



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 07:55 pm GMT

PDB ID : 2CXE
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	trunk30967
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk30967

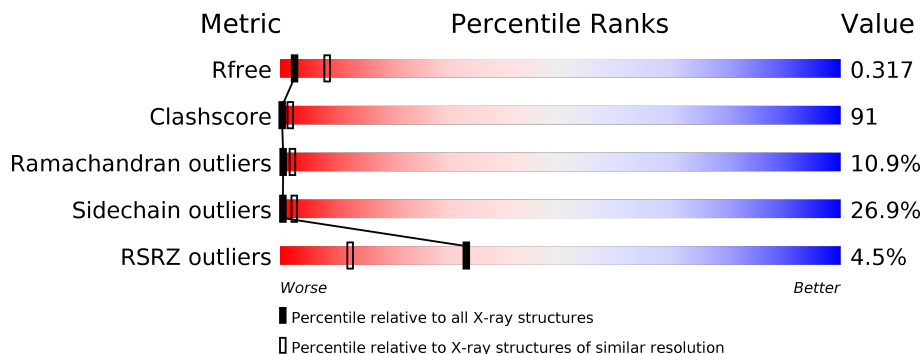
1 Overall quality at a glance

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}	111664	1851 (3.00-3.00)
Clashscore	122126	2167 (3.00-3.00)
Ramachandran outliers	120053	2101 (3.00-3.00)
Sidechain outliers	120020	2104 (3.00-3.00)
RSRZ outliers	108989	1751 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	
1	B	430	
1	C	430	
1	D	430	

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			

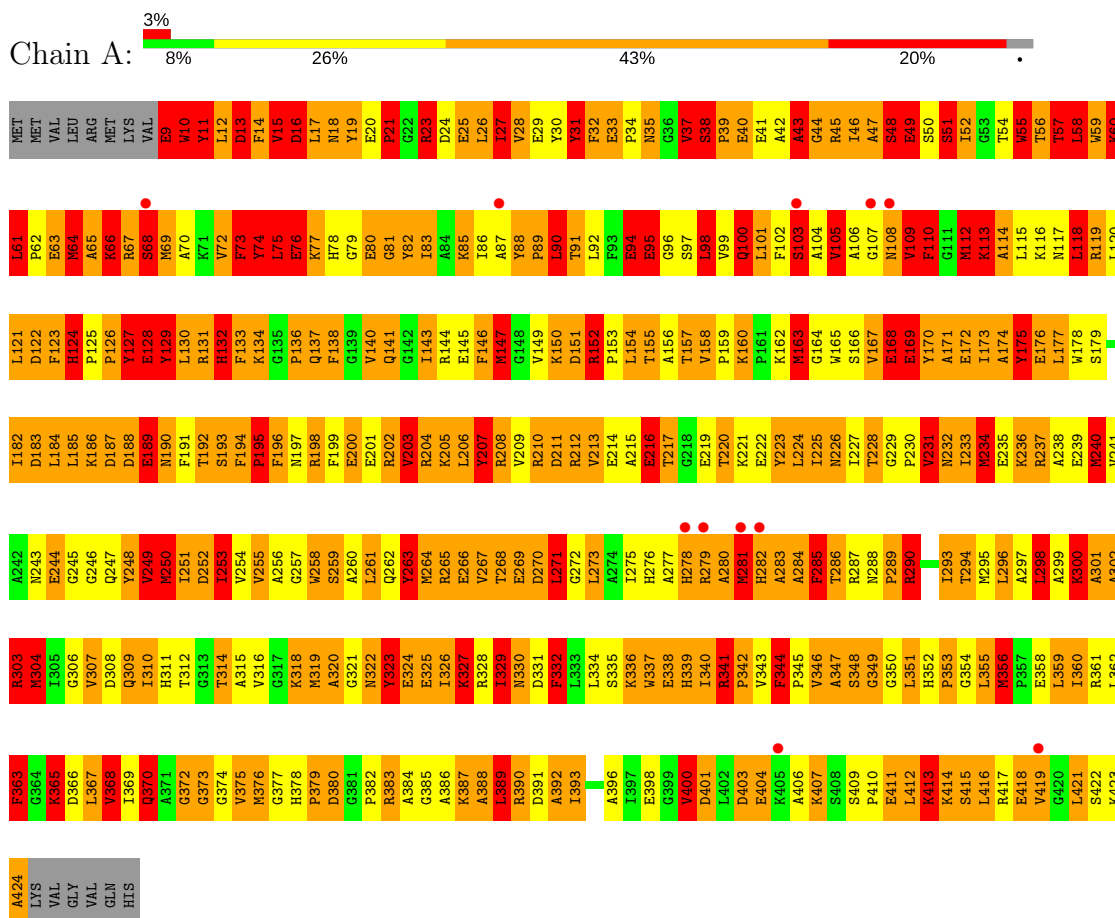
- Molecule 2 is water.

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		

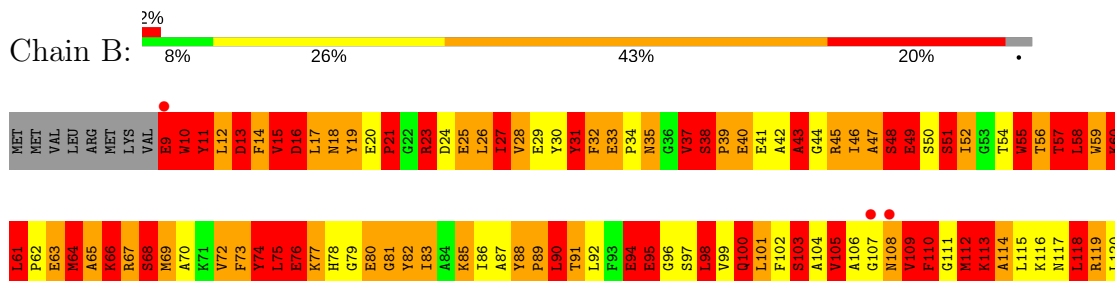
3 Residue-property plots

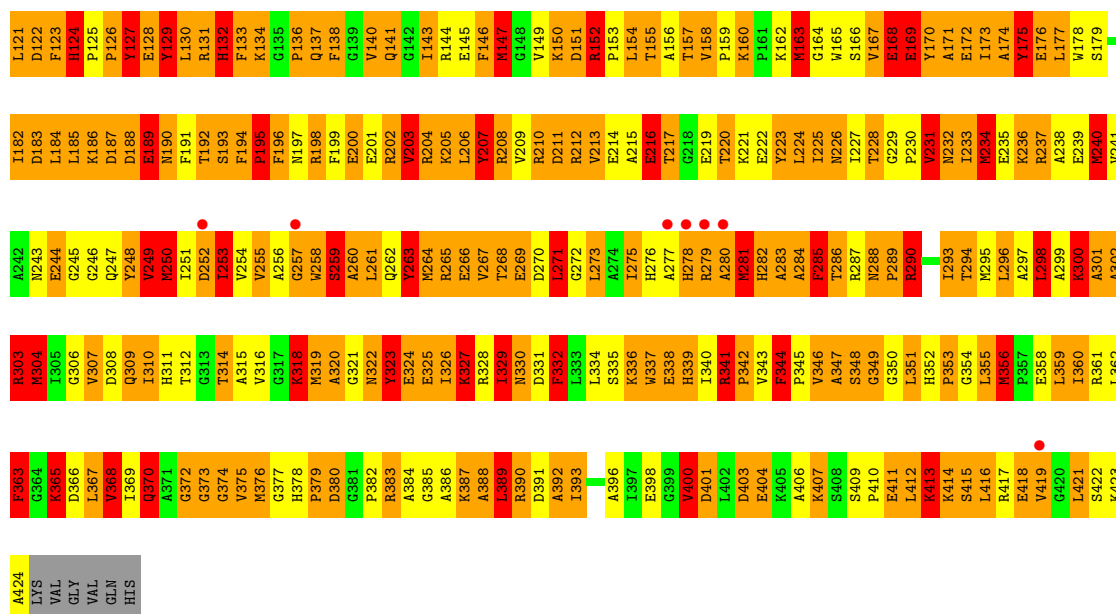
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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

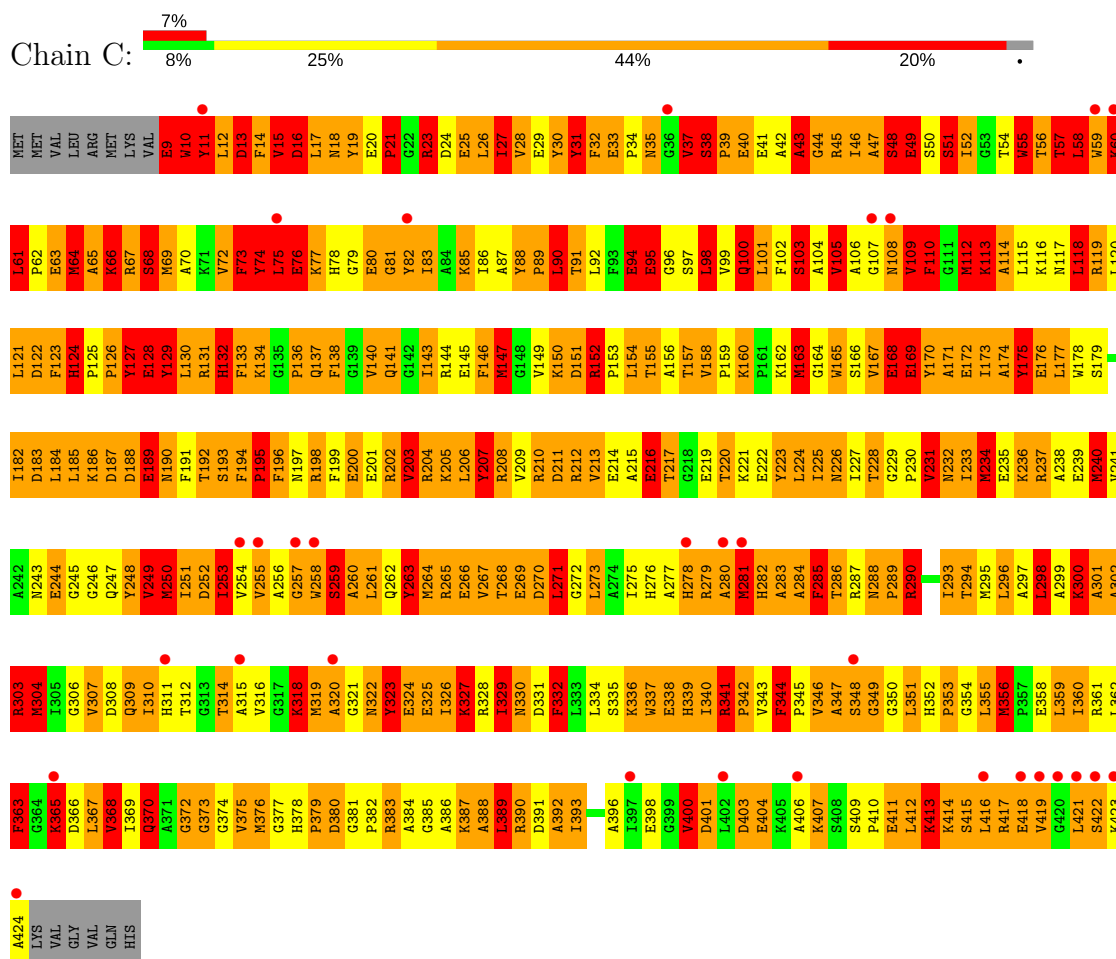


• Molecule 1: Ribulose biphosphate carboxylase





• 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 – 2.91	Depositor EDS
% Data completeness (in resolution range)	85.7 (46.72-3.00) 83.9 (46.72-2.91)	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)	0.31 , 57.5	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	0.91	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	3.39	375/3365 (11.1%)	2.81	308/4546 (6.8%)
1	B	3.39	379/3365 (11.3%)	2.81	310/4546 (6.8%)
1	C	3.39	377/3365 (11.2%)	2.81	310/4546 (6.8%)
1	D	3.39	374/3365 (11.1%)	2.81	307/4546 (6.8%)
All	All	3.39	1505/13460 (11.2%)	2.81	1235/18184 (6.8%)

