280:ALA:C	2.30	0.74
1:C:31:TYR:HB2	1:C:121:LEU:HD21	1.70	0.74
1:D:74:TYR:HD2	1:D:75:LEU:N	1.84	0.74
1:B:14:PHE:CE2	1:B:48:SER:HA	2.22	0.74
1:B:31:TYR:HB2	1:B:121:LEU:HD21	1.70	0.74
1:B:131:ARG:HA	1:B:339:HIS:HE1	1.49	0.74
1:B:216:GLU:C	1:B:216:GLU:N	2.45	0.74
1:A:216:GLU:C	1:A:216:GLU:N	2.45	0.73
1:B:216:GLU:CD	1:B:216:GLU:HA	2.13	0.73
1:C:279:ARG:O	1:C:280:ALA:C	2.31	0.73
1:B:279:ARG:HD3	1:B:295:MET:CE	2.18	0.73
1:B:279:ARG:O	1:B:280:ALA:C	2.31	0.73
1:A:14:PHE:CE2	1:A:48:SER:HA	2.22	0.73
1:A:31:TYR:HB2	1:A:121:LEU:HD21	1.70	0.73
1:A:178:TRP:HB3	1:A:213:VAL:HG11	1.70	0.73
1:A:231:VAL:HG13	1:A:234:MET:CE	2.19	0.73
1:B:231:VAL:HG13	1:B:234:MET:CE	2.19	0.73
1:C:216:GLU:C	1:C:216:GLU:N	2.45	0.73
1:B:194:PHE:O	1:B:195:PRO:C	2.28	0.73
1:B:318:LYS:HE2	1:C:113:LYS:HZ2	1.51	0.73
1:D:279:ARG:HD3	1:D:295:MET:CE	2.18	0.73
1:D:31:TYR:HB2	1:D:121:LEU:HD21	1.70	0.73
1:C:194:PHE:O	1:C:195:PRO:C	2.28	0.73
1:C:231:VAL:HG13	1:C:234:MET:CE	2.19	0.73
1:C:279:ARG:HD3	1:C:295:MET:CE	2.18	0.73
1:A:279:ARG:HD3	1:A:295:MET:CE	2.18	0.73
1:B:232:ASN:OD1	1:B:233:ILE:HG12	1.89	0.73
1:A:311:HIS:CD2	1:A:346:VAL:HG11	2.24	0.73
1:C:128:GLU:HG2	1:D:128:GLU:CG	2.19	0.73
1:D:216:GLU:CD	1:D:216:GLU:HA	2.13	0.72
1:A:232:ASN:OD1	1:A:233:ILE:HG12	1.89	0.72
1:B:205:LYS:O	1:B:209:VAL:HG23	1.90	0.72
1:C:178:TRP:HB3	1:C:213:VAL:HG11	1.70	0.72
1:C:232:ASN:OD1	1:C:233:ILE:HG12	1.89	0.72
1:D:231:VAL:HG13	1:D:234:MET:CE	2.19	0.72
1:B:59:TRP:CZ2	1:C:176:GLU:HG3	2.25	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:HIS:CD2	1:B:346:VAL:HG11	2.24	0.72
1:D:311:HIS:CD2	1:D:346:VAL:HG11	2.24	0.72
1:B:82:TYR:N	1:B:82:TYR:CD2	2.57	0.72
1:C:144:ARG:HG2	1:C:149:VAL:O	1.89	0.72
1:D:117:ASN:HD22	1:D:290:ARG:CB	2.02	0.72
1:A:144:ARG:HG2	1:A:149:VAL:O	1.89	0.72
1:C:74:TYR:HE2	1:C:76:GLU:H	1.38	0.72
1:B:110:PHE:HB2	1:C:283:ALA:HB3	1.72	0.72
1:B:178:TRP:HB3	1:B:213:VAL:HG11	1.70	0.72
1:D:178:TRP:HB3	1:D:213:VAL:HG11	1.70	0.72
1:B:90:LEU:HD21	1:B:126:PRO:HG3	1.72	0.72
1:B:113:LYS:HZ2	1:C:318:LYS:HE2	1.55	0.72
1:B:144:ARG:HG2	1:B:149:VAL:O	1.89	0.72
1:D:82:TYR:CD2	1:D:82:TYR:N	2.57	0.72
1:D:205:LYS:O	1:D:209:VAL:HG23	1.90	0.72
1:D:232:ASN:OD1	1:D:233:ILE:HG12	1.89	0.72
1:A:82:TYR:CD2	1:A:82:TYR:N	2.57	0.72
1:A:207:TYR:O	1:A:210:ARG:HB3	1.90	0.72
1:B:134:LYS:NZ	1:B:266:GLU:CG	2.53	0.72
1:A:14:PHE:O	1:A:72:VAL:HG23	1.90	0.72
1:B:31:TYR:HD1	1:B:32:PHE:N	1.88	0.72
1:B:117:ASN:HD22	1:B:290:ARG:CB	2.02	0.72
1:C:128:GLU:HG2	1:D:128:GLU:HG2	1.72	0.72
1:A:134:LYS:NZ	1:A:266:GLU:CG	2.53	0.71
1:C:14:PHE:O	1:C:72:VAL:HG23	1.90	0.71
1:B:323:TYR:HE2	1:B:362:LEU:HD22	1.54	0.71
1:C:117:ASN:HD22	1:C:290:ARG:CB	2.02	0.71
1:C:207:TYR:O	1:C:210:ARG:HB3	1.90	0.71
1:C:323:TYR:HE2	1:C:362:LEU:HD22	1.54	0.71
1:D:144:ARG:HG2	1:D:149:VAL:O	1.89	0.71
1:A:205:LYS:O	1:A:209:VAL:HG23	1.90	0.71
1:A:279:ARG:O	1:A:280:ALA:C	2.30	0.71
1:B:14:PHE:O	1:B:72:VAL:HG23	1.90	0.71
1:B:120:LEU:O	1:B:294:THR:CG2	2.38	0.71
1:C:311:HIS:CD2	1:C:346:VAL:HG11	2.24	0.71
1:D:14:PHE:O	1:D:72:VAL:HG23	1.90	0.71
1:D:31:TYR:HD1	1:D:32:PHE:N	1.89	0.71
1:D:134:LYS:NZ	1:D:266:GLU:CG	2.53	0.71
1:B:134:LYS:HZ1	1:B:266:GLU:CG	2.03	0.71
1:A:31:TYR:HD1	1:A:32:PHE:N	1.88	0.71
1:A:202:ARG:O	1:A:206:LEU:HD23	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:VAL:HG22	1:C:258:TRP:HB3	1.72	0.71
1:C:205:LYS:O	1:C:209:VAL:HG23	1.90	0.71
1:A:384:ALA:CB	1:A:411:GLU:HG2	2.20	0.71
1:B:259:SER:HB3	1:C:256:ALA:O	1.90	0.71
1:C:31:TYR:HD1	1:C:32:PHE:N	1.89	0.71
1:C:131:ARG:CG	1:C:132:HIS:HD1	2.04	0.71
1:C:134:LYS:NZ	1:C:266:GLU:CG	2.53	0.71
1:B:207:TYR:O	1:B:210:ARG:HB3	1.90	0.71
1:C:378:HIS:ND1	1:C:380:ASP:HB2	2.05	0.71
1:D:207:TYR:O	1:D:210:ARG:HB3	1.90	0.71
1:B:378:HIS:ND1	1:B:380:ASP:HB2	2.05	0.71
1:C:202:ARG:O	1:C:206:LEU:HD23	1.90	0.71
1:B:74:TYR:HE2	1:B:76:GLU:H	1.38	0.71
1:C:276:HIS:CD2	1:C:309:GLN:HE21	2.09	0.71
1:A:99:VAL:HG22	1:A:258:TRP:HB3	1.73	0.70
1:B:276:HIS:CD2	1:B:309:GLN:HE21	2.09	0.70
1:D:194:PHE:O	1:D:195:PRO:C	2.28	0.70
1:D:378:HIS:ND1	1:D:380:ASP:HB2	2.05	0.70
1:C:384:ALA:CB	1:C:411:GLU:HG2	2.20	0.70
1:D:278:HIS:ND1	1:D:311:HIS:HE1	1.90	0.70
1:A:11:TYR:CD1	1:A:11:TYR:N	2.60	0.70
1:C:90:LEU:HD21	1:C:126:PRO:HG3	1.72	0.70
2:C:451:HOH:O	1:D:23:ARG:HD2	1.90	0.70
1:D:90:LEU:HD21	1:D:126:PRO:HG3	1.72	0.70
1:B:202:ARG:O	1:B:206:LEU:HD23	1.90	0.70
1:C:82:TYR:CD2	1:C:82:TYR:N	2.57	0.70
1:C:254:VAL:HG12	1:C:281:MET:HE2	1.73	0.70
1:C:278:HIS:ND1	1:C:311:HIS:HE1	1.90	0.70
1:C:143:ILE:HD13	1:C:309:GLN:OE1	1.92	0.70
1:B:384:ALA:CB	1:B:411:GLU:HG2	2.20	0.70
1:C:252:ASP:HB3	1:C:255:VAL:HG23	1.74	0.70
1:C:419:VAL:CG2	1:C:419:VAL:HB	2.16	0.70
1:A:143:ILE:HD13	1:A:309:GLN:OE1	1.92	0.70
1:B:254:VAL:HG12	1:B:281:MET:HE2	1.73	0.70
1:A:90:LEU:HD21	1:A:126:PRO:HG3	1.72	0.70
1:A:117:ASN:HD22	1:A:290:ARG:CB	2.02	0.70
1:A:323:TYR:HE2	1:A:362:LEU:HD22	1.54	0.70
1:B:143:ILE:HD13	1:B:309:GLN:OE1	1.92	0.70
1:B:278:HIS:ND1	1:B:311:HIS:HE1	1.90	0.70
1:A:61:LEU:CD2	1:A:61:LEU:CD1	2.68	0.69
1:D:202:ARG:O	1:D:206:LEU:HD23	1.90	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:VAL:HG22	1:B:258:TRP:HB3	1.73	0.69
1:D:315:ALA:C	1:D:316:VAL:HG23	2.16	0.69
1:A:252:ASP:HB3	1:A:255:VAL:HG23	1.74	0.69
1:D:17:LEU:HD23	1:D:74:TYR:N	2.08	0.69
1:D:74:TYR:HE2	1:D:76:GLU:H	1.38	0.69
1:A:74:TYR:HE2	1:A:76:GLU:H	1.38	0.69
1:B:74:TYR:HD2	1:B:74:TYR:C	2.01	0.69
1:A:276:HIS:CD2	1:A:309:GLN:HE21	2.09	0.69
1:B:61:LEU:CD2	1:B:61:LEU:CD1	2.68	0.69
1:D:254:VAL:HG12	1:D:281:MET:HE2	1.73	0.69
1:D:276:HIS:CD2	1:D:309:GLN:HE21	2.09	0.69
1:A:315:ALA:C	1:A:316:VAL:HG23	2.16	0.69
1:A:378:HIS:ND1	1:A:380:ASP:HB2	2.05	0.69
1:B:9:GLU:N	1:B:56:THR:HG1	1.91	0.69
1:B:17:LEU:HD23	1:B:74:TYR:N	2.08	0.69
1:D:143:ILE:HD13	1:D:309:GLN:OE1	1.92	0.69
1:A:74:TYR:HD2	1:A:74:TYR:C	2.01	0.69
1:A:254:VAL:HG12	1:A:281:MET:HE2	1.73	0.69
1:A:278:HIS:ND1	1:A:311:HIS:HE1	1.90	0.69
1:A:365:LYS:HD3	1:A:365:LYS:N	2.06	0.69
1:D:120:LEU:O	1:D:294:THR:CG2	2.38	0.69
1:C:95:GLU:OE2	1:D:128:GLU:OE2	2.10	0.69
1:C:315:ALA:C	1:C:316:VAL:HG23	2.17	0.69
1:D:74:TYR:C	1:D:74:TYR:HD2	2.01	0.69
1:D:99:VAL:HG22	1:D:258:TRP:HB3	1.73	0.69
1:B:182:ILE:HG22	1:B:183:ASP:N	2.08	0.68
1:C:60:LYS:HG2	1:C:60:LYS:O	1.93	0.68
1:D:61:LEU:CD2	1:D:61:LEU:CD1	2.68	0.68
1:D:115:LEU:HD13	1:D:118:LEU:HD22	1.75	0.68
1:A:160:LYS:HZ1	1:A:373:GLY:N	1.91	0.68
1:D:384:ALA:CB	1:D:411:GLU:HG2	2.21	0.68
1:A:46:ILE:CG1	1:A:112:MET:HE1	2.23	0.68
1:B:92:LEU:CD2	1:C:163:MET:HE2	2.24	0.68
1:B:110:PHE:C	1:C:283:ALA:HB1	2.18	0.68
1:B:169:GLU:HG2	1:C:60:LYS:HZ3	1.58	0.68
1:C:17:LEU:HD23	1:C:74:TYR:N	2.08	0.68
1:D:343:VAL:HG12	1:D:344:PHE:N	2.08	0.68
1:A:17:LEU:HD23	1:A:74:TYR:N	2.08	0.68
1:B:113:LYS:HD2	1:B:113:LYS:N	2.07	0.68
1:B:346:VAL:HG22	1:B:368:VAL:HG21	1.76	0.68
1:A:10:TRP:C	1:A:12:LEU:H	2.02	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:ILE:HG12	1:B:112:MET:CE	2.24	0.68
1:B:46:ILE:CG1	1:B:112:MET:HE1	2.23	0.68
1:B:343:VAL:HG12	1:B:344:PHE:N	2.08	0.68
1:C:343:VAL:HG12	1:C:344:PHE:N	2.08	0.68
1:A:134:LYS:HZ1	1:A:266:GLU:CG	2.07	0.68
1:D:10:TRP:C	1:D:12:LEU:H	2.02	0.68
1:D:46:ILE:CG1	1:D:112:MET:HE1	2.23	0.68
1:A:115:LEU:HD13	1:A:118:LEU:HD22	1.75	0.68
1:B:252:ASP:HB3	1:B:255:VAL:HG23	1.74	0.68
1:C:9:GLU:N	1:C:56:THR:HG1	1.92	0.68
1:C:74:TYR:HD2	1:C:74:TYR:C	2.01	0.68
1:D:249:VAL:HG23	1:D:249:VAL:O	1.94	0.68
1:B:315:ALA:C	1:B:316:VAL:HG23	2.16	0.67
1:C:346:VAL:HG22	1:C:368:VAL:HG21	1.76	0.67
1:D:123:PHE:O	1:D:300:LYS:CE	2.42	0.67
1:B:115:LEU:HD13	1:B:118:LEU:HD22	1.75	0.67
1:C:123:PHE:O	1:C:300:LYS:CE	2.42	0.67
1:B:195:PRO:HG2	1:D:131:ARG:HB2	1.76	0.67
1:B:256:ALA:O	1:C:259:SER:HB3	1.93	0.67
1:D:252:ASP:HB3	1:D:255:VAL:HG23	1.74	0.67
1:D:323:TYR:HE2	1:D:362:LEU:HD22	1.54	0.67
1:B:123:PHE:O	1:B:300:LYS:CE	2.42	0.67
1:C:46:ILE:CG1	1:C:112:MET:HE1	2.23	0.67
1:D:55:TRP:CD2	1:D:57:THR:CG2	2.71	0.67
1:D:346:VAL:CG2	1:D:368:VAL:CG2	2.73	0.67
1:A:182:ILE:HG22	1:A:183:ASP:N	2.08	0.67
1:B:345:PRO:HD2	1:B:367:LEU:HD23	1.77	0.67
1:C:282:HIS:CD2	1:C:283:ALA:N	2.63	0.67
1:D:182:ILE:HG22	1:D:183:ASP:N	2.08	0.67
1:D:282:HIS:CD2	1:D:283:ALA:N	2.63	0.67
1:B:55:TRP:CD2	1:B:57:THR:CG2	2.71	0.67
1:B:94:GLU:OE1	1:C:192:THR:OG1	2.07	0.67
1:C:234:MET:CE	1:C:234:MET:CG	2.73	0.67
1:C:249:VAL:HG23	1:C:249:VAL:O	1.94	0.67
1:C:346:VAL:CG2	1:C:368:VAL:CG2	2.73	0.67
1:A:46:ILE:HG12	1:A:112:MET:CE	2.24	0.67
1:A:346:VAL:CG2	1:A:368:VAL:CG2	2.73	0.67
1:B:282:HIS:CD2	1:B:283:ALA:N	2.63	0.67
1:B:346:VAL:CG2	1:B:368:VAL:CG2	2.73	0.67
1:B:414:LYS:O	1:B:418:GLU:HB2	1.95	0.67
1:B:419:VAL:CG2	1:B:419:VAL:HB	2.16	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:LYS:O	1:A:60:LYS:HG2	1.93	0.67
1:B:321:GLY:O	1:B:323:TYR:N	2.28	0.67
1:C:154:LEU:HB2	1:C:368:VAL:HG13	1.77	0.67
1:D:321:GLY:O	1:D:323:TYR:N	2.28	0.67
1:D:345:PRO:HD2	1:D:367:LEU:HD23	1.77	0.67
1:A:282:HIS:CD2	1:A:283:ALA:N	2.63	0.67
1:D:134:LYS:HZ1	1:D:266:GLU:CG	2.08	0.67
1:D:346:VAL:HG22	1:D:368:VAL:HG21	1.76	0.67
1:A:123:PHE:O	1:A:300:LYS:CE	2.42	0.67
1:A:343:VAL:HG12	1:A:344:PHE:N	2.08	0.67
1:C:10:TRP:C	1:C:12:LEU:H	2.02	0.67
1:C:120:LEU:O	1:C:294:THR:CG2	2.38	0.67
1:A:227:ILE:O	1:A:234:MET:HG2	1.96	0.66
1:A:250:MET:CE	1:A:250:MET:CG	2.73	0.66
1:C:345:PRO:HD2	1:C:367:LEU:HD23	1.77	0.66
1:D:46:ILE:HG12	1:D:112:MET:CE	2.24	0.66
1:D:60:LYS:O	1:D:60:LYS:HG2	1.93	0.66
1:D:250:MET:CE	1:D:250:MET:CG	2.73	0.66
1:A:120:LEU:O	1:A:294:THR:CG2	2.38	0.66
1:A:345:PRO:HD2	1:A:367:LEU:HD23	1.77	0.66
1:A:414:LYS:O	1:A:418:GLU:HB2	1.95	0.66
1:B:234:MET:CE	1:B:234:MET:CG	2.73	0.66
1:C:182:ILE:HG22	1:C:183:ASP:N	2.08	0.66
1:C:250:MET:CE	1:C:250:MET:CG	2.73	0.66
1:C:365:LYS:HD3	1:C:365:LYS:N	2.06	0.66
1:B:10:TRP:C	1:B:12:LEU:H	2.02	0.66
1:B:154:LEU:HB2	1:B:368:VAL:HG13	1.77	0.66
1:B:250:MET:CE	1:B:250:MET:CG	2.73	0.66
1:C:115:LEU:HD13	1:C:118:LEU:HD22	1.75	0.66
1:C:321:GLY:O	1:C:323:TYR:N	2.28	0.66
1:B:60:LYS:O	1:B:60:LYS:HG2	1.93	0.66
1:B:146:PHE:CD2	1:B:147:MET:HG2	2.30	0.66
1:C:117:ASN:HB3	1:C:290:ARG:O	1.95	0.66
1:C:414:LYS:O	1:C:418:GLU:HB2	1.95	0.66
1:A:117:ASN:HB3	1:A:290:ARG:O	1.96	0.66
1:A:231:VAL:HG12	1:A:234:MET:HE3	1.78	0.66
1:B:160:LYS:HZ1	1:B:373:GLY:N	1.91	0.66
1:C:146:PHE:CD2	1:C:147:MET:HG2	2.30	0.66
1:A:323:TYR:O	1:A:323:TYR:CG	2.48	0.66
1:B:227:ILE:O	1:B:234:MET:HG2	1.96	0.66
1:B:249:VAL:O	1:B:249:VAL:HG23	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:GLY:HA3	1:C:257:GLY:HA3	1.78	0.66
1:C:227:ILE:O	1:C:234:MET:HG2	1.95	0.66
1:D:414:LYS:O	1:D:418:GLU:HB2	1.95	0.66
1:A:249:VAL:HG23	1:A:249:VAL:O	1.94	0.66
1:D:227:ILE:O	1:D:234:MET:HG2	1.95	0.66
1:A:321:GLY:O	1:A:323:TYR:N	2.28	0.66
1:B:117:ASN:HB3	1:B:290:ARG:O	1.96	0.66
1:A:234:MET:CE	1:A:234:MET:CG	2.73	0.66
1:C:134:LYS:HZ1	1:C:266:GLU:CG	2.09	0.66
1:C:231:VAL:HG12	1:C:234:MET:HE3	1.78	0.66
1:D:234:MET:CE	1:D:234:MET:CG	2.73	0.66
1:B:119:ARG:HB3	1:B:121:LEU:HD11	1.78	0.66
1:B:323:TYR:O	1:B:323:TYR:CG	2.48	0.66
1:A:146:PHE:CD2	1:A:147:MET:HG2	2.31	0.65
1:C:119:ARG:HB3	1:C:121:LEU:HD11	1.78	0.65
1:D:154:LEU:HB2	1:D:368:VAL:HG13	1.77	0.65
1:B:113:LYS:HZ2	1:C:318:LYS:CE	2.09	0.65
1:D:199:PHE:CG	1:D:237:ARG:HD3	2.32	0.65
1:C:199:PHE:CG	1:C:237:ARG:HD3	2.32	0.65
1:A:195:PRO:HG2	1:B:131:ARG:HB2	1.79	0.65
1:B:283:ALA:HB3	1:C:110:PHE:HB2	1.78	0.65
1:C:46:ILE:HG12	1:C:112:MET:CE	2.24	0.65
1:D:160:LYS:HZ1	1:D:373:GLY:N	1.95	0.65
1:D:117:ASN:HB3	1:D:290:ARG:O	1.96	0.65
1:D:119:ARG:HB3	1:D:121:LEU:HD11	1.78	0.65
1:D:146:PHE:CD2	1:D:147:MET:HG2	2.30	0.65
1:A:199:PHE:CG	1:A:237:ARG:HD3	2.32	0.65
1:A:278:HIS:CD2	1:A:280:ALA:HB2	2.32	0.65
1:D:9:GLU:N	1:D:56:THR:HG1	1.95	0.65
1:D:353:PRO:O	1:D:392:ALA:HB1	1.97	0.65
1:A:119:ARG:HB3	1:A:121:LEU:HD11	1.78	0.65
1:B:163:MET:HE2	1:C:92:LEU:CD2	2.27	0.65
1:C:282:HIS:CD2	1:C:283:ALA:H	2.15	0.65
1:C:353:PRO:O	1:C:392:ALA:HB1	1.97	0.65
1:A:154:LEU:HB2	1:A:368:VAL:HG13	1.77	0.65
1:D:323:TYR:O	1:D:323:TYR:CG	2.48	0.65
1:C:136:PRO:HB3	1:C:308:ASP:OD1	1.97	0.65
1:C:278:HIS:CD2	1:C:280:ALA:HB2	2.32	0.65
1:D:136:PRO:HB3	1:D:308:ASP:OD1	1.97	0.65
1:A:147:MET:HE3	1:A:147:MET:CB	2.19	0.64
1:B:12:LEU:HD21	1:B:41:GLU:HG3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:ILE:CG2	1:B:183:ASP:N	2.60	0.64
1:B:263:TYR:CD1	1:C:232:ASN:ND2	2.64	0.64
1:A:346:VAL:HG22	1:A:368:VAL:HG21	1.76	0.64
1:C:182:ILE:CG2	1:C:183:ASP:N	2.60	0.64
1:C:252:ASP:HB3	1:C:255:VAL:HG21	1.78	0.64
1:D:252:ASP:HB3	1:D:255:VAL:HG21	1.78	0.64
1:D:146:PHE:HD2	1:D:147:MET:HG2	1.63	0.64
1:A:55:TRP:CH2	1:A:58:LEU:CB	2.76	0.64
1:B:138:PHE:CD1	1:B:146:PHE:HE1	2.15	0.64
1:B:231:VAL:HG12	1:B:234:MET:HE3	1.78	0.64
1:D:282:HIS:CD2	1:D:283:ALA:H	2.15	0.64
1:D:278:HIS:CD2	1:D:280:ALA:HB2	2.32	0.64
1:A:160:LYS:NZ	1:A:373:GLY:H	1.96	0.64
1:B:147:MET:CE	1:B:147:MET:CG	2.76	0.64
1:B:282:HIS:CD2	1:B:283:ALA:H	2.15	0.64
1:C:134:LYS:NZ	1:C:266:GLU:HG3	2.13	0.64
1:C:147:MET:CE	1:C:147:MET:CG	2.76	0.64
1:C:323:TYR:O	1:C:323:TYR:CG	2.48	0.64
1:D:182:ILE:CG2	1:D:183:ASP:N	2.60	0.64
1:D:276:HIS:HD2	1:D:309:GLN:NE2	1.95	0.64
1:A:138:PHE:CD1	1:A:146:PHE:HE1	2.15	0.64
1:A:182:ILE:CG2	1:A:183:ASP:N	2.60	0.64
1:B:146:PHE:HD2	1:B:147:MET:HG2	1.63	0.64
1:B:278:HIS:CD2	1:B:280:ALA:HB2	2.32	0.64
1:C:138:PHE:CD1	1:C:146:PHE:HE1	2.15	0.64
1:D:113:LYS:HD2	1:D:113:LYS:N	2.07	0.64
1:D:138:PHE:CD1	1:D:146:PHE:HE1	2.15	0.64
1:D:231:VAL:HG12	1:D:234:MET:HE3	1.78	0.64
1:B:76:GLU:HG2	1:B:77:LYS:O	1.98	0.64
1:B:199:PHE:CG	1:B:237:ARG:HD3	2.32	0.64
1:B:252:ASP:HB3	1:B:255:VAL:HG21	1.78	0.64
1:B:341:ARG:CB	1:B:342:PRO:HD2	2.28	0.64
1:D:184:LEU:HD12	1:D:224:LEU:HD11	1.80	0.64
1:A:147:MET:CE	1:A:147:MET:CG	2.76	0.63
1:B:136:PRO:HB3	1:B:308:ASP:OD1	1.97	0.63
1:B:151:ASP:CG	1:B:151:ASP:CA	2.69	0.63
1:C:346:VAL:CG2	1:C:368:VAL:HG23	2.28	0.63
1:D:76:GLU:HG2	1:D:77:LYS:O	1.98	0.63
1:B:283:ALA:HB1	1:C:110:PHE:C	2.22	0.63
1:A:252:ASP:HB3	1:A:255:VAL:HG21	1.78	0.63
1:A:353:PRO:O	1:A:392:ALA:HB1	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:LEU:HD21	1:C:41:GLU:HG3	1.79	0.63
1:D:55:TRP:CH2	1:D:58:LEU:CB	2.76	0.63
1:D:134:LYS:NZ	1:D:266:GLU:HG3	2.13	0.63
1:D:151:ASP:CG	1:D:151:ASP:CA	2.69	0.63
1:A:202:ARG:NE	1:A:223:TYR:OH	2.26	0.63
1:A:282:HIS:CD2	1:A:283:ALA:H	2.15	0.63
1:B:353:PRO:O	1:B:392:ALA:HB1	1.97	0.63
1:C:15:VAL:HA	1:C:72:VAL:HG23	1.81	0.63
1:C:341:ARG:CB	1:C:342:PRO:HD2	2.28	0.63
1:D:12:LEU:HD21	1:D:41:GLU:HG3	1.79	0.63
1:A:146:PHE:HD2	1:A:147:MET:HG2	1.63	0.63
1:A:346:VAL:CG2	1:A:368:VAL:HG23	2.28	0.63
1:C:76:GLU:HG2	1:C:77:LYS:O	1.98	0.63
1:C:98:LEU:C	1:C:98:LEU:HD23	2.24	0.63
1:A:98:LEU:HD23	1:A:98:LEU:C	2.24	0.63
1:B:134:LYS:NZ	1:B:266:GLU:HG3	2.13	0.63
1:B:315:ALA:HB3	1:B:359:LEU:HD13	1.81	0.63
1:B:370:GLN:NE2	1:B:372:GLY:H	1.97	0.63
1:C:55:TRP:CH2	1:C:58:LEU:CB	2.76	0.63
1:C:61:LEU:CD2	1:C:61:LEU:CD1	2.68	0.63
1:C:113:LYS:HD2	1:C:113:LYS:N	2.07	0.63
1:D:315:ALA:HB3	1:D:359:LEU:HD13	1.81	0.63
1:A:134:LYS:NZ	1:A:266:GLU:HG3	2.13	0.63
1:B:11:TYR:CD2	1:B:45:ARG:CG	2.82	0.63
1:B:224:LEU:HD22	1:B:276:HIS:CG	2.34	0.63
1:C:224:LEU:HD22	1:C:276:HIS:CG	2.34	0.63
1:D:160:LYS:NZ	1:D:373:GLY:H	1.96	0.63
1:D:341:ARG:CB	1:D:342:PRO:HD2	2.28	0.63
1:A:76:GLU:HG2	1:A:77:LYS:O	1.98	0.63
1:A:133:PHE:CE2	1:A:304:MET:HE2	2.34	0.63
1:B:98:LEU:HD23	1:B:98:LEU:C	2.24	0.63
1:B:160:LYS:NZ	1:B:373:GLY:H	1.96	0.63
1:B:346:VAL:CG2	1:B:368:VAL:HG23	2.28	0.63
1:C:315:ALA:HB3	1:C:359:LEU:HD13	1.81	0.63
1:D:346:VAL:CG2	1:D:368:VAL:HG23	2.28	0.63
1:D:370:GLN:NE2	1:D:372:GLY:H	1.97	0.63
1:A:370:GLN:NE2	1:A:372:GLY:H	1.97	0.63
1:B:137:GLN:O	1:B:137:GLN:HG2	1.99	0.63
1:B:276:HIS:HD2	1:B:309:GLN:NE2	1.95	0.63
1:C:146:PHE:HD2	1:C:147:MET:HG2	1.63	0.63
1:A:136:PRO:HB3	1:A:308:ASP:OD1	1.97	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:TRP:CH2	1:C:176:GLU:HG3	2.34	0.62
1:A:12:LEU:HD21	1:A:41:GLU:HG3	1.79	0.62
1:C:229:GLY:O	1:C:234:MET:HG3	1.99	0.62
1:C:370:GLN:NE2	1:C:372:GLY:H	1.97	0.62
1:D:147:MET:CE	1:D:147:MET:CG	2.76	0.62
1:A:341:ARG:CB	1:A:342:PRO:HD2	2.28	0.62
1:B:389:LEU:O	1:B:393:ILE:HG13	2.00	0.62
1:C:276:HIS:HD2	1:C:309:GLN:NE2	1.95	0.62
1:B:208:ARG:NH2	1:D:145:GLU:OE2	2.28	0.62
1:C:137:GLN:O	1:C:137:GLN:HG2	1.99	0.62
1:C:184:LEU:HD12	1:C:224:LEU:HD11	1.80	0.62
1:D:98:LEU:HD23	1:D:98:LEU:C	2.24	0.62
1:B:184:LEU:HD12	1:B:224:LEU:HD11	1.80	0.62
1:C:46:ILE:HG22	1:C:86:ILE:HD12	1.81	0.62
1:C:133:PHE:CE2	1:C:304:MET:HE2	2.34	0.62
1:C:300:LYS:HD3	1:C:332:PHE:CZ	2.35	0.62
1:D:229:GLY:O	1:D:234:MET:HG3	1.99	0.62
1:A:137:GLN:HG2	1:A:137:GLN:O	1.99	0.62
1:A:184:LEU:HD12	1:A:224:LEU:HD11	1.80	0.62
1:A:310:ILE:O	1:A:346:VAL:HB	2.00	0.62
1:B:47:ALA:HB2	1:B:86:ILE:HD13	1.82	0.62
1:B:169:GLU:HG2	1:C:60:LYS:HZ1	1.63	0.62
1:C:151:ASP:CG	1:C:151:ASP:CA	2.69	0.62
1:B:300:LYS:HD3	1:B:332:PHE:CZ	2.35	0.62
1:D:217:THR:HG21	1:D:221:LYS:HE3	1.82	0.62
1:A:15:VAL:HA	1:A:72:VAL:HG23	1.81	0.62
1:A:389:LEU:O	1:A:393:ILE:HG13	2.00	0.62
1:B:133:PHE:CE2	1:B:304:MET:HE2	2.34	0.62
1:C:134:LYS:NZ	1:C:266:GLU:HG2	2.15	0.62
1:A:113:LYS:HD2	1:A:113:LYS:N	2.07	0.62
1:A:224:LEU:HD22	1:A:276:HIS:CG	2.34	0.62
1:B:134:LYS:NZ	1:B:266:GLU:HG2	2.15	0.62
1:D:15:VAL:HA	1:D:72:VAL:HG23	1.81	0.62
1:D:137:GLN:HG2	1:D:137:GLN:O	1.99	0.62
1:D:310:ILE:O	1:D:346:VAL:HB	2.00	0.62
1:D:365:LYS:HD3	1:D:365:LYS:N	2.06	0.62
1:B:27:ILE:CG2	1:B:86:ILE:O	2.48	0.62
1:B:60:LYS:CE	1:C:169:GLU:OE2	2.48	0.62
1:D:133:PHE:CE2	1:D:304:MET:HE2	2.34	0.62
1:D:300:LYS:HD3	1:D:332:PHE:CZ	2.35	0.62
1:A:276:HIS:HD2	1:A:309:GLN:NE2	1.95	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:ILE:HG22	1:B:86:ILE:HD12	1.81	0.61
1:B:152:ARG:HG3	1:B:152:ARG:NH1	2.14	0.61
1:D:224:LEU:HD22	1:D:276:HIS:CG	2.34	0.61
1:B:11:TYR:CD1	1:B:11:TYR:N	2.60	0.61
1:B:55:TRP:CH2	1:B:58:LEU:CB	2.76	0.61
1:C:131:ARG:HG2	1:C:132:HIS:HD1	1.65	0.61
1:C:310:ILE:O	1:C:346:VAL:HB	2.00	0.61
1:D:11:TYR:CD2	1:D:45:ARG:CG	2.82	0.61
1:A:134:LYS:NZ	1:A:266:GLU:HG2	2.15	0.61
1:A:300:LYS:HD3	1:A:332:PHE:CZ	2.35	0.61
1:B:15:VAL:HA	1:B:72:VAL:HG23	1.81	0.61
1:B:60:LYS:HZ1	1:C:169:GLU:HG2	1.63	0.61
1:B:229:GLY:O	1:B:234:MET:HG3	1.99	0.61
1:B:134:LYS:HZ1	1:B:266:GLU:HG3	1.65	0.61
1:B:217:THR:HG21	1:B:221:LYS:HE3	1.82	0.61
1:A:46:ILE:HG22	1:A:86:ILE:HD12	1.81	0.61
1:B:232:ASN:ND2	1:C:263:TYR:CD1	2.67	0.61
1:C:389:LEU:O	1:C:393:ILE:HG13	2.00	0.61
1:D:27:ILE:CG2	1:D:86:ILE:O	2.48	0.61
1:D:46:ILE:HG22	1:D:86:ILE:HD12	1.81	0.61
1:C:160:LYS:NZ	1:C:373:GLY:H	1.96	0.61
1:A:217:THR:HG21	1:A:221:LYS:HE3	1.82	0.61
1:A:315:ALA:HB3	1:A:359:LEU:HD13	1.81	0.61
1:D:419:VAL:HG12	1:D:419:VAL:O	2.01	0.61
1:A:16:ASP:C	1:A:16:ASP:OD2	2.44	0.61
1:A:229:GLY:O	1:A:234:MET:HG3	1.99	0.61
1:B:202:ARG:NE	1:B:223:TYR:OH	2.26	0.61
1:C:47:ALA:HB2	1:C:86:ILE:HD13	1.82	0.61
1:C:160:LYS:HZ1	1:C:373:GLY:N	1.97	0.61
1:D:12:LEU:CD2	1:D:41:GLU:HG3	2.31	0.61
1:A:308:ASP:C	1:A:309:GLN:HG3	2.26	0.61
1:B:60:LYS:HE2	1:C:169:GLU:OE2	2.01	0.61
1:B:310:ILE:O	1:B:346:VAL:HB	2.00	0.61
1:D:47:ALA:HB2	1:D:86:ILE:HD13	1.82	0.61
1:D:152:ARG:HG3	1:D:152:ARG:NH1	2.14	0.61
1:D:308:ASP:C	1:D:309:GLN:HG3	2.26	0.61
1:D:389:LEU:O	1:D:393:ILE:HG13	2.00	0.61
1:B:263:TYR:CE2	1:B:267:VAL:HG23	2.36	0.61
1:B:296:LEU:HD12	1:B:329:ILE:HA	1.83	0.61
1:C:12:LEU:CD2	1:C:41:GLU:HG3	2.31	0.61
1:C:217:THR:HG21	1:C:221:LYS:HE3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:417:ARG:HD3	2:C:481:HOH:O	1.59	0.61
1:D:134:LYS:NZ	1:D:266:GLU:HG2	2.15	0.61
1:A:47:ALA:HB2	1:A:86:ILE:HD13	1.82	0.60
1:A:152:ARG:HG3	1:A:152:ARG:NH1	2.14	0.60
1:B:16:ASP:OD2	1:B:16:ASP:C	2.44	0.60
1:C:263:TYR:CE2	1:C:267:VAL:HG23	2.36	0.60
1:D:263:TYR:C	1:D:263:TYR:HD2	2.09	0.60
1:A:263:TYR:CE2	1:A:267:VAL:HG23	2.36	0.60
1:B:263:TYR:C	1:B:263:TYR:HD2	2.10	0.60
1:C:152:ARG:HG3	1:C:152:ARG:NH1	2.14	0.60
1:C:263:TYR:C	1:C:263:TYR:HD2	2.10	0.60
1:D:296:LEU:HD12	1:D:329:ILE:HA	1.83	0.60
1:A:419:VAL:O	1:A:419:VAL:HG12	2.01	0.60
1:B:403:ASP:O	1:B:407:LYS:HG3	2.02	0.60
1:C:373:GLY:O	1:C:375:VAL:N	2.34	0.60
1:B:323:TYR:CD1	1:B:323:TYR:C	2.79	0.60
1:B:373:GLY:O	1:B:375:VAL:N	2.34	0.60
1:C:11:TYR:CD2	1:C:45:ARG:CG	2.82	0.60
1:C:160:LYS:O	1:C:376:MET:CE	2.49	0.60
1:C:403:ASP:O	1:C:407:LYS:HG3	2.02	0.60
1:A:160:LYS:O	1:A:376:MET:CE	2.49	0.60
1:B:160:LYS:O	1:B:376:MET:CE	2.49	0.60
1:B:419:VAL:O	1:B:419:VAL:HG12	2.01	0.60
1:C:311:HIS:HD2	1:C:346:VAL:HG12	1.65	0.60
1:C:419:VAL:O	1:C:419:VAL:HG12	2.01	0.60
1:D:160:LYS:O	1:D:376:MET:CE	2.49	0.60
1:A:151:ASP:CG	1:A:151:ASP:CA	2.69	0.60
1:B:311:HIS:CD2	1:B:346:VAL:CG1	2.79	0.60
1:C:296:LEU:HD12	1:C:329:ILE:HA	1.83	0.60
1:C:323:TYR:CD1	1:C:323:TYR:C	2.79	0.60
1:A:9:GLU:N	1:A:56:THR:HG1	1.99	0.60
1:A:12:LEU:CD2	1:A:41:GLU:HG3	2.31	0.60
1:A:311:HIS:HD2	1:A:346:VAL:HG12	1.65	0.60
1:D:263:TYR:CE2	1:D:267:VAL:HG23	2.36	0.60
1:D:323:TYR:CD1	1:D:323:TYR:C	2.79	0.60
1:B:300:LYS:O	1:B:301:ALA:C	2.45	0.60
1:A:27:ILE:CG2	1:A:86:ILE:O	2.48	0.60
1:A:323:TYR:CD1	1:A:323:TYR:C	2.79	0.60
1:C:202:ARG:NE	1:C:223:TYR:OH	2.26	0.60
1:D:15:VAL:HG13	1:D:72:VAL:CB	2.32	0.60