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 (1505) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	216	GLU	CG-CD	30.20	1.97	1.51
1	A	216	GLU	CG-CD	30.20	1.97	1.51
1	B	216	GLU	CG-CD	30.20	1.97	1.51
1	D	216	GLU	CG-CD	30.20	1.97	1.51
1	C	216	GLU	CD-OE2	22.83	1.50	1.25
1	B	216	GLU	CD-OE2	22.82	1.50	1.25
1	D	216	GLU	CD-OE2	22.82	1.50	1.25
1	A	216	GLU	CD-OE2	22.80	1.50	1.25
1	C	64	MET	SD-CE	20.95	2.95	1.77
1	A	64	MET	SD-CE	20.94	2.95	1.77
1	B	64	MET	SD-CE	20.93	2.95	1.77
1	D	64	MET	SD-CE	20.93	2.95	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	266	GLU	CD-OE1	17.53	1.45	1.25
1	B	266	GLU	CD-OE1	17.51	1.45	1.25
1	A	266	GLU	CD-OE1	17.50	1.45	1.25
1	C	266	GLU	CD-OE1	17.43	1.44	1.25
1	D	239	GLU	CD-OE2	17.25	1.44	1.25
1	C	239	GLU	CD-OE2	17.23	1.44	1.25
1	A	239	GLU	CD-OE2	17.20	1.44	1.25
1	B	239	GLU	CD-OE2	17.20	1.44	1.25
1	D	249	VAL	CB-CG1	-16.41	1.18	1.52
1	B	249	VAL	CB-CG1	-16.39	1.18	1.52
1	A	249	VAL	CB-CG1	-16.39	1.18	1.52
1	C	249	VAL	CB-CG1	-16.35	1.18	1.52
1	C	281	MET	SD-CE	16.12	2.68	1.77
1	D	281	MET	SD-CE	16.11	2.68	1.77
1	A	281	MET	SD-CE	16.11	2.68	1.77
1	B	281	MET	SD-CE	16.10	2.68	1.77
1	D	172	GLU	CG-CD	15.91	1.75	1.51
1	B	172	GLU	CG-CD	15.91	1.75	1.51
1	B	341	ARG	CZ-NH1	15.91	1.53	1.33
1	A	172	GLU	CG-CD	15.90	1.75	1.51
1	D	341	ARG	CZ-NH1	15.90	1.53	1.33
1	C	172	GLU	CG-CD	15.89	1.75	1.51
1	C	341	ARG	CZ-NH1	15.88	1.53	1.33
1	A	341	ARG	CZ-NH1	15.87	1.53	1.33
1	B	76	GLU	CD-OE2	15.80	1.43	1.25
1	D	76	GLU	CD-OE2	15.77	1.43	1.25
1	A	76	GLU	CD-OE2	15.74	1.43	1.25
1	B	200	GLU	CG-CD	15.69	1.75	1.51
1	C	200	GLU	CG-CD	15.68	1.75	1.51
1	C	76	GLU	CD-OE2	15.67	1.42	1.25
1	A	200	GLU	CG-CD	15.66	1.75	1.51
1	D	200	GLU	CG-CD	15.63	1.75	1.51
1	C	201	GLU	CD-OE2	15.43	1.42	1.25
1	D	201	GLU	CD-OE2	15.41	1.42	1.25
1	A	201	GLU	CD-OE2	15.40	1.42	1.25
1	B	266	GLU	CD-OE2	15.39	1.42	1.25
1	C	266	GLU	CD-OE2	15.38	1.42	1.25
1	A	266	GLU	CD-OE2	15.37	1.42	1.25
1	B	201	GLU	CD-OE2	15.36	1.42	1.25
1	D	266	GLU	CD-OE2	15.31	1.42	1.25
1	C	216	GLU	CD-OE1	14.70	1.41	1.25
1	B	216	GLU	CD-OE1	14.69	1.41	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	216	GLU	CD-OE1	14.66	1.41	1.25
1	D	216	GLU	CD-OE1	14.62	1.41	1.25
1	A	175	TYR	CD1-CE1	14.31	1.60	1.39
1	C	175	TYR	CD1-CE1	14.31	1.60	1.39
1	B	175	TYR	CD1-CE1	14.31	1.60	1.39
1	D	175	TYR	CD1-CE1	14.31	1.60	1.39
1	C	189	GLU	CD-OE1	14.10	1.41	1.25
1	A	189	GLU	CD-OE1	14.09	1.41	1.25
1	B	189	GLU	CD-OE1	14.08	1.41	1.25
1	D	189	GLU	CD-OE1	14.07	1.41	1.25
1	C	269	GLU	CG-CD	13.64	1.72	1.51
1	B	269	GLU	CG-CD	13.64	1.72	1.51
1	A	269	GLU	CG-CD	13.62	1.72	1.51
1	D	269	GLU	CG-CD	13.62	1.72	1.51
1	B	76	GLU	CG-CD	13.61	1.72	1.51
1	C	76	GLU	CG-CD	13.60	1.72	1.51
1	D	76	GLU	CG-CD	13.59	1.72	1.51
1	A	76	GLU	CG-CD	13.59	1.72	1.51
1	D	325	GLU	CD-OE2	13.56	1.40	1.25
1	B	80	GLU	CD-OE1	13.51	1.40	1.25
1	A	80	GLU	CD-OE1	13.51	1.40	1.25
1	A	325	GLU	CD-OE2	13.49	1.40	1.25
1	B	325	GLU	CD-OE2	13.48	1.40	1.25
1	C	325	GLU	CD-OE2	13.46	1.40	1.25
1	C	80	GLU	CD-OE1	13.46	1.40	1.25
1	A	141	GLN	CG-CD	13.46	1.82	1.51
1	B	141	GLN	CG-CD	13.46	1.81	1.51
1	D	141	GLN	CG-CD	13.45	1.81	1.51
1	C	141	GLN	CG-CD	13.44	1.81	1.51
1	D	80	GLU	CD-OE1	13.43	1.40	1.25
1	B	172	GLU	CD-OE1	13.39	1.40	1.25
1	C	172	GLU	CD-OE1	13.36	1.40	1.25
1	B	80	GLU	CG-CD	13.35	1.72	1.51
1	D	80	GLU	CG-CD	13.34	1.72	1.51
1	A	172	GLU	CD-OE1	13.34	1.40	1.25
1	B	63	GLU	CD-OE1	13.34	1.40	1.25
1	A	80	GLU	CG-CD	13.31	1.72	1.51
1	D	63	GLU	CD-OE1	13.29	1.40	1.25
1	C	63	GLU	CD-OE1	13.28	1.40	1.25
1	C	80	GLU	CG-CD	13.28	1.71	1.51
1	D	172	GLU	CD-OE1	13.28	1.40	1.25
1	A	63	GLU	CD-OE1	13.27	1.40	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	168	GLU	CD-OE2	13.08	1.40	1.25
1	A	168	GLU	CD-OE2	13.02	1.40	1.25
1	B	168	GLU	CD-OE2	13.01	1.40	1.25
1	C	168	GLU	CD-OE2	13.01	1.40	1.25
1	D	186	LYS	CE-NZ	12.71	1.80	1.49
1	A	186	LYS	CE-NZ	12.70	1.80	1.49
1	C	186	LYS	CE-NZ	12.69	1.80	1.49
1	B	186	LYS	CE-NZ	12.68	1.80	1.49
1	D	172	GLU	CD-OE2	12.68	1.39	1.25
1	D	319	MET	SD-CE	12.63	2.48	1.77
1	A	319	MET	SD-CE	12.63	2.48	1.77
1	C	172	GLU	CD-OE2	12.63	1.39	1.25
1	B	319	MET	SD-CE	12.62	2.48	1.77
1	C	319	MET	SD-CE	12.62	2.48	1.77
1	A	172	GLU	CD-OE2	12.62	1.39	1.25
1	B	172	GLU	CD-OE2	12.61	1.39	1.25
1	B	57	THR	CA-CB	12.30	1.85	1.53
1	D	57	THR	CA-CB	12.29	1.85	1.53
1	A	57	THR	CA-CB	12.28	1.85	1.53
1	C	57	THR	CA-CB	12.28	1.85	1.53
1	C	307	VAL	CB-CG2	-12.06	1.27	1.52
1	A	307	VAL	CB-CG2	-12.06	1.27	1.52
1	B	168	GLU	CG-CD	12.05	1.70	1.51
1	B	307	VAL	CB-CG2	-12.05	1.27	1.52
1	D	307	VAL	CB-CG2	-12.04	1.27	1.52
1	A	168	GLU	CG-CD	12.04	1.70	1.51
1	C	168	GLU	CG-CD	12.04	1.70	1.51
1	D	168	GLU	CG-CD	12.01	1.70	1.51
1	D	151	ASP	CB-CG	11.92	1.76	1.51
1	C	151	ASP	CB-CG	11.91	1.76	1.51
1	B	151	ASP	CB-CG	11.91	1.76	1.51
1	A	151	ASP	CB-CG	11.91	1.76	1.51
1	B	347	ALA	CA-CB	-11.60	1.28	1.52
1	C	66	LYS	CD-CE	11.60	1.80	1.51
1	D	66	LYS	CD-CE	11.59	1.80	1.51
1	A	347	ALA	CA-CB	-11.59	1.28	1.52
1	C	347	ALA	CA-CB	-11.59	1.28	1.52
1	A	66	LYS	CD-CE	11.57	1.80	1.51
1	B	66	LYS	CD-CE	11.57	1.80	1.51
1	D	347	ALA	CA-CB	-11.56	1.28	1.52
1	C	145	GLU	CG-CD	11.34	1.69	1.51
1	B	145	GLU	CG-CD	11.33	1.69	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	145	GLU	CG-CD	11.33	1.69	1.51
1	A	145	GLU	CG-CD	11.31	1.69	1.51
1	D	419	VAL	CB-CG2	11.03	1.76	1.52
1	A	419	VAL	CB-CG2	11.03	1.76	1.52
1	B	419	VAL	CB-CG2	11.02	1.75	1.52
1	D	226	ASN	C-O	11.00	1.44	1.23
1	D	324	GLU	CG-CD	11.00	1.68	1.51
1	C	226	ASN	C-O	11.00	1.44	1.23
1	C	419	VAL	CB-CG2	10.99	1.75	1.52
1	A	226	ASN	C-O	10.99	1.44	1.23
1	B	226	ASN	C-O	10.99	1.44	1.23
1	A	324	GLU	CG-CD	10.98	1.68	1.51
1	C	324	GLU	CG-CD	10.98	1.68	1.51
1	B	324	GLU	CG-CD	10.96	1.68	1.51
1	D	404	GLU	CD-OE2	10.93	1.37	1.25
1	C	404	GLU	CD-OE2	10.91	1.37	1.25
1	B	404	GLU	CD-OE2	10.90	1.37	1.25
1	A	404	GLU	CD-OE2	10.89	1.37	1.25
1	D	104	ALA	CA-CB	-10.88	1.29	1.52
1	B	104	ALA	CA-CB	-10.85	1.29	1.52
1	A	104	ALA	CA-CB	-10.84	1.29	1.52
1	C	104	ALA	CA-CB	-10.84	1.29	1.52
1	D	95	GLU	CD-OE1	10.75	1.37	1.25
1	C	95	GLU	CD-OE1	10.75	1.37	1.25
1	A	95	GLU	CD-OE1	10.75	1.37	1.25
1	B	95	GLU	CD-OE1	10.73	1.37	1.25
1	D	300	LYS	CD-CE	10.72	1.78	1.51
1	C	300	LYS	CD-CE	10.70	1.78	1.51
1	A	300	LYS	CD-CE	10.70	1.77	1.51
1	B	300	LYS	CD-CE	10.70	1.77	1.51
1	B	145	GLU	CD-OE1	10.53	1.37	1.25
1	A	233	ILE	CA-CB	-10.52	1.30	1.54
1	C	233	ILE	CA-CB	-10.52	1.30	1.54
1	B	233	ILE	CA-CB	-10.51	1.30	1.54
1	D	233	ILE	CA-CB	-10.51	1.30	1.54
1	D	91	THR	C-O	10.51	1.43	1.23
1	A	145	GLU	CD-OE1	10.50	1.37	1.25
1	C	145	GLU	CD-OE1	10.50	1.37	1.25
1	B	91	THR	C-O	10.49	1.43	1.23
1	C	91	THR	C-O	10.49	1.43	1.23
1	D	145	GLU	CD-OE1	10.49	1.37	1.25
1	A	91	THR	C-O	10.47	1.43	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	404	GLU	CD-OE1	10.35	1.37	1.25
1	D	198	ARG	NE-CZ	10.34	1.46	1.33
1	C	404	GLU	CD-OE1	10.34	1.37	1.25
1	A	404	GLU	CD-OE1	10.34	1.37	1.25
1	B	68	SER	CA-CB	10.32	1.68	1.52
1	B	266	GLU	CA-CB	-10.32	1.31	1.53
1	B	404	GLU	CD-OE1	10.32	1.36	1.25
1	B	198	ARG	NE-CZ	10.31	1.46	1.33
1	C	266	GLU	CA-CB	-10.31	1.31	1.53
1	A	266	GLU	CA-CB	-10.30	1.31	1.53
1	D	266	GLU	CA-CB	-10.30	1.31	1.53
1	A	198	ARG	NE-CZ	10.29	1.46	1.33
1	A	68	SER	CA-CB	10.28	1.68	1.52
1	D	68	SER	CA-CB	10.27	1.68	1.52
1	C	68	SER	CA-CB	10.27	1.68	1.52
1	A	189	GLU	CD-OE2	10.26	1.36	1.25
1	C	198	ARG	NE-CZ	10.26	1.46	1.33
1	B	189	GLU	CD-OE2	10.25	1.36	1.25
1	C	189	GLU	CD-OE2	10.24	1.36	1.25
1	D	189	GLU	CD-OE2	10.23	1.36	1.25
1	D	358	GLU	CD-OE2	10.14	1.36	1.25
1	B	302	ALA	CA-CB	-10.13	1.31	1.52
1	A	358	GLU	CD-OE2	10.12	1.36	1.25
1	C	302	ALA	CA-CB	-10.12	1.31	1.52
1	B	358	GLU	CD-OE2	10.11	1.36	1.25
1	A	302	ALA	CA-CB	-10.09	1.31	1.52
1	D	302	ALA	CA-CB	-10.07	1.31	1.52
1	C	358	GLU	CD-OE2	10.02	1.36	1.25
1	D	267	VAL	CB-CG1	-9.96	1.31	1.52
1	A	222	GLU	CB-CG	-9.96	1.33	1.52
1	D	222	GLU	CB-CG	-9.95	1.33	1.52
1	B	222	GLU	CB-CG	-9.94	1.33	1.52
1	C	194	PHE	CE2-CZ	9.94	1.56	1.37
1	B	267	VAL	CB-CG1	-9.94	1.31	1.52
1	A	267	VAL	CB-CG1	-9.94	1.31	1.52
1	C	222	GLU	CB-CG	-9.93	1.33	1.52
1	C	267	VAL	CB-CG1	-9.93	1.31	1.52
1	D	194	PHE	CE2-CZ	9.90	1.56	1.37
1	A	194	PHE	CE2-CZ	9.89	1.56	1.37
1	B	419	VAL	CB-CG1	9.87	1.73	1.52
1	C	419	VAL	CB-CG1	9.87	1.73	1.52
1	B	194	PHE	CE2-CZ	9.86	1.56	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	419	VAL	CB-CG1	9.85	1.73	1.52
1	B	160	LYS	CD-CE	9.85	1.75	1.51
1	D	419	VAL	CB-CG1	9.85	1.73	1.52
1	C	160	LYS	CD-CE	9.84	1.75	1.51
1	A	160	LYS	CD-CE	9.83	1.75	1.51
1	D	160	LYS	CD-CE	9.81	1.75	1.51
1	A	361	ARG	CZ-NH2	9.73	1.45	1.33
1	C	348	SER	CA-CB	9.73	1.67	1.52
1	C	361	ARG	CZ-NH2	9.73	1.45	1.33
1	B	361	ARG	CZ-NH2	9.72	1.45	1.33
1	D	361	ARG	CZ-NH2	9.71	1.45	1.33
1	B	348	SER	CA-CB	9.69	1.67	1.52
1	B	40	GLU	CD-OE2	9.69	1.36	1.25
1	C	40	GLU	CD-OE2	9.69	1.36	1.25
1	A	40	GLU	CD-OE2	9.67	1.36	1.25
1	A	348	SER	CA-CB	9.67	1.67	1.52
1	D	40	GLU	CD-OE2	9.67	1.36	1.25
1	D	266	GLU	CB-CG	-9.66	1.33	1.52
1	D	348	SER	CA-CB	9.66	1.67	1.52
1	A	266	GLU	CB-CG	-9.65	1.33	1.52
1	B	266	GLU	CB-CG	-9.65	1.33	1.52
1	C	266	GLU	CB-CG	-9.64	1.33	1.52
1	D	424	ALA	CA-CB	9.57	1.72	1.52
1	A	424	ALA	CA-CB	9.57	1.72	1.52
1	C	424	ALA	CA-CB	9.56	1.72	1.52
1	B	424	ALA	CA-CB	9.55	1.72	1.52
1	D	31	TYR	CE2-CZ	9.53	1.50	1.38
1	B	31	TYR	CE2-CZ	9.51	1.50	1.38
1	A	31	TYR	CE2-CZ	9.48	1.50	1.38
1	B	167	VAL	CB-CG2	9.47	1.72	1.52
1	A	167	VAL	CB-CG2	9.46	1.72	1.52
1	C	167	VAL	CB-CG2	9.46	1.72	1.52
1	B	82	TYR	CB-CG	-9.45	1.37	1.51
1	C	31	TYR	CE2-CZ	9.45	1.50	1.38
1	D	167	VAL	CB-CG2	9.45	1.72	1.52
1	A	207	TYR	CG-CD1	9.44	1.51	1.39
1	A	82	TYR	CB-CG	-9.43	1.37	1.51
1	A	182	ILE	CA-CB	-9.43	1.33	1.54
1	B	182	ILE	CA-CB	-9.43	1.33	1.54
1	B	306	GLY	C-O	9.42	1.38	1.23
1	C	182	ILE	CA-CB	-9.41	1.33	1.54
1	C	207	TYR	CG-CD1	9.40	1.51	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	336	LYS	CD-CE	9.40	1.74	1.51
1	D	182	ILE	CA-CB	-9.40	1.33	1.54
1	D	82	TYR	CB-CG	-9.40	1.37	1.51
1	D	207	TYR	CG-CD1	9.40	1.51	1.39
1	A	306	GLY	C-O	9.39	1.38	1.23
1	A	336	LYS	CD-CE	9.39	1.74	1.51
1	C	336	LYS	CD-CE	9.39	1.74	1.51
1	C	82	TYR	CB-CG	-9.39	1.37	1.51
1	C	216	GLU	CA-C	9.39	1.77	1.52
1	D	216	GLU	CA-C	9.38	1.77	1.52
1	C	306	GLY	C-O	9.38	1.38	1.23
1	D	336	LYS	CD-CE	9.38	1.74	1.51
1	A	216	GLU	CA-C	9.38	1.77	1.52
1	D	306	GLY	C-O	9.38	1.38	1.23
1	B	216	GLU	CA-C	9.37	1.77	1.52
1	B	207	TYR	CG-CD1	9.37	1.51	1.39
1	D	175	TYR	CZ-OH	9.33	1.53	1.37
1	B	175	TYR	CZ-OH	9.30	1.53	1.37
1	A	175	TYR	CZ-OH	9.29	1.53	1.37
1	C	175	TYR	CZ-OH	9.27	1.53	1.37
1	D	348	SER	CB-OG	9.15	1.54	1.42
1	A	348	SER	CB-OG	9.12	1.54	1.42
1	B	263	TYR	CD1-CE1	9.11	1.53	1.39
1	D	263	TYR	CD1-CE1	9.10	1.52	1.39
1	A	263	TYR	CD1-CE1	9.09	1.52	1.39
1	B	348	SER	CB-OG	9.09	1.54	1.42
1	C	263	TYR	CD1-CE1	9.07	1.52	1.39
1	C	348	SER	CB-OG	9.05	1.54	1.42
1	B	346	VAL	CB-CG2	-8.99	1.33	1.52
1	C	346	VAL	CB-CG2	-8.97	1.34	1.52
1	C	11	TYR	CE2-CZ	8.97	1.50	1.38
1	A	11	TYR	CE2-CZ	8.97	1.50	1.38
1	D	11	TYR	CE2-CZ	8.97	1.50	1.38
1	A	346	VAL	CB-CG2	-8.96	1.34	1.52
1	D	63	GLU	CD-OE2	8.96	1.35	1.25
1	C	77	LYS	CD-CE	8.95	1.73	1.51
1	A	63	GLU	CD-OE2	8.95	1.35	1.25
1	D	175	TYR	CD2-CE2	8.95	1.52	1.39
1	B	11	TYR	CE2-CZ	8.94	1.50	1.38
1	B	77	LYS	CD-CE	8.94	1.73	1.51
1	D	346	VAL	CB-CG2	-8.94	1.34	1.52
1	A	77	LYS	CD-CE	8.92	1.73	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	175	TYR	CD2-CE2	8.91	1.52	1.39
1	D	77	LYS	CD-CE	8.91	1.73	1.51
1	B	175	TYR	CD2-CE2	8.90	1.52	1.39
1	C	63	GLU	CD-OE2	8.90	1.35	1.25
1	A	203	VAL	CB-CG2	-8.89	1.34	1.52
1	A	244	GLU	CG-CD	-8.88	1.38	1.51
1	D	244	GLU	CG-CD	-8.88	1.38	1.51
1	C	203	VAL	CB-CG2	-8.88	1.34	1.52
1	B	203	VAL	CB-CG2	-8.87	1.34	1.52
1	B	244	GLU	CG-CD	-8.87	1.38	1.51
1	D	203	VAL	CB-CG2	-8.86	1.34	1.52
1	C	175	TYR	CD2-CE2	8.86	1.52	1.39
1	B	63	GLU	CD-OE2	8.85	1.35	1.25
1	C	244	GLU	CG-CD	-8.85	1.38	1.51
1	A	66	LYS	CG-CD	8.77	1.82	1.52
1	D	66	LYS	CG-CD	8.76	1.82	1.52
1	B	66	LYS	CG-CD	8.75	1.82	1.52
1	C	66	LYS	CG-CD	8.75	1.82	1.52
1	C	68	SER	CB-OG	8.68	1.53	1.42
1	A	240	MET	CG-SD	8.67	2.03	1.81
1	B	240	MET	CG-SD	8.67	2.03	1.81
1	C	18	ASN	CB-CG	8.67	1.71	1.51
1	B	18	ASN	CB-CG	8.67	1.71	1.51
1	A	18	ASN	CB-CG	8.66	1.71	1.51
1	D	240	MET	CG-SD	8.66	2.03	1.81
1	C	49	GLU	CG-CD	8.66	1.65	1.51
1	C	240	MET	CG-SD	8.65	2.03	1.81
1	D	18	ASN	CB-CG	8.65	1.71	1.51
1	B	11	TYR	CG-CD1	8.64	1.50	1.39
1	A	68	SER	CB-OG	8.63	1.53	1.42
1	D	68	SER	CB-OG	8.62	1.53	1.42
1	A	49	GLU	CG-CD	8.62	1.64	1.51
1	A	11	TYR	CG-CD1	8.61	1.50	1.39
1	B	387	LYS	CD-CE	8.61	1.72	1.51
1	C	244	GLU	CD-OE1	8.61	1.35	1.25
1	D	244	GLU	CD-OE1	8.61	1.35	1.25
1	D	387	LYS	CD-CE	8.61	1.72	1.51
1	A	31	TYR	CD2-CE2	8.60	1.52	1.39
1	D	136	PRO	CG-CD	8.60	1.79	1.50
1	D	49	GLU	CG-CD	8.60	1.64	1.51
1	C	31	TYR	CD2-CE2	8.60	1.52	1.39
1	A	387	LYS	CD-CE	8.60	1.72	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	68	SER	CB-OG	8.59	1.53	1.42
1	C	11	TYR	CG-CD1	8.59	1.50	1.39
1	C	136	PRO	CG-CD	8.59	1.79	1.50
1	B	244	GLU	CD-OE1	8.59	1.35	1.25
1	D	31	TYR	CD2-CE2	8.59	1.52	1.39
1	A	136	PRO	CG-CD	8.58	1.78	1.50
1	A	244	GLU	CD-OE1	8.58	1.35	1.25
1	B	49	GLU	CG-CD	8.58	1.64	1.51
1	D	398	GLU	CD-OE1	8.57	1.35	1.25
1	B	31	TYR	CD2-CE2	8.57	1.52	1.39
1	C	387	LYS	CD-CE	8.57	1.72	1.51
1	B	136	PRO	CG-CD	8.56	1.78	1.50
1	D	11	TYR	CG-CD1	8.56	1.50	1.39
1	D	320	ALA	CA-CB	8.54	1.70	1.52
1	A	398	GLU	CD-OE1	8.54	1.35	1.25
1	C	398	GLU	CD-OE1	8.53	1.35	1.25
1	B	398	GLU	CD-OE1	8.53	1.35	1.25
1	C	20	GLU	CD-OE1	8.52	1.35	1.25
1	C	171	ALA	CA-CB	8.52	1.70	1.52
1	C	320	ALA	CA-CB	8.51	1.70	1.52
1	A	320	ALA	CA-CB	8.50	1.70	1.52
1	B	320	ALA	CA-CB	8.49	1.70	1.52
1	A	20	GLU	CD-OE1	8.48	1.34	1.25
1	A	171	ALA	CA-CB	8.48	1.70	1.52
1	D	20	GLU	CD-OE1	8.48	1.34	1.25
1	D	171	ALA	CA-CB	8.47	1.70	1.52
1	B	200	GLU	CD-OE2	8.47	1.34	1.25
1	B	20	GLU	CD-OE1	8.47	1.34	1.25
1	D	200	GLU	CD-OE2	8.45	1.34	1.25
1	A	200	GLU	CD-OE2	8.45	1.34	1.25
1	B	171	ALA	CA-CB	8.45	1.70	1.52
1	C	63	GLU	CG-CD	8.41	1.64	1.51
1	D	285	PHE	CB-CG	8.40	1.65	1.51
1	C	56	THR	CA-CB	8.40	1.75	1.53
1	C	200	GLU	CD-OE2	8.40	1.34	1.25
1	D	63	GLU	CG-CD	8.40	1.64	1.51
1	D	56	THR	CA-CB	8.40	1.75	1.53
1	C	285	PHE	CB-CG	8.39	1.65	1.51
1	A	285	PHE	CB-CG	8.39	1.65	1.51
1	B	56	THR	CA-CB	8.39	1.75	1.53
1	B	63	GLU	CG-CD	8.39	1.64	1.51
1	A	56	THR	CA-CB	8.39	1.75	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	63	GLU	CG-CD	8.39	1.64	1.51
1	D	419	VAL	CA-CB	8.35	1.72	1.54
1	B	419	VAL	CA-CB	8.34	1.72	1.54
1	A	419	VAL	CA-CB	8.33	1.72	1.54
1	B	285	PHE	CB-CG	8.32	1.65	1.51
1	C	419	VAL	CA-CB	8.32	1.72	1.54
1	D	320	ALA	C-O	8.28	1.39	1.23
1	C	320	ALA	C-O	8.28	1.39	1.23
1	A	320	ALA	C-O	8.26	1.39	1.23
1	B	320	ALA	C-O	8.26	1.39	1.23
1	B	169	GLU	CD-OE2	8.23	1.34	1.25
1	A	169	GLU	CD-OE2	8.21	1.34	1.25
1	C	10	TRP	CE2-CZ2	8.21	1.53	1.39
1	A	10	TRP	CE2-CZ2	8.17	1.53	1.39
1	C	169	GLU	CD-OE2	8.15	1.34	1.25
1	D	40	GLU	CD-OE1	8.14	1.34	1.25
1	D	169	GLU	CD-OE2	8.14	1.34	1.25
1	C	40	GLU	CD-OE1	8.13	1.34	1.25
1	B	129	TYR	CE2-CZ	8.13	1.49	1.38
1	D	10	TRP	CE2-CZ2	8.12	1.53	1.39
1	A	40	GLU	CD-OE1	8.12	1.34	1.25
1	B	10	TRP	CE2-CZ2	8.12	1.53	1.39
1	D	346	VAL	CA-CB	-8.12	1.37	1.54
1	C	129	TYR	CE2-CZ	8.11	1.49	1.38
1	A	129	TYR	CE2-CZ	8.10	1.49	1.38
1	A	346	VAL	CA-CB	-8.10	1.37	1.54
1	C	404	GLU	CG-CD	8.10	1.64	1.51
1	C	346	VAL	CA-CB	-8.09	1.37	1.54
1	C	207	TYR	CD2-CE2	8.09	1.51	1.39
1	D	168	GLU	CB-CG	8.09	1.67	1.52
1	B	40	GLU	CD-OE1	8.08	1.34	1.25
1	D	404	GLU	CG-CD	8.07	1.64	1.51
1	D	129	TYR	CE2-CZ	8.07	1.49	1.38
1	B	346	VAL	CA-CB	-8.06	1.37	1.54
1	A	168	GLU	CB-CG	8.06	1.67	1.52
1	A	404	GLU	CG-CD	8.06	1.64	1.51
1	B	168	GLU	CB-CG	8.05	1.67	1.52
1	B	212	ARG	CZ-NH1	8.05	1.43	1.33
1	B	207	TYR	CD2-CE2	8.04	1.51	1.39
1	B	404	GLU	CG-CD	8.04	1.64	1.51
1	A	207	TYR	CD2-CE2	8.04	1.51	1.39
1	D	207	TYR	CD2-CE2	8.03	1.51	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	328	ARG	NE-CZ	8.03	1.43	1.33
1	A	328	ARG	NE-CZ	8.02	1.43	1.33
1	C	168	GLU	CB-CG	8.02	1.67	1.52
1	B	247	GLN	CG-CD	8.01	1.69	1.51
1	C	212	ARG	CZ-NH1	8.01	1.43	1.33
1	A	212	ARG	CZ-NH1	8.00	1.43	1.33
1	D	85	LYS	CE-NZ	8.00	1.69	1.49
1	A	85	LYS	CE-NZ	8.00	1.69	1.49
1	C	85	LYS	CE-NZ	8.00	1.69	1.49
1	D	247	GLN	CG-CD	8.00	1.69	1.51
1	C	328	ARG	NE-CZ	8.00	1.43	1.33
1	D	328	ARG	NE-CZ	7.99	1.43	1.33
1	A	247	GLN	CG-CD	7.99	1.69	1.51
1	D	212	ARG	CZ-NH1	7.98	1.43	1.33
1	B	85	LYS	CE-NZ	7.96	1.69	1.49
1	B	398	GLU	CG-CD	7.96	1.63	1.51
1	C	247	GLN	CG-CD	7.96	1.69	1.51
1	D	271	LEU	CG-CD2	-7.92	1.22	1.51
1	D	398	GLU	CG-CD	7.92	1.63	1.51
1	A	271	LEU	CG-CD2	-7.92	1.22	1.51
1	B	175	TYR	CE1-CZ	7.92	1.48	1.38
1	B	271	LEU	CG-CD2	-7.92	1.22	1.51
1	C	175	TYR	CE1-CZ	7.91	1.48	1.38
1	C	398	GLU	CG-CD	7.91	1.63	1.51
1	C	271	LEU	CG-CD2	-7.91	1.22	1.51
1	D	123	PHE	CD1-CE1	7.91	1.55	1.39
1	D	20	GLU	C-O	7.90	1.38	1.23
1	A	175	TYR	CE1-CZ	7.90	1.48	1.38
1	A	398	GLU	CG-CD	7.90	1.63	1.51
1	B	20	GLU	C-O	7.89	1.38	1.23
1	C	123	PHE	CD1-CE1	7.88	1.55	1.39
1	A	123	PHE	CD1-CE1	7.88	1.55	1.39
1	D	338	GLU	C-O	7.87	1.38	1.23
1	A	20	GLU	C-O	7.87	1.38	1.23
1	C	198	ARG	CZ-NH1	7.87	1.43	1.33
1	B	338	GLU	C-O	7.87	1.38	1.23
1	B	123	PHE	CD1-CE1	7.86	1.54	1.39
1	D	76	GLU	CB-CG	7.86	1.67	1.52
1	B	76	GLU	CB-CG	7.86	1.67	1.52
1	D	175	TYR	CE1-CZ	7.85	1.48	1.38
1	A	198	ARG	CZ-NH1	7.84	1.43	1.33
1	C	20	GLU	C-O	7.84	1.38	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	338	GLU	C-O	7.84	1.38	1.23
1	B	151	ASP	CG-OD1	7.84	1.43	1.25
1	B	198	ARG	CZ-NH1	7.83	1.43	1.33
1	C	151	ASP	CG-OD1	7.83	1.43	1.25
1	A	151	ASP	CG-OD1	7.83	1.43	1.25
1	C	338	GLU	C-O	7.83	1.38	1.23
1	A	76	GLU	CB-CG	7.83	1.67	1.52
1	D	151	ASP	CG-OD1	7.82	1.43	1.25
1	D	198	ARG	CZ-NH1	7.79	1.43	1.33
1	C	76	GLU	CB-CG	7.79	1.67	1.52
1	D	366	ASP	CB-CG	7.78	1.68	1.51
1	B	220	THR	C-O	7.78	1.38	1.23
1	B	69	MET	SD-CE	7.78	2.21	1.77
1	A	220	THR	C-O	7.77	1.38	1.23
1	C	69	MET	SD-CE	7.77	2.21	1.77
1	A	69	MET	SD-CE	7.76	2.21	1.77
1	D	220	THR	C-O	7.76	1.38	1.23
1	D	69	MET	SD-CE	7.76	2.21	1.77
1	C	220	THR	C-O	7.75	1.38	1.23
1	A	244	GLU	CD-OE2	7.75	1.34	1.25
1	C	244	GLU	CD-OE2	7.74	1.34	1.25
1	A	366	ASP	CB-CG	7.73	1.68	1.51
1	C	222	GLU	CD-OE1	7.73	1.34	1.25
1	A	255	VAL	CB-CG2	7.73	1.69	1.52
1	C	366	ASP	CB-CG	7.73	1.68	1.51
1	C	255	VAL	CB-CG2	7.72	1.69	1.52
1	D	244	GLU	CD-OE2	7.72	1.34	1.25
1	B	255	VAL	CB-CG2	7.72	1.69	1.52
1	D	255	VAL	CB-CG2	7.72	1.69	1.52
1	B	366	ASP	CB-CG	7.72	1.68	1.51
1	C	248	TYR	CD2-CE2	-7.71	1.27	1.39
1	B	56	THR	CA-C	7.71	1.73	1.52
1	D	56	THR	CA-C	7.70	1.73	1.52
1	A	56	THR	CA-C	7.70	1.73	1.52
1	C	214	GLU	CB-CG	-7.70	1.37	1.52
1	A	222	GLU	CD-OE1	7.69	1.34	1.25
1	A	214	GLU	CB-CG	-7.68	1.37	1.52
1	B	158	VAL	CB-CG2	-7.68	1.36	1.52
1	D	214	GLU	CB-CG	-7.68	1.37	1.52
1	A	346	VAL	C-O	7.68	1.38	1.23
1	C	56	THR	CA-C	7.67	1.73	1.52
1	C	158	VAL	CB-CG2	-7.67	1.36	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	244	GLU	CD-OE2	7.67	1.34	1.25
1	B	214	GLU	CB-CG	-7.67	1.37	1.52
1	D	346	VAL	C-O	7.67	1.38	1.23
1	A	55	TRP	CB-CG	-7.67	1.36	1.50
1	A	158	VAL	CB-CG2	-7.66	1.36	1.52
1	B	55	TRP	CB-CG	-7.66	1.36	1.50
1	A	248	TYR	CD2-CE2	-7.66	1.27	1.39
1	C	47	ALA	C-O	-7.66	1.08	1.23
1	D	158	VAL	CB-CG2	-7.66	1.36	1.52
1	D	222	GLU	CD-OE1	7.66	1.34	1.25
1	A	47	ALA	C-O	-7.66	1.08	1.23
1	B	346	VAL	C-O	7.66	1.37	1.23
1	D	248	TYR	CD2-CE2	-7.66	1.27	1.39
1	D	47	ALA	C-O	-7.66	1.08	1.23
1	C	346	VAL	C-O	7.65	1.37	1.23
1	C	55	TRP	CB-CG	-7.65	1.36	1.50
1	B	222	GLU	CD-OE1	7.65	1.34	1.25
1	B	47	ALA	C-O	-7.64	1.08	1.23
1	D	216	GLU	CB-CG	7.64	1.66	1.52
1	D	55	TRP	CB-CG	-7.64	1.36	1.50
1	B	324	GLU	CD-OE2	7.63	1.34	1.25
1	B	248	TYR	CD2-CE2	-7.62	1.27	1.39
1	A	327	LYS	CD-CE	7.62	1.70	1.51
1	C	327	LYS	CD-CE	7.62	1.70	1.51
1	A	216	GLU	CB-CG	7.62	1.66	1.52
1	B	327	LYS	CD-CE	7.61	1.70	1.51
1	D	327	LYS	CD-CE	7.61	1.70	1.51
1	C	216	GLU	CB-CG	7.60	1.66	1.52
1	D	160	LYS	CE-NZ	7.60	1.68	1.49
1	C	160	LYS	CE-NZ	7.59	1.68	1.49
1	D	269	GLU	CD-OE2	7.59	1.34	1.25
1	A	160	LYS	CE-NZ	7.59	1.68	1.49
1	B	216	GLU	CB-CG	7.59	1.66	1.52
1	B	269	GLU	CD-OE2	7.59	1.33	1.25
1	A	324	GLU	CD-OE2	7.58	1.33	1.25
1	B	160	LYS	CE-NZ	7.58	1.68	1.49
1	C	324	GLU	CD-OE2	7.57	1.33	1.25
1	C	269	GLU	CD-OE2	7.57	1.33	1.25
1	A	269	GLU	CD-OE2	7.57	1.33	1.25
1	C	208	ARG	NE-CZ	7.56	1.42	1.33
1	B	208	ARG	NE-CZ	7.54	1.42	1.33
1	A	208	ARG	NE-CZ	7.54	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	324	GLU	CD-OE2	7.53	1.33	1.25
1	D	208	ARG	NE-CZ	7.52	1.42	1.33
1	B	170	TYR	CD2-CE2	7.51	1.50	1.39
1	D	230	PRO	C-O	7.51	1.38	1.23
1	B	230	PRO	C-O	7.50	1.38	1.23
1	A	230	PRO	C-O	7.48	1.38	1.23
1	C	346	VAL	CB-CG1	-7.48	1.37	1.52
1	A	170	TYR	CD2-CE2	7.47	1.50	1.39
1	B	188	ASP	CB-CG	7.47	1.67	1.51
1	C	170	TYR	CD2-CE2	7.47	1.50	1.39
1	A	188	ASP	CB-CG	7.46	1.67	1.51
1	A	346	VAL	CB-CG1	-7.46	1.37	1.52
1	D	188	ASP	CB-CG	7.46	1.67	1.51
1	D	346	VAL	CB-CG1	-7.46	1.37	1.52
1	D	170	TYR	CD2-CE2	7.46	1.50	1.39
1	C	134	LYS	CD-CE	7.45	1.69	1.51
1	C	230	PRO	C-O	7.45	1.38	1.23
1	C	188	ASP	CB-CG	7.45	1.67	1.51
1	D	134	LYS	CD-CE	7.44	1.69	1.51
1	A	134	LYS	CD-CE	7.43	1.69	1.51
1	B	346	VAL	CB-CG1	-7.42	1.37	1.52
1	C	10	TRP	CD2-CE3	7.42	1.51	1.40
1	C	358	GLU	CG-CD	7.41	1.63	1.51
1	B	134	LYS	CD-CE	7.40	1.69	1.51
1	A	10	TRP	CD2-CE3	7.39	1.51	1.40
1	B	358	GLU	CG-CD	7.38	1.63	1.51
1	B	10	TRP	CD2-CE3	7.38	1.51	1.40
1	D	10	TRP	CD2-CE3	7.37	1.51	1.40
1	A	358	GLU	CG-CD	7.37	1.63	1.51
1	B	328	ARG	CZ-NH1	7.36	1.42	1.33
1	B	239	GLU	CG-CD	7.35	1.62	1.51
1	C	239	GLU	CG-CD	7.35	1.62	1.51
1	D	358	GLU	CG-CD	7.35	1.62	1.51
1	B	341	ARG	CZ-NH2	7.33	1.42	1.33
1	A	239	GLU	CG-CD	7.32	1.62	1.51
1	D	49	GLU	CD-OE1	7.32	1.33	1.25
1	A	328	ARG	CZ-NH1	7.31	1.42	1.33
1	C	328	ARG	CZ-NH1	7.31	1.42	1.33
1	D	123	PHE	CD2-CE2	7.30	1.53	1.39
1	A	35	ASN	C-O	7.30	1.37	1.23
1	A	341	ARG	CZ-NH2	7.30	1.42	1.33
1	D	35	ASN	C-O	7.29	1.37	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	328	ARG	CZ-NH1	7.29	1.42	1.33
1	B	35	ASN	C-O	7.28	1.37	1.23
1	D	239	GLU	CG-CD	7.28	1.62	1.51
1	B	49	GLU	CD-OE1	7.28	1.33	1.25
1	B	123	PHE	CD2-CE2	7.28	1.53	1.39
1	D	341	ARG	CZ-NH2	7.28	1.42	1.33
1	A	123	PHE	CD2-CE2	7.28	1.53	1.39
1	C	35	ASN	C-O	7.28	1.37	1.23
1	C	123	PHE	CD2-CE2	7.27	1.53	1.39
1	A	49	GLU	CD-OE1	7.27	1.33	1.25
1	D	263	TYR	CD2-CE2	7.26	1.50	1.39
1	A	263	TYR	CD2-CE2	7.25	1.50	1.39
1	C	49	GLU	CD-OE1	7.25	1.33	1.25
1	B	263	TYR	CD2-CE2	7.24	1.50	1.39
1	C	341	ARG	CZ-NH2	7.23	1.42	1.33
1	C	263	TYR	CD2-CE2	7.22	1.50	1.39
1	A	375	VAL	CB-CG2	-7.19	1.37	1.52
1	C	329	ILE	C-O	-7.18	1.09	1.23
1	B	375	VAL	CB-CG2	-7.17	1.37	1.52
1	C	375	VAL	CB-CG2	-7.16	1.37	1.52
1	D	59	TRP	CE3-CZ3	7.15	1.50	1.38
1	D	375	VAL	CB-CG2	-7.15	1.37	1.52
1	B	59	TRP	CE3-CZ3	7.15	1.50	1.38
1	A	329	ILE	C-O	-7.14	1.09	1.23
1	C	59	TRP	CE3-CZ3	7.14	1.50	1.38
1	A	59	TRP	CE3-CZ3	7.13	1.50	1.38
1	D	329	ILE	C-O	-7.13	1.09	1.23
1	B	329	ILE	C-O	-7.12	1.09	1.23
1	D	423	LYS	CB-CG	7.10	1.71	1.52
1	D	234	MET	SD-CE	7.10	2.17	1.77
1	C	423	LYS	CB-CG	7.10	1.71	1.52
1	C	59	TRP	CD2-CE3	7.09	1.50	1.40
1	B	59	TRP	CD2-CE3	7.09	1.50	1.40
1	A	234	MET	SD-CE	7.09	2.17	1.77
1	B	234	MET	SD-CE	7.09	2.17	1.77
1	A	423	LYS	CB-CG	7.09	1.71	1.52
1	B	423	LYS	CB-CG	7.09	1.71	1.52
1	B	207	TYR	CD1-CE1	7.08	1.50	1.39
1	B	40	GLU	CG-CD	7.08	1.62	1.51
1	C	234	MET	SD-CE	7.08	2.17	1.77
1	C	324	GLU	CD-OE1	7.07	1.33	1.25
1	D	207	TYR	CD1-CE1	7.07	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	59	TRP	CD2-CE3	7.06	1.50	1.40
1	D	324	GLU	CD-OE1	7.06	1.33	1.25
1	C	40	GLU	CG-CD	7.06	1.62	1.51
1	D	40	GLU	CG-CD	7.06	1.62	1.51
1	A	40	GLU	CG-CD	7.05	1.62	1.51
1	A	207	TYR	CD1-CE1	7.04	1.50	1.39
1	C	207	TYR	CD1-CE1	7.04	1.50	1.39
1	C	249	VAL	CB-CG2	-7.03	1.38	1.52
1	B	249	VAL	CB-CG2	-7.02	1.38	1.52
1	B	324	GLU	CD-OE1	7.02	1.33	1.25
1	A	324	GLU	CD-OE1	7.02	1.33	1.25
1	C	61	LEU	CG-CD2	7.01	1.77	1.51
1	A	249	VAL	CB-CG2	-7.01	1.38	1.52
1	D	59	TRP	CD2-CE3	7.01	1.50	1.40
1	D	31	TYR	CG-CD2	7.00	1.48	1.39
1	A	61	LEU	CG-CD2	7.00	1.77	1.51
1	D	61	LEU	CG-CD2	7.00	1.77	1.51
1	B	61	LEU	CG-CD2	7.00	1.77	1.51
1	D	249	VAL	CB-CG2	-6.99	1.38	1.52
1	D	134	LYS	CE-NZ	6.97	1.66	1.49
1	A	134	LYS	CE-NZ	6.97	1.66	1.49
1	D	82	TYR	CD1-CE1	-6.97	1.28	1.39
1	B	328	ARG	N-CA	6.96	1.60	1.46
1	D	328	ARG	N-CA	6.96	1.60	1.46
1	C	261	LEU	N-CA	6.96	1.60	1.46
1	A	328	ARG	N-CA	6.96	1.60	1.46
1	A	31	TYR	CG-CD2	6.95	1.48	1.39
1	A	82	TYR	CD1-CE1	-6.95	1.28	1.39
1	B	82	TYR	CD1-CE1	-6.95	1.28	1.39
1	B	134	LYS	CE-NZ	6.95	1.66	1.49
1	C	31	TYR	CG-CD2	6.95	1.48	1.39
1	B	48	SER	CB-OG	6.94	1.51	1.42
1	C	82	TYR	CD1-CE1	-6.94	1.28	1.39
1	B	31	TYR	CG-CD2	6.94	1.48	1.39
1	A	261	LEU	N-CA	6.93	1.60	1.46
1	C	134	LYS	CE-NZ	6.93	1.66	1.49
1	D	48	SER	CB-OG	6.93	1.51	1.42
1	D	261	LEU	N-CA	6.93	1.60	1.46
1	A	56	THR	C-O	6.93	1.36	1.23
1	C	328	ARG	N-CA	6.92	1.60	1.46
1	C	56	THR	C-O	6.92	1.36	1.23
1	D	56	THR	C-O	6.92	1.36	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	48	SER	CB-OG	6.92	1.51	1.42
1	B	56	THR	C-O	6.91	1.36	1.23
1	C	48	SER	CB-OG	6.91	1.51	1.42
1	B	261	LEU	N-CA	6.89	1.60	1.46
1	A	56	THR	N-CA	6.84	1.60	1.46
1	C	56	THR	N-CA	6.83	1.60	1.46
1	D	418	GLU	CD-OE2	6.83	1.33	1.25
1	D	32	PHE	CB-CG	-6.82	1.39	1.51
1	B	56	THR	N-CA	6.82	1.59	1.46
1	C	32	PHE	CB-CG	-6.82	1.39	1.51
1	B	32	PHE	CB-CG	-6.82	1.39	1.51
1	A	32	PHE	CB-CG	-6.82	1.39	1.51
1	B	103	SER	CB-OG	6.81	1.51	1.42
1	B	198	ARG	CD-NE	6.81	1.58	1.46
1	D	56	THR	N-CA	6.80	1.59	1.46
1	C	198	ARG	CD-NE	6.80	1.58	1.46
1	A	198	ARG	CD-NE	6.79	1.57	1.46
1	C	103	SER	CB-OG	6.79	1.51	1.42
1	A	103	SER	CB-OG	6.78	1.51	1.42
1	D	95	GLU	N-CA	6.78	1.59	1.46
1	C	95	GLU	N-CA	6.78	1.59	1.46
1	D	129	TYR	C-O	6.78	1.36	1.23
1	A	95	GLU	N-CA	6.77	1.59	1.46
1	B	418	GLU	CD-OE2	6.77	1.33	1.25
1	C	418	GLU	CD-OE2	6.77	1.33	1.25
1	B	95	GLU	N-CA	6.77	1.59	1.46
1	C	18	ASN	CG-ND2	6.77	1.49	1.32
1	D	103	SER	CB-OG	6.76	1.51	1.42
1	D	200	GLU	CD-OE1	6.76	1.33	1.25
1	D	198	ARG	CD-NE	6.76	1.57	1.46
1	D	18	ASN	CG-ND2	6.76	1.49	1.32
1	D	284	ALA	CA-CB	-6.76	1.38	1.52
1	B	273	LEU	C-O	6.75	1.36	1.23
1	A	284	ALA	CA-CB	-6.75	1.38	1.52
1	B	129	TYR	C-O	6.75	1.36	1.23
1	A	18	ASN	CG-ND2	6.75	1.49	1.32
1	A	418	GLU	CD-OE2	6.75	1.33	1.25
1	C	284	ALA	CA-CB	-6.75	1.38	1.52
1	B	284	ALA	CA-CB	-6.74	1.38	1.52
1	B	18	ASN	CG-ND2	6.74	1.49	1.32
1	A	273	LEU	C-O	6.74	1.36	1.23
1	A	129	TYR	C-O	6.74	1.36	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	270	ASP	CG-OD2	6.74	1.40	1.25
1	B	200	GLU	CD-OE1	6.73	1.33	1.25
1	C	129	TYR	C-O	6.73	1.36	1.23
1	B	15	VAL	CB-CG1	-6.72	1.38	1.52
1	D	48	SER	CA-CB	6.72	1.63	1.52
1	D	273	LEU	C-O	6.72	1.36	1.23
1	D	15	VAL	CB-CG1	-6.72	1.38	1.52
1	A	15	VAL	CB-CG1	-6.71	1.38	1.52
1	C	273	LEU	C-O	6.71	1.36	1.23
1	C	270	ASP	CG-OD2	6.71	1.40	1.25
1	A	270	ASP	CG-OD2	6.71	1.40	1.25
1	C	15	VAL	CB-CG1	-6.71	1.38	1.52
1	D	270	ASP	CG-OD2	6.70	1.40	1.25
1	B	48	SER	CA-CB	6.70	1.63	1.52
1	A	48	SER	CA-CB	6.70	1.62	1.52
1	C	200	GLU	CD-OE1	6.70	1.33	1.25
1	D	56	THR	CB-CG2	6.69	1.74	1.52
1	C	110	PHE	CB-CG	-6.68	1.40	1.51
1	A	200	GLU	CD-OE1	6.68	1.33	1.25
1	C	320	ALA	C-N	6.68	1.45	1.33
1	A	56	THR	CB-CG2	6.68	1.74	1.52
1	D	110	PHE	CB-CG	-6.68	1.40	1.51
1	C	48	SER	CA-CB	6.68	1.62	1.52
1	C	289	PRO	C-O	6.68	1.36	1.23
1	A	289	PRO	C-O	6.67	1.36	1.23
1	C	56	THR	CB-CG2	6.67	1.74	1.52
1	B	320	ALA	C-N	6.67	1.45	1.33
1	B	56	THR	CB-CG2	6.67	1.74	1.52
1	A	320	ALA	C-N	6.66	1.45	1.33
1	B	289	PRO	C-O	6.66	1.36	1.23
1	D	208	ARG	CZ-NH1	6.66	1.41	1.33
1	D	289	PRO	C-O	6.66	1.36	1.23
1	A	110	PHE	CB-CG	-6.65	1.40	1.51
1	B	110	PHE	CB-CG	-6.65	1.40	1.51
1	A	208	ARG	CZ-NH1	6.64	1.41	1.33
1	C	61	LEU	CA-C	6.64	1.70	1.52
1	D	61	LEU	CA-C	6.64	1.70	1.52
1	D	320	ALA	C-N	6.63	1.45	1.33
1	A	61	LEU	CA-C	6.62	1.70	1.52
1	B	61	LEU	CA-C	6.62	1.70	1.52
1	B	208	ARG	CZ-NH1	6.62	1.41	1.33
1	C	208	ARG	CZ-NH1	6.62	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	411	GLU	CG-CD	6.61	1.61	1.51
1	B	411	GLU	CG-CD	6.59	1.61	1.51
1	C	105	VAL	CA-CB	-6.59	1.41	1.54
1	B	129	TYR	CG-CD2	6.59	1.47	1.39
1	C	411	GLU	CG-CD	6.59	1.61	1.51
1	D	411	GLU	CG-CD	6.58	1.61	1.51
1	B	366	ASP	CG-OD1	6.58	1.40	1.25
1	D	129	TYR	CG-CD2	6.57	1.47	1.39
1	D	192	THR	CB-CG2	-6.56	1.30	1.52
1	D	328	ARG	CG-CD	6.56	1.68	1.51
1	A	129	TYR	CG-CD2	6.56	1.47	1.39
1	B	192	THR	CB-CG2	-6.56	1.30	1.52
1	B	105	VAL	CA-CB	-6.56	1.41	1.54
1	A	105	VAL	CA-CB	-6.55	1.41	1.54
1	C	366	ASP	CG-OD1	6.54	1.40	1.25
1	D	105	VAL	CA-CB	-6.54	1.41	1.54
1	A	192	THR	CB-CG2	-6.54	1.30	1.52
1	A	366	ASP	CG-OD1	6.54	1.40	1.25
1	B	328	ARG	CG-CD	6.54	1.68	1.51
1	C	192	THR	CB-CG2	-6.53	1.30	1.52
1	A	328	ARG	CG-CD	6.53	1.68	1.51
1	C	328	ARG	CG-CD	6.53	1.68	1.51
1	C	290	ARG	CG-CD	6.53	1.68	1.51
1	B	290	ARG	CG-CD	6.52	1.68	1.51
1	C	129	TYR	CG-CD2	6.52	1.47	1.39
1	C	85	LYS	CD-CE	6.52	1.67	1.51
1	D	366	ASP	CG-OD1	6.52	1.40	1.25
1	B	116	LYS	CE-NZ	6.51	1.65	1.49
1	D	290	ARG	CG-CD	6.51	1.68	1.51
1	A	290	ARG	CG-CD	6.51	1.68	1.51
1	A	116	LYS	CE-NZ	6.51	1.65	1.49
1	B	85	LYS	CD-CE	6.50	1.67	1.51
1	C	116	LYS	CE-NZ	6.49	1.65	1.49
1	C	301	ALA	CA-CB	-6.49	1.38	1.52
1	D	116	LYS	CE-NZ	6.49	1.65	1.49
1	A	301	ALA	CA-CB	-6.49	1.38	1.52
1	A	85	LYS	CD-CE	6.48	1.67	1.51
1	B	301	ALA	CA-CB	-6.48	1.38	1.52
1	D	280	ALA	C-O	6.48	1.35	1.23
1	D	301	ALA	CA-CB	-6.48	1.38	1.52
1	D	336	LYS	CE-NZ	6.48	1.65	1.49
1	D	368	VAL	CB-CG2	-6.48	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	85	LYS	CD-CE	6.47	1.67	1.51
1	A	368	VAL	CB-CG2	-6.47	1.39	1.52
1	C	45	ARG	CZ-NH2	6.47	1.41	1.33
1	C	368	VAL	CB-CG2	-6.46	1.39	1.52
1	C	336	LYS	CE-NZ	6.46	1.65	1.49
1	A	336	LYS	CE-NZ	6.46	1.65	1.49
1	A	280	ALA	C-O	6.46	1.35	1.23
1	C	280	ALA	C-O	6.45	1.35	1.23
1	A	212	ARG	C-O	6.45	1.35	1.23
1	C	212	ARG	C-O	6.45	1.35	1.23
1	A	45	ARG	CZ-NH2	6.45	1.41	1.33
1	C	59	TRP	CZ3-CH2	6.44	1.50	1.40
1	B	368	VAL	CB-CG2	-6.44	1.39	1.52
1	D	212	ARG	C-O	6.44	1.35	1.23
1	B	280	ALA	C-O	6.43	1.35	1.23
1	D	45	ARG	CZ-NH2	6.43	1.41	1.33
1	B	336	LYS	CE-NZ	6.43	1.65	1.49
1	B	260	ALA	N-CA	-6.43	1.33	1.46
1	C	310	ILE	CA-CB	-6.43	1.40	1.54
1	B	122	ASP	CG-OD2	6.43	1.40	1.25
1	D	122	ASP	CG-OD2	6.43	1.40	1.25
1	B	310	ILE	CA-CB	-6.42	1.40	1.54
1	D	310	ILE	CA-CB	-6.42	1.40	1.54
1	A	310	ILE	CA-CB	-6.42	1.40	1.54
1	B	212	ARG	C-O	6.42	1.35	1.23
1	B	216	GLU	CA-CB	6.42	1.68	1.53
1	D	59	TRP	CZ3-CH2	6.42	1.50	1.40
1	D	368	VAL	CB-CG1	-6.42	1.39	1.52
1	C	241	VAL	CB-CG2	-6.42	1.39	1.52
1	A	59	TRP	CZ3-CH2	6.42	1.50	1.40
1	A	260	ALA	N-CA	-6.42	1.33	1.46
1	A	122	ASP	CG-OD2	6.41	1.40	1.25
1	C	354	GLY	C-O	6.41	1.33	1.23
1	B	368	VAL	CB-CG1	-6.41	1.39	1.52
1	D	136	PRO	CA-C	-6.41	1.40	1.52
1	B	132	HIS	C-O	-6.41	1.11	1.23
1	A	368	VAL	CB-CG1	-6.41	1.39	1.52
1	D	241	VAL	CB-CG2	-6.41	1.39	1.52
1	A	132	HIS	C-O	-6.40	1.11	1.23
1	A	241	VAL	CB-CG2	-6.40	1.39	1.52
1	B	45	ARG	CZ-NH2	6.40	1.41	1.33
1	C	285	PHE	CG-CD1	6.40	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	132	HIS	C-O	-6.40	1.11	1.23
1	A	216	GLU	CA-CB	6.39	1.68	1.53
1	D	354	GLY	C-O	6.39	1.33	1.23
1	B	285	PHE	CG-CD1	6.39	1.48	1.38
1	A	136	PRO	CA-C	-6.39	1.40	1.52
1	A	246	GLY	C-O	6.38	1.33	1.23
1	C	368	VAL	CB-CG1	-6.38	1.39	1.52
1	D	151	ASP	C-O	6.38	1.35	1.23
1	D	246	GLY	C-O	6.38	1.33	1.23
1	D	285	PHE	CG-CD1	6.38	1.48	1.38
1	C	151	ASP	C-O	6.38	1.35	1.23
1	D	260	ALA	N-CA	-6.38	1.33	1.46
1	C	122	ASP	CG-OD2	6.38	1.40	1.25
1	C	260	ALA	N-CA	-6.38	1.33	1.46
1	D	216	GLU	CA-CB	6.38	1.68	1.53
1	A	354	GLY	C-O	6.38	1.33	1.23
1	B	59	TRP	CZ3-CH2	6.38	1.50	1.40
1	B	241	VAL	CB-CG2	-6.37	1.39	1.52
1	C	136	PRO	CA-C	-6.37	1.40	1.52
1	C	413	LYS	CD-CE	6.37	1.67	1.51
1	A	151	ASP	C-O	6.37	1.35	1.23
1	B	354	GLY	C-O	6.37	1.33	1.23
1	B	88	TYR	CG-CD2	6.36	1.47	1.39
1	B	136	PRO	CA-C	-6.36	1.40	1.52
1	C	246	GLY	C-O	6.36	1.33	1.23
1	B	151	ASP	C-O	6.36	1.35	1.23
1	C	132	HIS	C-O	-6.36	1.11	1.23
1	C	216	GLU	CA-CB	6.36	1.68	1.53
1	A	95	GLU	CA-CB	6.36	1.68	1.53
1	B	246	GLY	C-O	6.36	1.33	1.23
1	A	285	PHE	CG-CD1	6.35	1.48	1.38
1	D	95	GLU	CA-CB	6.35	1.68	1.53
1	A	413	LYS	CD-CE	6.35	1.67	1.51
1	B	95	GLU	CA-CB	6.35	1.68	1.53
1	C	14	PHE	CG-CD2	-6.35	1.29	1.38
1	D	413	LYS	CD-CE	6.34	1.67	1.51
1	D	344	PHE	CD2-CE2	6.33	1.51	1.39
1	C	95	GLU	CA-CB	6.33	1.67	1.53
1	C	344	PHE	CD2-CE2	6.32	1.51	1.39
1	A	14	PHE	CG-CD2	-6.32	1.29	1.38
1	B	413	LYS	CD-CE	6.32	1.67	1.51
1	D	88	TYR	CG-CD2	6.31	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	14	PHE	CG-CD2	-6.30	1.29	1.38
1	A	344	PHE	CD2-CE2	6.30	1.51	1.39
1	C	37	VAL	CB-CG2	6.30	1.66	1.52
1	A	37	VAL	CB-CG2	6.30	1.66	1.52
1	A	304	MET	SD-CE	6.30	2.13	1.77
1	B	186	LYS	C-O	-6.30	1.11	1.23
1	D	304	MET	SD-CE	6.30	2.13	1.77
1	B	16	ASP	CB-CG	-6.29	1.38	1.51
1	B	304	MET	SD-CE	6.29	2.13	1.77
1	B	344	PHE	CD2-CE2	6.29	1.51	1.39
1	C	186	LYS	C-O	-6.29	1.11	1.23
1	C	304	MET	SD-CE	6.29	2.13	1.77
1	D	37	VAL	CB-CG2	6.29	1.66	1.52
1	A	88	TYR	CG-CD2	6.28	1.47	1.39
1	A	16	ASP	CB-CG	-6.28	1.38	1.51
1	A	186	LYS	C-O	-6.28	1.11	1.23
1	C	16	ASP	CB-CG	-6.28	1.38	1.51
1	D	186	LYS	C-O	-6.27	1.11	1.23
1	B	37	VAL	CB-CG2	6.27	1.66	1.52
1	C	88	TYR	CE1-CZ	6.27	1.46	1.38
1	B	88	TYR	CE1-CZ	6.27	1.46	1.38
1	A	88	TYR	CE1-CZ	6.26	1.46	1.38
1	D	16	ASP	CB-CG	-6.25	1.38	1.51
1	D	14	PHE	CG-CD2	-6.25	1.29	1.38
1	C	88	TYR	CG-CD2	6.25	1.47	1.39
1	C	325	GLU	CG-CD	6.24	1.61	1.51
1	D	88	TYR	CE1-CZ	6.24	1.46	1.38
1	B	325	GLU	CG-CD	6.24	1.61	1.51
1	A	288	ASN	CB-CG	-6.23	1.36	1.51
1	A	325	GLU	CG-CD	6.22	1.61	1.51
1	C	288	ASN	CB-CG	-6.22	1.36	1.51
1	D	288	ASN	CB-CG	-6.21	1.36	1.51
1	B	332	PHE	CD2-CE2	6.21	1.51	1.39
1	B	288	ASN	CB-CG	-6.21	1.36	1.51
1	A	133	PHE	CE2-CZ	-6.20	1.25	1.37
1	C	133	PHE	CE2-CZ	-6.20	1.25	1.37
1	D	325	GLU	CG-CD	6.20	1.61	1.51
1	D	398	GLU	CD-OE2	6.20	1.32	1.25
1	C	332	PHE	CD2-CE2	6.19	1.51	1.39
1	C	392	ALA	CA-CB	6.19	1.65	1.52
1	A	332	PHE	CD2-CE2	6.19	1.51	1.39
1	B	250	MET	N-CA	6.19	1.58	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	133	PHE	CE2-CZ	-6.19	1.25	1.37
1	B	392	ALA	CA-CB	6.18	1.65	1.52
1	A	392	ALA	CA-CB	6.18	1.65	1.52
1	A	398	GLU	CD-OE2	6.18	1.32	1.25
1	D	133	PHE	CE2-CZ	-6.18	1.25	1.37
1	B	14	PHE	CB-CG	-6.16	1.40	1.51
1	C	398	GLU	CD-OE2	6.16	1.32	1.25
1	B	398	GLU	CD-OE2	6.16	1.32	1.25
1	A	250	MET	N-CA	6.15	1.58	1.46
1	D	332	PHE	CD2-CE2	6.15	1.51	1.39
1	C	21	PRO	CA-CB	6.14	1.65	1.53
1	D	392	ALA	CA-CB	6.14	1.65	1.52
1	A	129	TYR	CZ-OH	6.14	1.48	1.37
1	C	14	PHE	CB-CG	-6.14	1.41	1.51
1	A	14	PHE	CB-CG	-6.14	1.41	1.51
1	C	250	MET	N-CA	6.13	1.58	1.46
1	D	250	MET	N-CA	6.13	1.58	1.46
1	C	129	TYR	CZ-OH	6.13	1.48	1.37
1	A	21	PRO	CA-CB	6.13	1.65	1.53
1	D	366	ASP	CA-C	-6.13	1.37	1.52
1	B	21	PRO	CA-CB	6.12	1.65	1.53
1	B	129	TYR	CZ-OH	6.12	1.48	1.37
1	C	243	ASN	CG-OD1	6.12	1.37	1.24
1	D	223	TYR	CE1-CZ	-6.12	1.30	1.38
1	A	243	ASN	CG-OD1	6.12	1.37	1.24
1	D	14	PHE	CB-CG	-6.12	1.41	1.51
1	B	223	TYR	CE1-CZ	-6.11	1.30	1.38
1	B	243	ASN	CG-OD1	6.11	1.37	1.24
1	D	375	VAL	CA-CB	-6.11	1.42	1.54
1	D	21	PRO	CA-CB	6.11	1.65	1.53
1	C	113	LYS	CB-CG	6.11	1.69	1.52
1	D	129	TYR	CZ-OH	6.11	1.48	1.37
1	D	243	ASN	CG-OD1	6.11	1.37	1.24
1	A	375	VAL	CA-CB	-6.10	1.42	1.54
1	A	176	GLU	CB-CG	6.10	1.63	1.52
1	B	113	LYS	CB-CG	6.10	1.69	1.52
1	D	176	GLU	CB-CG	6.10	1.63	1.52
1	A	366	ASP	CA-C	-6.10	1.37	1.52
1	B	375	VAL	CA-CB	-6.10	1.42	1.54
1	A	223	TYR	CE1-CZ	-6.10	1.30	1.38
1	A	113	LYS	CB-CG	6.09	1.69	1.52
1	D	113	LYS	CB-CG	6.09	1.69	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	375	VAL	CA-CB	-6.09	1.42	1.54
1	B	366	ASP	CA-C	-6.09	1.37	1.52
1	B	176	GLU	CB-CG	6.09	1.63	1.52
1	C	366	ASP	CA-C	-6.08	1.37	1.52
1	D	300	LYS	CE-NZ	6.08	1.64	1.49
1	A	300	LYS	CE-NZ	6.07	1.64	1.49
1	C	176	GLU	CB-CG	6.07	1.63	1.52
1	C	300	LYS	CE-NZ	6.07	1.64	1.49
1	C	223	TYR	CE1-CZ	-6.06	1.30	1.38
1	B	354	GLY	CA-C	6.05	1.61	1.51
1	D	354	GLY	CA-C	6.05	1.61	1.51
1	B	389	LEU	CG-CD2	-6.04	1.29	1.51
1	B	300	LYS	CE-NZ	6.04	1.64	1.49
1	D	389	LEU	CG-CD2	-6.03	1.29	1.51
1	A	389	LEU	CG-CD2	-6.03	1.29	1.51
1	A	354	GLY	CA-C	6.03	1.61	1.51
1	C	354	GLY	CA-C	6.02	1.61	1.51
1	C	389	LEU	CG-CD2	-6.02	1.29	1.51
1	D	77	LYS	CE-NZ	6.02	1.64	1.49
1	A	77	LYS	CE-NZ	6.01	1.64	1.49