1:D:300:LYS:O	1:D:301:ALA:C	2.45	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:373:GLY:O	1:D:375:VAL:N	2.34	0.60
1:A:55:TRP:CZ3	1:A:58:LEU:N	2.70	0.59
1:A:296:LEU:HD12	1:A:329:ILE:HA	1.83	0.59
1:B:12:LEU:CD2	1:B:41:GLU:HG3	2.31	0.59
1:C:308:ASP:C	1:C:309:GLN:HG3	2.26	0.59
1:A:300:LYS:O	1:A:301:ALA:C	2.45	0.59
1:B:365:LYS:HD3	1:B:365:LYS:N	2.06	0.59
1:C:162:LYS:O	1:C:163:MET:HG2	2.03	0.59
1:A:373:GLY:O	1:A:375:VAL:N	2.34	0.59
1:D:16:ASP:C	1:D:16:ASP:OD2	2.44	0.59
1:A:195:PRO:CG	1:B:131:ARG:HB2	2.32	0.59
1:C:27:ILE:CG2	1:C:86:ILE:O	2.48	0.59
1:C:204:ARG:O	1:C:208:ARG:CD	2.50	0.59
1:C:15:VAL:HG13	1:C:72:VAL:CB	2.32	0.59
1:C:15:VAL:HG13	1:C:72:VAL:HB	1.85	0.59
1:D:122:ASP:OD1	1:D:300:LYS:HE2	2.03	0.59
1:B:15:VAL:HG13	1:B:72:VAL:HB	1.85	0.59
1:B:122:ASP:OD1	1:B:300:LYS:HE2	2.03	0.59
1:C:224:LEU:HD22	1:C:276:HIS:CD2	2.38	0.59
1:D:15:VAL:HG13	1:D:72:VAL:HB	1.85	0.59
1:A:162:LYS:O	1:A:163:MET:HG2	2.03	0.59
1:A:204:ARG:O	1:A:208:ARG:CD	2.50	0.59
1:A:403:ASP:O	1:A:407:LYS:HG3	2.02	0.59
1:B:15:VAL:HG13	1:B:72:VAL:CB	2.32	0.59
1:D:162:LYS:O	1:D:163:MET:HG2	2.03	0.59
1:D:419:VAL:CG2	1:D:419:VAL:HB	2.16	0.59
1:B:308:ASP:O	1:B:309:GLN:HG3	2.03	0.59
1:C:300:LYS:O	1:C:301:ALA:C	2.45	0.59
1:D:224:LEU:HD22	1:D:276:HIS:CD2	2.38	0.59
1:A:122:ASP:OD1	1:A:300:LYS:HE2	2.03	0.59
1:B:155:THR:O	1:B:183:ASP:HB2	2.03	0.59
1:B:249:VAL:O	1:B:249:VAL:CG2	2.50	0.59
1:D:155:THR:O	1:D:183:ASP:HB2	2.03	0.59
1:D:199:PHE:CD2	1:D:237:ARG:HD3	2.38	0.59
1:D:403:ASP:O	1:D:407:LYS:HG3	2.02	0.59
1:A:15:VAL:HG13	1:A:72:VAL:HB	1.85	0.58
1:A:308:ASP:O	1:A:309:GLN:HG3	2.03	0.58
1:B:10:TRP:C	1:B:12:LEU:N	2.60	0.58
1:B:224:LEU:HD22	1:B:276:HIS:CD2	2.38	0.58
1:C:308:ASP:O	1:C:309:GLN:HG3	2.03	0.58
1:C:359:LEU:O	1:C:363:PHE:HD1	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:321:GLY:O	1:D:322:ASN:C	2.46	0.58
1:A:15:VAL:HG13	1:A:72:VAL:CB	2.32	0.58
1:B:110:PHE:CB	1:C:283:ALA:HB3	2.34	0.58
1:B:162:LYS:O	1:B:163:MET:HG2	2.03	0.58
1:B:226:ASN:ND2	1:B:228:THR:OG1	2.32	0.58
1:C:199:PHE:CD2	1:C:237:ARG:HD3	2.38	0.58
1:C:263:TYR:HE2	1:C:267:VAL:HG23	1.69	0.58
1:C:303:ARG:NH2	1:C:342:PRO:CA	2.46	0.58
1:D:10:TRP:C	1:D:12:LEU:N	2.60	0.58
1:A:359:LEU:O	1:A:363:PHE:HD1	1.86	0.58
1:B:308:ASP:C	1:B:309:GLN:HG3	2.26	0.58
1:B:359:LEU:O	1:B:363:PHE:HD1	1.86	0.58
1:A:11:TYR:CD2	1:A:45:ARG:CG	2.82	0.58
1:A:188:ASP:OD1	1:A:190:ASN:HB2	2.03	0.58
1:B:199:PHE:CD2	1:B:237:ARG:HD3	2.38	0.58
1:C:122:ASP:OD1	1:C:300:LYS:HE2	2.03	0.58
1:C:162:LYS:C	1:C:163:MET:HG2	2.29	0.58
1:D:188:ASP:OD1	1:D:190:ASN:HB2	2.03	0.58
1:D:308:ASP:O	1:D:309:GLN:HG3	2.03	0.58
1:B:141:GLN:CD	1:B:141:GLN:HA	2.29	0.58
1:B:346:VAL:CG2	1:B:368:VAL:HG21	2.34	0.58
1:C:346:VAL:CG2	1:C:368:VAL:HG21	2.34	0.58
1:D:123:PHE:CZ	1:D:300:LYS:CG	2.79	0.58
1:D:263:TYR:HE2	1:D:267:VAL:HG23	1.69	0.58
1:A:152:ARG:HG3	1:A:152:ARG:HH11	1.68	0.58
1:A:162:LYS:C	1:A:163:MET:HG2	2.29	0.58
1:B:162:LYS:C	1:B:163:MET:HG2	2.29	0.58
1:C:131:ARG:HG3	1:C:132:HIS:HD1	1.68	0.58
1:A:123:PHE:CZ	1:A:300:LYS:CG	2.79	0.58
1:A:131:ARG:HG3	1:A:132:HIS:ND1	2.19	0.58
1:A:199:PHE:CD2	1:A:237:ARG:HD3	2.38	0.58
1:A:224:LEU:HD22	1:A:276:HIS:CD2	2.38	0.58
1:A:321:GLY:O	1:A:322:ASN:C	2.46	0.58
1:B:321:GLY:O	1:B:322:ASN:C	2.46	0.58
1:A:147:MET:HE3	1:A:220:THR:CG2	2.34	0.58
1:B:131:ARG:HG3	1:B:132:HIS:ND1	2.19	0.58
1:C:249:VAL:O	1:C:249:VAL:CG2	2.50	0.58
1:D:147:MET:HE3	1:D:220:THR:CG2	2.34	0.58
1:D:311:HIS:HD2	1:D:346:VAL:HG12	1.65	0.58
1:A:346:VAL:CG2	1:A:368:VAL:HG21	2.34	0.58
1:B:147:MET:HE3	1:B:147:MET:CB	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:PRO:CG	1:D:131:ARG:HB2	2.33	0.58
1:C:225:ILE:O	1:C:250:MET:HB3	2.04	0.58
1:C:55:TRP:CZ3	1:C:58:LEU:N	2.70	0.58
1:C:158:VAL:HG11	1:C:188:ASP:HB2	1.86	0.58
1:C:226:ASN:ND2	1:C:228:THR:OG1	2.32	0.58
1:D:112:MET:CE	1:D:115:LEU:HD11	2.31	0.58
1:D:158:VAL:HG11	1:D:188:ASP:HB2	1.86	0.58
1:A:141:GLN:CD	1:A:141:GLN:HA	2.29	0.57
1:A:375:VAL:HG13	1:A:385:GLY:O	2.03	0.57
1:B:263:TYR:HE2	1:B:267:VAL:HG23	1.69	0.57
1:C:141:GLN:CD	1:C:141:GLN:HA	2.29	0.57
1:D:160:LYS:CD	1:D:160:LYS:HE3	2.18	0.57
1:B:55:TRP:CZ3	1:B:58:LEU:N	2.70	0.57
1:B:204:ARG:O	1:B:208:ARG:CD	2.50	0.57
1:C:336:LYS:HD3	1:C:337:TRP:N	2.19	0.57
1:D:131:ARG:HG3	1:D:132:HIS:ND1	2.19	0.57
1:D:375:VAL:HG13	1:D:385:GLY:O	2.03	0.57
1:A:168:GLU:O	1:A:171:ALA:N	2.37	0.57
1:C:168:GLU:O	1:C:171:ALA:N	2.37	0.57
1:C:188:ASP:OD1	1:C:190:ASN:HB2	2.03	0.57
1:D:141:GLN:CD	1:D:141:GLN:HA	2.29	0.57
1:A:155:THR:O	1:A:183:ASP:HB2	2.03	0.57
1:B:112:MET:CE	1:B:115:LEU:HD11	2.31	0.57
1:B:375:VAL:HG13	1:B:385:GLY:O	2.03	0.57
1:C:131:ARG:HG3	1:C:132:HIS:ND1	2.19	0.57
1:C:155:THR:O	1:C:183:ASP:HB2	2.03	0.57
1:C:160:LYS:NZ	1:C:373:GLY:N	2.53	0.57
1:D:55:TRP:CZ3	1:D:58:LEU:N	2.70	0.57
1:D:346:VAL:CG2	1:D:368:VAL:HG21	2.34	0.57
1:A:158:VAL:HG11	1:A:188:ASP:HB2	1.86	0.57
1:B:158:VAL:HG11	1:B:188:ASP:HB2	1.86	0.57
1:B:225:ILE:O	1:B:250:MET:HB3	2.04	0.57
1:D:21:PRO:HA	1:D:25:GLU:OE2	2.05	0.57
1:D:144:ARG:CG	1:D:149:VAL:O	2.52	0.57
1:D:168:GLU:O	1:D:171:ALA:N	2.38	0.57
1:A:55:TRP:CD2	1:A:57:THR:CG2	2.71	0.57
1:B:188:ASP:OD1	1:B:190:ASN:HB2	2.03	0.57
1:C:55:TRP:CG	1:C:57:THR:HG23	2.39	0.57
1:C:375:VAL:HG13	1:C:385:GLY:O	2.03	0.57
1:D:152:ARG:HG3	1:D:152:ARG:HH11	1.68	0.57
1:D:359:LEU:O	1:D:363:PHE:HD1	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:PHE:N	1:A:102:PHE:CD1	2.73	0.57
1:A:225:ILE:O	1:A:250:MET:HB3	2.04	0.57
1:C:58:LEU:O	1:C:58:LEU:HD13	2.05	0.57
1:B:60:LYS:HZ3	1:C:169:GLU:HG2	1.70	0.57
1:B:77:LYS:HA	1:B:82:TYR:CD1	2.40	0.57
1:B:336:LYS:HD3	1:B:337:TRP:N	2.19	0.57
1:D:162:LYS:C	1:D:163:MET:HG2	2.29	0.57
1:D:253:ILE:CD1	1:D:277:ALA:CB	2.74	0.57
1:A:58:LEU:HD13	1:A:58:LEU:O	2.05	0.57
1:A:263:TYR:HE2	1:A:267:VAL:HG23	1.69	0.57
1:B:102:PHE:N	1:B:102:PHE:CD1	2.73	0.57
1:B:144:ARG:CG	1:B:149:VAL:O	2.53	0.57
1:C:147:MET:HE3	1:C:220:THR:CG2	2.34	0.57
1:A:55:TRP:CG	1:A:57:THR:HG23	2.39	0.56
1:A:112:MET:HA	1:A:113:LYS:HD2	1.87	0.56
1:A:263:TYR:C	1:A:263:TYR:HD2	2.10	0.56
1:B:160:LYS:NZ	1:B:373:GLY:N	2.53	0.56
1:C:21:PRO:HA	1:C:25:GLU:OE2	2.05	0.56
1:C:77:LYS:HA	1:C:82:TYR:CD1	2.40	0.56
1:C:152:ARG:HG3	1:C:152:ARG:HH11	1.68	0.56
1:A:77:LYS:HA	1:A:82:TYR:CD1	2.40	0.56
1:A:303:ARG:NH2	1:A:342:PRO:CA	2.46	0.56
1:A:336:LYS:HD3	1:A:337:TRP:N	2.19	0.56
1:B:112:MET:HA	1:B:113:LYS:HD2	1.87	0.56
1:B:152:ARG:HG3	1:B:152:ARG:HH11	1.68	0.56
1:C:112:MET:HA	1:C:113:LYS:HD2	1.87	0.56
1:C:123:PHE:CZ	1:C:300:LYS:CG	2.79	0.56
1:C:144:ARG:CG	1:C:149:VAL:O	2.53	0.56
1:C:311:HIS:CD2	1:C:346:VAL:CG1	2.79	0.56
1:D:58:LEU:HD13	1:D:58:LEU:O	2.05	0.56
1:D:336:LYS:HD3	1:D:337:TRP:N	2.19	0.56
1:B:55:TRP:CG	1:B:57:THR:HG23	2.39	0.56
1:C:321:GLY:O	1:C:322:ASN:C	2.46	0.56
1:D:156:ALA:O	1:D:370:GLN:HA	2.05	0.56
1:D:206:LEU:HA	1:D:209:VAL:CG2	2.36	0.56
1:D:249:VAL:O	1:D:249:VAL:CG2	2.50	0.56
1:A:21:PRO:HA	1:A:25:GLU:OE2	2.05	0.56
1:A:249:VAL:O	1:A:249:VAL:CG2	2.50	0.56
1:B:168:GLU:O	1:B:171:ALA:N	2.37	0.56
1:B:311:HIS:HD2	1:B:346:VAL:HG12	1.65	0.56
1:C:16:ASP:C	1:C:16:ASP:OD2	2.44	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:PRO:HA	1:B:25:GLU:OE2	2.05	0.56
1:B:156:ALA:O	1:B:370:GLN:HA	2.06	0.56
1:B:206:LEU:HA	1:B:209:VAL:CG2	2.36	0.56
1:D:160:LYS:NZ	1:D:373:GLY:N	2.53	0.56
1:D:225:ILE:O	1:D:250:MET:HB3	2.04	0.56
1:A:120:LEU:HD13	1:A:120:LEU:C	2.31	0.56
1:B:120:LEU:HD13	1:B:120:LEU:C	2.31	0.56
1:B:123:PHE:CZ	1:B:300:LYS:CG	2.79	0.56
1:D:77:LYS:HA	1:D:82:TYR:CD1	2.40	0.56
1:D:202:ARG:NE	1:D:223:TYR:OH	2.26	0.56
1:B:15:VAL:CG1	1:B:72:VAL:HB	2.36	0.56
1:B:72:VAL:HG13	1:B:86:ILE:HG12	1.88	0.56
1:C:117:ASN:ND2	1:C:290:ARG:CB	2.63	0.56
1:D:55:TRP:CG	1:D:57:THR:HG23	2.39	0.56
1:C:253:ILE:CD1	1:C:277:ALA:CB	2.75	0.56
1:A:74:TYR:CE2	1:A:76:GLU:N	2.74	0.56
1:A:206:LEU:HA	1:A:209:VAL:CG2	2.36	0.56
1:D:72:VAL:HG13	1:D:86:ILE:HG12	1.88	0.56
1:D:298:LEU:C	1:D:300:LYS:N	2.63	0.56
1:A:60:LYS:O	1:A:61:LEU:C	2.49	0.55
1:A:144:ARG:CG	1:A:149:VAL:O	2.53	0.55
1:A:160:LYS:NZ	1:A:373:GLY:N	2.53	0.55
1:B:141:GLN:CD	1:B:141:GLN:CA	2.79	0.55
1:C:15:VAL:CG1	1:C:72:VAL:HB	2.36	0.55
1:D:23:ARG:HE	1:D:23:ARG:N	2.00	0.55
1:A:156:ALA:O	1:A:370:GLN:HA	2.05	0.55
1:A:172:GLU:CD	1:A:172:GLU:CB	2.72	0.55
1:A:325:GLU:O	1:A:326:ILE:C	2.49	0.55
1:B:60:LYS:O	1:B:61:LEU:C	2.49	0.55
1:C:60:LYS:O	1:C:61:LEU:C	2.49	0.55
1:A:64:MET:CE	1:A:64:MET:SD	2.95	0.55
1:B:253:ILE:CD1	1:B:277:ALA:CB	2.74	0.55
1:C:141:GLN:CD	1:C:141:GLN:CA	2.79	0.55
1:D:60:LYS:O	1:D:61:LEU:C	2.49	0.55
1:D:74:TYR:CE2	1:D:76:GLU:N	2.74	0.55
1:B:58:LEU:O	1:B:58:LEU:HD13	2.05	0.55
1:B:147:MET:HE3	1:B:220:THR:CG2	2.34	0.55
1:D:226:ASN:ND2	1:D:228:THR:OG1	2.32	0.55
1:A:78:HIS:HB3	1:A:83:ILE:HG12	1.89	0.55
1:A:253:ILE:CD1	1:A:277:ALA:CB	2.74	0.55
1:A:384:ALA:HB1	1:A:411:GLU:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352:HIS:HB2	1:B:353:PRO:CD	2.32	0.55
1:C:120:LEU:C	1:C:120:LEU:HD13	2.31	0.55
1:D:78:HIS:HB3	1:D:83:ILE:HG12	1.89	0.55
1:B:64:MET:CE	1:B:64:MET:SD	2.95	0.55
1:B:271:LEU:HD12	1:B:273:LEU:HD12	1.89	0.55
1:C:23:ARG:HD2	2:D:449:HOH:O	2.05	0.55
1:D:102:PHE:N	1:D:102:PHE:CD1	2.73	0.55
1:D:141:GLN:CD	1:D:141:GLN:CA	2.79	0.55
1:A:112:MET:HE3	1:A:115:LEU:CD1	2.30	0.55
1:A:112:MET:CE	1:A:115:LEU:HD11	2.31	0.55
1:B:160:LYS:H	1:B:376:MET:CE	2.07	0.55
1:C:325:GLU:O	1:C:326:ILE:C	2.49	0.55
1:D:43:ALA:CB	1:D:75:LEU:HD22	2.37	0.55
1:D:112:MET:HA	1:D:113:LYS:HD2	1.87	0.55
1:A:298:LEU:C	1:A:300:LYS:N	2.63	0.55
1:C:74:TYR:CE2	1:C:76:GLU:N	2.74	0.55
1:C:315:ALA:C	1:C:316:VAL:CG2	2.80	0.55
1:D:81:GLY:C	1:D:82:TYR:CD2	2.85	0.55
1:D:352:HIS:CD2	1:D:419:VAL:HG21	2.42	0.55
1:A:28:VAL:HG23	1:A:88:TYR:CE2	2.41	0.55
1:B:352:HIS:CD2	1:B:419:VAL:HG21	2.42	0.55
1:C:156:ALA:O	1:C:370:GLN:HA	2.05	0.55
1:C:206:LEU:HA	1:C:209:VAL:CG2	2.36	0.55
1:C:300:LYS:HD3	1:C:332:PHE:CE1	2.42	0.55
1:C:352:HIS:CD2	1:C:419:VAL:HG21	2.42	0.55
1:D:64:MET:CE	1:D:64:MET:SD	2.95	0.55
1:D:120:LEU:HD13	1:D:120:LEU:C	2.31	0.55
1:D:315:ALA:C	1:D:316:VAL:CG2	2.80	0.55
1:A:15:VAL:CG1	1:A:72:VAL:HB	2.36	0.55
1:A:37:VAL:HG12	1:A:41:GLU:OE2	2.07	0.55
1:A:81:GLY:C	1:A:82:TYR:CD2	2.85	0.55
1:A:183:ASP:C	1:A:184:LEU:HD23	2.32	0.55
1:B:183:ASP:C	1:B:184:LEU:HD23	2.32	0.55
1:B:384:ALA:HB1	1:B:411:GLU:HB3	1.88	0.55
1:C:81:GLY:C	1:C:82:TYR:CD2	2.85	0.55
1:C:102:PHE:CD1	1:C:102:PHE:N	2.73	0.55
1:C:112:MET:CE	1:C:115:LEU:HD11	2.31	0.55
1:A:162:LYS:HD2	1:A:188:ASP:OD2	2.07	0.54
1:B:112:MET:HE3	1:B:115:LEU:CD1	2.30	0.54
1:C:64:MET:CE	1:C:64:MET:SD	2.95	0.54
1:C:128:GLU:OE2	1:D:95:GLU:OE2	2.24	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:384:ALA:HB1	1:C:411:GLU:HB3	1.88	0.54
1:D:112:MET:HE3	1:D:115:LEU:CD1	2.30	0.54
1:D:160:LYS:H	1:D:376:MET:CE	2.07	0.54
1:A:30:TYR:CE1	1:A:120:LEU:CD2	2.90	0.54
1:A:43:ALA:CB	1:A:75:LEU:HD22	2.37	0.54
1:A:141:GLN:CD	1:A:141:GLN:CA	2.79	0.54
1:A:315:ALA:O	1:A:316:VAL:CG2	2.55	0.54
1:C:72:VAL:HG13	1:C:86:ILE:HG12	1.88	0.54
1:D:37:VAL:HG12	1:D:41:GLU:OE2	2.08	0.54
1:D:315:ALA:O	1:D:316:VAL:CG2	2.55	0.54
1:A:315:ALA:C	1:A:316:VAL:CG2	2.80	0.54
1:A:419:VAL:CG2	1:A:419:VAL:HB	2.16	0.54
1:B:98:LEU:O	1:B:101:LEU:HB3	2.08	0.54
1:B:315:ALA:C	1:B:316:VAL:CG2	2.80	0.54
1:C:37:VAL:HG12	1:C:41:GLU:OE2	2.07	0.54
1:C:160:LYS:H	1:C:376:MET:CE	2.07	0.54
1:C:298:LEU:C	1:C:300:LYS:N	2.63	0.54
1:C:315:ALA:O	1:C:316:VAL:CG2	2.55	0.54
1:D:15:VAL:CG1	1:D:72:VAL:HB	2.36	0.54
1:D:183:ASP:C	1:D:184:LEU:HD23	2.32	0.54
1:D:300:LYS:HD3	1:D:332:PHE:CE1	2.42	0.54
1:D:327:LYS:HD3	1:D:331:ASP:OD1	2.08	0.54
1:A:49:GLU:HB3	1:A:109:VAL:HG23	1.90	0.54
1:A:174:ALA:O	1:A:175:TYR:C	2.49	0.54
1:A:271:LEU:HD12	1:A:273:LEU:HD12	1.89	0.54
1:C:11:TYR:CD1	1:C:11:TYR:N	2.59	0.54
1:C:286:THR:HG22	1:C:293:ILE:O	2.08	0.54
1:C:351:LEU:CD2	1:C:359:LEU:HD21	2.37	0.54
1:D:98:LEU:O	1:D:101:LEU:HB3	2.08	0.54
1:D:384:ALA:HB1	1:D:411:GLU:HB3	1.88	0.54
1:A:69:MET:O	1:A:89:PRO:HG3	2.08	0.54
1:B:30:TYR:CE1	1:B:120:LEU:CD2	2.90	0.54
1:B:43:ALA:CB	1:B:75:LEU:HD22	2.37	0.54
1:B:76:GLU:CG	1:B:77:LYS:H	2.21	0.54
1:B:300:LYS:HD3	1:B:332:PHE:CE1	2.42	0.54
1:C:28:VAL:HG23	1:C:88:TYR:CE2	2.41	0.54
1:D:271:LEU:HD12	1:D:273:LEU:HD12	1.89	0.54
1:A:327:LYS:HD3	1:A:331:ASP:OD1	2.08	0.54
1:B:28:VAL:HG23	1:B:88:TYR:CE2	2.41	0.54
1:B:69:MET:O	1:B:89:PRO:HG3	2.08	0.54
1:C:43:ALA:CB	1:C:75:LEU:HD22	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76:GLU:CG	1:C:77:LYS:H	2.21	0.54
1:C:183:ASP:C	1:C:184:LEU:HD23	2.32	0.54
1:A:72:VAL:HG13	1:A:86:ILE:HG12	1.88	0.54
1:A:233:ILE:O	1:A:237:ARG:N	2.39	0.54
1:A:352:HIS:CD2	1:A:419:VAL:HG21	2.42	0.54
1:B:37:VAL:HG12	1:B:41:GLU:OE2	2.07	0.54
1:B:62:PRO:HG3	1:C:165:TRP:CE3	2.41	0.54
1:B:81:GLY:C	1:B:82:TYR:CD2	2.85	0.54
1:B:162:LYS:HD2	1:B:188:ASP:OD2	2.07	0.54
1:B:279:ARG:HH11	1:B:295:MET:HE2	1.73	0.54
1:B:298:LEU:C	1:B:300:LYS:N	2.63	0.54
1:C:23:ARG:HE	1:C:23:ARG:N	2.00	0.54
1:C:49:GLU:HB3	1:C:109:VAL:HG23	1.90	0.54
1:D:160:LYS:CD	1:D:160:LYS:HE2	2.18	0.54
1:A:377:GLY:O	1:A:378:HIS:C	2.49	0.54
1:B:232:ASN:O	1:B:236:LYS:HG3	2.08	0.54
1:B:315:ALA:O	1:B:316:VAL:CG2	2.55	0.54
1:C:98:LEU:O	1:C:101:LEU:HB3	2.08	0.54
1:C:279:ARG:HH11	1:C:295:MET:HE2	1.73	0.54
1:D:204:ARG:O	1:D:208:ARG:CD	2.50	0.54
1:D:279:ARG:HH11	1:D:295:MET:HE2	1.73	0.54
1:D:325:GLU:O	1:D:326:ILE:C	2.49	0.54
1:D:351:LEU:CD2	1:D:359:LEU:HD21	2.37	0.54
1:A:76:GLU:CG	1:A:77:LYS:H	2.21	0.54
1:A:311:HIS:CD2	1:A:346:VAL:CG1	2.79	0.54
1:C:30:TYR:CE1	1:C:120:LEU:CD2	2.90	0.54
1:D:30:TYR:CE1	1:D:120:LEU:CD2	2.90	0.54
1:D:162:LYS:HD2	1:D:188:ASP:OD2	2.07	0.54
1:D:286:THR:HG22	1:D:293:ILE:O	2.08	0.54
1:A:160:LYS:CD	1:A:160:LYS:HE2	2.18	0.54
1:A:232:ASN:O	1:A:236:LYS:HG3	2.08	0.54
1:B:318:LYS:CE	1:C:113:LYS:NZ	2.69	0.54
1:C:162:LYS:HD2	1:C:188:ASP:OD2	2.07	0.54
1:D:49:GLU:HB3	1:D:109:VAL:HG23	1.90	0.54
1:D:232:ASN:O	1:D:236:LYS:HG3	2.08	0.54
1:D:281:MET:O	1:D:281:MET:CG	2.54	0.54
1:D:336:LYS:HD3	1:D:338:GLU:H	1.73	0.54
1:A:300:LYS:HD3	1:A:332:PHE:CE1	2.42	0.53
1:B:113:LYS:O	1:B:115:LEU:N	2.41	0.53
1:B:318:LYS:NZ	1:C:113:LYS:NZ	2.57	0.53
1:B:327:LYS:HD3	1:B:331:ASP:OD1	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:VAL:HG21	1:C:114:ALA:HB1	1.90	0.53
1:C:298:LEU:C	1:C:300:LYS:H	2.16	0.53
1:A:319:MET:C	1:A:321:GLY:H	2.16	0.53
1:B:37:VAL:HG21	1:B:114:ALA:HB1	1.90	0.53
1:B:288:ASN:ND2	1:C:288:ASN:ND2	2.56	0.53
1:B:336:LYS:HD3	1:B:338:GLU:H	1.73	0.53
1:C:78:HIS:HB3	1:C:83:ILE:HG12	1.89	0.53
1:C:119:ARG:HB3	1:C:121:LEU:CD1	2.38	0.53
1:C:232:ASN:O	1:C:236:LYS:HG3	2.08	0.53
1:D:119:ARG:HB3	1:D:121:LEU:CD1	2.38	0.53
1:A:98:LEU:O	1:A:101:LEU:HB3	2.08	0.53
1:A:413:LYS:O	1:A:416:LEU:HB2	2.08	0.53
1:B:92:LEU:HD23	1:C:163:MET:HE2	1.89	0.53
1:C:112:MET:HE3	1:C:115:LEU:CD1	2.30	0.53
1:D:113:LYS:O	1:D:115:LEU:N	2.41	0.53
1:D:286:THR:HG21	1:D:295:MET:HA	1.91	0.53
1:A:286:THR:HG22	1:A:293:ILE:O	2.08	0.53
1:A:351:LEU:CD2	1:A:359:LEU:HD21	2.37	0.53
1:B:325:GLU:O	1:B:326:ILE:C	2.49	0.53
1:B:336:LYS:O	1:B:337:TRP:HB2	2.08	0.53
1:C:174:ALA:O	1:C:175:TYR:C	2.49	0.53
1:D:11:TYR:CD1	1:D:11:TYR:N	2.60	0.53
1:D:37:VAL:HG21	1:D:114:ALA:HB1	1.90	0.53
1:A:9:GLU:O	1:A:9:GLU:HG2	2.05	0.53
1:B:32:PHE:CD2	1:B:34:PRO:HD3	2.44	0.53
1:B:49:GLU:HB3	1:B:109:VAL:HG23	1.90	0.53
1:C:32:PHE:CD2	1:C:34:PRO:HD3	2.44	0.53
1:C:352:HIS:HB2	1:C:353:PRO:CD	2.32	0.53
1:B:225:ILE:HG13	1:B:226:ASN:H	1.74	0.53
1:B:286:THR:HG22	1:B:293:ILE:O	2.08	0.53
1:C:160:LYS:CD	1:C:160:LYS:HE3	2.18	0.53
1:C:271:LEU:HD12	1:C:273:LEU:HD12	1.89	0.53
1:C:327:LYS:HD3	1:C:331:ASP:OD1	2.08	0.53
1:C:336:LYS:O	1:C:337:TRP:HB2	2.08	0.53
1:C:413:LYS:O	1:C:416:LEU:HB2	2.08	0.53
1:D:28:VAL:HG23	1:D:88:TYR:CE2	2.41	0.53
1:A:32:PHE:CD2	1:A:34:PRO:HD3	2.44	0.53
1:A:281:MET:O	1:A:281:MET:CG	2.54	0.53
1:B:113:LYS:HD3	1:C:318:LYS:HE3	1.91	0.53
1:B:286:THR:HG21	1:B:295:MET:HA	1.91	0.53
1:B:351:LEU:CD2	1:B:359:LEU:HD21	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:98:LEU:HD11	1:C:301:ALA:CB	2.36	0.53
1:C:102:PHE:N	1:C:102:PHE:HD1	2.07	0.53
1:C:147:MET:HE3	1:C:147:MET:CB	2.19	0.53
1:D:147:MET:HE3	1:D:147:MET:CB	2.19	0.53
1:A:102:PHE:O	1:A:103:SER:C	2.49	0.53
1:B:74:TYR:CE2	1:B:76:GLU:N	2.74	0.53
1:C:172:GLU:CD	1:C:172:GLU:CB	2.72	0.53
1:D:278:HIS:CG	1:D:311:HIS:HE1	2.26	0.53
1:A:37:VAL:HG21	1:A:114:ALA:HB1	1.90	0.53
1:A:336:LYS:O	1:A:337:TRP:HB2	2.08	0.53
1:B:153:PRO:HB2	1:B:369:ILE:HD11	1.91	0.53
1:B:302:ALA:O	1:B:307:VAL:HG22	2.09	0.53
1:B:377:GLY:O	1:B:378:HIS:C	2.49	0.53
1:C:56:THR:CB	1:C:56:THR:C	2.81	0.53
1:C:69:MET:O	1:C:89:PRO:HG3	2.08	0.53
1:D:76:GLU:CG	1:D:77:LYS:H	2.21	0.53
1:A:113:LYS:O	1:A:115:LEU:N	2.41	0.53
1:B:131:ARG:CG	1:B:132:HIS:ND1	2.72	0.53
1:C:319:MET:C	1:C:321:GLY:H	2.17	0.53
1:D:298:LEU:C	1:D:300:LYS:H	2.16	0.53
1:A:119:ARG:HB3	1:A:121:LEU:CD1	2.38	0.52
1:A:302:ALA:O	1:A:307:VAL:HG22	2.09	0.52
1:B:78:HIS:HB3	1:B:83:ILE:HG12	1.89	0.52
1:B:163:MET:HE2	1:C:92:LEU:HD23	1.91	0.52
1:D:131:ARG:CG	1:D:132:HIS:ND1	2.72	0.52
1:D:352:HIS:HB2	1:D:353:PRO:CD	2.33	0.52
1:B:278:HIS:CG	1:B:311:HIS:HE1	2.26	0.52
1:B:283:ALA:HB3	1:C:110:PHE:CB	2.38	0.52
1:B:413:LYS:O	1:B:416:LEU:HB2	2.08	0.52
1:C:336:LYS:HD3	1:C:338:GLU:H	1.73	0.52
1:D:32:PHE:CD2	1:D:34:PRO:HD3	2.44	0.52
1:D:69:MET:O	1:D:89:PRO:HG3	2.08	0.52
1:A:336:LYS:HD3	1:A:338:GLU:H	1.73	0.52
1:B:102:PHE:N	1:B:102:PHE:HD1	2.07	0.52
1:B:174:ALA:O	1:B:175:TYR:C	2.49	0.52
1:B:192:THR:OG1	1:B:193:SER:N	2.41	0.52
1:B:215:ALA:O	1:B:216:GLU:O	2.28	0.52
1:B:319:MET:C	1:B:321:GLY:H	2.16	0.52
1:C:113:LYS:O	1:C:115:LEU:N	2.41	0.52
1:D:102:PHE:N	1:D:102:PHE:HD1	2.07	0.52
1:D:413:LYS:O	1:D:416:LEU:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:ARG:HB3	1:B:121:LEU:CD1	2.38	0.52
1:C:302:ALA:O	1:C:307:VAL:HG22	2.09	0.52
1:D:233:ILE:O	1:D:237:ARG:N	2.39	0.52
1:A:153:PRO:HB2	1:A:369:ILE:HD11	1.91	0.52
1:B:315:ALA:O	1:B:316:VAL:HG23	2.09	0.52
1:A:56:THR:CB	1:A:56:THR:C	2.81	0.52
1:B:298:LEU:C	1:B:300:LYS:H	2.16	0.52
1:C:102:PHE:O	1:C:103:SER:C	2.49	0.52
1:C:157:THR:HG21	1:C:177:LEU:HD21	1.92	0.52
1:A:131:ARG:CG	1:A:132:HIS:ND1	2.72	0.52
1:B:345:PRO:HB2	1:B:367:LEU:CD2	2.40	0.52
1:C:211:ASP:O	1:C:212:ARG:C	2.52	0.52
1:D:302:ALA:O	1:D:307:VAL:HG22	2.09	0.52
1:A:211:ASP:O	1:A:212:ARG:C	2.53	0.52
1:A:278:HIS:CG	1:A:311:HIS:HE1	2.27	0.52
1:C:278:HIS:CG	1:C:311:HIS:HE1	2.27	0.52
1:D:319:MET:C	1:D:321:GLY:H	2.17	0.52
1:D:389:LEU:O	1:D:389:LEU:HD12	2.10	0.52
1:A:157:THR:HG21	1:A:177:LEU:HD21	1.92	0.52
1:A:215:ALA:O	1:A:216:GLU:O	2.28	0.52
1:A:227:ILE:O	1:A:227:ILE:HG13	2.07	0.52
2:B:466:HOH:O	1:C:281:MET:HE1	2.10	0.52
1:C:389:LEU:O	1:C:389:LEU:HD12	2.10	0.52
1:D:147:MET:CE	1:D:220:THR:HG22	2.39	0.52
1:D:303:ARG:NH2	1:D:342:PRO:CA	2.46	0.52
1:D:345:PRO:HB2	1:D:367:LEU:CD2	2.40	0.52
1:A:286:THR:HG21	1:A:295:MET:HA	1.91	0.52
1:C:315:ALA:O	1:C:316:VAL:HG23	2.09	0.52
1:D:153:PRO:HB2	1:D:369:ILE:HD11	1.91	0.52
1:A:102:PHE:N	1:A:102:PHE:HD1	2.07	0.51
1:A:315:ALA:O	1:A:316:VAL:HG23	2.09	0.51
1:B:113:LYS:NZ	1:C:318:LYS:CE	2.73	0.51
1:D:278:HIS:CG	1:D:311:HIS:CE1	2.99	0.51
1:D:336:LYS:O	1:D:337:TRP:HB2	2.08	0.51
1:A:226:ASN:ND2	1:A:228:THR:OG1	2.32	0.51
1:B:56:THR:CB	1:B:56:THR:C	2.81	0.51
1:B:233:ILE:O	1:B:237:ARG:N	2.39	0.51
1:D:172:GLU:CD	1:D:172:GLU:CB	2.72	0.51
1:D:315:ALA:O	1:D:316:VAL:HG23	2.09	0.51
1:A:389:LEU:O	1:A:389:LEU:HD12	2.10	0.51
1:D:174:ALA:O	1:D:175:TYR:C	2.49	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:215:ALA:O	1:D:216:GLU:O	2.28	0.51
1:A:23:ARG:HE	1:A:23:ARG:N	2.00	0.51
1:A:345:PRO:HB2	1:A:367:LEU:CD2	2.40	0.51
1:B:98:LEU:HD11	1:B:301:ALA:CB	2.36	0.51
1:B:157:THR:HG21	1:B:177:LEU:HD21	1.92	0.51
1:B:288:ASN:HD21	1:C:288:ASN:HD21	1.58	0.51
1:C:286:THR:HG21	1:C:295:MET:HA	1.91	0.51
1:A:279:ARG:HH11	1:A:295:MET:HE2	1.73	0.51
1:C:59:TRP:CG	1:C:60:LYS:N	2.79	0.51
1:C:153:PRO:HB2	1:C:369:ILE:HD11	1.91	0.51
1:C:157:THR:HG21	1:C:177:LEU:CD2	2.41	0.51
1:C:215:ALA:O	1:C:216:GLU:O	2.28	0.51
1:C:345:PRO:HB2	1:C:367:LEU:CD2	2.40	0.51
1:C:377:GLY:O	1:C:378:HIS:C	2.49	0.51
1:A:59:TRP:CG	1:A:60:LYS:N	2.79	0.51
1:A:192:THR:OG1	1:A:193:SER:N	2.41	0.51
1:B:95:GLU:OE1	1:B:132:HIS:CE1	2.64	0.51
1:B:178:TRP:CD1	1:B:221:LYS:HB3	2.46	0.51
1:B:278:HIS:CG	1:B:311:HIS:CE1	2.98	0.51
1:C:178:TRP:CD1	1:C:221:LYS:HB3	2.46	0.51
1:D:157:THR:HG21	1:D:177:LEU:HD21	1.92	0.51
1:D:227:ILE:O	1:D:227:ILE:HG13	2.07	0.51
1:C:131:ARG:CG	1:C:132:HIS:ND1	2.72	0.51
1:D:151:ASP:O	1:D:152:ARG:O	2.28	0.51
1:A:178:TRP:CD1	1:A:221:LYS:HB3	2.46	0.51
1:A:279:ARG:CD	1:A:295:MET:HE2	2.39	0.51
1:B:59:TRP:CG	1:B:60:LYS:N	2.79	0.51
1:B:384:ALA:HB1	1:B:411:GLU:CB	2.41	0.51
1:A:151:ASP:O	1:A:152:ARG:O	2.28	0.51
1:B:102:PHE:O	1:B:103:SER:C	2.49	0.51
1:B:172:GLU:CD	1:B:172:GLU:CB	2.72	0.51
1:C:151:ASP:O	1:C:152:ARG:O	2.28	0.51
1:C:352:HIS:O	1:C:353:PRO:C	2.54	0.51
1:D:233:ILE:O	1:D:233:ILE:HG22	2.07	0.51
1:D:347:ALA:HB3	1:D:369:ILE:HA	1.93	0.51
1:A:298:LEU:C	1:A:300:LYS:H	2.16	0.51
1:B:151:ASP:O	1:B:152:ARG:O	2.28	0.51
1:D:178:TRP:CD1	1:D:221:LYS:HB3	2.46	0.51
1:A:278:HIS:CG	1:A:311:HIS:CE1	2.99	0.50