1	C	96	GLY	CA-C	6.01	1.61	1.51
1	C	77	LYS	CE-NZ	6.00	1.64	1.49
1	A	188	ASP	C-O	-6.00	1.11	1.23
1	B	188	ASP	C-O	-5.99	1.11	1.23
1	B	320	ALA	CA-C	5.99	1.68	1.52
1	D	320	ALA	CA-C	5.99	1.68	1.52
1	B	77	LYS	CE-NZ	5.98	1.64	1.49
1	D	96	GLY	CA-C	5.98	1.61	1.51
1	B	253	ILE	CB-CG2	-5.98	1.34	1.52
1	D	188	ASP	C-O	-5.98	1.11	1.23
1	A	253	ILE	CB-CG2	-5.97	1.34	1.52
1	A	96	GLY	CA-C	5.97	1.61	1.51
1	A	320	ALA	CA-C	5.97	1.68	1.52
1	C	253	ILE	CB-CG2	-5.97	1.34	1.52
1	B	170	TYR	CE1-CZ	-5.97	1.30	1.38
1	C	170	TYR	CE1-CZ	-5.97	1.30	1.38
1	C	188	ASP	C-O	-5.96	1.12	1.23
1	D	51	SER	CA-CB	-5.96	1.44	1.52
1	D	253	ILE	CB-CG2	-5.96	1.34	1.52
1	B	116	LYS	CD-CE	5.96	1.66	1.51
1	D	116	LYS	CD-CE	5.95	1.66	1.51
1	A	116	LYS	CD-CE	5.94	1.66	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	96	GLY	CA-C	5.94	1.61	1.51
1	C	320	ALA	CA-C	5.94	1.68	1.52
1	D	208	ARG	CD-NE	5.94	1.56	1.46
1	D	365	LYS	CD-CE	5.94	1.66	1.51
1	B	208	ARG	CD-NE	5.93	1.56	1.46
1	C	365	LYS	CD-CE	5.93	1.66	1.51
1	A	208	ARG	CD-NE	5.93	1.56	1.46
1	C	116	LYS	CD-CE	5.93	1.66	1.51
1	A	170	TYR	CE1-CZ	-5.92	1.30	1.38
1	A	365	LYS	CD-CE	5.92	1.66	1.51
1	A	51	SER	CA-CB	-5.92	1.44	1.52
1	C	208	ARG	CD-NE	5.92	1.56	1.46
1	B	365	LYS	CD-CE	5.91	1.66	1.51
1	C	51	SER	CA-CB	-5.90	1.44	1.52
1	D	170	TYR	CE1-CZ	-5.90	1.30	1.38
1	C	407	LYS	CE-NZ	5.89	1.63	1.49
1	C	380	ASP	C-O	5.89	1.34	1.23
1	D	261	LEU	CG-CD2	-5.89	1.30	1.51
1	B	370	GLN	CG-CD	-5.89	1.37	1.51
1	C	424	ALA	N-CA	5.89	1.58	1.46
1	D	212	ARG	NE-CZ	5.89	1.40	1.33
1	D	370	GLN	CG-CD	-5.88	1.37	1.51
1	A	261	LEU	CG-CD2	-5.88	1.30	1.51
1	B	51	SER	CA-CB	-5.88	1.44	1.52
1	A	424	ALA	N-CA	5.88	1.58	1.46
1	B	261	LEU	CG-CD2	-5.88	1.30	1.51
1	C	212	ARG	NE-CZ	5.88	1.40	1.33
1	B	309	GLN	CB-CG	-5.88	1.36	1.52
1	B	380	ASP	C-O	5.88	1.34	1.23
1	A	380	ASP	C-O	5.87	1.34	1.23
1	C	261	LEU	CG-CD2	-5.87	1.30	1.51
1	B	424	ALA	N-CA	5.87	1.58	1.46
1	A	370	GLN	CG-CD	-5.87	1.37	1.51
1	D	309	GLN	CB-CG	-5.86	1.36	1.52
1	B	147	MET	CA-CB	-5.86	1.41	1.53
1	D	380	ASP	C-O	5.86	1.34	1.23
1	A	407	LYS	CE-NZ	5.86	1.63	1.49
1	A	309	GLN	CB-CG	-5.86	1.36	1.52
1	B	407	LYS	CE-NZ	5.85	1.63	1.49
1	D	208	ARG	CG-CD	5.85	1.66	1.51
1	D	407	LYS	CE-NZ	5.85	1.63	1.49
1	A	208	ARG	CG-CD	5.85	1.66	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	424	ALA	N-CA	5.84	1.58	1.46
1	C	208	ARG	CG-CD	5.84	1.66	1.51
1	C	370	GLN	CG-CD	-5.84	1.37	1.51
1	C	309	GLN	CB-CG	-5.84	1.36	1.52
1	A	212	ARG	NE-CZ	5.83	1.40	1.33
1	B	208	ARG	CG-CD	5.83	1.66	1.51
1	A	147	MET	CA-CB	-5.82	1.41	1.53
1	C	147	MET	CA-CB	-5.82	1.41	1.53
1	C	75	LEU	CG-CD1	-5.81	1.30	1.51
1	D	147	MET	CA-CB	-5.81	1.41	1.53
1	B	212	ARG	NE-CZ	5.80	1.40	1.33
1	A	75	LEU	CG-CD1	-5.80	1.30	1.51
1	C	60	LYS	CA-C	5.79	1.68	1.52
1	D	75	LEU	CG-CD1	-5.79	1.30	1.51
1	D	328	ARG	CZ-NH2	5.79	1.40	1.33
1	B	60	LYS	CA-C	5.79	1.68	1.52
1	A	60	LYS	CA-C	5.79	1.68	1.52
1	B	75	LEU	CG-CD1	-5.79	1.30	1.51
1	B	108	ASN	CB-CG	-5.79	1.37	1.51
1	B	358	GLU	CB-CG	5.78	1.63	1.52
1	D	60	LYS	CA-C	5.78	1.68	1.52
1	C	328	ARG	CZ-NH2	5.77	1.40	1.33
1	B	137	GLN	CD-NE2	5.77	1.47	1.32
1	D	108	ASN	CB-CG	-5.77	1.37	1.51
1	C	137	GLN	CD-NE2	5.76	1.47	1.32
1	D	137	GLN	CD-NE2	5.76	1.47	1.32
1	A	108	ASN	CB-CG	-5.76	1.37	1.51
1	A	358	GLU	CB-CG	5.76	1.63	1.52
1	C	285	PHE	CE2-CZ	5.76	1.48	1.37
1	A	137	GLN	CD-NE2	5.76	1.47	1.32
1	A	328	ARG	CZ-NH2	5.75	1.40	1.33
1	D	285	PHE	CE2-CZ	5.75	1.48	1.37
1	C	127	TYR	CZ-OH	5.75	1.47	1.37
1	D	127	TYR	CE2-CZ	5.75	1.46	1.38
1	B	127	TYR	CE2-CZ	5.75	1.46	1.38
1	A	127	TYR	CE2-CZ	5.75	1.46	1.38
1	C	358	GLU	CB-CG	5.74	1.63	1.52
1	A	285	PHE	CE2-CZ	5.74	1.48	1.37
1	D	164	GLY	CA-C	5.74	1.61	1.51
1	B	285	PHE	CE2-CZ	5.74	1.48	1.37
1	D	358	GLU	CB-CG	5.74	1.63	1.52
1	A	164	GLY	CA-C	5.73	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	164	GLY	CA-C	5.73	1.61	1.51
1	C	108	ASN	CB-CG	-5.73	1.37	1.51
1	C	127	TYR	CE2-CZ	5.73	1.46	1.38
1	D	376	MET	C-O	5.72	1.34	1.23
1	A	127	TYR	CZ-OH	5.71	1.47	1.37
1	C	55	TRP	CA-CB	-5.71	1.41	1.53
1	B	413	LYS	CE-NZ	5.71	1.63	1.49
1	C	164	GLY	CA-C	5.71	1.60	1.51
1	D	127	TYR	CZ-OH	5.71	1.47	1.37
1	A	55	TRP	CA-CB	-5.70	1.41	1.53
1	B	55	TRP	CA-CB	-5.70	1.41	1.53
1	B	127	TYR	CZ-OH	5.70	1.47	1.37
1	D	413	LYS	CE-NZ	5.70	1.63	1.49
1	A	413	LYS	CE-NZ	5.70	1.63	1.49
1	D	55	TRP	CA-CB	-5.70	1.41	1.53
1	B	376	MET	C-O	5.70	1.34	1.23
1	C	89	PRO	C-O	5.70	1.34	1.23
1	A	376	MET	C-O	5.69	1.34	1.23
1	B	89	PRO	C-O	5.69	1.34	1.23
1	C	271	LEU	CG-CD1	-5.68	1.30	1.51
1	C	57	THR	CA-C	5.68	1.67	1.52
1	C	413	LYS	CE-NZ	5.68	1.63	1.49
1	A	89	PRO	C-O	5.68	1.34	1.23
1	D	57	THR	CA-C	5.68	1.67	1.52
1	B	57	THR	CA-C	5.68	1.67	1.52
1	B	328	ARG	CZ-NH2	5.68	1.40	1.33
1	D	219	GLU	CD-OE2	5.67	1.31	1.25
1	A	57	THR	CA-C	5.67	1.67	1.52
1	B	258	TRP	CZ3-CH2	5.67	1.49	1.40
1	C	9	GLU	CG-CD	-5.67	1.43	1.51
1	D	258	TRP	CZ3-CH2	5.67	1.49	1.40
1	B	219	GLU	CD-OE2	5.67	1.31	1.25
1	A	271	LEU	CG-CD1	-5.66	1.30	1.51
1	D	271	LEU	CG-CD1	-5.66	1.30	1.51
1	A	258	TRP	CZ3-CH2	5.65	1.49	1.40
1	C	376	MET	C-O	5.64	1.34	1.23
1	D	89	PRO	C-O	5.64	1.34	1.23
1	A	219	GLU	CD-OE2	5.64	1.31	1.25
1	B	271	LEU	CG-CD1	-5.64	1.30	1.51
1	C	258	TRP	CZ3-CH2	5.64	1.49	1.40
1	B	258	TRP	N-CA	5.62	1.57	1.46
1	C	219	GLU	CD-OE2	5.62	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	258	TRP	N-CA	5.62	1.57	1.46
1	D	9	GLU	CG-CD	-5.62	1.43	1.51
1	A	9	GLU	CG-CD	-5.62	1.43	1.51
1	A	258	TRP	N-CA	5.62	1.57	1.46
1	D	212	ARG	CB-CG	5.60	1.67	1.52
1	B	29	GLU	CD-OE1	5.59	1.31	1.25
1	C	258	TRP	N-CA	5.59	1.57	1.46
1	A	29	GLU	CD-OE1	5.59	1.31	1.25
1	C	29	GLU	CD-OE1	5.58	1.31	1.25
1	C	67	ARG	CG-CD	5.58	1.66	1.51
1	A	67	ARG	CG-CD	5.58	1.65	1.51
1	B	67	ARG	CG-CD	5.58	1.65	1.51
1	D	29	GLU	CD-OE1	5.58	1.31	1.25
1	A	212	ARG	CB-CG	5.58	1.67	1.52
1	B	212	ARG	CB-CG	5.57	1.67	1.52
1	B	9	GLU	CG-CD	-5.56	1.43	1.51
1	B	207	TYR	CZ-OH	5.56	1.47	1.37
1	C	212	ARG	CB-CG	5.56	1.67	1.52
1	D	396	ALA	CA-CB	5.56	1.64	1.52
1	C	329	ILE	CA-CB	-5.56	1.42	1.54
1	D	67	ARG	CG-CD	5.56	1.65	1.51
1	B	94	GLU	CD-OE2	5.56	1.31	1.25
1	B	329	ILE	CA-CB	-5.55	1.42	1.54
1	D	285	PHE	CD1-CE1	5.55	1.50	1.39
1	C	51	SER	CB-OG	-5.55	1.35	1.42
1	A	207	TYR	CZ-OH	5.55	1.47	1.37
1	D	338	GLU	CD-OE1	5.55	1.31	1.25
1	A	285	PHE	CD1-CE1	5.54	1.50	1.39
1	A	329	ILE	CA-CB	-5.54	1.42	1.54
1	D	207	TYR	CZ-OH	5.54	1.47	1.37
1	A	396	ALA	CA-CB	5.54	1.64	1.52
1	B	165	TRP	CB-CG	-5.54	1.40	1.50
1	C	207	TYR	CZ-OH	5.54	1.47	1.37
1	C	396	ALA	CA-CB	5.54	1.64	1.52
1	B	396	ALA	CA-CB	5.53	1.64	1.52
1	D	329	ILE	CA-CB	-5.53	1.42	1.54
1	A	337	TRP	CE3-CZ3	5.53	1.47	1.38
1	C	285	PHE	CD1-CE1	5.53	1.50	1.39
1	C	165	TRP	CB-CG	-5.53	1.40	1.50
1	A	94	GLU	CD-OE2	5.52	1.31	1.25
1	A	267	VAL	CB-CG2	-5.52	1.41	1.52
1	B	285	PHE	CD1-CE1	5.52	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	165	TRP	CB-CG	-5.51	1.40	1.50
1	B	323	TYR	CD1-CE1	5.51	1.47	1.39
1	D	267	VAL	CB-CG2	-5.51	1.41	1.52
1	B	415	SER	CA-CB	5.51	1.61	1.52
1	A	415	SER	CA-CB	5.51	1.61	1.52
1	C	138	PHE	CA-CB	-5.51	1.41	1.53
1	B	267	VAL	CB-CG2	-5.51	1.41	1.52
1	C	140	VAL	CB-CG2	-5.51	1.41	1.52
1	D	94	GLU	CD-OE2	5.50	1.31	1.25
1	A	51	SER	CB-OG	-5.50	1.35	1.42
1	B	138	PHE	CA-CB	-5.50	1.41	1.53
1	C	338	GLU	CD-OE1	5.50	1.31	1.25
1	A	138	PHE	CA-CB	-5.50	1.41	1.53
1	A	338	GLU	CD-OE1	5.50	1.31	1.25
1	C	94	GLU	CD-OE2	5.50	1.31	1.25
1	B	337	TRP	CE3-CZ3	5.50	1.47	1.38
1	C	323	TYR	CD1-CE1	5.50	1.47	1.39
1	C	337	TRP	CE3-CZ3	5.50	1.47	1.38
1	D	138	PHE	CA-CB	-5.50	1.41	1.53
1	D	337	TRP	CE3-CZ3	5.50	1.47	1.38
1	C	415	SER	CA-CB	5.50	1.61	1.52
1	B	51	SER	CB-OG	-5.49	1.35	1.42
1	D	165	TRP	CB-CG	-5.49	1.40	1.50
1	B	338	GLU	CD-OE1	5.49	1.31	1.25
1	C	267	VAL	CB-CG2	-5.49	1.41	1.52
1	D	235	GLU	CA-C	-5.48	1.38	1.52
1	D	323	TYR	CD1-CE1	5.48	1.47	1.39
1	A	323	TYR	CD1-CE1	5.48	1.47	1.39
1	B	140	VAL	CB-CG2	-5.48	1.41	1.52
1	A	217	THR	CA-CB	5.48	1.67	1.53
1	A	140	VAL	CB-CG2	-5.47	1.41	1.52
1	D	51	SER	CB-OG	-5.47	1.35	1.42
1	A	235	GLU	CA-C	-5.46	1.38	1.52
1	B	235	GLU	CA-C	-5.46	1.38	1.52
1	D	415	SER	CA-CB	5.46	1.61	1.52
1	C	217	THR	CA-CB	5.46	1.67	1.53
1	D	217	THR	CA-CB	5.46	1.67	1.53
1	B	217	THR	CA-CB	5.45	1.67	1.53
1	C	235	GLU	CA-C	-5.45	1.38	1.52
1	D	140	VAL	CB-CG2	-5.45	1.41	1.52
1	D	241	VAL	C-O	5.44	1.33	1.23
1	B	241	VAL	C-O	5.44	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	401	ASP	CG-OD2	5.44	1.37	1.25
1	D	10	TRP	CG-CD1	5.42	1.44	1.36
1	C	241	VAL	C-O	5.41	1.33	1.23
1	A	241	VAL	C-O	5.41	1.33	1.23
1	A	401	ASP	CG-OD2	5.41	1.37	1.25
1	B	401	ASP	CG-OD2	5.40	1.37	1.25
1	B	10	TRP	CG-CD1	5.40	1.44	1.36
1	B	59	TRP	CG-CD1	5.40	1.44	1.36
1	D	401	ASP	CG-OD2	5.40	1.37	1.25
1	A	355	LEU	CG-CD1	-5.39	1.31	1.51
1	A	10	TRP	CG-CD1	5.39	1.44	1.36
1	B	355	LEU	CG-CD1	-5.39	1.31	1.51
1	C	355	LEU	CG-CD1	-5.39	1.31	1.51
1	A	383	ARG	CZ-NH2	5.38	1.40	1.33
1	C	83	ILE	CB-CG2	-5.38	1.36	1.52
1	D	355	LEU	CG-CD1	-5.38	1.31	1.51
1	C	383	ARG	CZ-NH2	5.38	1.40	1.33
1	C	59	TRP	CD2-CE2	5.38	1.47	1.41
1	D	361	ARG	CG-CD	5.38	1.65	1.51
1	D	383	ARG	CZ-NH2	5.37	1.40	1.33
1	C	10	TRP	CG-CD1	5.37	1.44	1.36
1	D	59	TRP	CD2-CE2	5.37	1.47	1.41
1	C	361	ARG	CG-CD	5.37	1.65	1.51
1	A	361	ARG	CG-CD	5.37	1.65	1.51
1	C	59	TRP	CG-CD1	5.37	1.44	1.36
1	A	59	TRP	CG-CD1	5.36	1.44	1.36
1	B	361	ARG	CG-CD	5.36	1.65	1.51
1	B	383	ARG	CZ-NH2	5.36	1.40	1.33
1	B	83	ILE	CB-CG2	-5.36	1.36	1.52
1	A	83	ILE	CB-CG2	-5.35	1.36	1.52
1	D	83	ILE	CB-CG2	-5.35	1.36	1.52
1	B	10	TRP	CE3-CZ3	5.35	1.47	1.38
1	B	275	ILE	CA-CB	-5.34	1.42	1.54
1	D	59	TRP	CG-CD1	5.34	1.44	1.36
1	D	10	TRP	CE3-CZ3	5.34	1.47	1.38
1	A	10	TRP	CE3-CZ3	5.34	1.47	1.38
1	D	154	LEU	C-O	5.34	1.33	1.23
1	B	154	LEU	C-O	5.32	1.33	1.23
1	C	275	ILE	CA-CB	-5.32	1.42	1.54
1	D	275	ILE	CA-CB	-5.32	1.42	1.54
1	A	59	TRP	CD2-CE2	5.32	1.47	1.41
1	A	154	LEU	C-O	5.32	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	275	ILE	CA-CB	-5.32	1.42	1.54
1	C	10	TRP	CE3-CZ3	5.32	1.47	1.38
1	B	228	THR	C-O	-5.30	1.13	1.23
1	C	154	LEU	C-O	5.30	1.33	1.23
1	B	147	MET	SD-CE	5.30	2.07	1.77
1	C	147	MET	SD-CE	5.30	2.07	1.77
1	A	147	MET	SD-CE	5.30	2.07	1.77
1	C	20	GLU	CG-CD	5.30	1.59	1.51
1	C	204	ARG	CZ-NH1	5.30	1.40	1.33
1	D	147	MET	SD-CE	5.30	2.07	1.77
1	C	312	THR	C-O	5.29	1.33	1.23
1	D	228	THR	C-O	-5.29	1.13	1.23
1	A	368	VAL	CA-CB	-5.29	1.43	1.54
1	B	59	TRP	CD2-CE2	5.29	1.47	1.41
1	A	124	HIS	C-O	5.28	1.33	1.23
1	A	312	THR	C-O	5.28	1.33	1.23
1	B	124	HIS	C-O	5.28	1.33	1.23
1	C	368	VAL	CA-CB	-5.28	1.43	1.54
1	A	228	THR	C-O	-5.28	1.13	1.23
1	B	368	VAL	CA-CB	-5.28	1.43	1.54
1	C	349	GLY	C-O	5.28	1.32	1.23
1	A	204	ARG	CZ-NH1	5.28	1.40	1.33
1	C	406	ALA	C-O	5.28	1.33	1.23
1	B	204	ARG	CZ-NH1	5.28	1.40	1.33
1	D	368	VAL	CA-CB	-5.28	1.43	1.54
1	A	341	ARG	NE-CZ	5.27	1.40	1.33
1	B	260	ALA	CA-CB	-5.27	1.41	1.52
1	B	341	ARG	NE-CZ	5.27	1.39	1.33
1	C	341	ARG	NE-CZ	5.27	1.39	1.33
1	D	88	TYR	N-CA	5.27	1.56	1.46
1	D	204	ARG	CZ-NH1	5.27	1.40	1.33
1	A	260	ALA	CA-CB	-5.27	1.41	1.52
1	D	43	ALA	CA-CB	5.27	1.63	1.52
1	D	312	THR	C-O	5.27	1.33	1.23
1	B	406	ALA	C-O	5.27	1.33	1.23
1	D	349	GLY	C-O	5.27	1.32	1.23
1	D	124	HIS	C-O	5.26	1.33	1.23
1	B	88	TYR	N-CA	5.26	1.56	1.46
1	C	124	HIS	C-O	5.26	1.33	1.23
1	C	260	ALA	CA-CB	-5.26	1.41	1.52
1	A	88	TYR	N-CA	5.26	1.56	1.46
1	C	122	ASP	CB-CG	5.26	1.62	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	349	GLY	C-O	5.25	1.32	1.23
1	D	260	ALA	CA-CB	-5.25	1.41	1.52
1	B	312	THR	C-O	5.25	1.33	1.23
1	A	20	GLU	CG-CD	5.25	1.59	1.51
1	C	43	ALA	CA-CB	5.25	1.63	1.52
1	C	27	ILE	CG1-CD1	5.25	1.86	1.50
1	A	122	ASP	CB-CG	5.25	1.62	1.51
1	A	349	GLY	C-O	5.25	1.32	1.23
1	A	419	VAL	C-O	5.25	1.33	1.23
1	D	27	ILE	CG1-CD1	5.24	1.86	1.50
1	D	28	VAL	CB-CG2	-5.24	1.41	1.52
1	A	27	ILE	CG1-CD1	5.24	1.86	1.50
1	D	100	GLN	CG-CD	5.24	1.63	1.51
1	A	43	ALA	CA-CB	5.24	1.63	1.52
1	A	100	GLN	CG-CD	5.24	1.63	1.51
1	B	27	ILE	CG1-CD1	5.24	1.86	1.50
1	B	100	GLN	CG-CD	5.24	1.63	1.51
1	C	228	THR	C-O	-5.24	1.13	1.23
1	D	236	LYS	CB-CG	5.24	1.66	1.52
1	C	100	GLN	CG-CD	5.24	1.63	1.51
1	A	406	ALA	C-O	5.24	1.33	1.23
1	B	43	ALA	CA-CB	5.24	1.63	1.52
1	B	122	ASP	CB-CG	5.24	1.62	1.51
1	C	28	VAL	CB-CG2	-5.23	1.41	1.52
1	D	122	ASP	CB-CG	5.23	1.62	1.51
1	A	28	VAL	CB-CG2	-5.23	1.41	1.52
1	B	20	GLU	CG-CD	5.23	1.59	1.51
1	C	368	VAL	C-O	5.23	1.33	1.23
1	D	419	VAL	C-O	5.23	1.33	1.23
1	A	368	VAL	C-O	5.22	1.33	1.23
1	C	360	ILE	CA-CB	-5.22	1.42	1.54
1	D	240	MET	CA-C	-5.22	1.39	1.52
1	D	406	ALA	C-O	5.22	1.33	1.23
1	A	236	LYS	CB-CG	5.22	1.66	1.52
1	B	360	ILE	CA-CB	-5.22	1.42	1.54
1	B	113	LYS	CG-CD	5.22	1.70	1.52
1	C	88	TYR	N-CA	5.22	1.56	1.46
1	C	236	LYS	CB-CG	5.22	1.66	1.52
1	C	240	MET	CA-C	-5.22	1.39	1.52
1	D	360	ILE	CA-CB	-5.22	1.42	1.54
1	B	419	VAL	C-O	5.22	1.33	1.23
1	B	189	GLU	CG-CD	5.22	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	419	VAL	C-O	5.22	1.33	1.23
1	A	113	LYS	CG-CD	5.21	1.70	1.52
1	A	189	GLU	CG-CD	5.21	1.59	1.51
1	C	94	GLU	CG-CD	5.21	1.59	1.51
1	C	113	LYS	CG-CD	5.21	1.70	1.52
1	A	94	GLU	CG-CD	5.21	1.59	1.51
1	A	360	ILE	CA-CB	-5.21	1.42	1.54
1	A	240	MET	CA-C	-5.21	1.39	1.52
1	B	240	MET	CA-C	-5.21	1.39	1.52
1	D	20	GLU	CG-CD	5.21	1.59	1.51
1	B	28	VAL	CB-CG2	-5.21	1.42	1.52
1	C	250	MET	SD-CE	5.21	2.07	1.77
1	D	113	LYS	CG-CD	5.21	1.70	1.52
1	B	236	LYS	CB-CG	5.21	1.66	1.52
1	D	189	GLU	CG-CD	5.21	1.59	1.51
1	B	250	MET	SD-CE	5.20	2.06	1.77
1	D	65	ALA	CA-C	-5.20	1.39	1.52
1	A	250	MET	SD-CE	5.20	2.06	1.77
1	B	329	ILE	CB-CG2	-5.20	1.36	1.52
1	D	250	MET	SD-CE	5.20	2.06	1.77
1	D	329	ILE	CB-CG2	-5.20	1.36	1.52
1	D	368	VAL	C-O	5.20	1.33	1.23
1	C	189	GLU	CG-CD	5.20	1.59	1.51
1	B	65	ALA	CA-C	-5.19	1.39	1.52
1	C	130	LEU	CG-CD1	-5.19	1.32	1.51
1	D	94	GLU	CG-CD	5.18	1.59	1.51
1	A	329	ILE	CB-CG2	-5.18	1.36	1.52
1	B	368	VAL	C-O	5.18	1.33	1.23
1	C	329	ILE	CB-CG2	-5.18	1.36	1.52
1	A	77	LYS	CG-CD	5.18	1.70	1.52
1	C	65	ALA	CA-C	-5.18	1.39	1.52
1	D	77	LYS	CG-CD	5.18	1.70	1.52
1	D	341	ARG	NE-CZ	5.18	1.39	1.33
1	A	130	LEU	CG-CD1	-5.18	1.32	1.51
1	C	77	LYS	CG-CD	5.18	1.70	1.52
1	D	224	LEU	C-O	-5.18	1.13	1.23
1	A	65	ALA	CA-C	-5.18	1.39	1.52
1	B	94	GLU	CG-CD	5.18	1.59	1.51
1	B	77	LYS	CG-CD	5.17	1.70	1.52
1	C	224	LEU	C-O	-5.17	1.13	1.23
1	D	130	LEU	CG-CD1	-5.17	1.32	1.51
1	B	224	LEU	C-O	-5.17	1.13	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	275	ILE	C-O	-5.16	1.13	1.23
1	C	275	ILE	C-O	-5.16	1.13	1.23
1	B	275	ILE	C-O	-5.16	1.13	1.23
1	D	275	ILE	C-O	-5.16	1.13	1.23
1	A	224	LEU	C-O	-5.15	1.13	1.23
1	B	130	LEU	CG-CD1	-5.15	1.32	1.51
1	C	328	ARG	CD-NE	5.14	1.55	1.46
1	D	328	ARG	CD-NE	5.14	1.55	1.46
1	B	260	ALA	C-O	-5.14	1.13	1.23
1	A	160	LYS	C-N	5.13	1.44	1.34
1	C	160	LYS	C-N	5.13	1.44	1.34
1	A	57	THR	N-CA	5.12	1.56	1.46
1	A	328	ARG	CD-NE	5.12	1.55	1.46
1	B	328	ARG	CD-NE	5.12	1.55	1.46
1	C	57	THR	N-CA	5.12	1.56	1.46
1	B	198	ARG	CZ-NH2	5.11	1.39	1.33
1	B	57	THR	N-CA	5.11	1.56	1.46
1	C	355	LEU	CG-CD2	-5.11	1.32	1.51
1	A	400	VAL	CB-CG2	-5.11	1.42	1.52
1	A	260	ALA	C-O	-5.10	1.13	1.23
1	D	57	THR	N-CA	5.10	1.56	1.46
1	D	258	TRP	CE3-CZ3	5.10	1.47	1.38
1	A	355	LEU	CG-CD2	-5.09	1.33	1.51
1	B	220	THR	CA-CB	-5.09	1.40	1.53
1	C	400	VAL	CB-CG2	-5.09	1.42	1.52
1	D	355	LEU	CG-CD2	-5.09	1.33	1.51
1	A	198	ARG	CZ-NH2	5.09	1.39	1.33
1	B	400	VAL	CB-CG2	-5.09	1.42	1.52
1	B	160	LYS	C-N	5.09	1.44	1.34
1	B	258	TRP	CE3-CZ3	5.09	1.47	1.38
1	D	260	ALA	C-O	-5.09	1.13	1.23
1	B	355	LEU	CG-CD2	-5.09	1.33	1.51
1	C	258	TRP	CE3-CZ3	5.09	1.47	1.38
1	D	220	THR	CA-CB	-5.08	1.40	1.53
1	D	302	ALA	N-CA	-5.08	1.36	1.46
1	D	407	LYS	CD-CE	5.08	1.64	1.51
1	A	220	THR	CA-CB	-5.08	1.40	1.53
1	C	198	ARG	CZ-NH2	5.08	1.39	1.33
1	D	160	LYS	C-N	5.08	1.44	1.34
1	D	400	VAL	CB-CG2	-5.08	1.42	1.52
1	C	174	ALA	CA-CB	-5.08	1.41	1.52
1	A	103	SER	C-O	5.08	1.32	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	260	ALA	C-O	-5.08	1.13	1.23
1	A	302	ALA	N-CA	-5.07	1.36	1.46
1	B	407	LYS	CD-CE	5.07	1.64	1.51
1	A	258	TRP	CE3-CZ3	5.07	1.47	1.38
1	B	252	ASP	CA-C	-5.07	1.39	1.52
1	B	11	TYR	CE1-CZ	5.07	1.45	1.38
1	C	407	LYS	CD-CE	5.07	1.64	1.51
1	D	174	ALA	CA-CB	-5.07	1.41	1.52
1	D	198	ARG	CZ-NH2	5.07	1.39	1.33
1	A	174	ALA	CA-CB	-5.07	1.41	1.52
1	B	103	SER	C-O	5.07	1.32	1.23
1	A	407	LYS	CD-CE	5.07	1.64	1.51
1	B	302	ALA	N-CA	-5.07	1.36	1.46
1	C	90	LEU	C-O	-5.07	1.13	1.23
1	C	220	THR	CA-CB	-5.07	1.40	1.53
1	D	157	THR	CA-CB	-5.07	1.40	1.53
1	B	157	THR	CA-CB	-5.06	1.40	1.53
1	B	174	ALA	CA-CB	-5.06	1.41	1.52
1	C	302	ALA	N-CA	-5.06	1.36	1.46
1	A	90	LEU	C-O	-5.06	1.13	1.23
1	D	252	ASP	CA-C	-5.06	1.39	1.52
1	D	90	LEU	C-O	-5.06	1.13	1.23
1	D	103	SER	C-O	5.06	1.32	1.23
1	A	157	THR	CA-CB	-5.05	1.40	1.53
1	B	45	ARG	CZ-NH1	5.05	1.39	1.33
1	B	90	LEU	C-O	-5.05	1.13	1.23
1	C	157	THR	CA-CB	-5.05	1.40	1.53
1	C	318	LYS	CB-CG	5.05	1.66	1.52
1	A	252	ASP	CA-C	-5.05	1.39	1.52
1	A	319	MET	CB-CG	5.05	1.67	1.51
1	C	319	MET	CB-CG	5.05	1.67	1.51
1	D	266	GLU	N-CA	-5.04	1.36	1.46
1	D	318	LYS	CB-CG	5.04	1.66	1.52
1	A	266	GLU	N-CA	-5.04	1.36	1.46
1	A	318	LYS	CB-CG	5.04	1.66	1.52
1	D	319	MET	CB-CG	5.04	1.67	1.51
1	C	113	LYS	CA-C	5.04	1.66	1.52
1	B	23	ARG	CZ-NH1	5.04	1.39	1.33
1	B	367	LEU	CG-CD1	-5.04	1.33	1.51
1	C	252	ASP	CA-C	-5.04	1.39	1.52
1	D	9	GLU	N-CA	5.04	1.56	1.46
1	D	11	TYR	CE1-CZ	5.04	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	11	TYR	CE1-CZ	5.03	1.45	1.38
1	B	319	MET	CB-CG	5.03	1.67	1.51
1	A	367	LEU	CG-CD1	-5.03	1.33	1.51
1	C	103	SER	C-O	5.03	1.32	1.23
1	C	23	ARG	CZ-NH1	5.03	1.39	1.33
1	C	266	GLU	N-CA	-5.03	1.36	1.46
1	C	367	LEU	CG-CD1	-5.02	1.33	1.51
1	B	266	GLU	N-CA	-5.02	1.36	1.46
1	B	318	LYS	CB-CG	5.02	1.66	1.52
1	C	278	HIS	CA-C	-5.02	1.39	1.52
1	B	101	LEU	CG-CD2	-5.02	1.33	1.51
1	D	367	LEU	CG-CD1	-5.01	1.33	1.51
1	C	9	GLU	N-CA	5.01	1.56	1.46
1	A	113	LYS	CA-C	5.01	1.66	1.52
1	D	101	LEU	CG-CD2	-5.01	1.33	1.51
1	B	113	LYS	CA-C	5.01	1.66	1.52
1	C	30	TYR	CG-CD1	-5.01	1.32	1.39
1	A	9	GLU	N-CA	5.01	1.56	1.46
1	C	367	LEU	CG-CD2	5.01	1.70	1.51
1	B	9	GLU	N-CA	5.01	1.56	1.46
1	A	101	LEU	CG-CD2	-5.00	1.33	1.51
1	B	367	LEU	CG-CD2	5.00	1.70	1.51
1	B	383	ARG	CZ-NH1	5.00	1.39	1.33

All (1235) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	341	ARG	NE-CZ-NH2	-23.96	108.32	120.30
1	B	341	ARG	NE-CZ-NH2	-23.93	108.34	120.30
1	C	341	ARG	NE-CZ-NH2	-23.92	108.34	120.30
1	D	341	ARG	NE-CZ-NH2	-23.85	108.37	120.30
1	D	366	ASP	CB-CG-OD2	-19.20	101.02	118.30
1	A	366	ASP	CB-CG-OD2	-19.18	101.04	118.30
1	C	366	ASP	CB-CG-OD2	-19.15	101.07	118.30
1	B	366	ASP	CB-CG-OD2	-19.15	101.07	118.30
1	A	366	ASP	CB-CG-OD1	18.18	134.66	118.30
1	C	366	ASP	CB-CG-OD1	18.18	134.66	118.30
1	B	366	ASP	CB-CG-OD1	18.17	134.65	118.30
1	D	366	ASP	CB-CG-OD1	18.16	134.65	118.30
1	D	208	ARG	NE-CZ-NH1	17.94	129.27	120.30
1	A	208	ARG	NE-CZ-NH1	17.86	129.23	120.30
1	C	208	ARG	NE-CZ-NH1	17.85	129.22	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	208	ARG	NE-CZ-NH1	17.80	129.20	120.30
1	D	270	ASP	CB-CG-OD2	16.86	133.47	118.30
1	A	270	ASP	CB-CG-OD2	16.84	133.46	118.30
1	B	270	ASP	CB-CG-OD2	16.84	133.45	118.30
1	C	270	ASP	CB-CG-OD2	16.83	133.44	118.30
1	D	237	ARG	NE-CZ-NH2	-16.80	111.90	120.30
1	A	237	ARG	NE-CZ-NH2	-16.75	111.93	120.30
1	B	237	ARG	NE-CZ-NH2	-16.74	111.93	120.30
1	C	237	ARG	NE-CZ-NH2	-16.69	111.95	120.30
1	B	198	ARG	NE-CZ-NH1	16.48	128.54	120.30
1	A	198	ARG	NE-CZ-NH1	16.45	128.53	120.30
1	D	198	ARG	NE-CZ-NH1	16.42	128.51	120.30
1	C	198	ARG	NE-CZ-NH1	16.40	128.50	120.30
1	B	131	ARG	NE-CZ-NH2	-15.30	112.65	120.30
1	A	131	ARG	NE-CZ-NH2	-15.21	112.69	120.30
1	C	131	ARG	NE-CZ-NH2	-15.17	112.71	120.30
1	D	131	ARG	NE-CZ-NH2	-15.13	112.74	120.30
1	A	341	ARG	NE-CZ-NH1	15.11	127.86	120.30
1	D	341	ARG	NE-CZ-NH1	15.11	127.86	120.30
1	C	341	ARG	NE-CZ-NH1	15.09	127.84	120.30
1	B	341	ARG	NE-CZ-NH1	15.08	127.84	120.30
1	C	237	ARG	NE-CZ-NH1	14.86	127.73	120.30
1	A	237	ARG	NE-CZ-NH1	14.79	127.69	120.30
1	B	237	ARG	NE-CZ-NH1	14.77	127.68	120.30
1	D	237	ARG	NE-CZ-NH1	14.75	127.68	120.30
1	C	244	GLU	OE1-CD-OE2	14.13	140.26	123.30
1	B	244	GLU	OE1-CD-OE2	14.12	140.24	123.30
1	A	244	GLU	OE1-CD-OE2	14.10	140.22	123.30
1	D	244	GLU	OE1-CD-OE2	14.09	140.21	123.30
1	B	270	ASP	CB-CG-OD1	-14.04	105.67	118.30
1	D	270	ASP	CB-CG-OD1	-14.03	105.67	118.30
1	A	270	ASP	CB-CG-OD1	-14.02	105.68	118.30
1	C	270	ASP	CB-CG-OD1	-14.02	105.69	118.30
1	A	391	ASP	CB-CG-OD1	-13.13	106.48	118.30
1	C	391	ASP	CB-CG-OD1	-13.12	106.49	118.30
1	B	391	ASP	CB-CG-OD1	-13.11	106.50	118.30
1	D	403	ASP	CB-CG-OD1	-13.11	106.50	118.30
1	D	391	ASP	CB-CG-OD1	-13.10	106.51	118.30
1	A	239	GLU	CG-CD-OE1	-13.09	92.11	118.30
1	D	239	GLU	CG-CD-OE1	-13.09	92.11	118.30
1	B	239	GLU	CG-CD-OE1	-13.09	92.12	118.30
1	C	239	GLU	CG-CD-OE1	-13.08	92.14	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	403	ASP	CB-CG-OD1	-13.07	106.54	118.30
1	B	403	ASP	CB-CG-OD1	-13.07	106.54	118.30
1	C	403	ASP	CB-CG-OD1	-13.07	106.54	118.30
1	C	391	ASP	CB-CG-OD2	12.47	129.52	118.30
1	A	391	ASP	CB-CG-OD2	12.44	129.49	118.30
1	B	391	ASP	CB-CG-OD2	12.43	129.49	118.30
1	B	212	ARG	NE-CZ-NH1	12.41	126.50	120.30
1	D	391	ASP	CB-CG-OD2	12.39	129.45	118.30
1	A	212	ARG	NE-CZ-NH1	12.39	126.49	120.30
1	D	212	ARG	NE-CZ-NH1	12.36	126.48	120.30
1	C	212	ARG	NE-CZ-NH1	12.30	126.45	120.30
1	C	16	ASP	CB-CG-OD1	-12.28	107.25	118.30
1	A	16	ASP	CB-CG-OD1	-12.26	107.26	118.30
1	B	16	ASP	CB-CG-OD1	-12.26	107.27	118.30
1	D	16	ASP	CB-CG-OD1	-12.24	107.28	118.30
1	B	380	ASP	CB-CG-OD2	-12.16	107.36	118.30
1	A	380	ASP	CB-CG-OD2	-12.16	107.36	118.30
1	D	380	ASP	CB-CG-OD2	-12.15	107.37	118.30
1	C	380	ASP	CB-CG-OD2	-12.14	107.37	118.30
1	C	328	ARG	NE-CZ-NH1	11.82	126.21	120.30
1	D	328	ARG	NE-CZ-NH1	11.78	126.19	120.30
1	A	328	ARG	NE-CZ-NH1	11.75	126.17	120.30
1	B	328	ARG	NE-CZ-NH1	11.68	126.14	120.30
1	D	92	LEU	CB-CG-CD1	-11.67	91.17	111.00
1	A	92	LEU	CB-CG-CD1	-11.65	91.20	111.00
1	B	92	LEU	CB-CG-CD1	-11.65	91.20	111.00
1	C	92	LEU	CB-CG-CD1	-11.63	91.22	111.00
1	C	152	ARG	NE-CZ-NH1	11.59	126.09	120.30
1	A	152	ARG	NE-CZ-NH1	11.53	126.07	120.30
1	C	151	ASP	CB-CG-OD1	11.52	128.67	118.30
1	B	152	ARG	NE-CZ-NH1	11.51	126.06	120.30
1	D	152	ARG	NE-CZ-NH1	11.51	126.06	120.30
1	A	151	ASP	CB-CG-OD1	11.50	128.65	118.30
1	B	151	ASP	CB-CG-OD1	11.50	128.65	118.30
1	D	151	ASP	CB-CG-OD1	11.48	128.63	118.30
1	D	403	ASP	CB-CG-OD2	11.44	128.59	118.30
1	B	403	ASP	CB-CG-OD2	11.43	128.59	118.30
1	C	403	ASP	CB-CG-OD2	11.41	128.57	118.30
1	A	403	ASP	CB-CG-OD2	11.40	128.56	118.30
1	B	356	MET	CG-SD-CE	11.33	118.33	100.20
1	C	356	MET	CG-SD-CE	11.33	118.33	100.20
1	D	356	MET	CG-SD-CE	11.33	118.32	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	356	MET	CG-SD-CE	11.32	118.32	100.20
1	D	376	MET	CG-SD-CE	-11.17	82.33	100.20
1	C	376	MET	CG-SD-CE	-11.16	82.34	100.20
1	A	390	ARG	NE-CZ-NH2	-11.16	114.72	120.30
1	A	376	MET	CG-SD-CE	-11.16	82.35	100.20
1	B	376	MET	CG-SD-CE	-11.14	82.37	100.20
1	D	390	ARG	NE-CZ-NH2	-11.12	114.74	120.30
1	B	390	ARG	NE-CZ-NH2	-11.11	114.75	120.30
1	C	390	ARG	NE-CZ-NH2	-11.03	114.79	120.30
1	D	275	ILE	CG1-CB-CG2	-11.00	87.21	111.40
1	B	275	ILE	CG1-CB-CG2	-10.99	87.22	111.40
1	C	275	ILE	CG1-CB-CG2	-10.99	87.22	111.40
1	A	275	ILE	CG1-CB-CG2	-10.98	87.23	111.40
1	B	130	LEU	CB-CG-CD2	10.95	129.61	111.00
1	A	130	LEU	CB-CG-CD2	10.95	129.61	111.00
1	D	130	LEU	CB-CG-CD2	10.93	129.59	111.00
1	C	130	LEU	CB-CG-CD2	10.91	129.55	111.00
1	A	160	LYS	CD-CE-NZ	10.80	136.54	111.70
1	D	160	LYS	CD-CE-NZ	10.79	136.52	111.70
1	B	160	LYS	CD-CE-NZ	10.79	136.52	111.70
1	C	160	LYS	CD-CE-NZ	10.79	136.51	111.70
1	D	64	MET	CG-SD-CE	10.67	117.27	100.20
1	A	64	MET	CG-SD-CE	10.67	117.27	100.20
1	B	64	MET	CG-SD-CE	10.66	117.26	100.20
1	C	64	MET	CG-SD-CE	10.66	117.26	100.20
1	B	101	LEU	CB-CG-CD2	-10.65	92.89	111.00
1	C	101	LEU	CB-CG-CD2	-10.65	92.89	111.00
1	D	101	LEU	CB-CG-CD2	-10.65	92.90	111.00
1	A	101	LEU	CB-CG-CD2	-10.64	92.92	111.00
1	C	279	ARG	NE-CZ-NH1	10.58	125.59	120.30
1	A	279	ARG	NE-CZ-NH1	10.53	125.57	120.30
1	B	279	ARG	NE-CZ-NH1	10.53	125.56	120.30
1	D	279	ARG	NE-CZ-NH1	10.48	125.54	120.30
1	B	119	ARG	NE-CZ-NH1	-10.34	115.13	120.30
1	B	361	ARG	NE-CZ-NH1	-10.32	115.14	120.30
1	C	361	ARG	NE-CZ-NH1	-10.32	115.14	120.30
1	A	361	ARG	NE-CZ-NH1	-10.31	115.14	120.30
1	D	361	ARG	NE-CZ-NH1	-10.31	115.15	120.30
1	A	119	ARG	NE-CZ-NH1	-10.30	115.15	120.30
1	C	119	ARG	NE-CZ-NH1	-10.29	115.16	120.30
1	D	119	ARG	NE-CZ-NH1	-10.24	115.18	120.30
1	B	201	GLU	CG-CD-OE1	-10.14	98.02	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	201	GLU	CG-CD-OE1	-10.11	98.08	118.30
1	D	201	GLU	CG-CD-OE1	-10.10	98.10	118.30
1	C	201	GLU	CG-CD-OE1	-10.10	98.11	118.30
1	B	188	ASP	CB-CG-OD2	10.08	127.37	118.30
1	C	188	ASP	CB-CG-OD2	10.06	127.35	118.30
1	A	188	ASP	CB-CG-OD2	10.05	127.34	118.30
1	D	290	ARG	NE-CZ-NH2	10.04	125.32	120.30
1	D	188	ASP	CB-CG-OD2	10.02	127.32	118.30
1	A	290	ARG	NE-CZ-NH2	10.02	125.31	120.30
1	A	265	ARG	NE-CZ-NH1	-9.96	115.32	120.30
1	D	265	ARG	NE-CZ-NH1	-9.95	115.32	120.30
1	B	265	ARG	NE-CZ-NH1	-9.95	115.33	120.30
1	C	265	ARG	NE-CZ-NH1	-9.94	115.33	120.30
1	B	290	ARG	NE-CZ-NH2	9.94	125.27	120.30
1	D	310	ILE	CG1-CB-CG2	9.91	133.21	111.40
1	A	310	ILE	CG1-CB-CG2	9.90	133.18	111.40
1	B	310	ILE	CG1-CB-CG2	9.89	133.15	111.40
1	C	310	ILE	CG1-CB-CG2	9.89	133.15	111.40
1	C	290	ARG	NE-CZ-NH2	9.87	125.23	120.30
1	D	222	GLU	CG-CD-OE2	-9.77	98.77	118.30
1	C	222	GLU	CG-CD-OE2	-9.76	98.78	118.30
1	A	222	GLU	CG-CD-OE2	-9.76	98.78	118.30
1	B	222	GLU	CG-CD-OE2	-9.75	98.79	118.30
1	B	208	ARG	NE-CZ-NH2	-9.69	115.45	120.30
1	D	239	GLU	CG-CD-OE2	9.67	137.65	118.30
1	D	208	ARG	NE-CZ-NH2	-9.67	115.47	120.30
1	A	239	GLU	CG-CD-OE2	9.66	137.62	118.30
1	A	208	ARG	NE-CZ-NH2	-9.65	115.47	120.30
1	B	239	GLU	CG-CD-OE2	9.64	137.59	118.30
1	C	239	GLU	CG-CD-OE2	9.64	137.57	118.30
1	C	208	ARG	NE-CZ-NH2	-9.62	115.49	120.30
1	D	367	LEU	CB-CG-CD1	-9.56	94.75	111.00
1	A	367	LEU	CB-CG-CD1	-9.54	94.78	111.00
1	C	367	LEU	CB-CG-CD1	-9.53	94.80	111.00
1	B	367	LEU	CB-CG-CD1	-9.51	94.83	111.00
1	C	202	ARG	NE-CZ-NH2	9.39	125.00	120.30
1	D	85	LYS	CD-CE-NZ	9.34	133.18	111.70
1	B	85	LYS	CD-CE-NZ	9.33	133.16	111.70
1	C	264	MET	CG-SD-CE	9.33	115.12	100.20
1	D	264	MET	CG-SD-CE	9.33	115.12	100.20
1	A	85	LYS	CD-CE-NZ	9.32	133.14	111.70
1	B	167	VAL	CG1-CB-CG2	9.32	125.82	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	202	ARG	NE-CZ-NH2	9.32	124.96	120.30
1	A	264	MET	CG-SD-CE	9.32	115.11	100.20
1	B	264	MET	CG-SD-CE	9.32	115.11	100.20
1	C	85	LYS	CD-CE-NZ	9.32	133.13	111.70
1	A	167	VAL	CG1-CB-CG2	9.30	125.78	110.90
1	D	167	VAL	CG1-CB-CG2	9.29	125.77	110.90
1	D	202	ARG	NE-CZ-NH2	9.29	124.94	120.30
1	C	167	VAL	CG1-CB-CG2	9.29	125.75	110.90
1	B	202	ARG	NE-CZ-NH2	9.28	124.94	120.30
1	C	141	GLN	N-CA-CB	-9.05	94.31	110.60
1	A	141	GLN	N-CA-CB	-9.01	94.38	110.60
1	D	141	GLN	N-CA-CB	-9.01	94.38	110.60
1	B	141	GLN	N-CA-CB	-8.99	94.41	110.60
1	D	298	LEU	CB-CG-CD2	-8.97	95.74	111.00
1	A	298	LEU	CB-CG-CD2	-8.97	95.75	111.00
1	B	298	LEU	CB-CG-CD2	-8.97	95.75	111.00
1	C	298	LEU	CB-CG-CD2	-8.95	95.78	111.00
1	C	216	GLU	CB-CA-C	8.92	128.25	110.40
1	D	216	GLU	CB-CA-C	8.91	128.23	110.40
1	A	216	GLU	CB-CA-C	8.91	128.22	110.40
1	B	216	GLU	CB-CA-C	8.91	128.21	110.40
1	B	211	ASP	CB-CG-OD1	-8.90	110.28	118.30
1	A	94	GLU	N-CA-C	-8.89	87.01	111.00
1	B	94	GLU	N-CA-C	-8.89	87.00	111.00
1	D	94	GLU	N-CA-C	-8.88	87.01	111.00
1	D	211	ASP	CB-CG-OD1	-8.88	110.30	118.30
1	A	211	ASP	CB-CG-OD1	-8.88	110.31	118.30
1	C	94	GLU	N-CA-C	-8.88	87.02	111.00
1	C	211	ASP	CB-CG-OD1	-8.85	110.34	118.30
1	D	24	ASP	CB-CG-OD2	8.78	126.21	118.30
1	D	367	LEU	CA-CB-CG	-8.77	95.12	115.30
1	C	367	LEU	CA-CB-CG	-8.77	95.13	115.30
1	A	367	LEU	CA-CB-CG	-8.76	95.14	115.30
1	B	367	LEU	CA-CB-CG	-8.76	95.16	115.30
1	C	24	ASP	CB-CG-OD2	8.74	126.17	118.30
1	A	24	ASP	CB-CG-OD2	8.74	126.17	118.30
1	B	24	ASP	CB-CG-OD2	8.71	126.14	118.30
1	B	266	GLU	OE1-CD-OE2	8.71	133.75	123.30
1	C	266	GLU	OE1-CD-OE2	8.71	133.75	123.30
1	A	266	GLU	OE1-CD-OE2	8.68	133.72	123.30
1	D	266	GLU	OE1-CD-OE2	8.68	133.71	123.30
1	D	259	SER	N-CA-CB	-8.65	97.53	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	259	SER	N-CA-CB	-8.64	97.54	110.50
1	A	259	SER	N-CA-CB	-8.63	97.55	110.50
1	B	259	SER	N-CA-CB	-8.63	97.55	110.50
1	D	80	GLU	CG-CD-OE1	8.50	135.30	118.30
1	B	80	GLU	CG-CD-OE1	8.49	135.27	118.30
1	C	80	GLU	CG-CD-OE1	8.48	135.26	118.30
1	A	80	GLU	CG-CD-OE1	8.48	135.26	118.30
1	B	296	LEU	CB-CG-CD2	-8.47	96.60	111.00
1	A	296	LEU	CB-CG-CD2	-8.45	96.63	111.00
1	C	233	ILE	CG1-CB-CG2	8.45	130.00	111.40
1	D	296	LEU	CB-CG-CD2	-8.45	96.64	111.00
1	C	296	LEU	CB-CG-CD2	-8.44	96.66	111.00
1	A	233	ILE	CG1-CB-CG2	8.43	129.95	111.40
1	B	233	ILE	CG1-CB-CG2	8.42	129.93	111.40
1	D	233	ILE	CG1-CB-CG2	8.42	129.93	111.40
1	D	212	ARG	NE-CZ-NH2	-8.40	116.10	120.30
1	A	212	ARG	NE-CZ-NH2	-8.35	116.12	120.30
1	C	95	GLU	N-CA-CB	8.32	125.57	110.60
1	C	212	ARG	NE-CZ-NH2	-8.32	116.14	120.30
1	A	95	GLU	N-CA-CB	8.30	125.53	110.60
1	B	95	GLU	N-CA-CB	8.29	125.53	110.60
1	B	212	ARG	NE-CZ-NH2	-8.29	116.16	120.30
1	D	95	GLU	N-CA-CB	8.29	125.52	110.60
1	D	407	LYS	CD-CE-NZ	8.29	130.76	111.70
1	C	198	ARG	CD-NE-CZ	8.28	135.20	123.60
1	B	407	LYS	CD-CE-NZ	8.28	130.75	111.70
1	A	407	LYS	CD-CE-NZ	8.28	130.74	111.70
1	C	407	LYS	CD-CE-NZ	8.27	130.71	111.70
1	A	198	ARG	CD-NE-CZ	8.25	135.15	123.60
1	D	198	ARG	CD-NE-CZ	8.25	135.15	123.60
1	A	91	THR	CA-C-N	-8.23	99.10	117.20
1	B	198	ARG	CD-NE-CZ	8.23	135.12	123.60
1	B	91	THR	CA-C-N	-8.22	99.11	117.20
1	C	91	THR	CA-C-N	-8.22	99.12	117.20
1	D	17	LEU	CA-CB-CG	-8.22	96.40	115.30
1	A	17	LEU	CA-CB-CG	-8.22	96.40	115.30
1	D	91	THR	CA-C-N	-8.21	99.14	117.20
1	B	17	LEU	CA-CB-CG	-8.21	96.43	115.30
1	C	17	LEU	CA-CB-CG	-8.21	96.43	115.30
1	C	61	LEU	CB-CG-CD2	8.17	124.89	111.00
1	A	61	LEU	CB-CG-CD2	8.16	124.88	111.00
1	D	61	LEU	CB-CG-CD2	8.16	124.88	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	61	LEU	CB-CG-CD2	8.16	124.87	111.00
1	B	314	THR	N-CA-C	8.15	133.00	111.00
1	D	216	GLU	OE1-CD-OE2	-8.13	113.54	123.30
1	A	216	GLU	OE1-CD-OE2	-8.13	113.55	123.30
1	A	314	THR	N-CA-C	8.13	132.94	111.00
1	D	314	THR	N-CA-C	8.13	132.94	111.00
1	C	314	THR	N-CA-C	8.12	132.94	111.00
1	D	175	TYR	CE1-CZ-OH	8.11	142.00	120.10
1	C	175	TYR	CE1-CZ-OH	8.11	141.98	120.10
1	C	216	GLU	OE1-CD-OE2	-8.10	113.58	123.30
1	A	175	TYR	CE1-CZ-OH	8.10	141.96	120.10
1	B	216	GLU	OE1-CD-OE2	-8.10	113.58	123.30
1	B	175	TYR	CE1-CZ-OH	8.09	141.95	120.10
1	A	413	LYS	CD-CE-NZ	8.07	130.27	111.70
1	B	413	LYS	CD-CE-NZ	8.07	130.27	111.70
1	D	413	LYS	CD-CE-NZ	8.07	130.27	111.70
1	C	413	LYS	CD-CE-NZ	8.06	130.25	111.70
1	B	119	ARG	CG-CD-NE	-8.03	94.93	111.80
1	A	119	ARG	CG-CD-NE	-8.03	94.94	111.80
1	C	119	ARG	CG-CD-NE	-8.03	94.94	111.80
1	D	119	ARG	CG-CD-NE	-8.03	94.95	111.80
1	D	289	PRO	N-CA-C	7.97	132.83	112.10
1	C	289	PRO	N-CA-C	7.97	132.81	112.10
1	B	289	PRO	N-CA-C	7.96	132.81	112.10
1	A	289	PRO	N-CA-C	7.96	132.79	112.10
1	D	307	VAL	CG1-CB-CG2	-7.96	98.17	110.90
1	B	307	VAL	CG1-CB-CG2	-7.95	98.18	110.90
1	C	147	MET	CA-CB-CG	-7.94	99.80	113.30
1	C	307	VAL	CG1-CB-CG2	-7.94	98.20	110.90
1	A	147	MET	CA-CB-CG	-7.94	99.81	113.30
1	A	307	VAL	CG1-CB-CG2	-7.93	98.20	110.90
1	D	147	MET	CA-CB-CG	-7.93	99.81	113.30
1	B	147	MET	CA-CB-CG	-7.93	99.82	113.30
1	C	61	LEU	CB-CG-CD1	-7.88	97.61	111.00
1	A	290	ARG	NE-CZ-NH1	-7.87	116.36	120.30
1	B	290	ARG	NE-CZ-NH1	-7.87	116.36	120.30
1	A	61	LEU	CB-CG-CD1	-7.87	97.63	111.00
1	B	61	LEU	CB-CG-CD1	-7.87	97.63	111.00
1	D	61	LEU	CB-CG-CD1	-7.85	97.66	111.00
1	C	261	LEU	CB-CA-C	-7.84	95.31	110.20
1	D	290	ARG	NE-CZ-NH1	-7.84	116.38	120.30
1	A	261	LEU	CB-CA-C	-7.83	95.32	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	261	LEU	CB-CA-C	-7.83	95.33	110.20
1	D	261	LEU	CB-CA-C	-7.83	95.33	110.20
1	C	290	ARG	NE-CZ-NH1	-7.81	116.40	120.30
1	C	298	LEU	CB-CG-CD1	7.80	124.27	111.00
1	A	298	LEU	CB-CG-CD1	7.79	124.24	111.00
1	D	298	LEU	CB-CG-CD1	7.78	124.23	111.00
1	B	298	LEU	CB-CG-CD1	7.78	124.23	111.00
1	D	92	LEU	CB-CG-CD2	7.78	124.22	111.00
1	C	92	LEU	CB-CG-CD2	7.77	124.21	111.00
1	A	92	LEU	CB-CG-CD2	7.76	124.19	111.00
1	B	92	LEU	CB-CG-CD2	7.75	124.17	111.00
1	B	85	LYS	N-CA-C	-7.72	90.16	111.00
1	A	85	LYS	N-CA-C	-7.70	90.21	111.00
1	C	85	LYS	N-CA-C	-7.69	90.24	111.00
1	D	85	LYS	N-CA-C	-7.69	90.24	111.00
1	C	172	GLU	N-CA-CB	-7.63	96.87	110.60
1	B	172	GLU	N-CA-CB	-7.62	96.88	110.60
1	A	172	GLU	N-CA-CB	-7.60	96.92	110.60
1	D	172	GLU	N-CA-CB	-7.60	96.92	110.60
1	A	189	GLU	OE1-CD-OE2	7.56	132.37	123.30
1	B	189	GLU	OE1-CD-OE2	7.55	132.36	123.30
1	C	189	GLU	OE1-CD-OE2	7.55	132.36	123.30
1	D	189	GLU	OE1-CD-OE2	7.54	132.35	123.30
1	C	293	ILE	CG1-CB-CG2	7.53	127.96	111.40
1	D	222	GLU	CG-CD-OE1	7.52	133.35	118.30
1	B	293	ILE	CG1-CB-CG2	7.52	127.94	111.40
1	A	222	GLU	CG-CD-OE1	7.52	133.33	118.30
1	A	293	ILE	CG1-CB-CG2	7.52	127.94	111.40
1	B	222	GLU	CG-CD-OE1	7.52	133.33	118.30
1	C	222	GLU	CG-CD-OE1	7.51	133.32	118.30
1	C	58	LEU	CB-CG-CD2	-7.51	98.24	111.00
1	D	58	LEU	CB-CG-CD2	-7.50	98.24	111.00
1	D	389	LEU	CB-CG-CD2	-7.50	98.24	111.00
1	D	293	ILE	CG1-CB-CG2	7.50	127.90	111.40
1	A	58	LEU	CB-CG-CD2	-7.50	98.26	111.00
1	A	389	LEU	CB-CG-CD2	-7.50	98.26	111.00
1	B	58	LEU	CB-CG-CD2	-7.49	98.26	111.00
1	C	389	LEU	CB-CG-CD2	-7.49	98.26	111.00
1	B	389	LEU	CB-CG-CD2	-7.49	98.27	111.00
1	B	157	THR	N-CA-CB	-7.48	96.09	110.30
1	C	26	LEU	CA-CB-CG	-7.47	98.11	115.30
1	A	157	THR	N-CA-CB	-7.46	96.12	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	157	THR	N-CA-CB	-7.46	96.12	110.30
1	A	26	LEU	CA-CB-CG	-7.46	98.14	115.30
1	D	26	LEU	CA-CB-CG	-7.46	98.14	115.30
1	B	26	LEU	CA-CB-CG	-7.46	98.15	115.30
1	D	157	THR	N-CA-CB	-7.45	96.15	110.30
1	D	201	GLU	CG-CD-OE2	7.45	133.19	118.30
1	A	201	GLU	CG-CD-OE2	7.44	133.18	118.30
1	B	201	GLU	CG-CD-OE2	7.44	133.18	118.30
1	C	201	GLU	CG-CD-OE2	7.44	133.18	118.30
1	C	217	THR	N-CA-C	7.43	131.06	111.00
1	D	217	THR	N-CA-C	7.43	131.05	111.00
1	A	217	THR	N-CA-C	7.42	131.05	111.00
1	B	217	THR	N-CA-C	7.42	131.04	111.00
1	B	303	ARG	NE-CZ-NH1	-7.42	116.59	120.30
1	A	303	ARG	NE-CZ-NH1	-7.41	116.59	120.30
1	D	303	ARG	NE-CZ-NH1	-7.39	116.60	120.30
1	C	303	ARG	NE-CZ-NH1	-7.34	116.63	120.30
1	D	244	GLU	CA-CB-CG	-7.33	97.27	113.40
1	A	244	GLU	CA-CB-CG	-7.33	97.28	113.40
1	C	244	GLU	CA-CB-CG	-7.33	97.28	113.40
1	A	168	GLU	CG-CD-OE2	7.32	132.94	118.30
1	B	168	GLU	CG-CD-OE2	7.31	132.92	118.30
1	C	168	GLU	CG-CD-OE2	7.31	132.92	118.30
1	B	244	GLU	CA-CB-CG	-7.31	97.32	113.40
1	D	168	GLU	CG-CD-OE2	7.31	132.92	118.30
1	B	211	ASP	CB-CG-OD2	7.31	124.88	118.30
1	A	68	SER	CA-CB-OG	7.30	130.92	111.20
1	D	68	SER	CA-CB-OG	7.30	130.92	111.20
1	A	211	ASP	CB-CG-OD2	7.30	124.87	118.30
1	C	68	SER	CA-CB-OG	7.30	130.90	111.20
1	B	68	SER	CA-CB-OG	7.29	130.89	111.20
1	B	55	TRP	C-N-CA	7.28	139.90	121.70
1	D	211	ASP	CB-CG-OD2	7.28	124.85	118.30
1	C	55	TRP	C-N-CA	7.28	139.90	121.70
1	B	208	ARG	CD-NE-CZ	7.28	133.79	123.60
1	A	55	TRP	C-N-CA	7.27	139.88	121.70
1	A	208	ARG	CD-NE-CZ	7.27	133.78	123.60
1	C	208	ARG	CD-NE-CZ	7.27	133.78	123.60
1	D	55	TRP	C-N-CA	7.27	139.88	121.70
1	C	211	ASP	CB-CG-OD2	7.26	124.84	118.30
1	D	208	ARG	CD-NE-CZ	7.24	133.73	123.60
1	B	9	GLU	OE1-CD-OE2	7.21	131.95	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	370	GLN	CA-CB-CG	-7.21	97.54	113.40
1	C	370	GLN	CA-CB-CG	-7.20	97.56	113.40
1	B	370	GLN	CA-CB-CG	-7.20	97.57	113.40
1	D	370	GLN	CA-CB-CG	-7.20	97.57	113.40
1	B	390	ARG	NE-CZ-NH1	7.19	123.89	120.30
1	A	9	GLU	OE1-CD-OE2	7.17	131.91	123.30
1	D	338	GLU	O-C-N	7.17	134.16	122.70
1	C	9	GLU	OE1-CD-OE2	7.16	131.89	123.30
1	A	338	GLU	O-C-N	7.15	134.14	122.70
1	C	207	TYR	CB-CG-CD1	7.15	125.29	121.00
1	C	338	GLU	O-C-N	7.15	134.14	122.70
1	B	338	GLU	O-C-N	7.13	134.11	122.70
1	C	411	GLU	OE1-CD-OE2	-7.13	114.75	123.30