1:A:352:HIS:HB2	1:A:353:PRO:CD	2.32	0.50
1:B:58:LEU:HG	1:C:381:GLY:HA2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:MET:HE2	1:C:92:LEU:HD22	1.93	0.50
1:C:95:GLU:OE1	1:C:132:HIS:CE1	2.64	0.50
1:C:227:ILE:O	1:C:227:ILE:HG13	2.07	0.50
1:D:34:PRO:HB3	1:D:37:VAL:HG23	1.93	0.50
1:D:47:ALA:HB1	1:D:70:ALA:HB3	1.93	0.50
1:D:95:GLU:OE1	1:D:132:HIS:CE1	2.64	0.50
1:D:117:ASN:ND2	1:D:290:ARG:CB	2.63	0.50
1:B:28:VAL:HG11	1:B:30:TYR:CZ	2.47	0.50
1:B:51:SER:OG	1:B:52:ILE:N	2.41	0.50
1:B:110:PHE:C	1:C:283:ALA:CB	2.83	0.50
1:C:233:ILE:O	1:C:237:ARG:N	2.39	0.50
1:A:56:THR:CA	1:A:56:THR:CG2	2.87	0.50
1:A:157:THR:HG21	1:A:177:LEU:CD2	2.41	0.50
1:B:34:PRO:HB3	1:B:37:VAL:HG23	1.93	0.50
1:B:281:MET:O	1:B:281:MET:CG	2.54	0.50
1:C:10:TRP:CE3	1:C:10:TRP:CA	2.91	0.50
1:C:28:VAL:HG11	1:C:30:TYR:CZ	2.46	0.50
1:C:278:HIS:CG	1:C:311:HIS:CE1	2.98	0.50
1:C:281:MET:O	1:C:281:MET:CG	2.54	0.50
1:C:384:ALA:HB1	1:C:411:GLU:CB	2.41	0.50
1:D:343:VAL:HG12	1:D:344:PHE:H	1.76	0.50
1:A:137:GLN:O	1:A:137:GLN:CG	2.60	0.50
1:A:347:ALA:HB3	1:A:369:ILE:HA	1.93	0.50
1:B:10:TRP:CE3	1:B:10:TRP:CA	2.91	0.50
1:B:294:THR:C	1:B:296:LEU:N	2.68	0.50
1:B:347:ALA:HB3	1:B:369:ILE:HA	1.93	0.50
1:D:98:LEU:HD11	1:D:301:ALA:CB	2.36	0.50
1:D:157:THR:HG21	1:D:177:LEU:CD2	2.41	0.50
1:A:212:ARG:O	1:A:216:GLU:HB2	2.12	0.50
1:A:286:THR:HG22	1:A:295:MET:N	2.27	0.50
1:B:55:TRP:CH2	1:C:376:MET:O	2.65	0.50
1:B:92:LEU:HD22	1:C:163:MET:HE2	1.92	0.50
1:B:389:LEU:O	1:B:389:LEU:HD12	2.10	0.50
1:C:212:ARG:O	1:C:216:GLU:HB2	2.12	0.50
1:C:343:VAL:HG12	1:C:344:PHE:H	1.76	0.50
1:A:75:LEU:C	1:A:75:LEU:HD12	2.37	0.50
1:C:47:ALA:HB1	1:C:70:ALA:HB3	1.93	0.50
1:C:347:ALA:HB3	1:C:369:ILE:HA	1.93	0.50
1:D:384:ALA:HB1	1:D:411:GLU:CB	2.41	0.50
1:A:28:VAL:HG11	1:A:30:TYR:CZ	2.47	0.50
1:A:47:ALA:HB1	1:A:70:ALA:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:GLU:OE1	1:A:132:HIS:CE1	2.64	0.50
1:A:147:MET:CE	1:A:220:THR:HG22	2.39	0.50
1:B:15:VAL:HG13	1:B:72:VAL:HG23	1.92	0.50
1:B:157:THR:HG21	1:B:177:LEU:CD2	2.41	0.50
1:B:176:GLU:HG3	1:C:59:TRP:CH2	2.46	0.50
1:B:206:LEU:HA	1:B:209:VAL:HG23	1.94	0.50
1:B:233:ILE:O	1:B:233:ILE:HG22	2.07	0.50
1:B:286:THR:HG22	1:B:295:MET:N	2.27	0.50
1:B:343:VAL:HG12	1:B:344:PHE:H	1.76	0.50
1:C:34:PRO:HB3	1:C:37:VAL:HG23	1.93	0.50
1:C:51:SER:OG	1:C:52:ILE:N	2.41	0.50
1:C:137:GLN:HB2	1:C:265:ARG:CZ	2.42	0.50
1:D:28:VAL:HG11	1:D:30:TYR:CZ	2.47	0.50
1:A:294:THR:C	1:A:296:LEU:N	2.68	0.50
1:A:343:VAL:HG12	1:A:344:PHE:H	1.76	0.50
1:B:212:ARG:O	1:B:216:GLU:HB2	2.12	0.50
1:C:138:PHE:CD1	1:C:146:PHE:CE1	2.99	0.50
1:A:10:TRP:CE3	1:A:10:TRP:CA	2.91	0.49
1:A:34:PRO:HB3	1:A:37:VAL:HG23	1.94	0.49
1:A:384:ALA:HB1	1:A:411:GLU:CB	2.41	0.49
1:B:137:GLN:O	1:B:137:GLN:CG	2.60	0.49
1:C:268:THR:HB	1:C:273:LEU:O	2.12	0.49
1:D:137:GLN:O	1:D:137:GLN:CG	2.60	0.49
1:D:294:THR:C	1:D:296:LEU:N	2.68	0.49
1:A:51:SER:OG	1:A:52:ILE:N	2.41	0.49
1:B:279:ARG:CD	1:B:295:MET:HE2	2.39	0.49
1:D:268:THR:HB	1:D:273:LEU:O	2.12	0.49
1:D:286:THR:HG22	1:D:295:MET:N	2.27	0.49
1:B:113:LYS:NZ	1:C:318:LYS:NZ	2.60	0.49
1:B:147:MET:CE	1:B:220:THR:HG22	2.39	0.49
1:B:160:LYS:CD	1:B:160:LYS:HE3	2.18	0.49
1:B:352:HIS:O	1:B:353:PRO:C	2.54	0.49
1:C:137:GLN:O	1:C:137:GLN:CG	2.60	0.49
1:C:300:LYS:HD2	1:C:337:TRP:CH2	2.47	0.49
1:D:21:PRO:O	1:D:21:PRO:HG2	2.13	0.49
1:D:102:PHE:O	1:D:103:SER:C	2.49	0.49
1:A:38:SER:HB2	1:A:40:GLU:H	1.77	0.49
1:A:225:ILE:HG13	1:A:226:ASN:H	1.74	0.49
1:B:47:ALA:HB1	1:B:70:ALA:HB3	1.93	0.49
1:B:130:LEU:HG	1:B:130:LEU:O	2.13	0.49
1:B:211:ASP:O	1:B:212:ARG:C	2.52	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:THR:HB	1:B:273:LEU:O	2.12	0.49
1:D:38:SER:HB2	1:D:40:GLU:H	1.77	0.49
1:D:59:TRP:CG	1:D:60:LYS:N	2.79	0.49
1:D:75:LEU:C	1:D:75:LEU:HD12	2.37	0.49
1:D:134:LYS:HZ2	1:D:266:GLU:HG3	1.78	0.49
1:C:279:ARG:CD	1:C:295:MET:HE2	2.39	0.49
1:D:55:TRP:CH2	1:D:58:LEU:N	2.76	0.49
1:A:15:VAL:HG13	1:A:72:VAL:HG23	1.91	0.49
1:A:130:LEU:HG	1:A:130:LEU:O	2.13	0.49
1:A:268:THR:HB	1:A:273:LEU:O	2.12	0.49
1:B:9:GLU:O	1:B:9:GLU:HG2	2.05	0.49
1:B:38:SER:HB2	1:B:40:GLU:H	1.77	0.49
1:C:94:GLU:HG2	1:C:97:SER:CB	2.40	0.49
1:D:51:SER:OG	1:D:52:ILE:N	2.41	0.49
1:D:137:GLN:HB2	1:D:265:ARG:CZ	2.42	0.49
1:D:212:ARG:O	1:D:216:GLU:HB2	2.12	0.49
1:D:300:LYS:HD2	1:D:337:TRP:CH2	2.47	0.49
1:D:311:HIS:CD2	1:D:346:VAL:CG1	2.79	0.49
1:D:377:GLY:O	1:D:378:HIS:C	2.49	0.49
1:A:19:TYR:HD1	1:A:21:PRO:HD3	1.78	0.49
1:B:19:TYR:HD1	1:B:21:PRO:HD3	1.78	0.49
1:B:138:PHE:CD1	1:B:146:PHE:CE1	2.99	0.49
1:B:293:ILE:CG2	1:B:297:ALA:HB3	2.43	0.49
1:C:38:SER:HB2	1:C:40:GLU:H	1.77	0.49
1:C:75:LEU:C	1:C:75:LEU:HD12	2.37	0.49
1:D:19:TYR:HD1	1:D:21:PRO:HD3	1.78	0.49
1:A:98:LEU:HD11	1:A:301:ALA:CB	2.36	0.49
1:A:293:ILE:CG2	1:A:297:ALA:HB3	2.43	0.49
1:B:45:ARG:HA	1:B:48:SER:HB3	1.95	0.49
1:B:343:VAL:CG1	1:B:344:PHE:N	2.75	0.49
1:C:45:ARG:HA	1:C:48:SER:HB3	1.95	0.49
1:C:55:TRP:CD2	1:C:57:THR:CG2	2.71	0.49
1:C:130:LEU:O	1:C:130:LEU:HG	2.13	0.49
1:C:215:ALA:C	1:C:216:GLU:C	2.81	0.49
1:D:205:LYS:O	1:D:209:VAL:CG2	2.61	0.49
1:D:206:LEU:HA	1:D:209:VAL:HG23	1.94	0.49
1:D:211:ASP:O	1:D:212:ARG:C	2.53	0.49
1:A:137:GLN:HB2	1:A:265:ARG:CZ	2.42	0.49
1:B:21:PRO:HG2	1:B:21:PRO:O	2.13	0.49
1:B:32:PHE:HE2	1:B:42:ALA:HB3	1.78	0.49
1:B:32:PHE:C	1:B:33:GLU:HG3	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:LYS:HD2	1:B:337:TRP:CH2	2.47	0.49
1:B:336:LYS:CE	1:B:336:LYS:HD3	2.20	0.49
1:C:32:PHE:C	1:C:33:GLU:HG3	2.37	0.49
1:C:205:LYS:O	1:C:209:VAL:CG2	2.61	0.49
1:A:32:PHE:HE2	1:A:42:ALA:HB3	1.78	0.49
1:A:254:VAL:HG23	1:A:279:ARG:HA	1.95	0.49
1:C:254:VAL:HG23	1:C:279:ARG:HA	1.95	0.49
1:C:286:THR:HG22	1:C:295:MET:N	2.27	0.49
1:D:279:ARG:CD	1:D:295:MET:HE2	2.39	0.49
1:D:293:ILE:CG2	1:D:297:ALA:HB3	2.43	0.49
1:A:206:LEU:HA	1:A:209:VAL:HG23	1.94	0.48
1:A:351:LEU:HD12	1:A:351:LEU:N	2.28	0.48
1:B:227:ILE:O	1:B:227:ILE:HG13	2.07	0.48
1:B:283:ALA:CB	1:C:110:PHE:C	2.86	0.48
1:C:178:TRP:CZ2	1:C:185:LEU:HB2	2.48	0.48
1:C:220:THR:CG2	1:C:221:LYS:N	2.76	0.48
1:D:45:ARG:O	1:D:46:ILE:C	2.56	0.48
1:D:64:MET:HG3	1:D:64:MET:O	2.12	0.48
1:D:118:LEU:HD12	1:D:119:ARG:N	2.28	0.48
1:A:118:LEU:HD12	1:A:119:ARG:N	2.28	0.48
1:A:138:PHE:CD1	1:A:146:PHE:CE1	2.99	0.48
1:B:176:GLU:HG3	1:C:59:TRP:CZ2	2.48	0.48
1:C:56:THR:CA	1:C:56:THR:CG2	2.87	0.48
1:C:64:MET:O	1:C:64:MET:HG3	2.12	0.48
1:D:215:ALA:C	1:D:216:GLU:C	2.81	0.48
1:D:254:VAL:HG23	1:D:279:ARG:HA	1.95	0.48
1:A:21:PRO:O	1:A:21:PRO:HG2	2.13	0.48
1:A:178:TRP:CZ2	1:A:185:LEU:HB2	2.48	0.48
1:A:300:LYS:HD2	1:A:337:TRP:CH2	2.47	0.48
1:B:257:GLY:CA	1:C:257:GLY:HA3	2.43	0.48
1:B:303:ARG:NH2	1:B:342:PRO:CA	2.46	0.48
1:C:52:ILE:HD13	1:C:69:MET:HG2	1.96	0.48
1:C:206:LEU:HA	1:C:209:VAL:HG23	1.94	0.48
1:D:178:TRP:CZ2	1:D:185:LEU:HB2	2.48	0.48
1:D:351:LEU:HD12	1:D:351:LEU:N	2.28	0.48
1:A:45:ARG:HA	1:A:48:SER:HB3	1.95	0.48
1:A:206:LEU:HD22	1:A:206:LEU:N	2.29	0.48
1:B:75:LEU:HD12	1:B:75:LEU:C	2.37	0.48
1:B:83:ILE:O	1:B:83:ILE:HG22	2.14	0.48
1:B:178:TRP:CZ2	1:B:185:LEU:HB2	2.48	0.48
1:B:281:MET:HE1	2:C:469:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:189:GLU:HA	1:C:250:MET:CE	2.44	0.48
1:A:352:HIS:O	1:A:353:PRO:C	2.54	0.48
1:B:27:ILE:HG23	1:B:87:ALA:HA	1.96	0.48
1:B:55:TRP:HZ2	1:C:377:GLY:HA2	1.78	0.48
1:B:119:ARG:O	1:B:121:LEU:HD13	2.14	0.48
1:B:193:SER:OG	1:B:199:PHE:N	2.46	0.48
1:B:215:ALA:C	1:B:216:GLU:C	2.81	0.48
1:C:21:PRO:O	1:C:21:PRO:HG2	2.13	0.48
1:D:119:ARG:O	1:D:121:LEU:HD13	2.14	0.48
1:A:52:ILE:HD13	1:A:69:MET:HG2	1.96	0.48
1:A:94:GLU:HG2	1:A:97:SER:CB	2.40	0.48
1:B:137:GLN:HB2	1:B:265:ARG:CZ	2.42	0.48
1:B:189:GLU:HA	1:B:250:MET:CE	2.44	0.48
1:B:205:LYS:O	1:B:209:VAL:CG2	2.61	0.48
1:C:19:TYR:HD1	1:C:21:PRO:HD3	1.78	0.48
1:C:83:ILE:O	1:C:83:ILE:HG22	2.14	0.48
1:C:119:ARG:O	1:C:121:LEU:HD13	2.14	0.48
1:D:10:TRP:CE3	1:D:10:TRP:CA	2.91	0.48
1:D:45:ARG:HA	1:D:48:SER:HB3	1.95	0.48
1:D:296:LEU:HB2	1:D:329:ILE:HG12	1.95	0.48
1:A:45:ARG:O	1:A:46:ILE:C	2.56	0.48
1:A:64:MET:HG3	1:A:64:MET:O	2.12	0.48
1:A:215:ALA:C	1:A:216:GLU:C	2.81	0.48
1:A:296:LEU:HB2	1:A:329:ILE:HG12	1.96	0.48
1:B:64:MET:HG3	1:B:64:MET:O	2.12	0.48
1:C:9:GLU:O	1:C:9:GLU:HG2	2.05	0.48
1:C:189:GLU:HB3	1:C:278:HIS:CE1	2.49	0.48
1:D:27:ILE:HG23	1:D:87:ALA:HA	1.96	0.48
1:D:32:PHE:C	1:D:33:GLU:HG3	2.37	0.48
1:D:56:THR:CB	1:D:56:THR:C	2.81	0.48
1:D:352:HIS:O	1:D:353:PRO:C	2.54	0.48
1:A:32:PHE:C	1:A:33:GLU:HG3	2.37	0.48
1:A:220:THR:CG2	1:A:221:LYS:N	2.76	0.48
1:B:118:LEU:HD12	1:B:119:ARG:N	2.28	0.48
1:C:118:LEU:HD12	1:C:119:ARG:N	2.28	0.48
1:C:124:HIS:HA	1:C:125:PRO:HD3	1.45	0.48
1:D:166:SER:OG	1:D:169:GLU:HG3	2.14	0.48
1:D:189:GLU:HA	1:D:250:MET:CE	2.44	0.48
1:D:193:SER:OG	1:D:199:PHE:N	2.46	0.48
1:A:27:ILE:HG23	1:A:87:ALA:HA	1.96	0.48
1:B:189:GLU:HB3	1:B:278:HIS:CE1	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:294:THR:C	1:C:296:LEU:N	2.68	0.48
1:A:83:ILE:O	1:A:83:ILE:HG22	2.14	0.48
1:A:189:GLU:HB3	1:A:278:HIS:CE1	2.49	0.48
1:B:57:THR:CA	1:B:57:THR:CG2	2.87	0.48
1:C:130:LEU:C	1:C:132:HIS:H	2.22	0.48
1:C:293:ILE:CG2	1:C:297:ALA:HB3	2.43	0.48
1:C:294:THR:O	1:C:295:MET:C	2.57	0.48
1:D:206:LEU:HD22	1:D:206:LEU:N	2.29	0.48
1:D:343:VAL:CG1	1:D:344:PHE:N	2.76	0.48
1:A:130:LEU:C	1:A:132:HIS:H	2.22	0.47
1:B:273:LEU:HA	1:B:273:LEU:HD23	1.66	0.47
1:D:52:ILE:HD13	1:D:69:MET:HG2	1.96	0.47
1:A:193:SER:OG	1:A:199:PHE:N	2.46	0.47
1:A:279:ARG:HD3	1:A:295:MET:HE1	1.96	0.47
1:B:130:LEU:C	1:B:132:HIS:H	2.22	0.47
1:B:167:VAL:HG23	1:B:196:PHE:O	2.14	0.47
1:B:254:VAL:HG23	1:B:279:ARG:HA	1.95	0.47
1:B:294:THR:O	1:B:295:MET:C	2.57	0.47
1:B:296:LEU:HB2	1:B:329:ILE:HG12	1.95	0.47
1:C:134:LYS:HZ2	1:C:266:GLU:HG3	1.77	0.47
1:C:193:SER:OG	1:C:199:PHE:N	2.46	0.47
1:D:138:PHE:CD1	1:D:146:PHE:CE1	2.99	0.47
1:D:225:ILE:HG13	1:D:226:ASN:H	1.74	0.47
1:D:294:THR:O	1:D:295:MET:C	2.57	0.47
1:A:88:TYR:HA	1:A:89:PRO:HD3	1.69	0.47
1:A:166:SER:OG	1:A:169:GLU:HG3	2.14	0.47
1:A:294:THR:O	1:A:295:MET:C	2.57	0.47
1:B:108:ASN:N	1:B:108:ASN:OD1	2.48	0.47
1:C:57:THR:CA	1:C:57:THR:CG2	2.87	0.47
1:C:170:TYR:CE1	1:C:191:PHE:HE1	2.33	0.47
1:C:351:LEU:N	1:C:351:LEU:HD12	2.28	0.47
1:A:108:ASN:OD1	1:A:108:ASN:N	2.48	0.47
1:A:263:TYR:HE2	1:A:267:VAL:CG2	2.27	0.47
1:B:254:VAL:O	1:B:281:MET:HE2	2.14	0.47
1:B:318:LYS:HE3	1:C:113:LYS:HD3	1.97	0.47
1:C:166:SER:OG	1:C:169:GLU:HG3	2.14	0.47
1:C:206:LEU:HD22	1:C:206:LEU:N	2.29	0.47
1:C:296:LEU:HB2	1:C:329:ILE:HG12	1.95	0.47
1:D:130:LEU:HG	1:D:130:LEU:O	2.13	0.47
1:D:254:VAL:O	1:D:281:MET:HE2	2.14	0.47
1:A:55:TRP:CH2	1:A:58:LEU:N	2.76	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:LEU:N	1:B:206:LEU:HD22	2.29	0.47
1:C:45:ARG:O	1:C:46:ILE:C	2.56	0.47
1:C:167:VAL:HG23	1:C:196:PHE:O	2.15	0.47
1:D:32:PHE:HE2	1:D:42:ALA:HB3	1.78	0.47
1:A:119:ARG:O	1:A:121:LEU:HD13	2.14	0.47
1:A:170:TYR:CE1	1:A:191:PHE:HE1	2.33	0.47
1:B:30:TYR:CE1	1:B:120:LEU:HD22	2.50	0.47
1:B:351:LEU:HD12	1:B:351:LEU:N	2.28	0.47
1:C:192:THR:OG1	1:C:193:SER:N	2.41	0.47
1:D:9:GLU:HG2	1:D:9:GLU:O	2.05	0.47
1:D:400:VAL:H	1:D:400:VAL:HG23	1.42	0.47
1:A:195:PRO:HG2	1:B:131:ARG:HE	1.80	0.47
1:A:273:LEU:HA	1:A:273:LEU:HD23	1.66	0.47
1:B:166:SER:OG	1:B:169:GLU:HG3	2.14	0.47
1:C:233:ILE:O	1:C:233:ILE:HG22	2.07	0.47
1:C:253:ILE:HD12	1:C:253:ILE:HG21	1.62	0.47
1:D:170:TYR:CE1	1:D:191:PHE:HE1	2.33	0.47
1:D:189:GLU:HB3	1:D:278:HIS:CE1	2.49	0.47
1:D:263:TYR:HE2	1:D:267:VAL:CG2	2.28	0.47
1:A:154:LEU:HA	1:A:154:LEU:HD23	1.40	0.47
1:C:160:LYS:HZ2	1:C:373:GLY:CA	2.28	0.47
1:C:263:TYR:HE2	1:C:267:VAL:CG2	2.27	0.47
1:C:343:VAL:CG1	1:C:344:PHE:N	2.75	0.47
1:D:46:ILE:HA	1:D:112:MET:HE1	1.97	0.47
1:A:57:THR:CA	1:A:57:THR:CG2	2.87	0.47
1:A:189:GLU:HA	1:A:250:MET:CE	2.44	0.47
1:C:32:PHE:HE2	1:C:42:ALA:HB3	1.78	0.47
1:C:58:LEU:O	1:C:58:LEU:CD1	2.63	0.47
1:C:147:MET:CE	1:C:220:THR:HG22	2.39	0.47
1:C:252:ASP:CB	1:C:255:VAL:CG2	2.89	0.47
1:C:271:LEU:H	1:C:271:LEU:HG	1.47	0.47
1:D:57:THR:CA	1:D:57:THR:CG2	2.87	0.47
1:A:167:VAL:HG23	1:A:196:PHE:O	2.14	0.47
1:B:52:ILE:HD13	1:B:69:MET:HG2	1.96	0.47
1:B:56:THR:CA	1:B:56:THR:CG2	2.87	0.47
1:C:46:ILE:HA	1:C:112:MET:HE1	1.97	0.47
1:C:383:ARG:O	1:C:383:ARG:HG2	2.15	0.47
1:D:130:LEU:C	1:D:132:HIS:H	2.22	0.47
1:A:30:TYR:CE1	1:A:120:LEU:HD22	2.50	0.46
1:B:58:LEU:O	1:B:58:LEU:CD1	2.63	0.46
1:C:225:ILE:HG13	1:C:226:ASN:H	1.74	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:167:VAL:HG23	1:D:196:PHE:O	2.15	0.46
1:A:46:ILE:HA	1:A:112:MET:HE1	1.97	0.46
1:C:30:TYR:CE1	1:C:120:LEU:HD22	2.50	0.46
1:C:254:VAL:O	1:C:281:MET:HE2	2.14	0.46
1:D:58:LEU:O	1:D:58:LEU:CD1	2.63	0.46
1:D:282:HIS:C	1:D:284:ALA:H	2.24	0.46
1:D:378:HIS:HE1	1:D:380:ASP:CB	2.14	0.46
1:A:11:TYR:CE2	1:A:45:ARG:HG2	2.51	0.46
1:A:254:VAL:O	1:A:281:MET:HE2	2.14	0.46
1:A:279:ARG:O	1:A:281:MET:N	2.48	0.46
1:B:125:PRO:HA	1:B:126:PRO:HD2	1.69	0.46
1:B:268:THR:HG23	1:B:268:THR:H	1.42	0.46
1:B:282:HIS:C	1:B:284:ALA:H	2.24	0.46
1:C:27:ILE:HG23	1:C:87:ALA:HA	1.96	0.46
1:C:268:THR:HG23	1:C:268:THR:H	1.42	0.46
1:C:409:SER:HA	1:C:410:PRO:HD2	1.63	0.46
1:D:383:ARG:O	1:D:383:ARG:HG2	2.15	0.46
1:A:343:VAL:CG1	1:A:344:PHE:N	2.76	0.46
1:B:220:THR:CG2	1:B:221:LYS:N	2.76	0.46
1:B:275:ILE:HG21	1:B:275:ILE:HD13	1.17	0.46
1:D:47:ALA:HB2	1:D:86:ILE:HG21	1.97	0.46
1:B:138:PHE:CE1	1:B:146:PHE:HE1	2.34	0.46
1:B:263:TYR:HE2	1:B:267:VAL:CG2	2.28	0.46
1:C:47:ALA:HB2	1:C:86:ILE:HG21	1.97	0.46
1:C:279:ARG:O	1:C:281:MET:N	2.48	0.46
1:D:110:PHE:HE1	1:D:293:ILE:HD11	1.81	0.46
1:D:154:LEU:CB	1:D:368:VAL:HG13	2.44	0.46
1:B:336:LYS:CE	1:B:336:LYS:HD2	2.20	0.46
1:B:341:ARG:HB2	1:B:342:PRO:HD2	1.98	0.46
1:D:26:LEU:HD12	1:D:124:HIS:O	2.16	0.46
1:A:26:LEU:HD12	1:A:124:HIS:O	2.16	0.46
1:A:153:PRO:HB2	1:A:369:ILE:CD1	2.46	0.46
1:A:182:ILE:HG12	1:A:386:ALA:HB1	1.98	0.46
1:A:188:ASP:C	1:A:190:ASN:H	2.19	0.46
1:A:401:ASP:CB	1:A:404:GLU:HG2	2.36	0.46
1:B:46:ILE:HA	1:B:112:MET:HE1	1.97	0.46
1:B:383:ARG:O	1:B:383:ARG:HG2	2.15	0.46
1:B:388:ALA:C	1:B:390:ARG:N	2.74	0.46
1:C:44:GLY:O	1:C:45:ARG:C	2.57	0.46
1:C:188:ASP:C	1:C:190:ASN:H	2.19	0.46
1:D:387:LYS:HE3	2:D:465:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:ILE:O	1:A:233:ILE:HG22	2.07	0.46
1:A:409:SER:HB3	1:A:412:LEU:HB3	1.98	0.46
1:B:47:ALA:HB2	1:B:86:ILE:HG21	1.97	0.46
1:B:55:TRP:CZ2	1:C:376:MET:O	2.69	0.46
1:B:170:TYR:CE1	1:B:191:PHE:HE1	2.33	0.46
1:B:279:ARG:O	1:B:281:MET:N	2.48	0.46
1:B:285:PHE:HB3	1:C:284:ALA:O	2.15	0.46
1:C:32:PHE:CE2	1:C:42:ALA:HB3	2.51	0.46
1:C:64:MET:HE1	1:D:338:GLU:HA	1.97	0.46
1:C:154:LEU:CB	1:C:368:VAL:HG13	2.44	0.46
1:C:187:ASP:OD1	1:C:223:TYR:HE1	1.99	0.46
1:D:56:THR:CA	1:D:56:THR:CG2	2.87	0.46
1:A:189:GLU:CB	1:A:278:HIS:CE1	2.99	0.46
1:A:210:ARG:HD3	1:A:221:LYS:O	2.16	0.46
1:A:390:ARG:HD2	1:A:390:ARG:HA	1.83	0.46
1:B:257:GLY:HA3	1:C:257:GLY:CA	2.42	0.46
1:B:409:SER:HB3	1:B:412:LEU:HB3	1.98	0.46
1:C:138:PHE:CE1	1:C:146:PHE:HE1	2.34	0.46
1:C:144:ARG:NH1	1:C:150:LYS:O	2.49	0.46
1:C:160:LYS:CE	1:C:160:LYS:CG	2.84	0.46
1:C:189:GLU:CB	1:C:278:HIS:CE1	2.99	0.46
1:C:210:ARG:HD3	1:C:221:LYS:O	2.16	0.46
1:D:44:GLY:O	1:D:45:ARG:C	2.57	0.46
1:D:177:LEU:HD23	1:D:177:LEU:HA	1.75	0.46
1:A:58:LEU:O	1:A:58:LEU:CD1	2.63	0.46
1:A:187:ASP:OD1	1:A:223:TYR:HE1	1.99	0.46
1:B:45:ARG:O	1:B:46:ILE:C	2.56	0.46
1:B:182:ILE:HG12	1:B:386:ALA:HB1	1.98	0.46
1:B:189:GLU:CB	1:B:278:HIS:CE1	2.99	0.46
1:B:373:GLY:O	1:B:374:GLY:C	2.59	0.46
1:D:175:TYR:CE2	1:D:213:VAL:CG2	2.99	0.46
1:A:282:HIS:C	1:A:284:ALA:H	2.24	0.45
1:B:55:TRP:CE2	1:B:57:THR:HG21	2.51	0.45
1:B:113:LYS:HZ1	1:C:318:LYS:NZ	2.14	0.45
1:B:282:HIS:CG	1:B:283:ALA:N	2.84	0.45
1:B:296:LEU:N	1:B:329:ILE:HD11	2.31	0.45
1:C:175:TYR:CE2	1:C:213:VAL:CG2	2.99	0.45
1:D:15:VAL:HG13	1:D:72:VAL:HG23	1.92	0.45
1:D:30:TYR:CE1	1:D:120:LEU:HD22	2.50	0.45
1:D:32:PHE:CE2	1:D:42:ALA:HB3	2.51	0.45
1:D:83:ILE:O	1:D:83:ILE:HG22	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:188:ASP:C	1:D:190:ASN:H	2.19	0.45
1:D:282:HIS:CG	1:D:283:ALA:N	2.84	0.45
1:A:252:ASP:CB	1:A:255:VAL:CG2	2.89	0.45
1:B:26:LEU:HD12	1:B:124:HIS:O	2.16	0.45
1:B:111:GLY:O	1:B:112:MET:C	2.60	0.45
1:C:26:LEU:HD12	1:C:124:HIS:O	2.16	0.45
1:C:392:ALA:HB2	1:C:412:LEU:HD13	1.99	0.45
1:D:144:ARG:NH1	1:D:150:LYS:O	2.49	0.45
1:D:182:ILE:HG12	1:D:386:ALA:HB1	1.98	0.45
1:D:220:THR:CG2	1:D:221:LYS:N	2.76	0.45
1:D:341:ARG:HB2	1:D:342:PRO:HD2	1.98	0.45
1:A:144:ARG:NH1	1:A:150:LYS:O	2.49	0.45
1:B:144:ARG:NH1	1:B:150:LYS:O	2.49	0.45
1:B:154:LEU:HA	1:B:154:LEU:HD23	1.40	0.45
1:B:175:TYR:CE2	1:B:213:VAL:CG2	2.99	0.45
1:B:210:ARG:HD3	1:B:221:LYS:O	2.16	0.45
1:D:138:PHE:CE1	1:D:146:PHE:HE1	2.34	0.45
1:D:153:PRO:HB2	1:D:369:ILE:CD1	2.46	0.45
1:A:44:GLY:O	1:A:45:ARG:C	2.57	0.45
1:A:110:PHE:HE1	1:A:293:ILE:HD11	1.81	0.45
1:A:175:TYR:CE2	1:A:213:VAL:CG2	2.99	0.45
1:A:383:ARG:O	1:A:383:ARG:HG2	2.15	0.45
1:C:273:LEU:HD23	1:C:273:LEU:HA	1.66	0.45
1:C:278:HIS:CD2	1:C:280:ALA:CB	2.99	0.45
1:C:282:HIS:C	1:C:284:ALA:H	2.24	0.45
1:D:108:ASN:OD1	1:D:108:ASN:N	2.48	0.45
1:A:32:PHE:CE2	1:A:42:ALA:HB3	2.51	0.45
1:A:47:ALA:HB2	1:A:86:ILE:HG21	1.97	0.45
1:A:124:HIS:HA	1:A:125:PRO:HD3	1.45	0.45
1:A:130:LEU:O	1:A:339:HIS:CE1	2.70	0.45
1:A:392:ALA:HB2	1:A:412:LEU:HD13	1.99	0.45
1:B:11:TYR:HD2	1:B:45:ARG:HA	1.82	0.45
1:B:32:PHE:CE2	1:B:42:ALA:HB3	2.51	0.45
1:B:154:LEU:CB	1:B:368:VAL:HG13	2.44	0.45
1:B:192:THR:OG1	1:C:94:GLU:OE1	2.19	0.45
1:B:404:GLU:O	1:B:407:LYS:HB2	2.16	0.45
1:C:108:ASN:N	1:C:108:ASN:OD1	2.48	0.45
1:C:153:PRO:HB2	1:C:369:ILE:CD1	2.46	0.45
1:C:409:SER:HB3	1:C:412:LEU:HB3	1.98	0.45
1:D:386:ALA:O	1:D:387:LYS:C	2.57	0.45
1:A:17:LEU:CD2	1:A:74:TYR:N	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:PHE:CE1	1:A:146:PHE:HE1	2.34	0.45
1:A:322:ASN:O	1:A:324:GLU:N	2.50	0.45
1:A:378:HIS:HE1	1:A:380:ASP:CB	2.14	0.45
1:B:153:PRO:HB2	1:B:369:ILE:CD1	2.46	0.45
1:B:187:ASP:OD1	1:B:223:TYR:HE1	1.99	0.45
1:B:206:LEU:CA	1:B:209:VAL:HG23	2.47	0.45
1:B:269:GLU:OE1	1:B:269:GLU:HA	2.16	0.45
1:B:271:LEU:H	1:B:271:LEU:HG	1.47	0.45
1:C:98:LEU:HD23	1:C:99:VAL:N	2.32	0.45
1:C:168:GLU:O	1:C:169:GLU:C	2.60	0.45
1:C:322:ASN:O	1:C:324:GLU:N	2.50	0.45
1:C:404:GLU:O	1:C:407:LYS:HB2	2.16	0.45
1:D:43:ALA:HB1	1:D:72:VAL:HG11	1.99	0.45
1:D:404:GLU:O	1:D:407:LYS:HB2	2.16	0.45
1:D:419:VAL:O	1:D:419:VAL:CG1	2.65	0.45
1:A:105:VAL:O	1:A:105:VAL:CG2	2.41	0.45
1:A:186:LYS:NZ	1:A:278:HIS:CE1	2.85	0.45
1:A:202:ARG:HE	1:A:223:TYR:HH	1.58	0.45
1:B:110:PHE:HE1	1:B:293:ILE:HD11	1.81	0.45
1:B:266:GLU:O	1:B:269:GLU:CB	2.65	0.45
1:C:110:PHE:HE1	1:C:293:ILE:HD11	1.81	0.45
1:C:388:ALA:C	1:C:390:ARG:N	2.74	0.45
1:D:168:GLU:O	1:D:169:GLU:C	2.60	0.45
1:D:185:LEU:HD12	1:D:185:LEU:HA	1.68	0.45
1:D:269:GLU:OE1	1:D:269:GLU:HA	2.16	0.45
1:D:278:HIS:CD2	1:D:280:ALA:CB	2.99	0.45
1:A:11:TYR:HD2	1:A:45:ARG:HA	1.82	0.45
1:A:117:ASN:ND2	1:A:290:ARG:CB	2.63	0.45
1:A:160:LYS:H	1:A:376:MET:CE	2.07	0.45
1:A:205:LYS:O	1:A:209:VAL:CG2	2.61	0.45
1:A:375:VAL:CG1	1:A:385:GLY:C	2.85	0.45
1:A:387:LYS:HE3	2:A:466:HOH:O	2.16	0.45
1:B:263:TYR:HD1	1:C:232:ASN:ND2	2.14	0.45
1:C:125:PRO:HA	1:C:126:PRO:HD2	1.69	0.45
1:C:341:ARG:HB2	1:C:342:PRO:HD2	1.98	0.45
1:D:98:LEU:HD23	1:D:99:VAL:N	2.32	0.45
1:D:130:LEU:O	1:D:339:HIS:CE1	2.70	0.45
1:D:187:ASP:OD1	1:D:223:TYR:HE1	1.99	0.45
1:D:279:ARG:O	1:D:281:MET:N	2.48	0.45
1:D:409:SER:HB3	1:D:412:LEU:HB3	1.98	0.45
1:A:176:GLU:OE1	1:A:383:ARG:NH1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:LEU:HD23	1:A:177:LEU:HA	1.75	0.45
1:A:296:LEU:N	1:A:329:ILE:HD11	2.31	0.45
1:C:206:LEU:CA	1:C:209:VAL:HG23	2.47	0.45
1:C:279:ARG:HD3	1:C:295:MET:HE1	1.96	0.45
1:C:387:LYS:HE3	2:C:466:HOH:O	2.16	0.45
1:D:111:GLY:O	1:D:112:MET:C	2.60	0.45
1:D:168:GLU:O	1:D:170:TYR:N	2.50	0.45
1:D:189:GLU:CB	1:D:278:HIS:CE1	2.99	0.45
1:D:206:LEU:CA	1:D:209:VAL:HG23	2.47	0.45
1:A:43:ALA:HB1	1:A:72:VAL:HG11	1.99	0.45
1:A:168:GLU:O	1:A:170:TYR:N	2.50	0.45
1:A:175:TYR:O	1:A:179:SER:HB2	2.17	0.45
1:A:282:HIS:C	1:A:284:ALA:N	2.75	0.45
1:B:11:TYR:CE2	1:B:45:ARG:HG2	2.51	0.45
1:B:133:PHE:CD2	1:B:304:MET:HE2	2.52	0.45
1:B:168:GLU:O	1:B:169:GLU:C	2.60	0.45
1:B:186:LYS:NZ	1:B:278:HIS:CE1	2.85	0.45
1:B:419:VAL:CG2	1:B:419:VAL:CA	2.89	0.45
1:C:159:PRO:HB3	1:C:173:ILE:HD12	1.99	0.45
1:C:160:LYS:CD	1:C:160:LYS:HE2	2.18	0.45
1:C:297:ALA:O	1:C:300:LYS:HB3	2.17	0.45
1:D:11:TYR:HD2	1:D:45:ARG:HA	1.82	0.45
1:D:186:LYS:NZ	1:D:278:HIS:CE1	2.85	0.45
1:D:210:ARG:HD3	1:D:221:LYS:O	2.16	0.45
1:D:322:ASN:O	1:D:324:GLU:N	2.50	0.45
1:A:404:GLU:O	1:A:407:LYS:HB2	2.16	0.44
1:B:130:LEU:O	1:B:339:HIS:CE1	2.70	0.44
1:B:160:LYS:CD	1:B:160:LYS:HE2	2.18	0.44
1:B:232:ASN:ND2	1:C:263:TYR:HD1	2.15	0.44
1:C:43:ALA:HB1	1:C:72:VAL:HG11	1.99	0.44
1:C:186:LYS:NZ	1:C:278:HIS:CE1	2.85	0.44
1:C:296:LEU:N	1:C:329:ILE:HD11	2.31	0.44
1:C:378:HIS:HE1	1:C:380:ASP:CB	2.14	0.44
1:D:133:PHE:CD2	1:D:304:MET:HE2	2.52	0.44
1:D:296:LEU:N	1:D:329:ILE:HD11	2.31	0.44
1:A:168:GLU:O	1:A:169:GLU:C	2.60	0.44
1:A:266:GLU:O	1:A:269:GLU:CB	2.65	0.44
1:B:159:PRO:HB3	1:B:173:ILE:HD12	1.99	0.44
1:B:176:GLU:OE1	1:B:383:ARG:NH1	2.50	0.44
1:B:263:TYR:CD2	1:B:263:TYR:O	2.70	0.44
1:B:409:SER:HA	1:B:410:PRO:HD2	1.63	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:263:TYR:CD2	1:D:263:TYR:O	2.70	0.44
1:D:363:PHE:CD1	1:D:363:PHE:N	2.85	0.44
1:A:98:LEU:HD23	1:A:99:VAL:N	2.32	0.44
1:A:263:TYR:CD2	1:A:263:TYR:O	2.70	0.44
1:A:341:ARG:HB2	1:A:342:PRO:HD2	1.98	0.44
1:B:175:TYR:O	1:B:179:SER:HB2	2.18	0.44
1:B:322:ASN:O	1:B:324:GLU:N	2.50	0.44
1:B:387:LYS:HE3	2:B:463:HOH:O	2.16	0.44
1:C:15:VAL:HG13	1:C:72:VAL:HG23	1.92	0.44
1:C:55:TRP:CE2	1:C:57:THR:HG21	2.51	0.44
1:D:38:SER:C	1:D:40:GLU:H	2.26	0.44
1:D:373:GLY:O	1:D:374:GLY:C	2.59	0.44
1:A:133:PHE:CD2	1:A:304:MET:HE2	2.52	0.44
1:A:297:ALA:O	1:A:300:LYS:HB3	2.17	0.44
1:B:121:LEU:CD1	1:B:121:LEU:N	2.81	0.44
1:B:177:LEU:HA	1:B:177:LEU:HD23	1.75	0.44
1:B:288:ASN:HD21	1:C:288:ASN:ND2	2.16	0.44
1:C:176:GLU:OE1	1:C:383:ARG:NH1	2.50	0.44
1:C:269:GLU:OE1	1:C:269:GLU:HA	2.16	0.44
1:D:94:GLU:HG2	1:D:97:SER:CB	2.40	0.44
1:A:100:GLN:O	1:A:103:SER:N	2.51	0.44
1:A:340:ILE:H	1:A:340:ILE:HG12	1.50	0.44
1:B:43:ALA:HB1	1:B:72:VAL:HG11	1.99	0.44
1:B:278:HIS:CD2	1:B:280:ALA:CB	2.99	0.44
1:B:355:LEU:O	1:B:356:MET:C	2.60	0.44
1:C:10:TRP:O	1:C:11:TYR:C	2.61	0.44
1:C:133:PHE:CD2	1:C:304:MET:HE2	2.52	0.44
1:C:378:HIS:HA	1:C:379:PRO:HD2	1.61	0.44
1:C:390:ARG:HD2	1:C:390:ARG:HA	1.83	0.44
1:C:419:VAL:O	1:C:419:VAL:CG1	2.65	0.44
1:B:31:TYR:O	1:B:119:ARG:N	2.44	0.44
1:B:98:LEU:HD23	1:B:99:VAL:N	2.32	0.44
1:B:282:HIS:C	1:B:284:ALA:N	2.75	0.44
1:B:341:ARG:CB	1:B:342:PRO:CD	2.96	0.44
1:B:375:VAL:CG1	1:B:385:GLY:C	2.85	0.44
1:B:419:VAL:O	1:B:419:VAL:CG1	2.65	0.44
1:C:130:LEU:O	1:C:339:HIS:CE1	2.70	0.44
1:C:363:PHE:CD1	1:C:363:PHE:N	2.85	0.44
1:D:100:GLN:O	1:D:103:SER:N	2.51	0.44
1:A:134:LYS:HZ1	1:A:266:GLU:HG3	1.77	0.44
1:A:251:ILE:HG21	1:A:251:ILE:HD13	1.19	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:LEU:O	1:A:261:LEU:CD2	2.66	0.44
1:A:409:SER:HA	1:A:410:PRO:HD2	1.63	0.44
1:B:168:GLU:O	1:B:170:TYR:N	2.50	0.44
1:B:224:LEU:CD2	1:B:276:HIS:CD2	3.01	0.44
1:B:386:ALA:O	1:B:387:LYS:C	2.57	0.44
1:C:100:GLN:O	1:C:103:SER:N	2.51	0.44
1:C:266:GLU:O	1:C:269:GLU:CB	2.65	0.44
1:D:121:LEU:CD1	1:D:121:LEU:N	2.81	0.44
1:D:176:GLU:OE1	1:D:383:ARG:NH1	2.50	0.44
1:D:266:GLU:O	1:D:269:GLU:CB	2.65	0.44
1:D:273:LEU:HA	1:D:273:LEU:HD23	1.66	0.44
1:A:154:LEU:CB	1:A:368:VAL:HG13	2.44	0.44
1:A:224:LEU:CD2	1:A:276:HIS:CD2	3.01	0.44
1:B:17:LEU:CD2	1:B:74:TYR:N	2.79	0.44
1:B:44:GLY:O	1:B:45:ARG:C	2.57	0.44
1:B:279:ARG:HD3	1:B:295:MET:HE1	1.96	0.44
1:C:373:GLY:O	1:C:374:GLY:C	2.59	0.44
1:D:191:PHE:CD2	1:D:194:PHE:CE1	3.06	0.44
1:D:200:GLU:O	1:D:204:ARG:HG3	2.18	0.44
1:D:393:ILE:O	1:D:394:ASP:C	2.61	0.44
1:A:268:THR:HG23	1:A:268:THR:H	1.42	0.44
1:A:386:ALA:O	1:A:387:LYS:C	2.57	0.44
1:A:393:ILE:O	1:A:394:ASP:C	2.61	0.44
1:B:78:HIS:CB	1:B:83:ILE:HG12	2.48	0.44
1:B:188:ASP:C	1:B:190:ASN:H	2.19	0.44
1:B:261:LEU:CD2	1:B:261:LEU:O	2.66	0.44
1:C:78:HIS:CB	1:C:83:ILE:HG12	2.48	0.44
1:C:111:GLY:O	1:C:112:MET:C	2.60	0.44
1:C:175:TYR:O	1:C:179:SER:HB2	2.17	0.44
1:C:263:TYR:CD2	1:C:263:TYR:O	2.71	0.44
1:D:127:TYR:HB3	1:D:128:GLU:H	1.41	0.44
1:D:202:ARG:HE	1:D:223:TYR:HH	1.59	0.44
1:D:392:ALA:HB2	1:D:412:LEU:HD13	1.99	0.44
1:A:55:TRP:CE3	1:A:57:THR:HG23	2.48	0.43
1:A:199:PHE:CE1	1:A:203:VAL:HG11	2.53	0.43
1:A:206:LEU:CA	1:A:209:VAL:HG23	2.47	0.43
1:A:266:GLU:O	1:A:269:GLU:HB2	2.19	0.43
1:A:355:LEU:O	1:A:356:MET:C	2.61	0.43
1:A:388:ALA:C	1:A:390:ARG:N	2.74	0.43
1:B:23:ARG:HE	1:B:23:ARG:N	2.00	0.43
1:B:143:ILE:HD11	1:B:308:ASP:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:ALA:O	1:B:300:LYS:HB3	2.17	0.43
1:C:126:PRO:O	1:C:127:TYR:O	2.34	0.43
1:C:367:LEU:HD23	1:C:367:LEU:HA	1.63	0.43
1:D:270:ASP:N	1:D:270:ASP:OD1	2.51	0.43
1:D:297:ALA:O	1:D:300:LYS:HB3	2.17	0.43
1:D:355:LEU:O	1:D:356:MET:C	2.61	0.43
1:A:120:LEU:HD13	1:A:121:LEU:N	2.33	0.43
1:A:121:LEU:CD1	1:A:121:LEU:N	2.81	0.43
1:A:282:HIS:CG	1:A:283:ALA:N	2.84	0.43
1:A:373:GLY:O	1:A:374:GLY:C	2.59	0.43
1:B:55:TRP:NE1	1:B:57:THR:HG21	2.33	0.43
1:B:100:GLN:O	1:B:103:SER:N	2.51	0.43
1:B:288:ASN:ND2	1:C:288:ASN:HD21	2.14	0.43
1:B:363:PHE:CD1	1:B:363:PHE:N	2.85	0.43
1:B:390:ARG:HD2	1:B:390:ARG:HA	1.83	0.43
1:B:392:ALA:HB2	1:B:412:LEU:HD13	1.99	0.43
1:C:168:GLU:O	1:C:170:TYR:N	2.50	0.43
1:C:311:HIS:CD2	1:C:346:VAL:HG12	2.50	0.43
1:C:375:VAL:CG1	1:C:385:GLY:C	2.85	0.43
1:D:160:LYS:HZ2	1:D:373:GLY:CA	2.30	0.43
1:D:199:PHE:CE1	1:D:203:VAL:HG11	2.53	0.43
1:D:282:HIS:C	1:D:284:ALA:N	2.75	0.43
1:A:191:PHE:CD2	1:A:194:PHE:CE1	3.06	0.43
1:A:269:GLU:OE1	1:A:269:GLU:HA	2.16	0.43
1:B:199:PHE:CE1	1:B:203:VAL:HG11	2.53	0.43
1:B:200:GLU:O	1:B:204:ARG:HG3	2.18	0.43
1:B:261:LEU:O	1:B:261:LEU:HD22	2.19	0.43
1:C:11:TYR:HD2	1:C:45:ARG:HA	1.82	0.43
1:C:182:ILE:HG12	1:C:386:ALA:HB1	1.98	0.43
1:C:199:PHE:CE1	1:C:203:VAL:HG11	2.53	0.43
1:D:11:TYR:CE2	1:D:45:ARG:HG2	2.51	0.43
1:D:78:HIS:CB	1:D:83:ILE:HG12	2.48	0.43
1:D:261:LEU:O	1:D:261:LEU:CD2	2.66	0.43
1:A:79:GLY:O	1:A:81:GLY:N	2.51	0.43
1:A:185:LEU:HA	1:A:185:LEU:HD12	1.68	0.43
1:A:332:PHE:O	1:A:332:PHE:CG	2.63	0.43
1:B:30:TYR:CE1	1:B:120:LEU:HD23	2.53	0.43
1:B:393:ILE:HG21	1:B:393:ILE:HD13	1.81	0.43
1:C:30:TYR:CE1	1:C:120:LEU:HD23	2.53	0.43
1:C:121:LEU:CD1	1:C:121:LEU:N	2.81	0.43
1:C:191:PHE:HD2	1:C:194:PHE:CE1	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:LEU:CD2	1:C:276:HIS:CD2	3.01	0.43
1:C:355:LEU:O	1:C:356:MET:C	2.61	0.43
1:C:386:ALA:O	1:C:387:LYS:C	2.57	0.43
1:D:10:TRP:O	1:D:11:TYR:C	2.61	0.43
1:D:31:TYR:O	1:D:119:ARG:N	2.44	0.43
1:D:175:TYR:O	1:D:179:SER:HB2	2.18	0.43
1:D:224:LEU:CD2	1:D:276:HIS:CD2	3.01	0.43
1:D:261:LEU:O	1:D:261:LEU:HD22	2.19	0.43
1:A:159:PRO:HB3	1:A:173:ILE:HD12	1.99	0.43
1:A:341:ARG:CB	1:A:342:PRO:CD	2.96	0.43
1:B:266:GLU:O	1:B:269:GLU:HB2	2.19	0.43
1:C:55:TRP:CH2	1:C:58:LEU:N	2.76	0.43
1:C:171:ALA:O	1:C:172:GLU:C	2.61	0.43
1:C:341:ARG:CB	1:C:342:PRO:CD	2.96	0.43
1:D:27:ILE:O	1:D:123:PHE:HA	2.19	0.43
1:D:30:TYR:CE1	1:D:120:LEU:HD23	2.53	0.43
1:D:105:VAL:H	1:D:105:VAL:HG13	1.51	0.43
1:D:159:PRO:HB3	1:D:173:ILE:HD12	1.99	0.43
1:A:111:GLY:O	1:A:112:MET:C	2.60	0.43
1:A:171:ALA:O	1:A:172:GLU:C	2.61	0.43
1:B:94:GLU:HG2	1:B:97:SER:CB	2.40	0.43
1:B:191:PHE:CD2	1:B:194:PHE:CE1	3.06	0.43
1:B:284:ALA:O	1:C:285:PHE:HB3	2.19	0.43
1:C:17:LEU:CD2	1:C:74:TYR:N	2.80	0.43
1:C:191:PHE:CD2	1:C:194:PHE:CE1	3.06	0.43
1:C:251:ILE:HD13	1:C:251:ILE:HG21	1.19	0.43
1:C:261:LEU:CD2	1:C:261:LEU:O	2.66	0.43
1:A:200:GLU:O	1:A:204:ARG:HG3	2.18	0.43
1:A:213:VAL:HG13	1:A:217:THR:CG2	2.49	0.43
1:A:271:LEU:H	1:A:271:LEU:HG	1.47	0.43
1:B:191:PHE:HD2	1:B:194:PHE:CE1	2.36	0.43
1:C:27:ILE:O	1:C:123:PHE:HA	2.19	0.43
1:C:62:PRO:HB2	1:C:65:ALA:HB2	2.01	0.43
1:C:261:LEU:O	1:C:261:LEU:HD22	2.19	0.43
1:D:55:TRP:NE1	1:D:57:THR:HG21	2.33	0.43
1:A:160:LYS:CD	1:A:160:LYS:HE3	2.18	0.43
1:A:231:VAL:HA	1:A:234:MET:HE3	2.01	0.43
1:A:298:LEU:C	1:A:298:LEU:CD2	2.87	0.43
1:B:62:PRO:HB2	1:B:65:ALA:HB2	2.01	0.43
1:B:120:LEU:HD13	1:B:121:LEU:N	2.33	0.43
1:B:189:GLU:HA	1:B:250:MET:HE2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:ASP:CB	1:B:255:VAL:CG2	2.89	0.43
1:C:393:ILE:O	1:C:394:ASP:C	2.61	0.43
1:A:27:ILE:O	1:A:123:PHE:HA	2.19	0.43
1:A:39:PRO:O	1:A:75:LEU:CD2	2.58	0.43
1:A:55:TRP:NE1	1:A:57:THR:HG21	2.33	0.43
1:A:261:LEU:O	1:A:261:LEU:HD22	2.19	0.43
1:A:419:VAL:O	1:A:419:VAL:CG1	2.65	0.43
1:B:38:SER:C	1:B:40:GLU:H	2.26	0.43
1:B:171:ALA:O	1:B:172:GLU:C	2.61	0.43
1:C:189:GLU:HA	1:C:250:MET:HE2	2.01	0.43
1:C:231:VAL:CG1	1:C:234:MET:CE	2.84	0.43
1:D:17:LEU:CD2	1:D:74:TYR:N	2.79	0.43
1:D:126:PRO:O	1:D:127:TYR:O	2.34	0.43
1:A:363:PHE:CD1	1:A:363:PHE:N	2.85	0.43
1:B:27:ILE:O	1:B:123:PHE:HA	2.19	0.43
1:B:213:VAL:HG13	1:B:217:THR:CG2	2.49	0.43
1:C:120:LEU:HD13	1:C:121:LEU:N	2.33	0.43
1:C:200:GLU:O	1:C:204:ARG:HG3	2.18	0.43
1:D:125:PRO:HA	1:D:126:PRO:HD2	1.69	0.43
1:D:394:ASP:O	1:D:395:ALA:C	2.62	0.43
1:A:30:TYR:CE1	1:A:120:LEU:HD23	2.53	0.42
1:A:77:LYS:HA	1:A:82:TYR:HD1	1.84	0.42
1:A:298:LEU:HD23	1:A:299:ALA:N	2.33	0.42
1:B:170:TYR:O	1:B:171:ALA:C	2.62	0.42
1:B:393:ILE:O	1:B:394:ASP:C	2.61	0.42
1:B:401:ASP:OD1	1:B:403:ASP:HB2	2.20	0.42
1:C:11:TYR:CE2	1:C:45:ARG:HG2	2.50	0.42
1:A:19:TYR:HE1	1:A:21:PRO:CA	2.33	0.42
1:A:143:ILE:HD11	1:A:308:ASP:HB2	2.00	0.42
1:B:19:TYR:HE1	1:B:21:PRO:CA	2.32	0.42
1:C:286:THR:CG2	1:C:293:ILE:O	2.67	0.42
1:C:394:ASP:O	1:C:395:ALA:C	2.62	0.42
1:C:401:ASP:OD1	1:C:403:ASP:HB2	2.20	0.42
1:D:55:TRP:CE2	1:D:57:THR:HG21	2.51	0.42
1:D:213:VAL:HG13	1:D:217:THR:CG2	2.49	0.42
1:D:253:ILE:H	1:D:253:ILE:HG23	1.64	0.42
1:D:266:GLU:O	1:D:269:GLU:HB2	2.19	0.42
1:D:341:ARG:CB	1:D:342:PRO:CD	2.96	0.42
1:A:62:PRO:HB2	1:A:65:ALA:HB2	2.01	0.42
1:A:134:LYS:HZ2	1:A:266:GLU:HG3	1.81	0.42
1:A:278:HIS:CD2	1:A:280:ALA:CB	2.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:378:HIS:HE1	1:B:380:ASP:CB	2.14	0.42
1:C:38:SER:C	1:C:40:GLU:H	2.25	0.42
1:C:127:TYR:HB3	1:C:128:GLU:H	1.41	0.42
1:C:213:VAL:HG13	1:C:217:THR:CG2	2.49	0.42
1:C:220:THR:C	1:C:221:LYS:HG2	2.45	0.42
1:C:270:ASP:N	1:C:270:ASP:OD1	2.51	0.42
1:D:120:LEU:HD13	1:D:121:LEU:N	2.33	0.42
1:D:252:ASP:CB	1:D:255:VAL:HG21	2.48	0.42
1:D:388:ALA:C	1:D:390:ARG:N	2.74	0.42
1:D:390:ARG:HD2	1:D:390:ARG:HA	1.83	0.42
1:A:37:VAL:CG2	1:A:114:ALA:HB1	2.49	0.42
1:A:38:SER:C	1:A:40:GLU:H	2.25	0.42
1:A:220:THR:C	1:A:221:LYS:HG2	2.45	0.42
1:A:286:THR:CG2	1:A:293:ILE:O	2.67	0.42
1:B:258:TRP:HB2	1:C:255:VAL:O	2.19	0.42
1:B:322:ASN:OD1	1:B:324:GLU:HG2	2.20	0.42
1:C:282:HIS:CG	1:C:283:ALA:N	2.84	0.42
1:D:238:ALA:O	1:D:239:GLU:C	2.62	0.42
1:D:311:HIS:CD2	1:D:346:VAL:HG12	2.50	0.42
1:A:90:LEU:HD21	1:A:126:PRO:CG	2.46	0.42
1:A:94:GLU:CG	1:A:97:SER:HB3	2.43	0.42
1:A:322:ASN:OD1	1:A:324:GLU:HG2	2.20	0.42
1:A:401:ASP:OD1	1:A:403:ASP:HB2	2.20	0.42
1:B:62:PRO:O	1:B:63:GLU:C	2.63	0.42
1:B:220:THR:C	1:B:221:LYS:HG2	2.45	0.42
1:B:394:ASP:O	1:B:395:ALA:C	2.62	0.42
1:C:62:PRO:O	1:C:63:GLU:C	2.63	0.42
1:C:177:LEU:HA	1:C:177:LEU:HD23	1.75	0.42
1:C:191:PHE:CD2	1:C:194:PHE:HE1	2.38	0.42
1:D:191:PHE:HD2	1:D:194:PHE:CE1	2.36	0.42
1:D:316:VAL:O	1:D:317:GLY:C	2.62	0.42
1:D:364:GLY:C	1:D:366:ASP:H	2.28	0.42
1:D:401:ASP:OD1	1:D:403:ASP:HB2	2.20	0.42
1:D:401:ASP:CB	1:D:404:GLU:HG2	2.36	0.42
1:B:124:HIS:HA	1:B:125:PRO:HD3	1.45	0.42
1:C:19:TYR:HE1	1:C:21:PRO:CA	2.33	0.42
1:C:143:ILE:HD11	1:C:308:ASP:HB2	2.00	0.42
1:C:253:ILE:H	1:C:253:ILE:HG23	1.64	0.42
1:A:393:ILE:HG21	1:A:393:ILE:HD13	1.81	0.42
1:B:185:LEU:HA	1:B:185:LEU:HD12	1.68	0.42
1:C:266:GLU:O	1:C:269:GLU:HB2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:322:ASN:OD1	1:C:324:GLU:HG2	2.20	0.42
1:D:73:PHE:CD2	1:D:73:PHE:N	2.88	0.42
1:D:79:GLY:O	1:D:81:GLY:N	2.51	0.42
1:D:328:ARG:HB3	1:D:329:ILE:H	1.71	0.42
1:A:110:PHE:HZ	1:A:293:ILE:HD13	1.85	0.42
1:B:79:GLY:O	1:B:81:GLY:N	2.51	0.42
1:B:188:ASP:O	1:B:189:GLU:C	2.60	0.42
1:B:298:LEU:HD23	1:B:299:ALA:N	2.33	0.42
1:B:311:HIS:CD2	1:B:346:VAL:HG12	2.50	0.42
1:B:314:THR:CG2	1:B:348:SER:O	2.68	0.42
1:B:316:VAL:HG22	1:B:355:LEU:HD13	2.02	0.42
1:C:187:ASP:OD1	1:C:223:TYR:CE1	2.73	0.42
1:C:206:LEU:C	1:C:209:VAL:HG23	2.45	0.42
1:C:231:VAL:HA	1:C:234:MET:HE3	2.01	0.42
1:C:285:PHE:C	1:C:287:ARG:H	2.28	0.42
1:D:143:ILE:HD11	1:D:308:ASP:HB2	2.00	0.42
1:D:170:TYR:O	1:D:171:ALA:C	2.62	0.42
1:D:187:ASP:OD1	1:D:223:TYR:CE1	2.73	0.42
1:D:314:THR:CG2	1:D:348:SER:O	2.68	0.42
1:D:316:VAL:HG22	1:D:355:LEU:HD13	2.02	0.42
1:D:373:GLY:C	1:D:375:VAL:N	2.78	0.42
1:D:409:SER:HA	1:D:410:PRO:HD2	1.63	0.42
1:A:252:ASP:O	1:A:256:ALA:CB	2.68	0.42
1:A:316:VAL:O	1:A:317:GLY:C	2.62	0.42
1:B:168:GLU:C	1:B:170:TYR:N	2.77	0.42
1:C:37:VAL:CG2	1:C:114:ALA:HB1	2.49	0.42
1:C:79:GLY:O	1:C:81:GLY:N	2.51	0.42
1:C:316:VAL:O	1:C:317:GLY:C	2.62	0.42
1:D:191:PHE:CD2	1:D:194:PHE:HE1	2.38	0.42
1:D:231:VAL:HA	1:D:234:MET:HE3	2.01	0.42
1:D:252:ASP:O	1:D:256:ALA:CB	2.68	0.42
1:A:105:VAL:H	1:A:105:VAL:HG13	1.51	0.42
1:A:189:GLU:HA	1:A:250:MET:HE2	2.01	0.42
1:A:270:ASP:N	1:A:270:ASP:OD1	2.51	0.42
1:A:316:VAL:HG22	1:A:355:LEU:HD13	2.02	0.42
1:B:187:ASP:OD1	1:B:223:TYR:CE1	2.73	0.42
1:B:238:ALA:O	1:B:239:GLU:C	2.62	0.42
1:B:364:GLY:C	1:B:366:ASP:H	2.28	0.42
1:C:55:TRP:NE1	1:C:57:THR:HG21	2.33	0.42
1:C:110:PHE:HZ	1:C:293:ILE:HD13	1.85	0.42
1:C:163:MET:SD	1:C:190:ASN:HB3	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:ASP:O	1:C:256:ALA:CB	2.68	0.42
1:D:19:TYR:HE1	1:D:21:PRO:CA	2.33	0.42
1:D:110:PHE:HZ	1:D:293:ILE:HD13	1.85	0.42
1:D:124:HIS:HA	1:D:125:PRO:HD3	1.45	0.42
1:D:154:LEU:HA	1:D:154:LEU:HD23	1.40	0.42
1:A:168:GLU:C	1:A:168:GLU:OE1	2.63	0.41
1:A:187:ASP:OD1	1:A:223:TYR:CE1	2.73	0.41
1:A:191:PHE:HD2	1:A:194:PHE:CE1	2.36	0.41
1:B:90:LEU:HD21	1:B:126:PRO:CG	2.46	0.41
1:B:110:PHE:HZ	1:B:293:ILE:HD13	1.85	0.41
1:B:191:PHE:CD2	1:B:194:PHE:HE1	2.38	0.41
1:B:206:LEU:C	1:B:209:VAL:HG23	2.45	0.41
1:B:316:VAL:O	1:B:317:GLY:C	2.62	0.41
1:C:30:TYR:HE1	1:C:120:LEU:HD23	1.85	0.41
1:C:206:LEU:HA	1:C:209:VAL:HG21	2.01	0.41
1:D:30:TYR:HE1	1:D:120:LEU:HD23	1.85	0.41
1:D:127:TYR:O	1:D:128:GLU:C	2.63	0.41
1:D:189:GLU:HA	1:D:250:MET:HE2	2.01	0.41
1:D:252:ASP:CB	1:D:255:VAL:CG2	2.89	0.41
1:A:78:HIS:CB	1:A:83:ILE:HG12	2.48	0.41
1:A:206:LEU:HA	1:A:209:VAL:HG21	2.01	0.41
1:A:285:PHE:C	1:A:287:ARG:H	2.28	0.41
1:A:300:LYS:O	1:A:303:ARG:N	2.49	0.41
1:B:168:GLU:C	1:B:168:GLU:OE1	2.63	0.41
1:B:206:LEU:HA	1:B:209:VAL:HG21	2.01	0.41
1:B:343:VAL:CG1	1:B:344:PHE:H	2.34	0.41
1:C:168:GLU:C	1:C:170:TYR:N	2.77	0.41
1:C:170:TYR:O	1:C:171:ALA:C	2.62	0.41
1:C:237:ARG:HH21	1:C:237:ARG:HD2	1.56	0.41
1:D:90:LEU:HD21	1:D:126:PRO:CG	2.45	0.41
1:D:206:LEU:C	1:D:209:VAL:HG23	2.45	0.41
1:D:251:ILE:HG21	1:D:251:ILE:HD13	1.19	0.41
1:D:253:ILE:HD12	1:D:253:ILE:HG21	1.62	0.41
1:D:322:ASN:OD1	1:D:324:GLU:HG2	2.20	0.41
1:D:336:LYS:CE	1:D:336:LYS:HD3	2.20	0.41
1:A:73:PHE:N	1:A:73:PHE:CD2	2.88	0.41
1:A:191:PHE:CD2	1:A:194:PHE:HE1	2.38	0.41
1:A:311:HIS:CD2	1:A:346:VAL:HG12	2.50	0.41
1:A:373:GLY:C	1:A:375:VAL:N	2.78	0.41
1:B:117:ASN:ND2	1:B:290:ARG:CB	2.63	0.41
1:C:393:ILE:HG21	1:C:393:ILE:HD13	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:37:VAL:CG2	1:D:114:ALA:HB1	2.49	0.41
1:D:171:ALA:O	1:D:172:GLU:C	2.61	0.41
1:D:266:GLU:O	1:D:267:VAL:C	2.62	0.41
1:D:375:VAL:CG1	1:D:385:GLY:C	2.85	0.41
1:A:140:VAL:HG23	1:A:342:PRO:O	2.21	0.41
1:A:163:MET:SD	1:A:190:ASN:HB3	2.60	0.41
1:A:394:ASP:O	1:A:395:ALA:C	2.62	0.41
1:B:141:GLN:HA	1:B:141:GLN:OE1	2.20	0.41
1:B:252:ASP:O	1:B:256:ALA:CB	2.68	0.41
1:C:168:GLU:C	1:C:168:GLU:OE1	2.63	0.41
1:C:266:GLU:O	1:C:267:VAL:C	2.62	0.41
1:C:295:MET:HG3	1:C:329:ILE:HD13	2.02	0.41
1:C:295:MET:HG3	1:C:329:ILE:CD1	2.51	0.41
1:C:314:THR:CG2	1:C:348:SER:O	2.68	0.41
1:D:243:ASN:C	1:D:245:GLY:N	2.78	0.41
1:D:298:LEU:HD23	1:D:299:ALA:N	2.33	0.41
1:A:132:HIS:O	1:A:133:PHE:CD1	2.74	0.41
1:A:364:GLY:C	1:A:366:ASP:H	2.28	0.41
1:B:132:HIS:O	1:B:133:PHE:CD1	2.73	0.41
1:B:163:MET:SD	1:B:190:ASN:HB3	2.60	0.41
1:B:225:ILE:H	1:B:225:ILE:HG22	1.43	0.41
1:B:253:ILE:HD12	1:B:253:ILE:HG21	1.63	0.41
1:B:373:GLY:C	1:B:375:VAL:N	2.78	0.41
1:B:400:VAL:H	1:B:400:VAL:HG23	1.42	0.41
1:C:141:GLN:HA	1:C:141:GLN:OE1	2.20	0.41
1:C:336:LYS:O	1:C:337:TRP:CB	2.62	0.41
1:D:141:GLN:HA	1:D:141:GLN:OE1	2.20	0.41
1:D:166:SER:O	1:D:170:TYR:HB2	2.20	0.41
1:D:168:GLU:C	1:D:168:GLU:OE1	2.63	0.41
1:D:168:GLU:C	1:D:170:TYR:N	2.77	0.41
1:D:286:THR:CG2	1:D:293:ILE:O	2.67	0.41
1:A:30:TYR:HE1	1:A:120:LEU:HD23	1.85	0.41
1:A:32:PHE:CZ	1:A:43:ALA:HB2	2.56	0.41
1:A:314:THR:CG2	1:A:348:SER:O	2.68	0.41
1:B:19:TYR:C	1:B:19:TYR:CD1	2.99	0.41
1:B:30:TYR:HE1	1:B:120:LEU:HD23	1.85	0.41
1:B:126:PRO:O	1:B:127:TYR:O	2.34	0.41
1:B:140:VAL:HG23	1:B:342:PRO:O	2.21	0.41
1:C:32:PHE:CZ	1:C:43:ALA:HB2	2.56	0.41
1:C:169:GLU:O	1:C:173:ILE:HG22	2.21	0.41
1:C:238:ALA:O	1:C:239:GLU:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:282:HIS:C	1:C:284:ALA:N	2.75	0.41
1:C:298:LEU:HD23	1:C:299:ALA:N	2.33	0.41
1:C:373:GLY:C	1:C:375:VAL:N	2.78	0.41
1:D:378:HIS:HA	1:D:379:PRO:HD2	1.61	0.41
1:A:62:PRO:O	1:A:63:GLU:C	2.63	0.41
1:A:141:GLN:HA	1:A:141:GLN:OE1	2.20	0.41
1:A:243:ASN:C	1:A:245:GLY:N	2.78	0.41
1:A:400:VAL:H	1:A:400:VAL:HG23	1.42	0.41
1:B:127:TYR:O	1:B:128:GLU:C	2.63	0.41
1:B:182:ILE:HG22	1:B:184:LEU:N	2.36	0.41
1:B:286:THR:CG2	1:B:293:ILE:O	2.67	0.41
1:C:132:HIS:O	1:C:133:PHE:CD1	2.74	0.41
1:D:163:MET:SD	1:D:190:ASN:HB3	2.60	0.41
1:D:199:PHE:O	1:D:203:VAL:HG13	2.21	0.41
1:D:220:THR:C	1:D:221:LYS:HG2	2.45	0.41
1:D:367:LEU:HD23	1:D:367:LEU:HA	1.63	0.41
1:A:125:PRO:HA	1:A:126:PRO:HD2	1.69	0.41
1:A:166:SER:O	1:A:170:TYR:HB2	2.20	0.41
1:A:296:LEU:O	1:A:297:ALA:C	2.64	0.41
1:A:345:PRO:O	1:A:368:VAL:HG23	2.21	0.41
1:B:166:SER:O	1:B:170:TYR:HB2	2.20	0.41
1:B:199:PHE:O	1:B:203:VAL:HG13	2.21	0.41
1:B:318:LYS:NZ	1:C:113:LYS:HZ1	2.17	0.41
1:B:378:HIS:HA	1:B:379:PRO:HD2	1.61	0.41
1:D:110:PHE:CE1	1:D:293:ILE:HD11	2.56	0.41
1:D:130:LEU:C	1:D:132:HIS:N	2.79	0.41
1:D:132:HIS:O	1:D:133:PHE:CD1	2.73	0.41
1:D:140:VAL:HG23	1:D:342:PRO:O	2.21	0.41
1:D:152:ARG:H	1:D:152:ARG:HG2	1.75	0.41
1:D:237:ARG:HH21	1:D:237:ARG:HD2	1.56	0.41
1:A:55:TRP:CE2	1:A:57:THR:HG21	2.51	0.41
1:A:126:PRO:O	1:A:127:TYR:O	2.34	0.41
1:A:160:LYS:HZ2	1:A:373:GLY:CA	2.34	0.41
1:A:199:PHE:O	1:A:203:VAL:HG13	2.21	0.41
1:A:206:LEU:C	1:A:209:VAL:HG23	2.45	0.41
1:A:255:VAL:CG2	1:A:280:ALA:O	2.69	0.41
1:A:376:MET:HB3	1:A:376:MET:HE3	1.94	0.41
1:B:16:ASP:C	1:B:18:ASN:H	2.29	0.41
1:B:176:GLU:O	1:B:383:ARG:HG3	2.21	0.41
1:B:202:ARG:HE	1:B:223:TYR:HH	1.60	0.41
1:C:16:ASP:C	1:C:18:ASN:H	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:TYR:CD1	1:C:19:TYR:C	2.99	0.41
1:C:31:TYR:O	1:C:119:ARG:N	2.44	0.41
1:C:73:PHE:CD2	1:C:73:PHE:N	2.88	0.41
1:C:150:LYS:HG3	1:C:151:ASP:N	2.36	0.41
1:C:166:SER:O	1:C:170:TYR:HB2	2.20	0.41
1:C:345:PRO:O	1:C:368:VAL:HG23	2.21	0.41
1:C:401:ASP:CB	1:C:404:GLU:HG2	2.36	0.41
1:D:19:TYR:CD1	1:D:19:TYR:C	2.99	0.41
1:D:32:PHE:CZ	1:D:43:ALA:HB2	2.56	0.41
1:D:39:PRO:HG3	1:D:82:TYR:OH	2.21	0.41
1:D:52:ILE:O	1:D:52:ILE:CG1	2.69	0.41
1:D:128:GLU:OE1	1:D:128:GLU:HA	2.21	0.41
1:D:206:LEU:HA	1:D:209:VAL:HG21	2.01	0.41
1:D:255:VAL:CG2	1:D:280:ALA:O	2.69	0.41
1:D:295:MET:HG3	1:D:329:ILE:CD1	2.51	0.41
1:D:332:PHE:O	1:D:332:PHE:CG	2.63	0.41
1:A:19:TYR:CD1	1:A:19:TYR:C	2.99	0.41
1:A:39:PRO:HG3	1:A:82:TYR:OH	2.21	0.41
1:A:127:TYR:O	1:A:128:GLU:C	2.63	0.41
1:A:268:THR:HB	1:A:273:LEU:HB2	2.03	0.41
1:B:32:PHE:CZ	1:B:43:ALA:HB2	2.56	0.41
1:B:52:ILE:HD13	1:B:69:MET:CG	2.51	0.41
1:B:231:VAL:HA	1:B:234:MET:HE3	2.01	0.41
1:C:268:THR:HB	1:C:273:LEU:HB2	2.03	0.41
1:C:400:VAL:H	1:C:400:VAL:HG23	1.42	0.41
1:A:169:GLU:O	1:A:173:ILE:HG22	2.21	0.40
1:A:176:GLU:O	1:A:383:ARG:HG3	2.21	0.40
1:A:295:MET:HG3	1:A:329:ILE:CD1	2.51	0.40
1:A:367:LEU:HD23	1:A:367:LEU:HA	1.63	0.40
1:A:378:HIS:HA	1:A:379:PRO:HD2	1.61	0.40
1:B:37:VAL:CG2	1:B:114:ALA:HB1	2.49	0.40
1:B:58:LEU:HA	1:B:58:LEU:HD22	1.87	0.40
1:B:160:LYS:HZ2	1:B:373:GLY:CA	2.34	0.40
1:B:243:ASN:C	1:B:245:GLY:N	2.78	0.40
1:C:316:VAL:HG22	1:C:355:LEU:HD13	2.02	0.40
1:C:332:PHE:O	1:C:332:PHE:CG	2.63	0.40
1:C:336:LYS:CE	1:C:336:LYS:HD2	2.20	0.40
1:D:212:ARG:O	1:D:215:ALA:HB3	2.22	0.40
1:D:285:PHE:C	1:D:287:ARG:H	2.28	0.40
1:A:110:PHE:CE1	1:A:293:ILE:HD11	2.56	0.40
1:B:105:VAL:H	1:B:105:VAL:HG13	1.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:LEU:C	1:B:132:HIS:N	2.78	0.40
1:B:139:GLY:C	1:B:141:GLN:N	2.78	0.40
1:B:150:LYS:HG3	1:B:151:ASP:N	2.36	0.40
1:B:296:LEU:O	1:B:297:ALA:C	2.64	0.40
1:C:52:ILE:O	1:C:52:ILE:CG1	2.69	0.40
1:C:55:TRP:CG	1:C:57:THR:CG2	3.04	0.40
1:C:77:LYS:HA	1:C:82:TYR:HD1	1.84	0.40
1:C:364:GLY:C	1:C:366:ASP:H	2.28	0.40
1:D:16:ASP:C	1:D:18:ASN:H	2.29	0.40
1:D:55:TRP:CG	1:D:57:THR:CG2	3.04	0.40
1:D:62:PRO:HB2	1:D:65:ALA:HB2	2.01	0.40
1:D:279:ARG:HD3	1:D:295:MET:HE1	1.96	0.40
1:B:39:PRO:HG3	1:B:82:TYR:OH	2.21	0.40
1:B:295:MET:HG3	1:B:329:ILE:HD13	2.02	0.40
1:C:52:ILE:HD13	1:C:69:MET:CG	2.51	0.40
1:C:55:TRP:CE3	1:C:57:THR:HG23	2.48	0.40
1:C:154:LEU:HD23	1:C:154:LEU:HA	1.40	0.40
1:C:182:ILE:HG22	1:C:184:LEU:N	2.36	0.40
1:D:43:ALA:HB3	1:D:75:LEU:CD2	2.51	0.40
1:D:62:PRO:O	1:D:63:GLU:C	2.63	0.40
1:D:295:MET:HG3	1:D:329:ILE:HD13	2.02	0.40
1:D:343:VAL:CG1	1:D:344:PHE:H	2.34	0.40
1:A:252:ASP:CB	1:A:255:VAL:HG21	2.48	0.40
1:B:59:TRP:O	1:B:60:LYS:C	2.64	0.40
1:B:124:HIS:ND1	1:B:124:HIS:N	2.69	0.40
1:B:295:MET:HG3	1:B:329:ILE:CD1	2.51	0.40
1:C:39:PRO:HG3	1:C:82:TYR:OH	2.21	0.40
1:C:252:ASP:CB	1:C:255:VAL:HG21	2.48	0.40
1:C:340:ILE:H	1:C:340:ILE:HG12	1.50	0.40
1:D:77:LYS:HA	1:D:82:TYR:HD1	1.84	0.40
1:D:94:GLU:CG	1:D:97:SER:HB3	2.43	0.40
1:D:150:LYS:HG3	1:D:151:ASP:N	2.36	0.40
1:D:169:GLU:O	1:D:173:ILE:HG22	2.21	0.40
1:A:43:ALA:HB3	1:A:75:LEU:CD2	2.51	0.40
1:A:52:ILE:HD13	1:A:69:MET:CG	2.51	0.40
1:A:150:LYS:HG3	1:A:151:ASP:N	2.36	0.40
1:A:295:MET:HG3	1:A:329:ILE:HD13	2.02	0.40
1:C:110:PHE:CE1	1:C:293:ILE:HD11	2.56	0.40
1:C:296:LEU:O	1:C:297:ALA:C	2.64	0.40
1:C:343:VAL:CG1	1:C:344:PHE:H	2.34	0.40