1	A	244	GLU	CG-CD-OE2	-7.13	104.05	118.30
1	C	244	GLU	CG-CD-OE2	-7.13	104.05	118.30
1	D	244	GLU	CG-CD-OE2	-7.12	104.06	118.30
1	B	207	TYR	CB-CG-CD1	7.12	125.27	121.00
1	B	244	GLU	CG-CD-OE2	-7.12	104.07	118.30
1	A	207	TYR	CB-CG-CD1	7.12	125.27	121.00
1	D	9	GLU	OE1-CD-OE2	7.11	131.83	123.30
1	A	390	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	A	411	GLU	OE1-CD-OE2	-7.10	114.78	123.30
1	B	411	GLU	OE1-CD-OE2	-7.09	114.79	123.30
1	D	411	GLU	OE1-CD-OE2	-7.09	114.79	123.30
1	C	390	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	C	202	ARG	CG-CD-NE	7.07	126.65	111.80
1	A	202	ARG	CG-CD-NE	7.07	126.65	111.80
1	B	202	ARG	CG-CD-NE	7.06	126.63	111.80
1	D	207	TYR	CB-CG-CD1	7.06	125.24	121.00
1	D	390	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	D	202	ARG	CG-CD-NE	7.05	126.62	111.80
1	C	82	TYR	CB-CG-CD1	-7.03	116.78	121.00
1	B	58	LEU	N-CA-C	7.03	129.97	111.00
1	A	58	LEU	N-CA-C	7.02	129.97	111.00
1	C	58	LEU	N-CA-C	7.02	129.96	111.00
1	D	58	LEU	N-CA-C	7.02	129.95	111.00
1	B	175	TYR	CB-CG-CD1	6.99	125.20	121.00
1	D	130	LEU	O-C-N	-6.99	111.52	122.70
1	A	82	TYR	CB-CG-CD1	-6.99	116.81	121.00
1	A	231	VAL	CA-CB-CG1	-6.95	100.47	110.90
1	B	130	LEU	O-C-N	-6.95	111.58	122.70
1	B	231	VAL	CA-CB-CG1	-6.95	100.47	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	231	VAL	CA-CB-CG1	-6.95	100.47	110.90
1	D	231	VAL	CA-CB-CG1	-6.95	100.47	110.90
1	C	130	LEU	O-C-N	-6.95	111.58	122.70
1	A	129	TYR	CB-CG-CD1	-6.95	116.83	121.00
1	A	130	LEU	O-C-N	-6.95	111.59	122.70
1	C	129	TYR	CB-CG-CD1	-6.94	116.84	121.00
1	B	129	TYR	CB-CG-CD1	-6.93	116.84	121.00
1	A	175	TYR	CB-CG-CD1	6.93	125.16	121.00
1	D	80	GLU	CG-CD-OE2	-6.92	104.45	118.30
1	D	82	TYR	CB-CG-CD1	-6.92	116.85	121.00
1	B	82	TYR	CB-CG-CD1	-6.92	116.85	121.00
1	D	175	TYR	CB-CG-CD1	6.92	125.15	121.00
1	C	80	GLU	CG-CD-OE2	-6.91	104.48	118.30
1	D	129	TYR	CB-CG-CD1	-6.91	116.86	121.00
1	A	80	GLU	CG-CD-OE2	-6.90	104.50	118.30
1	B	80	GLU	CG-CD-OE2	-6.90	104.50	118.30
1	C	12	LEU	CB-CG-CD2	6.87	122.68	111.00
1	C	366	ASP	O-C-N	6.87	133.69	122.70
1	D	327	LYS	CD-CE-NZ	6.86	127.49	111.70
1	A	327	LYS	CD-CE-NZ	6.86	127.48	111.70
1	B	327	LYS	CD-CE-NZ	6.86	127.47	111.70
1	C	327	LYS	CD-CE-NZ	6.85	127.47	111.70
1	B	366	ASP	O-C-N	6.85	133.66	122.70
1	C	175	TYR	CB-CG-CD1	6.85	125.11	121.00
1	A	12	LEU	CB-CG-CD2	6.85	122.64	111.00
1	A	250	MET	CG-SD-CE	-6.84	89.25	100.20
1	B	12	LEU	CB-CG-CD2	6.84	122.63	111.00
1	D	12	LEU	CB-CG-CD2	6.84	122.63	111.00
1	A	366	ASP	O-C-N	6.84	133.64	122.70
1	D	250	MET	CG-SD-CE	-6.84	89.26	100.20
1	B	250	MET	CG-SD-CE	-6.83	89.27	100.20
1	C	250	MET	CG-SD-CE	-6.83	89.27	100.20
1	C	21	PRO	CA-N-CD	-6.83	101.94	111.50
1	A	21	PRO	CA-N-CD	-6.81	101.97	111.50
1	D	366	ASP	O-C-N	6.80	133.58	122.70
1	D	21	PRO	CA-N-CD	-6.80	101.98	111.50
1	B	21	PRO	CA-N-CD	-6.80	101.98	111.50
1	B	129	TYR	CB-CG-CD2	6.78	125.06	121.00
1	D	234	MET	CG-SD-CE	-6.77	89.36	100.20
1	A	234	MET	CG-SD-CE	-6.77	89.37	100.20
1	B	234	MET	CG-SD-CE	-6.76	89.38	100.20
1	C	234	MET	CG-SD-CE	-6.76	89.38	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	187	ASP	CB-CA-C	-6.76	96.88	110.40
1	B	187	ASP	CB-CA-C	-6.76	96.88	110.40
1	D	187	ASP	CB-CA-C	-6.75	96.89	110.40
1	A	187	ASP	CB-CA-C	-6.75	96.89	110.40
1	A	129	TYR	CB-CG-CD2	6.74	125.05	121.00
1	B	75	LEU	CB-CG-CD2	6.74	122.45	111.00
1	D	129	TYR	CB-CG-CD2	6.73	125.04	121.00
1	C	76	GLU	CG-CD-OE2	6.73	131.77	118.30
1	C	129	TYR	CB-CG-CD2	6.73	125.04	121.00
1	D	75	LEU	CB-CG-CD2	6.72	122.43	111.00
1	A	75	LEU	CB-CG-CD2	6.72	122.42	111.00
1	A	76	GLU	CG-CD-OE2	6.71	131.72	118.30
1	B	91	THR	CA-C-O	6.71	134.19	120.10
1	A	91	THR	CA-C-O	6.71	134.18	120.10
1	D	91	THR	CA-C-O	6.70	134.17	120.10
1	B	76	GLU	CG-CD-OE2	6.70	131.69	118.30
1	D	76	GLU	CG-CD-OE2	6.70	131.70	118.30
1	C	185	LEU	CB-CG-CD1	-6.70	99.62	111.00
1	C	75	LEU	CB-CG-CD2	6.69	122.37	111.00
1	A	185	LEU	CB-CG-CD1	-6.68	99.64	111.00
1	B	306	GLY	N-CA-C	6.68	129.81	113.10
1	C	91	THR	CA-C-O	6.68	134.14	120.10
1	C	306	GLY	N-CA-C	6.68	129.81	113.10
1	A	306	GLY	N-CA-C	6.68	129.80	113.10
1	D	185	LEU	CB-CG-CD1	-6.68	99.64	111.00
1	D	306	GLY	N-CA-C	6.68	129.79	113.10
1	B	185	LEU	CB-CG-CD1	-6.67	99.66	111.00
1	B	66	LYS	CB-CG-CD	6.66	128.91	111.60
1	A	66	LYS	CB-CG-CD	6.64	128.87	111.60
1	B	188	ASP	CB-CG-OD1	-6.64	112.32	118.30
1	D	66	LYS	CB-CG-CD	6.64	128.88	111.60
1	C	66	LYS	CB-CG-CD	6.64	128.86	111.60
1	D	188	ASP	CB-CG-OD1	-6.64	112.33	118.30
1	A	303	ARG	NE-CZ-NH2	6.62	123.61	120.30
1	D	303	ARG	NE-CZ-NH2	6.62	123.61	120.30
1	A	188	ASP	CB-CG-OD1	-6.61	112.36	118.30
1	C	152	ARG	NE-CZ-NH2	-6.61	117.00	120.30
1	C	188	ASP	CB-CG-OD1	-6.61	112.36	118.30
1	C	303	ARG	NE-CZ-NH2	6.59	123.60	120.30
1	D	387	LYS	CD-CE-NZ	6.59	126.86	111.70
1	A	387	LYS	CD-CE-NZ	6.58	126.84	111.70
1	B	355	LEU	CB-CG-CD1	-6.58	99.82	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	387	LYS	CD-CE-NZ	6.58	126.83	111.70
1	B	206	LEU	CB-CG-CD2	-6.57	99.83	111.00
1	B	387	LYS	CD-CE-NZ	6.57	126.81	111.70
1	B	95	GLU	CG-CD-OE2	-6.57	105.16	118.30
1	C	206	LEU	CB-CG-CD2	-6.57	99.83	111.00
1	D	355	LEU	CB-CG-CD1	-6.57	99.84	111.00
1	C	75	LEU	N-CA-C	-6.56	93.28	111.00
1	A	75	LEU	N-CA-C	-6.56	93.28	111.00
1	A	355	LEU	CB-CG-CD1	-6.56	99.84	111.00
1	B	303	ARG	NE-CZ-NH2	6.56	123.58	120.30
1	D	75	LEU	N-CA-C	-6.56	93.28	111.00
1	B	152	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	B	75	LEU	N-CA-C	-6.55	93.31	111.00
1	C	355	LEU	CB-CG-CD1	-6.55	99.86	111.00
1	A	95	GLU	CG-CD-OE2	-6.55	105.20	118.30
1	A	206	LEU	CB-CG-CD2	-6.55	99.87	111.00
1	A	152	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	D	95	GLU	CG-CD-OE2	-6.53	105.23	118.30
1	C	95	GLU	CG-CD-OE2	-6.53	105.24	118.30
1	D	206	LEU	CB-CG-CD2	-6.53	99.89	111.00
1	D	287	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	D	151	ASP	N-CA-C	6.51	128.58	111.00
1	D	152	ARG	NE-CZ-NH2	-6.51	117.04	120.30
1	A	151	ASP	N-CA-C	6.51	128.57	111.00
1	A	287	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	C	287	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	C	309	GLN	CA-CB-CG	-6.50	99.10	113.40
1	C	151	ASP	N-CA-C	6.50	128.55	111.00
1	D	309	GLN	CA-CB-CG	-6.50	99.11	113.40
1	B	151	ASP	N-CA-C	6.49	128.53	111.00
1	B	287	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	A	309	GLN	CA-CB-CG	-6.49	99.13	113.40
1	C	338	GLU	CA-C-N	-6.48	102.94	117.20
1	B	309	GLN	CA-CB-CG	-6.48	99.15	113.40
1	A	338	GLU	CA-C-N	-6.47	102.96	117.20
1	D	338	GLU	CA-C-N	-6.47	102.97	117.20
1	C	177	LEU	CB-CG-CD2	-6.46	100.03	111.00
1	D	177	LEU	CB-CG-CD2	-6.46	100.02	111.00
1	B	338	GLU	CA-C-N	-6.45	103.01	117.20
1	A	177	LEU	CB-CG-CD2	-6.45	100.04	111.00
1	B	175	TYR	CZ-CE2-CD2	6.45	125.60	119.80
1	A	126	PRO	CA-C-N	6.44	131.38	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	175	TYR	CZ-CE2-CD2	6.44	125.60	119.80
1	D	126	PRO	CA-C-N	6.44	131.37	117.20
1	B	126	PRO	CA-C-N	6.44	131.37	117.20
1	D	175	TYR	CZ-CE2-CD2	6.44	125.60	119.80
1	D	252	ASP	CB-CG-OD1	-6.44	112.51	118.30
1	C	126	PRO	CA-C-N	6.43	131.36	117.20
1	D	422	SER	CB-CA-C	-6.43	97.88	110.10
1	A	422	SER	CB-CA-C	-6.43	97.89	110.10
1	B	177	LEU	CB-CG-CD2	-6.42	100.08	111.00
1	D	158	VAL	N-CA-C	-6.42	93.67	111.00
1	A	175	TYR	CZ-CE2-CD2	6.42	125.57	119.80
1	B	422	SER	CB-CA-C	-6.41	97.91	110.10
1	C	422	SER	CB-CA-C	-6.41	97.92	110.10
1	A	158	VAL	N-CA-C	-6.41	93.70	111.00
1	C	252	ASP	CB-CG-OD1	-6.41	112.53	118.30
1	B	158	VAL	N-CA-C	-6.41	93.70	111.00
1	B	81	GLY	N-CA-C	-6.40	97.09	113.10
1	C	147	MET	C-N-CA	-6.40	108.85	122.30
1	B	44	GLY	N-CA-C	-6.40	97.10	113.10
1	C	158	VAL	N-CA-C	-6.40	93.72	111.00
1	D	81	GLY	N-CA-C	-6.39	97.11	113.10
1	D	44	GLY	N-CA-C	-6.39	97.12	113.10
1	A	44	GLY	N-CA-C	-6.39	97.12	113.10
1	A	81	GLY	N-CA-C	-6.39	97.12	113.10
1	A	147	MET	C-N-CA	-6.39	108.88	122.30
1	A	252	ASP	CB-CG-OD1	-6.39	112.55	118.30
1	B	147	MET	C-N-CA	-6.39	108.89	122.30
1	C	81	GLY	N-CA-C	-6.39	97.13	113.10
1	D	147	MET	C-N-CA	-6.39	108.89	122.30
1	C	44	GLY	N-CA-C	-6.38	97.15	113.10
1	B	252	ASP	CB-CG-OD1	-6.37	112.57	118.30
1	D	21	PRO	O-C-N	6.37	134.03	123.20
1	A	21	PRO	O-C-N	6.36	134.01	123.20
1	C	21	PRO	O-C-N	6.35	133.99	123.20
1	B	21	PRO	O-C-N	6.33	133.97	123.20
1	C	223	TYR	CA-CB-CG	6.33	125.42	113.40
1	A	223	TYR	CA-CB-CG	6.32	125.42	113.40
1	A	330	ASN	N-CA-C	6.32	128.07	111.00
1	B	223	TYR	CA-CB-CG	6.32	125.41	113.40
1	B	330	ASN	N-CA-C	6.32	128.05	111.00
1	C	330	ASN	N-CA-C	6.31	128.04	111.00
1	D	330	ASN	N-CA-C	6.31	128.04	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	223	TYR	CA-CB-CG	6.31	125.39	113.40
1	A	278	HIS	CA-C-N	-6.27	103.41	117.20
1	B	278	HIS	CA-C-N	-6.27	103.41	117.20
1	C	278	HIS	CA-C-N	-6.26	103.43	117.20
1	D	278	HIS	CA-C-N	-6.26	103.44	117.20
1	B	300	LYS	CG-CD-CE	6.25	130.64	111.90
1	D	300	LYS	CG-CD-CE	6.24	130.61	111.90
1	A	300	LYS	CG-CD-CE	6.23	130.59	111.90
1	C	300	LYS	CG-CD-CE	6.23	130.58	111.90
1	B	49	GLU	CA-CB-CG	-6.22	99.71	113.40
1	B	167	VAL	CA-CB-CG1	-6.22	101.56	110.90
1	D	416	LEU	CB-CG-CD1	-6.22	100.43	111.00
1	A	49	GLU	CA-CB-CG	-6.22	99.72	113.40
1	D	49	GLU	CA-CB-CG	-6.22	99.72	113.40
1	A	167	VAL	CA-CB-CG1	-6.21	101.58	110.90
1	D	167	VAL	CA-CB-CG1	-6.21	101.58	110.90
1	B	416	LEU	CB-CG-CD1	-6.21	100.44	111.00
1	A	416	LEU	CB-CG-CD1	-6.21	100.44	111.00
1	C	49	GLU	CA-CB-CG	-6.20	99.75	113.40
1	C	167	VAL	CA-CB-CG1	-6.20	101.60	110.90
1	C	416	LEU	CB-CG-CD1	-6.19	100.47	111.00
1	D	251	ILE	CG1-CB-CG2	-6.19	97.78	111.40
1	A	251	ILE	CG1-CB-CG2	-6.18	97.79	111.40
1	B	251	ILE	CG1-CB-CG2	-6.18	97.80	111.40
1	A	175	TYR	CG-CD2-CE2	6.18	126.25	121.30
1	C	251	ILE	CG1-CB-CG2	-6.18	97.80	111.40
1	C	175	TYR	CG-CD2-CE2	6.17	126.23	121.30
1	B	175	TYR	CG-CD2-CE2	6.16	126.23	121.30
1	C	69	MET	CG-SD-CE	6.15	110.04	100.20
1	D	69	MET	CG-SD-CE	6.14	110.02	100.20
1	A	69	MET	CG-SD-CE	6.14	110.02	100.20
1	B	69	MET	CG-SD-CE	6.13	110.01	100.20
1	C	367	LEU	CB-CA-C	-6.13	98.55	110.20
1	D	367	LEU	CB-CA-C	-6.13	98.55	110.20
1	C	196	PHE	N-CA-C	6.13	127.54	111.00
1	A	367	LEU	CB-CA-C	-6.12	98.56	110.20
1	B	194	PHE	C-N-CD	6.12	141.26	128.40
1	D	175	TYR	CG-CD2-CE2	6.12	126.20	121.30
1	D	255	VAL	CA-C-N	-6.12	103.73	117.20
1	A	255	VAL	CA-C-N	-6.12	103.73	117.20
1	A	196	PHE	N-CA-C	6.12	127.52	111.00
1	A	336	LYS	CG-CD-CE	6.12	130.25	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	336	LYS	CG-CD-CE	6.12	130.25	111.90
1	A	194	PHE	C-N-CD	6.12	141.24	128.40
1	D	196	PHE	N-CA-C	6.12	127.51	111.00
1	B	127	TYR	CB-CA-C	-6.11	98.17	110.40
1	C	127	TYR	CB-CA-C	-6.11	98.17	110.40
1	B	336	LYS	CG-CD-CE	6.11	130.24	111.90
1	C	194	PHE	C-N-CD	6.11	141.22	128.40
1	C	255	VAL	CA-C-N	-6.11	103.76	117.20
1	C	336	LYS	CG-CD-CE	6.11	130.22	111.90
1	A	127	TYR	CB-CA-C	-6.11	98.19	110.40
1	B	196	PHE	N-CA-C	6.11	127.48	111.00
1	D	127	TYR	CB-CA-C	-6.11	98.19	110.40
1	B	328	ARG	CD-NE-CZ	6.10	132.14	123.60
1	B	367	LEU	CB-CA-C	-6.10	98.61	110.20
1	C	186	LYS	CD-CE-NZ	6.10	125.72	111.70
1	D	20	GLU	N-CA-CB	6.09	121.57	110.60
1	B	255	VAL	CA-C-N	-6.09	103.80	117.20
1	D	194	PHE	C-N-CD	6.09	141.19	128.40
1	B	75	LEU	CB-CG-CD1	-6.09	100.65	111.00
1	A	20	GLU	N-CA-CB	6.08	121.55	110.60
1	D	328	ARG	CD-NE-CZ	6.08	132.12	123.60
1	A	328	ARG	CD-NE-CZ	6.08	132.11	123.60
1	B	186	LYS	CD-CE-NZ	6.08	125.69	111.70
1	A	186	LYS	CD-CE-NZ	6.08	125.68	111.70
1	B	20	GLU	N-CA-CB	6.08	121.54	110.60
1	C	20	GLU	N-CA-CB	6.07	121.52	110.60
1	D	75	LEU	CB-CG-CD1	-6.07	100.68	111.00
1	C	393	ILE	CG1-CB-CG2	-6.06	98.06	111.40
1	D	186	LYS	CD-CE-NZ	6.06	125.64	111.70
1	C	328	ARG	CD-NE-CZ	6.06	132.09	123.60
1	A	75	LEU	CB-CG-CD1	-6.06	100.70	111.00
1	C	266	GLU	CB-CG-CD	-6.06	97.84	114.20
1	A	266	GLU	CB-CG-CD	-6.06	97.85	114.20
1	B	266	GLU	CB-CG-CD	-6.05	97.86	114.20
1	A	393	ILE	CG1-CB-CG2	-6.05	98.08	111.40
1	D	266	GLU	CB-CG-CD	-6.05	97.86	114.20
1	D	393	ILE	CG1-CB-CG2	-6.05	98.09	111.40
1	B	393	ILE	CG1-CB-CG2	-6.05	98.10	111.40
1	C	75	LEU	CB-CG-CD1	-6.05	100.72	111.00
1	A	423	LYS	CA-CB-CG	6.04	126.68	113.40
1	B	423	LYS	CA-CB-CG	6.04	126.69	113.40
1	D	423	LYS	CA-CB-CG	6.04	126.68	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	423	LYS	CA-CB-CG	6.03	126.67	113.40
1	D	176	GLU	CG-CD-OE2	-6.02	106.25	118.30
1	B	176	GLU	CG-CD-OE2	-6.01	106.27	118.30
1	C	176	GLU	CG-CD-OE2	-6.01	106.28	118.30
1	A	176	GLU	CG-CD-OE2	-6.01	106.28	118.30
1	D	207	TYR	CZ-CE2-CD2	6.00	125.20	119.80
1	D	340	ILE	CG1-CB-CG2	5.99	124.58	111.40
1	B	340	ILE	CG1-CB-CG2	5.99	124.57	111.40
1	C	340	ILE	CG1-CB-CG2	5.99	124.57	111.40
1	A	207	TYR	CZ-CE2-CD2	5.98	125.19	119.80
1	A	340	ILE	CG1-CB-CG2	5.98	124.56	111.40
1	B	226	ASN	CA-C-N	-5.98	104.04	117.20
1	C	207	TYR	CZ-CE2-CD2	5.97	125.18	119.80
1	B	267	VAL	CG1-CB-CG2	-5.97	101.34	110.90
1	D	267	VAL	CG1-CB-CG2	-5.97	101.35	110.90
1	D	272	GLY	CA-C-N	-5.97	104.08	117.20
1	A	226	ASN	CA-C-N	-5.96	104.08	117.20
1	B	207	TYR	CZ-CE2-CD2	5.96	125.17	119.80
1	A	272	GLY	CA-C-N	-5.96	104.09	117.20
1	B	105	VAL	N-CA-C	5.96	127.08	111.00
1	C	9	GLU	CG-CD-OE1	-5.96	106.39	118.30
1	C	105	VAL	N-CA-C	5.96	127.08	111.00
1	A	105	VAL	N-CA-C	5.96	127.08	111.00
1	A	267	VAL	CG1-CB-CG2	-5.96	101.37	110.90
1	B	9	GLU	CG-CD-OE1	-5.95	106.39	118.30
1	C	267	VAL	CG1-CB-CG2	-5.95	101.38	110.90
1	C	272	GLY	CA-C-N	-5.95	104.11	117.20
1	D	226	ASN	CA-C-N	-5.95	104.11	117.20
1	D	105	VAL	N-CA-C	5.95	127.06	111.00
1	A	9	GLU	CG-CD-OE1	-5.95	106.41	118.30
1	C	226	ASN	CA-C-N	-5.94	104.13	117.20
1	B	272	GLY	CA-C-N	-5.94	104.14	117.20
1	B	214	GLU	CG-CD-OE1	5.93	130.17	118.30
1	D	183	ASP	CB-CG-OD1	-5.93	112.96	118.30
1	B	259	SER	CA-C-N	-5.93	104.16	117.20
1	D	9	GLU	CG-CD-OE1	-5.93	106.44	118.30
1	A	259	SER	CA-C-N	-5.92	104.17	117.20
1	C	259	SER	CA-C-N	-5.92	104.17	117.20
1	B	183	ASP	CB-CG-OD1	-5.92	112.97	118.30
1	D	259	SER	CA-C-N	-5.92	104.19	117.20
1	C	214	GLU	CG-CD-OE1	5.91	130.13	118.30
1	A	214	GLU	CG-CD-OE1	5.91	130.12	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	260	ALA	N-CA-CB	-5.91	101.83	110.10
1	D	214	GLU	CG-CD-OE1	5.90	130.09	118.30
1	C	183	ASP	CB-CG-OD1	-5.89	113.00	118.30
1	B	260	ALA	N-CA-CB	-5.89	101.86	110.10
1	B	269	GLU	O-C-N	5.89	132.12	122.70
1	A	183	ASP	CB-CG-OD1	-5.88	113.00	118.30
1	C	260	ALA	N-CA-CB	-5.88	101.86	110.10
1	C	269	GLU	O-C-N	5.88	132.12	122.70
1	A	269	GLU	O-C-N	5.88	132.10	122.70
1	A	260	ALA	N-CA-CB	-5.87	101.88	110.10
1	C	21	PRO	N-CD-CG	5.87	112.00	103.20
1	A	168	GLU	OE1-CD-OE2	-5.86	116.27	123.30
1	D	129	TYR	CE1-CZ-OH	-5.86	104.29	120.10
1	A	214	GLU	CA-CB-CG	-5.85	100.52	113.40
1	C	214	GLU	CA-CB-CG	-5.85	100.52	113.40
1	C	330	ASN	CB-CA-C	-5.85	98.70	110.40
1	B	214	GLU	CA-CB-CG	-5.85	100.54	113.40
1	D	214	GLU	CA-CB-CG	-5.85	100.53	113.40
1	D	269	GLU	O-C-N	5.85	132.06	122.70
1	B	129	TYR	CE1-CZ-OH	-5.85	104.32	120.10
1	A	21	PRO	N-CD-CG	5.84	111.97	103.20
1	B	330	ASN	CB-CA-C	-5.84	98.71	110.40
1	D	330	ASN	CB-CA-C	-5.84	98.71	110.40
1	A	129	TYR	CE1-CZ-OH	-5.84	104.32	120.10
1	B	25	GLU	CA-C-N	-5.84	104.35	117.20
1	C	168	GLU	OE1-CD-OE2	-5.84	116.29	123.30
1	A	330	ASN	CB-CA-C	-5.84	98.72	110.40
1	B	168	GLU	OE1-CD-OE2	-5.84	116.29	123.30
1	C	129	TYR	CE1-CZ-OH	-5.84	104.34	120.10
1	C	298	LEU	CA-CB-CG	5.84	128.72	115.30
1	D	25	GLU	CA-C-N	-5.84	104.36	117.20
1	D	168	GLU	OE1-CD-OE2	-5.83	116.30	123.30
1	A	298	LEU	CA-CB-CG	5.83	128.70	115.30
1	A	25	GLU	CA-C-N	-5.82	104.39	117.20
1	D	298	LEU	CA-CB-CG	5.82	128.69	115.30
1	D	21	PRO	N-CD-CG	5.82	111.93	103.20
1	B	239	GLU	OE1-CD-OE2	5.82	130.28	123.30
1	B	298	LEU	CA-CB-CG	5.82	128.68	115.30
1	C	239	GLU	OE1-CD-OE2	5.82	130.28	123.30
1	C	25	GLU	CA-C-N	-5.81	104.41	117.20
1	C	401	ASP	CB-CG-OD1	-5.81	113.07	118.30
1	B	21	PRO	N-CD-CG	5.81	111.92	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	226	ASN	CA-C-O	5.81	132.31	120.10
1	C	226	ASN	CA-C-O	5.81	132.29	120.10
1	A	239	GLU	OE1-CD-OE2	5.80	130.27	123.30
1	A	226	ASN	CA-C-O	5.80	132.28	120.10
1	D	141	GLN	CA-CB-CG	-5.80	100.64	113.40
1	C	141	GLN	CA-CB-CG	-5.79	100.65	113.40
1	A	141	GLN	CA-CB-CG	-5.79	100.66	113.40
1	A	401	ASP	CB-CG-OD1	-5.79	113.09	118.30
1	D	226	ASN	CA-C-O	5.78	132.24	120.10
1	D	239	GLU	OE1-CD-OE2	5.78	130.24	123.30
1	B	141	GLN	CA-CB-CG	-5.78	100.69	113.40
1	B	401	ASP	CB-CG-OD1	-5.78	113.10	118.30
1	D	401	ASP	CB-CG-OD1	-5.77	113.10	118.30
1	B	363	PHE	N-CA-C	5.77	126.57	111.00
1	C	363	PHE	N-CA-C	5.76	126.54	111.00
1	D	158	VAL	CB-CA-C	-5.76	100.46	111.40
1	D	363	PHE	N-CA-C	5.76	126.55	111.00
1	B	421	LEU	CA-CB-CG	5.75	128.53	115.30
1	C	158	VAL	CB-CA-C	-5.75	100.47	111.40
1	A	363	PHE	N-CA-C	5.75	126.53	111.00
1	C	280	ALA	C-N-CA	5.75	136.07	121.70
1	A	158	VAL	CB-CA-C	-5.74	100.49	111.40
1	A	421	LEU	CA-CB-CG	5.74	128.51	115.30
1	C	175	TYR	CE1-CZ-CE2	-5.74	110.61	119.80
1	B	298	LEU	CB-CA-C	5.74	121.11	110.20
1	D	175	TYR	CE1-CZ-CE2	-5.74	110.62	119.80
1	C	421	LEU	CA-CB-CG	5.74	128.50	115.30
1	D	421	LEU	CA-CB-CG	5.73	128.48	115.30
1	A	280	ALA	C-N-CA	5.73	136.03	121.70
1	B	280	ALA	C-N-CA	5.73	136.03	121.70
1	D	56	THR	C-N-CA	5.73	136.03	121.70
1	D	280	ALA	C-N-CA	5.73	136.03	121.70
1	D	298	LEU	CB-CA-C	5.73	121.09	110.20
1	A	175	TYR	CE1-CZ-CE2	-5.73	110.64	119.80
1	B	175	TYR	CE1-CZ-CE2	-5.72	110.64	119.80
1	C	76	GLU	CG-CD-OE1	-5.72	106.85	118.30
1	A	298	LEU	CB-CA-C	5.72	121.07	110.20
1	D	76	GLU	CG-CD-OE1	-5.72	106.86	118.30
1	A	76	GLU	CG-CD-OE1	-5.72	106.86	118.30
1	B	38	SER	CB-CA-C	-5.72	99.24	110.10
1	B	56	THR	C-N-CA	5.72	135.99	121.70
1	A	56	THR	C-N-CA	5.71	135.99	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	76	GLU	CG-CD-OE1	-5.71	106.87	118.30
1	B	158	VAL	CB-CA-C	-5.71	100.54	111.40
1	B	177	LEU	CB-CG-CD1	5.71	120.71	111.00
1	C	298	LEU	CB-CA-C	5.71	121.06	110.20
1	B	131	ARG	NH1-CZ-NH2	5.71	125.68	119.40
1	C	131	ARG	NH1-CZ-NH2	5.71	125.68	119.40
1	C	38	SER	CB-CA-C	-5.71	99.26	110.10