All (19) symmetry-related close contacts are listed below. The label for Atom-2 includes the

symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:THR:O	1:D:421:LEU:CD1[3_444]	0.58	1.62
1:C:422:SER:OG	1:D:424:ALA:O[3_444]	1.07	1.13
1:C:422:SER:OG	1:D:424:ALA:C[3_444]	1.34	0.86
1:A:23:ARG:NH1	1:B:23:ARG:NH2[2_555]	1.63	0.57
1:A:23:ARG:NH2	1:B:23:ARG:NH1[2_555]	1.66	0.54
1:B:9:GLU:OE1	1:D:421:LEU:CD2[3_444]	1.69	0.51
1:B:9:GLU:CD	1:D:421:LEU:CD2[3_444]	1.80	0.40
1:B:56:THR:C	1:D:421:LEU:CD1[3_444]	1.81	0.39
1:A:131:ARG:NH1	1:B:95:GLU:OE2[2_555]	1.90	0.30
1:A:95:GLU:OE2	1:B:131:ARG:NH1[2_555]	1.95	0.25
1:B:56:THR:O	1:D:421:LEU:CG[3_444]	1.98	0.22
1:A:424:ALA:CB	1:C:37:VAL:O[4_445]	2.03	0.17
2:A:469:HOH:O	2:A:469:HOH:O[2_555]	2.09	0.11
1:D:94:GLU:OE1	1:D:192:THR:OG1[2_555]	2.09	0.11
1:C:422:SER:CB	1:D:424:ALA:O[3_444]	2.11	0.09
1:B:9:GLU:OE2	1:D:421:LEU:CD2[3_444]	2.14	0.06
1:A:94:GLU:OE1	1:A:192:THR:OG1[2_555]	2.16	0.04
1:A:128:GLU:OE2	1:B:95:GLU:OE2[2_555]	2.17	0.03
2:D:468:HOH:O	2:D:468:HOH:O[2_555]	2.19	0.01