1	C	56	THR	C-N-CA	5.71	135.97	121.70
1	A	131	ARG	NH1-CZ-NH2	5.70	125.67	119.40
1	D	289	PRO	O-C-N	5.70	131.82	122.70
1	A	38	SER	CB-CA-C	-5.70	99.27	110.10
1	A	220	THR	OG1-CB-CG2	5.70	123.10	110.00
1	C	177	LEU	CB-CG-CD1	5.70	120.69	111.00
1	C	220	THR	OG1-CB-CG2	5.70	123.10	110.00
1	D	38	SER	CB-CA-C	-5.69	99.28	110.10
1	B	17	LEU	CA-C-N	-5.69	104.67	117.20
1	B	154	LEU	CA-CB-CG	-5.69	102.21	115.30
1	A	17	LEU	CA-C-N	-5.69	104.68	117.20
1	A	289	PRO	O-C-N	5.69	131.80	122.70
1	C	17	LEU	CA-C-N	-5.69	104.68	117.20
1	A	177	LEU	CB-CG-CD1	5.69	120.67	111.00
1	B	220	THR	OG1-CB-CG2	5.68	123.08	110.00
1	D	154	LEU	CA-CB-CG	-5.68	102.23	115.30
1	A	154	LEU	CA-CB-CG	-5.68	102.23	115.30
1	B	238	ALA	CB-CA-C	5.68	118.62	110.10
1	D	17	LEU	CA-C-N	-5.68	104.70	117.20
1	C	154	LEU	CA-CB-CG	-5.68	102.23	115.30
1	D	131	ARG	NH1-CZ-NH2	5.68	125.65	119.40
1	D	220	THR	OG1-CB-CG2	5.68	123.06	110.00
1	C	382	PRO	C-N-CA	-5.68	107.51	121.70
1	D	177	LEU	CB-CG-CD1	5.68	120.65	111.00
1	A	382	PRO	C-N-CA	-5.67	107.52	121.70
1	B	289	PRO	O-C-N	5.67	131.77	122.70
1	B	382	PRO	C-N-CA	-5.67	107.53	121.70
1	D	382	PRO	C-N-CA	-5.67	107.53	121.70
1	C	238	ALA	CB-CA-C	5.66	118.59	110.10
1	B	367	LEU	CB-CG-CD2	5.66	120.62	111.00
1	C	289	PRO	O-C-N	5.66	131.76	122.70
1	A	238	ALA	CB-CA-C	5.66	118.59	110.10
1	A	367	LEU	CB-CG-CD2	5.66	120.62	111.00
1	D	367	LEU	CB-CG-CD2	5.65	120.60	111.00
1	C	367	LEU	CB-CG-CD2	5.64	120.59	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	112	MET	CG-SD-CE	5.64	109.22	100.20
1	A	112	MET	CG-SD-CE	5.63	109.21	100.20
1	D	238	ALA	CB-CA-C	5.63	118.54	110.10
1	C	112	MET	CG-SD-CE	5.62	109.20	100.20
1	D	163	MET	N-CA-CB	5.61	120.71	110.60
1	B	112	MET	CG-SD-CE	5.61	109.17	100.20
1	B	145	GLU	OE1-CD-OE2	-5.60	116.58	123.30
1	B	66	LYS	CD-CE-NZ	5.59	124.56	111.70
1	C	247	GLN	N-CA-CB	5.59	120.66	110.60
1	D	150	LYS	C-N-CA	-5.59	107.73	121.70
1	B	150	LYS	C-N-CA	-5.59	107.73	121.70
1	C	150	LYS	C-N-CA	-5.59	107.73	121.70
1	C	163	MET	N-CA-CB	5.59	120.65	110.60
1	A	150	LYS	C-N-CA	-5.58	107.74	121.70
1	A	163	MET	N-CA-CB	5.58	120.65	110.60
1	B	424	ALA	N-CA-CB	5.58	117.92	110.10
1	A	66	LYS	CD-CE-NZ	5.57	124.52	111.70
1	A	145	GLU	OE1-CD-OE2	-5.57	116.61	123.30
1	C	66	LYS	CD-CE-NZ	5.57	124.52	111.70
1	C	424	ALA	N-CA-CB	5.57	117.90	110.10
1	B	247	GLN	N-CA-CB	5.57	120.63	110.60
1	C	289	PRO	CA-N-CD	-5.57	103.70	111.50
1	B	163	MET	N-CA-CB	5.57	120.63	110.60
1	D	424	ALA	N-CA-CB	5.57	117.90	110.10
1	A	247	GLN	N-CA-CB	5.57	120.62	110.60
1	D	247	GLN	N-CA-CB	5.57	120.62	110.60
1	A	424	ALA	N-CA-CB	5.56	117.89	110.10
1	C	145	GLU	OE1-CD-OE2	-5.56	116.62	123.30
1	D	145	GLU	OE1-CD-OE2	-5.56	116.63	123.30
1	A	289	PRO	CA-N-CD	-5.56	103.72	111.50
1	B	289	PRO	CA-N-CD	-5.56	103.72	111.50
1	D	66	LYS	CD-CE-NZ	5.55	124.47	111.70
1	A	189	GLU	N-CA-C	5.55	125.99	111.00
1	D	289	PRO	CA-N-CD	-5.55	103.74	111.50
1	D	189	GLU	N-CA-C	5.54	125.97	111.00
1	B	189	GLU	N-CA-C	5.54	125.96	111.00
1	C	189	GLU	N-CA-C	5.53	125.93	111.00
1	D	98	LEU	CB-CG-CD2	-5.52	101.61	111.00
1	A	98	LEU	CB-CG-CD2	-5.52	101.62	111.00
1	B	98	LEU	CB-CG-CD2	-5.52	101.62	111.00
1	C	98	LEU	CB-CG-CD2	-5.51	101.63	111.00
1	C	379	PRO	CA-N-CD	-5.50	103.80	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	119	ARG	NH1-CZ-NH2	5.50	125.44	119.40
1	B	214	GLU	CG-CD-OE2	-5.49	107.32	118.30
1	B	118	LEU	CB-CG-CD2	-5.49	101.67	111.00
1	A	119	ARG	NH1-CZ-NH2	5.49	125.44	119.40
1	B	204	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	C	314	THR	CA-C-N	-5.49	105.13	117.20
1	A	314	THR	CA-C-N	-5.49	105.13	117.20
1	D	176	GLU	CG-CD-OE1	5.49	129.27	118.30
1	D	119	ARG	NH1-CZ-NH2	5.48	125.43	119.40
1	A	118	LEU	CB-CG-CD2	-5.48	101.69	111.00
1	A	379	PRO	CA-N-CD	-5.48	103.83	111.50
1	A	176	GLU	CG-CD-OE1	5.48	129.25	118.30
1	C	214	GLU	CG-CD-OE2	-5.48	107.34	118.30
1	D	118	LEU	CB-CG-CD2	-5.48	101.69	111.00
1	D	379	PRO	CA-N-CD	-5.48	103.83	111.50
1	B	190	ASN	CA-C-N	-5.48	105.15	117.20
1	B	255	VAL	C-N-CA	5.47	135.38	121.70
1	A	214	GLU	CG-CD-OE2	-5.47	107.36	118.30
1	D	190	ASN	CA-C-N	-5.47	105.16	117.20
1	D	314	THR	CA-C-N	-5.47	105.16	117.20
1	C	118	LEU	CB-CG-CD2	-5.47	101.70	111.00
1	B	176	GLU	CG-CD-OE1	5.47	129.24	118.30
1	B	379	PRO	CA-N-CD	-5.47	103.84	111.50
1	A	190	ASN	CA-C-N	-5.47	105.17	117.20
1	B	314	THR	CA-C-N	-5.47	105.17	117.20
1	C	176	GLU	CG-CD-OE1	5.47	129.23	118.30
1	C	119	ARG	NH1-CZ-NH2	5.46	125.41	119.40
1	D	214	GLU	CG-CD-OE2	-5.46	107.38	118.30
1	C	190	ASN	CA-C-N	-5.46	105.19	117.20
1	C	255	VAL	C-N-CA	5.46	135.35	121.70
1	C	415	SER	CA-C-N	-5.46	105.20	117.20
1	A	204	ARG	NE-CZ-NH2	-5.45	117.57	120.30
1	A	255	VAL	C-N-CA	5.45	135.33	121.70
1	D	129	TYR	OH-CZ-CE2	5.45	134.82	120.10
1	A	216	GLU	CG-CD-OE2	5.45	129.20	118.30
1	C	155	THR	CA-CB-CG2	-5.45	104.77	112.40
1	D	255	VAL	C-N-CA	5.45	135.32	121.70
1	D	155	THR	CA-CB-CG2	-5.45	104.77	112.40
1	D	204	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	D	216	GLU	CG-CD-OE2	5.45	129.19	118.30
1	A	415	SER	CA-C-N	-5.44	105.23	117.20
1	B	155	THR	CA-CB-CG2	-5.44	104.78	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	155	THR	CA-CB-CG2	-5.44	104.78	112.40
1	A	279	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	C	216	GLU	CG-CD-OE2	5.44	129.18	118.30
1	C	281	MET	CB-CG-SD	5.44	128.72	112.40
1	D	415	SER	CA-C-N	-5.44	105.23	117.20
1	B	130	LEU	CB-CG-CD1	-5.44	101.76	111.00
1	B	216	GLU	CG-CD-OE2	5.44	129.17	118.30
1	B	415	SER	CA-C-N	-5.44	105.24	117.20
1	C	113	LYS	CB-CG-CD	5.44	125.74	111.60
1	D	130	LEU	CB-CG-CD1	-5.44	101.76	111.00
1	A	113	LYS	CB-CG-CD	5.43	125.73	111.60
1	B	281	MET	CB-CG-SD	5.43	128.70	112.40
1	D	281	MET	CB-CG-SD	5.43	128.70	112.40
1	A	129	TYR	OH-CZ-CE2	5.43	134.76	120.10
1	A	281	MET	CB-CG-SD	5.43	128.69	112.40
1	B	170	TYR	CB-CG-CD2	5.43	124.26	121.00
1	C	129	TYR	OH-CZ-CE2	5.43	134.76	120.10
1	D	113	LYS	CB-CG-CD	5.43	125.72	111.60
1	B	74	TYR	N-CA-C	-5.43	96.35	111.00
1	B	129	TYR	OH-CZ-CE2	5.43	134.75	120.10
1	C	204	ARG	NE-CZ-NH2	-5.43	117.59	120.30
1	C	170	TYR	CB-CG-CD2	5.42	124.25	121.00
1	B	257	GLY	C-N-CA	-5.42	108.14	121.70
1	A	257	GLY	C-N-CA	-5.42	108.15	121.70
1	D	257	GLY	C-N-CA	-5.42	108.15	121.70
1	D	279	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	B	113	LYS	CB-CG-CD	5.42	125.69	111.60
1	C	257	GLY	C-N-CA	-5.42	108.16	121.70
1	A	130	LEU	CB-CG-CD1	-5.42	101.79	111.00
1	D	46	ILE	CA-CB-CG1	-5.42	100.71	111.00
1	D	74	TYR	N-CA-C	-5.41	96.38	111.00
1	A	74	TYR	N-CA-C	-5.41	96.39	111.00
1	B	46	ILE	CA-CB-CG1	-5.41	100.72	111.00
1	C	74	TYR	N-CA-C	-5.41	96.40	111.00
1	C	130	LEU	CB-CG-CD1	-5.41	101.80	111.00
1	C	213	VAL	CG1-CB-CG2	-5.41	102.25	110.90
1	A	46	ILE	CA-CB-CG1	-5.41	100.73	111.00
1	A	59	TRP	CB-CA-C	-5.40	99.59	110.40
1	D	170	TYR	CB-CG-CD2	5.40	124.24	121.00
1	D	59	TRP	CB-CA-C	-5.40	99.60	110.40
1	B	59	TRP	CB-CA-C	-5.40	99.61	110.40
1	B	279	ARG	NE-CZ-NH2	-5.40	117.60	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	59	TRP	CB-CA-C	-5.40	99.61	110.40
1	C	46	ILE	CA-CB-CG1	-5.39	100.75	111.00
1	C	279	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	A	213	VAL	CG1-CB-CG2	-5.39	102.28	110.90
1	B	213	VAL	CG1-CB-CG2	-5.38	102.29	110.90
1	C	13	ASP	CB-CG-OD1	-5.38	113.45	118.30
1	A	147	MET	CG-SD-CE	-5.38	91.59	100.20
1	C	147	MET	CG-SD-CE	-5.38	91.59	100.20
1	D	213	VAL	CG1-CB-CG2	-5.38	102.29	110.90
1	B	27	ILE	CA-CB-CG2	-5.38	100.14	110.90
1	D	248	TYR	CD1-CE1-CZ	-5.38	114.96	119.80
1	A	170	TYR	CB-CG-CD2	5.37	124.22	121.00
1	A	27	ILE	CA-CB-CG2	-5.37	100.16	110.90
1	B	249	VAL	CA-CB-CG2	5.37	118.96	110.90
1	D	27	ILE	CA-CB-CG2	-5.37	100.16	110.90
1	C	249	VAL	CA-CB-CG2	5.37	118.95	110.90
1	B	13	ASP	CB-CG-OD1	-5.37	113.47	118.30
1	B	95	GLU	C-N-CA	-5.37	111.03	122.30
1	C	27	ILE	CA-CB-CG2	-5.37	100.17	110.90
1	C	383	ARG	CG-CD-NE	5.37	123.07	111.80
1	D	48	SER	N-CA-C	-5.36	96.52	111.00
1	A	383	ARG	CG-CD-NE	5.36	123.06	111.80
1	B	147	MET	CG-SD-CE	-5.36	91.62	100.20
1	D	147	MET	CG-SD-CE	-5.36	91.63	100.20
1	D	383	ARG	CG-CD-NE	5.36	123.05	111.80
1	B	383	ARG	CG-CD-NE	5.36	123.05	111.80
1	A	48	SER	N-CA-C	-5.35	96.55	111.00
1	A	249	VAL	CA-CB-CG2	5.35	118.93	110.90
1	C	48	SER	N-CA-C	-5.35	96.55	111.00
1	D	95	GLU	C-N-CA	-5.35	111.06	122.30
1	A	13	ASP	CB-CG-OD1	-5.34	113.49	118.30
1	A	95	GLU	C-N-CA	-5.34	111.08	122.30
1	A	160	LYS	N-CA-C	-5.34	96.57	111.00
1	B	48	SER	N-CA-C	-5.34	96.57	111.00
1	C	160	LYS	N-CA-C	-5.34	96.58	111.00
1	D	13	ASP	CB-CG-OD1	-5.34	113.49	118.30
1	D	249	VAL	CA-CB-CG2	5.34	118.91	110.90
1	B	160	LYS	N-CA-C	-5.34	96.58	111.00
1	D	160	LYS	N-CA-C	-5.34	96.59	111.00
1	D	90	LEU	CD1-CG-CD2	-5.34	94.49	110.50
1	D	107	GLY	CA-C-O	5.33	130.20	120.60
1	A	143	ILE	CG1-CB-CG2	-5.33	99.67	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	248	TYR	CD1-CE1-CZ	-5.33	115.00	119.80
1	B	269	GLU	CA-C-N	-5.33	105.47	117.20
1	C	95	GLU	C-N-CA	-5.33	111.11	122.30
1	D	275	ILE	CB-CA-C	-5.33	100.94	111.60
1	A	269	GLU	CA-C-N	-5.33	105.48	117.20
1	B	248	TYR	CD1-CE1-CZ	-5.33	115.00	119.80
1	C	107	GLY	CA-C-O	5.33	130.19	120.60
1	C	143	ILE	CG1-CB-CG2	-5.33	99.69	111.40
1	A	90	LEU	CD1-CG-CD2	-5.32	94.53	110.50
1	A	107	GLY	CA-C-O	5.32	130.18	120.60
1	C	269	GLU	CA-C-N	-5.32	105.50	117.20
1	D	143	ILE	CG1-CB-CG2	-5.32	99.70	111.40
1	B	143	ILE	CG1-CB-CG2	-5.32	99.70	111.40
1	B	90	LEU	CD1-CG-CD2	-5.32	94.55	110.50
1	C	90	LEU	CD1-CG-CD2	-5.32	94.55	110.50
1	D	269	GLU	CA-C-N	-5.32	105.51	117.20
1	B	196	PHE	C-N-CA	5.31	134.98	121.70
1	B	275	ILE	CB-CA-C	-5.31	100.98	111.60
1	C	248	TYR	CD1-CE1-CZ	-5.31	115.02	119.80
1	A	275	ILE	CB-CA-C	-5.31	100.98	111.60
1	B	107	GLY	CA-C-O	5.31	130.15	120.60
1	D	245	GLY	N-CA-C	5.31	126.37	113.10
1	C	196	PHE	C-N-CA	5.30	134.96	121.70
1	A	196	PHE	C-N-CA	5.30	134.95	121.70
1	C	275	ILE	CB-CA-C	-5.30	101.00	111.60
1	D	196	PHE	C-N-CA	5.30	134.95	121.70
1	D	314	THR	C-N-CA	5.30	134.94	121.70
1	C	109	VAL	CB-CA-C	5.29	121.45	111.40
1	B	109	VAL	CB-CA-C	5.29	121.45	111.40
1	B	136	PRO	O-C-N	5.29	131.16	122.70
1	C	245	GLY	N-CA-C	5.29	126.32	113.10
1	A	122	ASP	N-CA-C	-5.28	96.74	111.00
1	A	314	THR	C-N-CA	5.28	134.90	121.70
1	B	314	THR	C-N-CA	5.28	134.90	121.70
1	C	82	TYR	CB-CA-C	-5.28	99.84	110.40
1	D	122	ASP	N-CA-C	-5.28	96.74	111.00
1	A	245	GLY	N-CA-C	5.28	126.30	113.10
1	C	107	GLY	N-CA-C	5.28	126.30	113.10
1	C	314	THR	C-N-CA	5.28	134.90	121.70
1	D	61	LEU	CA-CB-CG	-5.28	103.16	115.30
1	A	61	LEU	CA-CB-CG	-5.28	103.17	115.30
1	B	61	LEU	CA-CB-CG	-5.27	103.17	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	122	ASP	N-CA-C	-5.27	96.76	111.00
1	C	122	ASP	N-CA-C	-5.27	96.76	111.00
1	A	109	VAL	CB-CA-C	5.27	121.42	111.40
1	D	107	GLY	N-CA-C	5.27	126.28	113.10
1	C	61	LEU	CA-CB-CG	-5.27	103.18	115.30
1	D	82	TYR	CB-CA-C	-5.27	99.86	110.40
1	A	107	GLY	N-CA-C	5.27	126.27	113.10
1	C	136	PRO	O-C-N	5.27	131.13	122.70
1	C	412	LEU	CB-CG-CD1	5.27	119.95	111.00
1	B	412	LEU	CB-CG-CD1	5.26	119.95	111.00
1	A	136	PRO	O-C-N	5.26	131.12	122.70
1	A	82	TYR	CB-CA-C	-5.26	99.88	110.40
1	A	412	LEU	CB-CG-CD1	5.26	119.94	111.00
1	D	339	HIS	CA-C-O	-5.26	109.06	120.10
1	B	82	TYR	CB-CA-C	-5.26	99.88	110.40
1	B	245	GLY	N-CA-C	5.26	126.24	113.10
1	B	107	GLY	N-CA-C	5.25	126.24	113.10
1	A	339	HIS	CA-C-O	-5.25	109.08	120.10
1	D	109	VAL	CB-CA-C	5.25	121.37	111.40
1	D	412	LEU	CB-CG-CD1	5.24	119.91	111.00
1	D	136	PRO	O-C-N	5.24	131.09	122.70
1	D	17	LEU	O-C-N	5.24	131.08	122.70
1	B	17	LEU	O-C-N	5.24	131.08	122.70
1	C	339	HIS	CA-C-O	-5.24	109.10	120.10
1	C	141	GLN	CB-CA-C	5.23	120.86	110.40
1	D	141	GLN	CB-CA-C	5.23	120.86	110.40
1	A	17	LEU	O-C-N	5.23	131.06	122.70
1	A	141	GLN	CB-CA-C	5.23	120.85	110.40
1	C	355	LEU	CB-CG-CD2	5.23	119.88	111.00
1	C	17	LEU	O-C-N	5.22	131.06	122.70
1	C	198	ARG	NH1-CZ-NH2	-5.22	113.65	119.40
1	D	217	THR	CA-CB-CG2	5.22	119.71	112.40
1	A	355	LEU	CB-CG-CD2	5.22	119.87	111.00
1	A	217	THR	CA-CB-CG2	5.21	119.70	112.40
1	B	217	THR	CA-CB-CG2	5.21	119.70	112.40
1	B	339	HIS	CA-C-O	-5.21	109.15	120.10
1	D	355	LEU	CB-CG-CD2	5.21	119.86	111.00
1	B	141	GLN	CB-CA-C	5.21	120.81	110.40
1	D	172	GLU	N-CA-C	5.21	125.06	111.00
1	B	355	LEU	CB-CG-CD2	5.20	119.85	111.00
1	C	217	THR	CA-CB-CG2	5.20	119.68	112.40
1	D	190	ASN	N-CA-CB	-5.20	101.23	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	190	ASN	N-CA-CB	-5.20	101.24	110.60
1	A	390	ARG	O-C-N	5.20	131.01	122.70
1	B	190	ASN	N-CA-CB	-5.20	101.25	110.60
1	B	390	ARG	O-C-N	5.20	131.01	122.70
1	C	236	LYS	CB-CG-CD	5.20	125.11	111.60
1	A	172	GLU	N-CA-C	5.19	125.02	111.00
1	A	198	ARG	NH1-CZ-NH2	-5.19	113.69	119.40
1	B	55	TRP	N-CA-C	5.19	125.01	111.00
1	C	172	GLU	N-CA-C	5.19	125.02	111.00
1	B	216	GLU	C-N-CA	5.19	134.67	121.70
1	C	190	ASN	N-CA-CB	-5.18	101.27	110.60
1	C	216	GLU	C-N-CA	5.18	134.66	121.70
1	D	390	ARG	O-C-N	5.18	131.00	122.70
1	C	390	ARG	O-C-N	5.18	130.99	122.70
1	D	55	TRP	N-CA-C	5.18	124.99	111.00
1	A	55	TRP	N-CA-C	5.18	124.98	111.00
1	A	216	GLU	C-N-CA	5.18	134.64	121.70
1	C	31	TYR	CB-CG-CD1	-5.18	117.89	121.00
1	B	236	LYS	CB-CG-CD	5.17	125.06	111.60
1	B	172	GLU	N-CA-C	5.17	124.97	111.00
1	C	55	TRP	N-CA-C	5.17	124.97	111.00
1	A	207	TYR	CB-CA-C	5.17	120.74	110.40
1	A	236	LYS	CB-CG-CD	5.17	125.05	111.60
1	B	198	ARG	NH1-CZ-NH2	-5.17	113.71	119.40
1	B	207	TYR	CB-CA-C	5.17	120.74	110.40
1	C	246	GLY	CA-C-O	-5.17	111.30	120.60
1	D	216	GLU	C-N-CA	5.17	134.63	121.70
1	D	207	TYR	CB-CA-C	5.17	120.73	110.40
1	A	246	GLY	CA-C-O	-5.16	111.31	120.60
1	B	75	LEU	CA-CB-CG	5.16	127.18	115.30
1	D	236	LYS	CB-CG-CD	5.16	125.03	111.60
1	B	198	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	C	265	ARG	N-CA-C	-5.16	97.06	111.00
1	A	417	ARG	CD-NE-CZ	5.16	130.82	123.60
1	B	246	GLY	CA-C-O	-5.16	111.31	120.60
1	D	198	ARG	NH1-CZ-NH2	-5.16	113.73	119.40
1	D	246	GLY	CA-C-O	-5.16	111.31	120.60
1	A	31	TYR	CB-CG-CD1	-5.15	117.91	121.00
1	A	77	LYS	CD-CE-NZ	5.15	123.55	111.70
1	D	77	LYS	CD-CE-NZ	5.15	123.55	111.70
1	D	198	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	B	77	LYS	CD-CE-NZ	5.15	123.54	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	207	TYR	CB-CA-C	5.15	120.70	110.40
1	A	265	ARG	N-CA-C	-5.15	97.10	111.00
1	A	75	LEU	CA-CB-CG	5.15	127.14	115.30
1	D	417	ARG	CD-NE-CZ	5.15	130.80	123.60
1	C	417	ARG	CD-NE-CZ	5.14	130.80	123.60
1	D	75	LEU	CA-CB-CG	5.14	127.13	115.30
1	B	265	ARG	N-CA-C	-5.14	97.11	111.00
1	C	77	LYS	CD-CE-NZ	5.14	123.53	111.70
1	B	31	TYR	CB-CG-CD1	-5.14	117.92	121.00
1	B	417	ARG	CD-NE-CZ	5.14	130.79	123.60
1	A	141	GLN	CA-C-N	-5.13	105.93	116.20
1	D	141	GLN	CA-C-N	-5.13	105.94	116.20
1	D	265	ARG	N-CA-C	-5.13	97.14	111.00
1	D	21	PRO	CA-C-N	-5.13	105.95	116.20
1	C	21	PRO	CA-C-N	-5.12	105.95	116.20
1	C	141	GLN	CA-C-N	-5.12	105.95	116.20
1	A	21	PRO	CA-C-N	-5.12	105.96	116.20
1	C	75	LEU	CA-CB-CG	5.12	127.08	115.30
1	B	141	GLN	CA-C-N	-5.12	105.97	116.20
1	B	21	PRO	CA-C-N	-5.11	105.97	116.20
1	B	109	VAL	CG1-CB-CG2	5.11	119.08	110.90
1	D	109	VAL	CG1-CB-CG2	5.11	119.08	110.90
1	A	109	VAL	CG1-CB-CG2	5.11	119.07	110.90
1	A	198	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	D	33	GLU	CA-CB-CG	-5.10	102.18	113.40
1	C	109	VAL	CG1-CB-CG2	5.10	119.05	110.90
1	D	259	SER	CA-C-O	5.09	130.80	120.10
1	C	383	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	A	293	ILE	CA-CB-CG2	-5.09	100.72	110.90
1	C	33	GLU	CA-CB-CG	-5.09	102.21	113.40
1	D	268	THR	CA-CB-CG2	-5.09	105.28	112.40
1	A	259	SER	CA-C-O	5.09	130.78	120.10
1	C	259	SER	CA-C-O	5.09	130.78	120.10
1	C	293	ILE	CA-CB-CG2	-5.08	100.73	110.90
1	A	33	GLU	CA-CB-CG	-5.08	102.22	113.40
1	B	259	SER	CA-C-O	5.08	130.77	120.10
1	B	33	GLU	CA-CB-CG	-5.08	102.22	113.40
1	B	268	THR	CA-CB-CG2	-5.08	105.29	112.40
1	B	293	ILE	CA-CB-CG2	-5.07	100.75	110.90
1	D	293	ILE	CA-CB-CG2	-5.07	100.76	110.90
1	D	31	TYR	CB-CG-CD1	-5.06	117.96	121.00
1	A	268	THR	CA-CB-CG2	-5.05	105.32	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	51	SER	CA-CB-OG	-5.05	97.56	111.20
1	C	268	THR	CA-CB-CG2	-5.05	105.33	112.40
1	A	51	SER	CA-CB-OG	-5.05	97.56	111.20
1	B	189	GLU	CG-CD-OE2	-5.05	108.20	118.30
1	C	51	SER	CA-CB-OG	-5.05	97.56	111.20
1	D	347	ALA	N-CA-CB	-5.05	103.03	110.10
1	A	189	GLU	CG-CD-OE2	-5.05	108.20	118.30
1	B	347	ALA	N-CA-CB	-5.05	103.03	110.10
1	C	105	VAL	CA-CB-CG1	-5.05	103.33	110.90
1	C	336	LYS	C-N-CA	-5.04	109.09	121.70
1	D	336	LYS	C-N-CA	-5.04	109.09	121.70
1	D	189	GLU	CG-CD-OE2	-5.04	108.22	118.30
1	A	336	LYS	C-N-CA	-5.04	109.11	121.70
1	C	189	GLU	CG-CD-OE2	-5.04	108.23	118.30
1	A	347	ALA	N-CA-CB	-5.03	103.05	110.10
1	B	360	ILE	CB-CA-C	-5.03	101.53	111.60
1	C	347	ALA	N-CA-CB	-5.03	103.05	110.10
1	D	51	SER	CA-CB-OG	-5.03	97.61	111.20
1	D	184	LEU	N-CA-C	5.03	124.58	111.00
1	A	105	VAL	CA-CB-CG1	-5.03	103.36	110.90
1	A	334	LEU	N-CA-C	5.03	124.58	111.00
1	A	360	ILE	CB-CA-C	-5.03	101.55	111.60
1	C	334	LEU	N-CA-C	5.03	124.57	111.00
1	B	334	LEU	N-CA-C	5.02	124.56	111.00
1	B	336	LYS	C-N-CA	-5.02	109.15	121.70
1	C	204	ARG	NE-CZ-NH1	-5.02	117.79	120.30
1	D	105	VAL	CA-CB-CG1	-5.02	103.37	110.90
1	D	334	LEU	N-CA-C	5.02	124.55	111.00
1	B	105	VAL	CA-CB-CG1	-5.02	103.37	110.90
1	C	360	ILE	CB-CA-C	-5.02	101.56	111.60
1	D	360	ILE	CB-CA-C	-5.02	101.56	111.60
1	B	288	ASN	N-CA-CB	-5.02	101.57	110.60
1	D	288	ASN	N-CA-CB	-5.02	101.57	110.60
1	A	184	LEU	N-CA-C	5.01	124.54	111.00
1	C	184	LEU	N-CA-C	5.01	124.54	111.00
1	A	224	LEU	CB-CG-CD1	5.01	119.52	111.00
1	C	88	TYR	CZ-CE2-CD2	-5.01	115.29	119.80
1	A	288	ASN	N-CA-CB	-5.01	101.58	110.60
1	B	184	LEU	N-CA-C	5.01	124.52	111.00
1	C	288	ASN	N-CA-CB	-5.01	101.59	110.60
1	C	224	LEU	CB-CG-CD1	5.00	119.51	111.00
1	B	95	GLU	CG-CD-OE1	5.00	128.31	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	224	LEU	CB-CG-CD1	5.00	119.50	111.00
1	B	396	ALA	N-CA-CB	5.00	117.10	110.10