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	414/430 (96%)	298 (72%)	71 (17%)	45 (11%)	0	1
1	B	414/430 (96%)	298 (72%)	71 (17%)	45 (11%)	0	1
1	C	414/430 (96%)	298 (72%)	71 (17%)	45 (11%)	0	1
1	D	414/430 (96%)	298 (72%)	71 (17%)	45 (11%)	0	1
All	All	1656/1720 (96%)	1192 (72%)	284 (17%)	180 (11%)	0	1

All (180) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	TYR
1	A	50	SER
1	A	60	LYS
1	A	114	ALA
1	A	128	GLU
1	A	152	ARG
1	A	189	GLU
1	A	322	ASN
1	B	11	TYR
1	B	50	SER
1	B	60	LYS
1	B	114	ALA
1	B	128	GLU
1	B	152	ARG
1	B	189	GLU
1	B	322	ASN
1	C	11	TYR
1	C	50	SER
1	C	60	LYS
1	C	114	ALA
1	C	128	GLU
1	C	152	ARG
1	C	189	GLU
1	C	322	ASN
1	D	11	TYR
1	D	50	SER
1	D	60	LYS
1	D	114	ALA
1	D	128	GLU
1	D	152	ARG
1	D	189	GLU
1	D	322	ASN
1	A	43	ALA
1	A	51	SER
1	A	90	LEU
1	A	127	TYR
1	A	216	GLU
1	A	281	MET
1	A	320	ALA
1	A	323	TYR
1	A	374	GLY
1	A	388	ALA
1	A	389	LEU

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Mol	Chain	Res	Type
1	A	414	LYS
1	B	43	ALA
1	B	51	SER
1	B	90	LEU
1	B	127	TYR
1	B	216	GLU
1	B	281	MET
1	B	320	ALA
1	B	323	TYR
1	B	374	GLY
1	B	388	ALA
1	B	389	LEU
1	B	414	LYS
1	C	43	ALA
1	C	51	SER
1	C	90	LEU
1	C	127	TYR
1	C	216	GLU
1	C	281	MET
1	C	320	ALA
1	C	323	TYR
1	C	374	GLY
1	C	388	ALA
1	C	389	LEU
1	C	414	LYS
1	D	43	ALA
1	D	51	SER
1	D	90	LEU
1	D	127	TYR
1	D	216	GLU
1	D	281	MET
1	D	320	ALA
1	D	323	TYR
1	D	374	GLY
1	D	388	ALA
1	D	389	LEU
1	D	414	LYS
1	A	23	ARG
1	A	49	GLU
1	A	55	TRP
1	A	63	GLU
1	A	112	MET

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Mol	Chain	Res	Type
1	A	169	GLU
1	A	283	ALA
1	B	23	ARG
1	B	49	GLU
1	B	55	TRP
1	B	63	GLU
1	B	112	MET
1	B	169	GLU
1	B	283	ALA
1	C	23	ARG
1	C	49	GLU
1	C	55	TRP
1	C	63	GLU
1	C	112	MET
1	C	169	GLU
1	C	283	ALA
1	D	23	ARG
1	D	49	GLU
1	D	55	TRP
1	D	63	GLU
1	D	112	MET
1	D	169	GLU
1	D	283	ALA
1	A	74	TYR
1	A	80	GLU
1	A	106	ALA
1	A	349	GLY
1	A	350	GLY
1	A	373	GLY
1	A	413	LYS
1	A	421	LEU
1	B	74	TYR
1	B	80	GLU
1	B	106	ALA
1	B	349	GLY
1	B	350	GLY
1	B	373	GLY
1	B	413	LYS
1	B	421	LEU
1	C	74	TYR
1	C	80	GLU
1	C	106	ALA

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Mol	Chain	Res	Type
1	C	349	GLY
1	C	350	GLY
1	C	373	GLY
1	C	413	LYS
1	C	421	LEU
1	D	74	TYR
1	D	80	GLU
1	D	106	ALA
1	D	349	GLY
1	D	350	GLY
1	D	373	GLY
1	D	413	LYS
1	D	421	LEU
1	A	64	MET
1	C	64	MET
1	D	64	MET
1	A	68	SER
1	A	195	PRO
1	B	64	MET
1	B	68	SER
1	B	195	PRO
1	C	68	SER
1	C	195	PRO
1	D	68	SER
1	D	195	PRO
1	A	105	VAL
1	B	105	VAL
1	C	105	VAL
1	C	329	ILE
1	D	105	VAL
1	A	329	ILE
1	B	329	ILE
1	D	329	ILE
1	A	356	MET
1	B	356	MET
1	C	356	MET
1	D	356	MET
1	A	326	ILE
1	A	353	PRO
1	A	372	GLY
1	A	400	VAL
1	B	353	PRO

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Mol	Chain	Res	Type
1	B	372	GLY
1	B	400	VAL
1	C	353	PRO
1	C	372	GLY
1	C	400	VAL
1	D	353	PRO
1	D	372	GLY
1	D	400	VAL
1	B	326	ILE
1	C	326	ILE
1	D	326	ILE

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	338/351 (96%)	238 (70%)	100 (30%)	0	2
1	B	338/351 (96%)	238 (70%)	100 (30%)	0	2
1	C	338/351 (96%)	238 (70%)	100 (30%)	0	2
1	D	338/351 (96%)	238 (70%)	100 (30%)	0	2
All	All	1352/1404 (96%)	952 (70%)	400 (30%)	0	2

All (400) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	GLU
1	A	10	TRP
1	A	15	VAL
1	A	16	ASP
1	A	18	ASN
1	A	21	PRO
1	A	23	ARG
1	A	27	ILE
1	A	31	TYR
1	A	37	VAL

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Mol	Chain	Res	Type
1	A	38	SER
1	A	39	PRO
1	A	48	SER
1	A	52	ILE
1	A	54	THR
1	A	55	TRP
1	A	57	THR
1	A	58	LEU
1	A	61	LEU
1	A	64	MET
1	A	66	LYS
1	A	67	ARG
1	A	68	SER
1	A	72	VAL
1	A	73	PHE
1	A	74	TYR
1	A	75	LEU
1	A	76	GLU
1	A	83	ILE
1	A	91	THR
1	A	94	GLU
1	A	95	GLU
1	A	98	LEU
1	A	100	GLN
1	A	103	SER
1	A	105	VAL
1	A	109	VAL
1	A	113	LYS
1	A	116	LYS
1	A	118	LEU
1	A	121	LEU
1	A	124	HIS
1	A	128	GLU
1	A	147	MET
1	A	152	ARG
1	A	160	LYS
1	A	163	MET
1	A	168	GLU
1	A	173	ILE
1	A	184	LEU
1	A	189	GLU
1	A	193	SER

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Mol	Chain	Res	Type
1	A	195	PRO
1	A	198	ARG
1	A	203	VAL
1	A	205	LYS
1	A	209	VAL
1	A	216	GLU
1	A	217	THR
1	A	225	ILE
1	A	231	VAL
1	A	232	ASN
1	A	234	MET
1	A	240	MET
1	A	244	GLU
1	A	249	VAL
1	A	250	MET
1	A	251	ILE
1	A	253	ILE
1	A	254	VAL
1	A	255	VAL
1	A	259	SER
1	A	262	GLN
1	A	269	GLU
1	A	271	LEU
1	A	286	THR
1	A	289	PRO
1	A	290	ARG
1	A	294	THR
1	A	298	LEU
1	A	303	ARG
1	A	314	THR
1	A	318	LYS
1	A	325	GLU
1	A	326	ILE
1	A	327	LYS
1	A	329	ILE
1	A	341	ARG
1	A	342	PRO
1	A	344	PHE
1	A	348	SER
1	A	351	LEU
1	A	359	LEU
1	A	360	ILE

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Mol	Chain	Res	Type
1	A	365	LYS
1	A	368	VAL
1	A	370	GLN
1	A	375	VAL
1	A	397	ILE
1	A	418	GLU
1	B	9	GLU
1	B	10	TRP
1	B	15	VAL
1	B	16	ASP
1	B	18	ASN
1	B	21	PRO
1	B	23	ARG
1	B	27	ILE
1	B	31	TYR
1	B	37	VAL
1	B	38	SER
1	B	39	PRO
1	B	48	SER
1	B	52	ILE
1	B	54	THR
1	B	55	TRP
1	B	57	THR
1	B	58	LEU
1	B	61	LEU
1	B	64	MET
1	B	66	LYS
1	B	67	ARG
1	B	68	SER
1	B	72	VAL
1	B	73	PHE
1	B	74	TYR
1	B	75	LEU
1	B	76	GLU
1	B	83	ILE
1	B	91	THR
1	B	94	GLU
1	B	95	GLU
1	B	98	LEU
1	B	100	GLN
1	B	103	SER
1	B	105	VAL

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Mol	Chain	Res	Type
1	B	109	VAL
1	B	113	LYS
1	B	116	LYS
1	B	118	LEU
1	B	121	LEU
1	B	124	HIS
1	B	128	GLU
1	B	147	MET
1	B	152	ARG
1	B	160	LYS
1	B	163	MET
1	B	168	GLU
1	B	173	ILE
1	B	184	LEU
1	B	189	GLU
1	B	193	SER
1	B	195	PRO
1	B	198	ARG
1	B	203	VAL
1	B	205	LYS
1	B	209	VAL
1	B	216	GLU
1	B	217	THR
1	B	225	ILE
1	B	231	VAL
1	B	232	ASN
1	B	234	MET
1	B	240	MET
1	B	244	GLU
1	B	249	VAL
1	B	250	MET
1	B	251	ILE
1	B	253	ILE
1	B	254	VAL
1	B	255	VAL
1	B	259	SER
1	B	262	GLN
1	B	269	GLU
1	B	271	LEU
1	B	286	THR
1	B	289	PRO
1	B	290	ARG

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Mol	Chain	Res	Type
1	B	294	THR
1	B	298	LEU
1	B	303	ARG
1	B	314	THR
1	B	318	LYS
1	B	325	GLU
1	B	326	ILE
1	B	327	LYS
1	B	329	ILE
1	B	341	ARG
1	B	342	PRO
1	B	344	PHE
1	B	348	SER
1	B	351	LEU
1	B	359	LEU
1	B	360	ILE
1	B	365	LYS
1	B	368	VAL
1	B	370	GLN
1	B	375	VAL
1	B	397	ILE
1	B	418	GLU
1	C	9	GLU
1	C	10	TRP
1	C	15	VAL
1	C	16	ASP
1	C	18	ASN
1	C	21	PRO
1	C	23	ARG
1	C	27	ILE
1	C	31	TYR
1	C	37	VAL
1	C	38	SER
1	C	39	PRO
1	C	48	SER
1	C	52	ILE
1	C	54	THR
1	C	55	TRP
1	C	57	THR
1	C	58	LEU
1	C	61	LEU
1	C	64	MET

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Mol	Chain	Res	Type
1	C	66	LYS
1	C	67	ARG
1	C	68	SER
1	C	72	VAL
1	C	73	PHE
1	C	74	TYR
1	C	75	LEU
1	C	76	GLU
1	C	83	ILE
1	C	91	THR
1	C	94	GLU
1	C	95	GLU
1	C	98	LEU
1	C	100	GLN
1	C	103	SER
1	C	105	VAL
1	C	109	VAL
1	C	113	LYS
1	C	116	LYS
1	C	118	LEU
1	C	121	LEU
1	C	124	HIS
1	C	128	GLU
1	C	147	MET
1	C	152	ARG
1	C	160	LYS
1	C	163	MET
1	C	168	GLU
1	C	173	ILE
1	C	184	LEU
1	C	189	GLU
1	C	193	SER
1	C	195	PRO
1	C	198	ARG
1	C	203	VAL
1	C	205	LYS
1	C	209	VAL
1	C	216	GLU
1	C	217	THR
1	C	225	ILE
1	C	231	VAL
1	C	232	ASN

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Mol	Chain	Res	Type
1	C	234	MET
1	C	240	MET
1	C	244	GLU
1	C	249	VAL
1	C	250	MET
1	C	251	ILE
1	C	253	ILE
1	C	254	VAL
1	C	255	VAL
1	C	259	SER
1	C	262	GLN
1	C	269	GLU
1	C	271	LEU
1	C	286	THR
1	C	289	PRO
1	C	290	ARG
1	C	294	THR
1	C	298	LEU
1	C	303	ARG
1	C	314	THR
1	C	318	LYS
1	C	325	GLU
1	C	326	ILE
1	C	327	LYS
1	C	329	ILE
1	C	341	ARG
1	C	342	PRO
1	C	344	PHE
1	C	348	SER
1	C	351	LEU
1	C	359	LEU
1	C	360	ILE
1	C	365	LYS
1	C	368	VAL
1	C	370	GLN
1	C	375	VAL
1	C	397	ILE
1	C	418	GLU
1	D	9	GLU
1	D	10	TRP
1	D	15	VAL
1	D	16	ASP

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Mol	Chain	Res	Type
1	D	18	ASN
1	D	21	PRO
1	D	23	ARG
1	D	27	ILE
1	D	31	TYR
1	D	37	VAL
1	D	38	SER
1	D	39	PRO
1	D	48	SER
1	D	52	ILE
1	D	54	THR
1	D	55	TRP
1	D	57	THR
1	D	58	LEU
1	D	61	LEU
1	D	64	MET
1	D	66	LYS
1	D	67	ARG
1	D	68	SER
1	D	72	VAL
1	D	73	PHE
1	D	74	TYR
1	D	75	LEU
1	D	76	GLU
1	D	83	ILE
1	D	91	THR
1	D	94	GLU
1	D	95	GLU
1	D	98	LEU
1	D	100	GLN
1	D	103	SER
1	D	105	VAL
1	D	109	VAL
1	D	113	LYS
1	D	116	LYS
1	D	118	LEU
1	D	121	LEU
1	D	124	HIS
1	D	128	GLU
1	D	147	MET
1	D	152	ARG
1	D	160	LYS

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Mol	Chain	Res	Type
1	D	163	MET
1	D	168	GLU
1	D	173	ILE
1	D	184	LEU
1	D	189	GLU
1	D	193	SER
1	D	195	PRO
1	D	198	ARG
1	D	203	VAL
1	D	205	LYS
1	D	209	VAL
1	D	216	GLU
1	D	217	THR
1	D	225	ILE
1	D	231	VAL
1	D	232	ASN
1	D	234	MET
1	D	240	MET
1	D	244	GLU
1	D	249	VAL
1	D	250	MET
1	D	251	ILE
1	D	253	ILE
1	D	254	VAL
1	D	255	VAL
1	D	259	SER
1	D	262	GLN
1	D	269	GLU
1	D	271	LEU
1	D	286	THR
1	D	289	PRO
1	D	290	ARG
1	D	294	THR
1	D	298	LEU
1	D	303	ARG
1	D	314	THR
1	D	318	LYS
1	D	325	GLU
1	D	326	ILE
1	D	327	LYS
1	D	329	ILE
1	D	341	ARG

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Mol	Chain	Res	Type
1	D	342	PRO
1	D	344	PHE
1	D	348	SER
1	D	351	LEU
1	D	359	LEU
1	D	360	ILE
1	D	365	LYS
1	D	368	VAL
1	D	370	GLN
1	D	375	VAL
1	D	397	ILE
1	D	418	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	35	ASN
1	A	100	GLN
1	A	117	ASN
1	A	124	HIS
1	A	137	GLN
1	A	226	ASN
1	A	243	ASN
1	A	247	GLN
1	A	276	HIS
1	A	282	HIS
1	A	311	HIS
1	A	330	ASN
1	A	370	GLN
1	B	35	ASN
1	B	100	GLN
1	B	124	HIS
1	B	137	GLN
1	B	226	ASN
1	B	243	ASN
1	B	247	GLN
1	B	276	HIS
1	B	282	HIS
1	B	288	ASN
1	B	311	HIS
1	B	330	ASN

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Mol	Chain	Res	Type
1	B	339	HIS
1	B	370	GLN
1	C	35	ASN
1	C	100	GLN
1	C	124	HIS
1	C	137	GLN
1	C	226	ASN
1	C	243	ASN
1	C	247	GLN
1	C	276	HIS
1	C	282	HIS
1	C	288	ASN
1	C	311	HIS
1	C	330	ASN
1	C	339	HIS
1	C	370	GLN
1	D	18	ASN
1	D	35	ASN
1	D	100	GLN
1	D	226	ASN
1	D	243	ASN
1	D	247	GLN
1	D	276	HIS
1	D	282	HIS
1	D	311	HIS
1	D	330	ASN
1	D	339	HIS
1	D	370	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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	416/430 (96%)	-0.52	1 (0%) 91 83	61, 89, 123, 154	0
1	B	416/430 (96%)	-0.50	1 (0%) 91 83	61, 89, 123, 154	0
1	C	416/430 (96%)	-0.47	0 100 100	61, 89, 123, 154	0
1	D	416/430 (96%)	-0.40	4 (0%) 79 59	61, 89, 123, 154	0
All	All	1664/1720 (96%)	-0.47	6 (0%) 88 76	61, 89, 123, 154	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	422	SER	3.1
1	B	419	VAL	3.0
1	D	420	GLY	2.8
1	D	56	THR	2.4
1	D	241	VAL	2.3
1	A	297	ALA	2.2

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.