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
1	C	129	TYR	Sidechain

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Mol	Chain	Res	Type	Group
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	584	7
1	B	3286	0	3271	637	11
1	C	3286	0	3269	654	4
1	D	3286	0	3269	598	10

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	52	0	0	1	1
2	B	51	0	0	1	0
2	C	52	0	0	5	0
2	D	49	0	0	2	1
All	All	13348	0	13080	2395	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 91.

All (2395) 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:CE	1:A:336:LYS:CD	1.74	1.65
1:C:160:LYS:CE	1:C:160:LYS:CD	1.75	1.63
1:A:56:THR:CB	1:A:56:THR:CA	1.75	1.63
1:C:56:THR:CB	1:C:56:THR:CA	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:CE	1:B:336:LYS:CD	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:CG2	1:C:419:VAL:CB	1.75	1.61
1:C:336:LYS:CD	1:C:336:LYS:CE	1.74	1.60
1:B:300:LYS:CD	1:B:300:LYS:CE	1.78	1.60
1:A:300:LYS:CD	1:A:300:LYS:CE	1.78	1.60
1:D:336:LYS:CE	1:D:336:LYS:CD	1.74	1.59
1:A:66:LYS:CD	1:A:66:LYS:CE	1.80	1.59
1:B:56:THR:CA	1:B:56:THR:CB	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:CE	1:B:160:LYS:CD	1.75	1.58
1:C:300:LYS:CD	1:C:300:LYS:CE	1.78	1.58
1:D:66:LYS:CD	1:D:66:LYS:CE	1.80	1.57
1:A:419:VAL:CG2	1:A:419:VAL:CB	1.76	1.57
1:D:160:LYS:NZ	1:D:160:LYS:CE	1.68	1.57
1:C:61:LEU:CD2	1:C:61:LEU:CG	1.77	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:CD	1:C:66:LYS:CG	1.82	1.55
1:A:66:LYS:CD	1:A:66:LYS:CG	1.82	1.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:LYS:CD	1:A:160:LYS:CE	1.75	1.55
1:A:61:LEU:CG	1:A:61:LEU:CD2	1.77	1.55
1:D:136:PRO:CG	1:D:136:PRO:CD	1.79	1.55
1:A:85:LYS:CE	1:A:85:LYS:NZ	1.69	1.55
1:B:61:LEU:CD2	1:B:61:LEU:CG	1.77	1.55
1:D:200:GLU:CG	1:D:200: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:C:66:LYS:CE	1:C:66:LYS:CD	1.80	1.54
1:B:160:LYS:CE	1:B:160:LYS:NZ	1.68	1.54
1:B:66:LYS:CG	1:B:66:LYS:CD	1.82	1.54
1:C:160:LYS:CE	1:C:160:LYS:NZ	1.68	1.54
1:C:172:GLU:CG	1:C:172:GLU:CD	1.75	1.53
1:A:160:LYS:NZ	1:A:160:LYS:CE	1.68	1.53
1:C:200:GLU:CD	1:C:200:GLU:CG	1.75	1.53
1:D:57:THR:CA	1:D:57:THR:CB	1.85	1.53
1:C:151:ASP:CG	1:C:151:ASP:CB	1.76	1.53
1:B:57:THR:CA	1:B:57:THR:CB	1.85	1.52
1:B:151:ASP:CB	1:B:151:ASP:CG	1.76	1.52
1:D:172:GLU:CD	1:D:172:GLU:CG	1.75	1.52
1:B:200:GLU:CD	1:B:200:GLU:CG	1.75	1.51
1:B:85:LYS:CE	1:B:85:LYS:NZ	1.68	1.51
1:B:216:GLU:C	1:B:216:GLU:CA	1.77	1.51
1:C:216:GLU:C	1:C:216:GLU:CA	1.77	1.50
1:A:151:ASP:CB	1:A:151:ASP:CG	1.76	1.50
1:D:27:ILE:CG1	1:D:27:ILE:CD1	1.86	1.50
1:B:27:ILE:CD1	1:B:27:ILE:CG1	1.86	1.50
1:A:172:GLU:CD	1:A:172:GLU:CG	1.75	1.50
1:B:172:GLU:CG	1:B:172:GLU:CD	1.75	1.50
1:A:57:THR:CB	1:A:57:THR:CA	1.85	1.49
1:A:200:GLU:CG	1:A:200:GLU:CD	1.75	1.49
1:A:216:GLU:C	1:A:216:GLU:CA	1.77	1.49
1:A:27:ILE:CG1	1:A:27:ILE:CD1	1.86	1.49
1:D:216:GLU:C	1:D:216:GLU:CA	1.77	1.49
1:D:151:ASP:CG	1:D:151:ASP:CB	1.76	1.49
1:C:27:ILE:CG1	1:C:27:ILE:CD1	1.86	1.47
1:D:356:MET:SD	1:D:356:MET:CE	2.03	1.47
1:B:141:GLN:CD	1:B:141:GLN:CG	1.82	1.47
1:C:136:PRO:CD	1:C:136:PRO:CG	1.79	1.46
1:D:240:MET:CG	1:D:240:MET:SD	2.03	1.46
1:C:240:MET:CG	1:C:240:MET:SD	2.03	1.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:356:MET:CE	1:C:356:MET:SD	2.03	1.46
1:A:240:MET:SD	1:A:240:MET:CG	2.03	1.46
1:A:141:GLN:CD	1:A:141:GLN:CG	1.82	1.46
1:A:356:MET:SD	1:A:356:MET:CE	2.03	1.46
1:C:141:GLN:CD	1:C:141:GLN:CG	1.82	1.45
1:B:240:MET:CG	1:B:240:MET:SD	2.03	1.45
1:D:141:GLN:CG	1:D:141:GLN:CD	1.82	1.44
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:CE	1:C:250:MET:SD	2.07	1.43
1:D:250:MET:SD	1:D:250:MET:CE	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:B:250:MET:SD	1:B:250:MET:CE	2.07	1.42
1:A:250:MET:SD	1:A:250:MET:CE	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:SD	1:D:147:MET:CE	2.07	1.41
1:C:186:LYS:CE	1:C:186:LYS:NZ	1.80	1.41
1:B:186:LYS:CE	1:B:186:LYS:NZ	1.80	1.41
1:C:147:MET:CE	1:C:147:MET:SD	2.07	1.40
1:B:304:MET:SD	1:B:304:MET:CE	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:A:147:MET:HB3	1:A:147:MET:CE	1.56	1.34
1:D:147:MET:HB3	1:D:147:MET:CE	1.56	1.33
1:A:216:GLU:CD	1:A:216:GLU:CG	1.97	1.33
1:B:147:MET:HB3	1:B:147:MET:CE	1.56	1.33
1:B:216:GLU:CG	1:B:216:GLU:CD	1.97	1.32
1:C:216:GLU:CD	1:C:216:GLU:CG	1.97	1.32
1:D:234:MET:SD	1:D:234:MET:CE	2.17	1.32
1:A:234:MET:CE	1:A:234:MET:SD	2.17	1.32
1:C:234:MET:SD	1:C:234:MET:CE	2.17	1.32
1:D:216:GLU:CD	1:D:216:GLU:CG	1.97	1.31
1:C:147:MET:CE	1:C:147:MET:HB3	1.56	1.31
1:B:234:MET:SD	1:B:234:MET:CE	2.17	1.30
1:D:69:MET:CE	1:D:69:MET:SD	2.21	1.29
1:C:69:MET:CE	1:C: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: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:378:HIS:CE1	1:D:380:ASP:HB2	1.78	1.18
1:D:55:TRP:CD2	1:D:57:THR:HG23	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: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: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:D:264:MET:O	1:D:268:THR:HG23	1.55	1.04
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:B:120:LEU:O	1:B:294:THR:HG23	1.56	1.04
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:MET:HB3	1:A:147:MET:HE3	1.05	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:303:ARG:HH21	1:D:342:PRO:HA	0.88	1.02
1:D:147:MET:HB3	1:D:147:MET:HE3	1.04	1.02
1:B:303:ARG:HH21	1:B:342:PRO:HA	0.88	1.02
1:C:147:MET:HE3	1:C:147:MET:HB3	1.02	1.02
1:C:319:MET:CE	1:C:319:MET:SD	2.48	1.01
1:D:319:MET:SD	1:D:319:MET:CE	2.48	1.01
1:A:319:MET:SD	1:A:319:MET:CE	2.48	1.01
1:B:110:PHE:O	1:C:283:ALA:HB1	1.61	1.01
1:A:365:LYS:HD3	1:A:365:LYS:H	1.26	1.01
1:A:113:LYS:HD2	1:A:113:LYS:H	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:CB	1:B:147:MET:CE	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:B:147:MET:HE3	1:B:147:MET:HB3	1.01	0.99
1:A:147:MET:CB	1:A:147:MET:CE	2.40	0.99
1:A:117:ASN:ND2	1:A:290:ARG:HB2	1.78	0.98
1:D:147:MET:CB	1:D:147:MET:CE	2.40	0.98
1:A:213:VAL:O	1:A:217:THR:HG23	1.61	0.98
1:C:365:LYS:HD3	1:C:365:LYS:H	1.26	0.98
1:D:117:ASN:ND2	1:D:290:ARG:HB2	1.78	0.98
1:C:147:MET:CE	1:C:147:MET:CB	2.40	0.98
1:C:117:ASN:ND2	1:C:290:ARG:HB2	1.78	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
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:B:147:MET:CB	1:B:147:MET:HE3	1.93	0.97
1:C:167:VAL:HG22	1:C:197:ASN:HA	1.46	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:113:LYS:HD2	1:D:113:LYS:H	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: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:365:LYS:HD3	1:D:365:LYS:H	1.26	0.96
1:D:55:TRP:CE2	1:D:57:THR:HG23	2.00	0.96
1:A:253:ILE:CD1	1:A:277:ALA:HB1	1.94	0.96
1:B:113:LYS:HD2	1:B:113:LYS:H	1.26	0.96
1:B:253:ILE:CD1	1:B:277:ALA:HB1	1.94	0.96
1:C:147:MET:HE3	1:C:147:MET:CB	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: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
1:C:352:HIS:HB2	1:C:353:PRO:HD2	1.50	0.94
1:D:147:MET:CB	1:D:147:MET:HE3	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:126:PRO:O	1:C:127:TYR:C	2.07	0.92
1:A:105:VAL:O	1:A:105:VAL:HG23	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:C:156:ALA:HB2	1:C:184:LEU:HB2	1.49	0.91
1:C:76:GLU:HG2	1:C:77:LYS:N	1.86	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:CD1	1:A:323:TYR:O	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:353:PRO:HG3	1:D:415:SER:OG	1.71	0.90
1:A:147:MET:CB	1:A:147:MET:HE3	1.96	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:D:126:PRO:O	1:D:127:TYR:C	2.07	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:199:PHE:CZ	1:D:225:ILE:HD11	2.08	0.89
1:D:76:GLU:HG2	1:D:77:LYS:N	1.86	0.89
1:A:199:PHE:CZ	1:A:225:ILE:HD11	2.08	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:PHE:CZ	1:B:225:ILE:HD11	2.08	0.89
1:B:23:ARG:HE	1:B:23:ARG:H	1.21	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:CD	1:D:113:LYS:H	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:H	1:D:23:ARG:HE	1.21	0.89
1:B:323:TYR:CE2	1:B:362:LEU:HD22	2.08	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:311:HIS:HD2	1:C:346:VAL:CG1	1.87	0.88
1:C:39:PRO:O	1:C:75:LEU:HD21	1.73	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:126:PRO:O	1:B:127:TYR:C	2.07	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:128:GLU:HG3	1:D:128:GLU:HG3	0.89	0.88
1:C:10:TRP:O	1:C:12:LEU:N	2.07	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
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:137:GLN:HB2	1:A:265:ARG:HH22	1.36	0.87
1:A:11:TYR:CD2	1:A:45:ARG:HG2	2.09	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:TRP:CE3	1:A:10:TRP:HA	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: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:B:10:TRP:HA	1:B:10:TRP:CE3	2.10	0.86
1:A:126:PRO:O	1:A:127:TYR:C	2.07	0.85
1:B:113:LYS:CD	1:B:113:LYS:H	1.85	0.85
1:B:351:LEU:HD23	1:B:359:LEU:CD2	2.05	0.85
1:C:10:TRP:CE3	1:C:10:TRP:HA	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:C:160:LYS:HZ1	1:C:373:GLY:H	1.24	0.85
1:B:61:LEU:CD2	1:B:61:LEU:HG	2.04	0.85
1:A:23:ARG:H	1:A:23:ARG:HE	1.21	0.85
1:A:61:LEU:HG	1:A:61:LEU:CD2	2.04	0.85
1:C:351:LEU:HD23	1:C:359:LEU:CD2	2.05	0.84
1:A:113:LYS:CD	1:A:113:LYS:H	1.85	0.84
1:B:253:ILE:HD13	1:B:277:ALA:CB	2.03	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: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:160:LYS:HZ1	1:B:373:GLY:H	1.22	0.83
1:B:98:LEU:HD11	1:B:301:ALA:HB1	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:252:ASP:HB3	1:A:255:VAL:CG2	2.08	0.83
1:A:123:PHE:CE1	1:A:300:LYS:HG2	2.13	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:HE3	1:A:10:TRP:HA	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:281:MET:HG2	1:D:281:MET:O	1.79	0.82
1:D:61:LEU:CD2	1:D:61:LEU:HG	2.04	0.82
1:D:10:TRP:HA	1:D:10:TRP:HE3	1.44	0.82
1:D:160:LYS:HZ1	1:D:373:GLY:H	1.27	0.82
1:A:28:VAL:CG2	1:A:88:TYR:CE2	2.60	0.82
1:C:10:TRP:HE3	1:C:10:TRP:HA	1.44	0.82
1:B:281:MET:SD	1:B:281:MET:CE	2.68	0.82
1:D:281:MET:SD	1:D:281:MET:CE	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:A:281:MET:CE	1:A:281:MET:SD	2.68	0.81
1:C:281:MET:CE	1:C:281:MET:SD	2.68	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: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:O	1:A:281:MET:HG2	1.79	0.81
1:D:98:LEU:HD11	1:D:301:ALA:HB1	1.60	0.81
1:D:276:HIS:HD2	1:D:309:GLN:HE21	1.27	0.81
1:C:281:MET:HG2	1:C:281:MET:O	1.79	0.81
1:C:98:LEU:HD11	1:C:301:ALA:HB1	1.60	0.81
1:B:169:GLU:OE2	1:C:60:LYS:HE2	1.81	0.81
1:B:27:ILE:HG23	1:B:86:ILE:O	1.80	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:B:276:HIS:HD2	1:B:309:GLN:HE21	1.27	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:121:LEU:HA	1:A:294:THR:HG21	1.65	0.79
1:A:55:TRP:HH2	1:A:58:LEU:CB	1.94	0.79
1:A:140:VAL:O	1:A:144:ARG:HB2	1.83	0.79
1:A:278:HIS:HD2	1:A:280:ALA:H	1.30	0.79
1:A:276:HIS:HD2	1:A:309:GLN:HE21	1.27	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: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:121:LEU:HA	1:C:294:THR:HG21	1.65	0.78
1:B:131:ARG:HA	1:B:339:HIS:CE1	2.18	0.78
1:C:131:ARG:HA	1:C:339:HIS:CE1	2.18	0.78
1:B:375:VAL:HG13	1:B:385:GLY:C	2.05	0.78
1:C:156:ALA:O	1:C:370:GLN:HG2	1.84	0.78
1:C:375:VAL:HG13	1:C:385:GLY:C	2.05	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:A:375:VAL:HG13	1:A:385:GLY:C	2.05	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:D:375:VAL:HG13	1:D:385:GLY:C	2.05	0.77
1:A:156:ALA:O	1:A:370:GLN:HG2	1.84	0.77
1:A:160:LYS:HZ1	1:A:373:GLY:H	1.32	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:TYR:O	1:C:129:TYR:N	2.17	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:B:127:TYR:O	1:B:129:TYR:N	2.18	0.77
1:C:35:ASN:OD1	1:C:35:ASN:O	2.03	0.77
1:B:169:GLU:OE2	1:C:60:LYS:CE	2.33	0.77
1:D:121:LEU:HA	1:D:294:THR:CG2	2.15	0.77
1:D:298:LEU:HD23	1:D:298:LEU:C	2.05	0.77
1:A:121:LEU:HA	1:A:294:THR:CG2	2.15	0.77
1:A:298:LEU:HD23	1:A:298:LEU:C	2.05	0.77
1:A:35:ASN:O	1:A:35:ASN:OD1	2.03	0.77
1:B:74:TYR:CD2	1:B:75:LEU:N	2.53	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: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: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:A:225:ILE:HG13	1:A:226:ASN:N	2.01	0.76
1:A:131:ARG:HA	1:A:339:HIS:HE1	1.49	0.76
1:B:35:ASN:O	1:B:35:ASN:OD1	2.03	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
1:A:74:TYR:HD2	1:A:75:LEU:N	1.84	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:298:LEU:HD23	1:C:298:LEU:C	2.05	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:B:26:LEU:HB3	1:B:88:TYR:HB2	1.67	0.75
1:C:76:GLU:CG	1:C:77:LYS:N	2.49	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:B:160:LYS:H	1:B:376:MET:HE2	1.51	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:131:ARG:HA	1:C:339:HIS:HE1	1.49	0.75
1:A:31:TYR:CD1	1:A:32:PHE:N	2.55	0.75
1:C:12:LEU:O	1:C:15:VAL:HG23	1.85	0.75
1:B:60:LYS:NZ	1:C:169:GLU:HG2	2.01	0.75
1:B:76:GLU:CG	1:B:77:LYS:N	2.49	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:D:14:PHE:CE2	1:D:48:SER:HA	2.21	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:279:ARG:HD3	1:D:295:MET:HE1	1.69	0.74
1:D:76:GLU:CG	1:D:77:LYS:N	2.49	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
1:B:298:LEU:C	1:B:298:LEU:HD23	2.05	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: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: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:14:PHE:CE2	1:B:48:SER:HA	2.22	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:TYR:C	1:B:31:TYR:CD1	2.61	0.73
1:C:31:TYR:C	1:C:31:TYR:HD1	1.91	0.73
1:B:113:LYS:HZ2	1:C:318:LYS:HE2	1.53	0.73
1:B:279:ARG:HD3	1:B:295:MET:CE	2.18	0.73
1:B:279:ARG:HD3	1:B:295:MET:HE1	1.70	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:A:14:PHE:CE2	1:A:48:SER:HA	2.22	0.73
1:D:31:TYR:CD1	1:D:31:TYR:C	2.61	0.73
1:B:231:VAL:HG13	1:B:234:MET:CE	2.19	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:B:31:TYR:C	1:B:31:TYR:HD1	1.91	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:A:31:TYR:HD1	1:A:31:TYR:C	1.91	0.73
1:B:232:ASN:OD1	1:B:233:ILE:HG12	1.89	0.73
1:C:31:TYR:CD1	1:C:31:TYR:C	2.61	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:C:263:TYR:C	1:C:263:TYR:CD2	2.63	0.72
1:C:279:ARG:HD3	1:C:295:MET:HE1	1.70	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
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:D:31:TYR:HD1	1:D:31:TYR:C	1.91	0.72
1:A:31:TYR:CD1	1:A:31:TYR:C	2.61	0.72
1:B:110:PHE:HB2	1:C:283:ALA:HB3	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:144:ARG:HG2	1:B:149:VAL:O	1.89	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:D:82:TYR:CD2	1:D:82:TYR:N	2.57	0.72
1:A:207:TYR:O	1:A:210:ARG:HB3	1.90	0.72
1:A:82:TYR:N	1:A:82:TYR:CD2	2.57	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:117:ASN:HD22	1:B:290:ARG:CB	2.02	0.72
1:B:31:TYR:HD1	1:B:32:PHE:N	1.88	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:207:TYR:O	1:C:210:ARG:HB3	1.90	0.71
1:C:117:ASN:HD22	1:C:290:ARG:CB	2.02	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:D:263:TYR:CD2	1:D:263:TYR:C	2.62	0.71
1:A:205:LYS:O	1:A:209:VAL:HG23	1.90	0.71
1:A:263:TYR:CD2	1:A:263:TYR:C	2.63	0.71
1:B:120:LEU:O	1:B:294:THR:CG2	2.38	0.71
1:B:14:PHE:O	1:B:72:VAL:HG23	1.90	0.71
1:C:311:HIS:CD2	1:C:346:VAL:HG11	2.24	0.71
1:D:134:LYS:NZ	1:D:266:GLU:CG	2.53	0.71
1:D:31:TYR:HD1	1:D:32:PHE:N	1.89	0.71
1:D:14:PHE:O	1:D:72:VAL:HG23	1.90	0.71
1:B:263:TYR:C	1:B:263:TYR:CD2	2.63	0.71
1:A:202:ARG:O	1:A:206:LEU:HD23	1.90	0.71
1:A:31:TYR:HD1	1:A:32:PHE:N	1.88	0.71
1:C:205:LYS:O	1:C:209:VAL:HG23	1.90	0.71
1:C:99:VAL:HG22	1:C:258:TRP:HB3	1.72	0.71
1:A:384:ALA:CB	1:A:411:GLU:HG2	2.20	0.71
1:A:9:GLU:N	1:A:56:THR:HG1	1.87	0.71
1:B:259:SER:HB3	1:C:256:ALA:O	1.90	0.71
1:C:134:LYS:NZ	1:C:266:GLU:CG	2.53	0.71
1:C:31:TYR:HD1	1:C:32:PHE:N	1.89	0.71
1:B:207:TYR:O	1:B:210:ARG:HB3	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:378:HIS:ND1	1:D:380:ASP:HB2	2.05	0.70
1:D:74:TYR:CD2	1:D:74:TYR:C	2.64	0.70
1:A:74:TYR:C	1:A:74:TYR:CD2	2.64	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
1:C:74:TYR:CD2	1:C:74:TYR:C	2.64	0.70
1:D:90:LEU:HD21	1:D:126:PRO:HG3	1.72	0.70
2:C:451:HOH:O	1:D:23:ARG:HD2	1.90	0.70
1:A:194:PHE:O	1:A:195:PRO:C	2.28	0.70
1:B:202:ARG:O	1:B:206:LEU:HD23	1.90	0.70
1:C:278:HIS:ND1	1:C:311:HIS:HE1	1.90	0.70
1:C:82:TYR:N	1:C:82:TYR:CD2	2.57	0.70
1:B:9:GLU:N	1:B:56:THR:HG1	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:D:131:ARG:CG	1:D:132:HIS:HD1	2.04	0.70
1:A:143:ILE:HD13	1:A:309:GLN:OE1	1.92	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:113:LYS:HZ2	1:C:318:LYS:CE	2.05	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:B:74:TYR:C	1:B:74:TYR:CD2	2.64	0.70
1:A:61:LEU:CD1	1:A:61:LEU:CD2	2.68	0.69
1:C:216:GLU:CD	1:C:216:GLU:HA	2.13	0.69
1:D:202:ARG:O	1:D:206:LEU:HD23	1.90	0.69
1:A:160:LYS:H	1:A:376:MET:HE2	1.57	0.69
1:B:99:VAL:HG22	1:B:258:TRP:HB3	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:216:GLU:N	1:D:216:GLU:C	2.45	0.69
1:A:216:GLU:CD	1:A:216:GLU:HA	2.13	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:279:ARG:O	1:D:280:ALA:C	2.30	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:A:216:GLU:N	1:A:216:GLU:C	2.45	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:276:HIS:CD2	1:D:309:GLN:HE21	2.09	0.69
1:D:46:ILE:HG12	1:D:112:MET:HE1	1.74	0.69
1:B:17:LEU:HD23	1:B:74:TYR:N	2.08	0.69
1:C:279:ARG:O	1:C:280:ALA:C	2.31	0.69
1:D:143:ILE:HD13	1:D:309:GLN:OE1	1.92	0.69
1:A:378:HIS:ND1	1:A:380:ASP:HB2	2.05	0.69
1:A:278:HIS:ND1	1:A:311:HIS:HE1	1.90	0.69
1:A:365:LYS:N	1:A:365:LYS:HD3	2.06	0.69
1:B:279:ARG:O	1:B:280:ALA:C	2.31	0.69
1:C:194:PHE:O	1:C:195:PRO:C	2.28	0.69
1:C:216:GLU:C	1:C:216:GLU:N	2.45	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: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:O	1:C:60:LYS:HG2	1.93	0.68
1:D:115:LEU:HD13	1:D:118:LEU:HD22	1.75	0.68
1:D:61:LEU:CD2	1:D:61:LEU:CD1	2.68	0.68
1:B:194:PHE:O	1:B:195:PRO:C	2.28	0.68
1:D:384:ALA:CB	1:D:411:GLU:HG2	2.21	0.68
1:B:216:GLU:CD	1:B:216:GLU:HA	2.13	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:46:ILE:HG12	1:B:112:MET:HE1	1.73	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:C:9:GLU:N	1:C:56:THR:HG1	1.91	0.68
1:D:160:LYS:H	1:D:376:MET:HE2	1.57	0.68
1:D:46:ILE:HG12	1:D:112:MET:CE	2.24	0.68
1:B:46:ILE:HG12	1:B:112:MET:CE	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:216:GLU:HA	1:D:216:GLU:CD	2.13	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: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:D:249:VAL:HG23	1:D:249:VAL:O	1.94	0.68
1:A:160:LYS:H	1:A:376:MET:CE	2.07	0.67
1:A:46:ILE:HG12	1:A:112:MET:CE	2.24	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:A:279:ARG:HD3	1:A:295:MET:HE1	1.76	0.67
1:B:256:ALA:O	1:C:259:SER:HB3	1.93	0.67
1:B:195:PRO:HG2	1:D:131:ARG:HB2	1.76	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:D:346:VAL:CG2	1:D:368:VAL:CG2	2.73	0.67
1:D:55:TRP:CD2	1:D:57:THR:CG2	2.71	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:160:LYS:H	1:C:376:MET:HE2	1.58	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:CG	1:C:234:MET:CE	2.73	0.67
1:C:249:VAL:O	1:C:249:VAL:HG23	1.94	0.67
1:C:346:VAL:CG2	1:C:368:VAL:CG2	2.73	0.67
1:B:169:GLU:HG2	1:C:60:LYS:HZ3	1.59	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:HB	1:B:419:VAL:CG2	2.16	0.67
1:A:60:LYS:HG2	1:A:60:LYS:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:345:PRO:HD2	1:D:367:LEU:HD23	1.77	0.67
1:A:279:ARG:O	1:A:280:ALA:C	2.30	0.67
1:A:282:HIS:CD2	1:A:283:ALA:N	2.63	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:46:ILE:HG12	1:C:112:MET:HE1	1.76	0.67
1:C:120:LEU:O	1:C:294:THR:CG2	2.38	0.67
1:C:46:ILE:HG12	1:C:112:MET:CE	2.24	0.67
1:A:227:ILE:O	1:A:234:MET:HG2	1.96	0.66
1:A:250:MET:CG	1:A:250:MET:CE	2.73	0.66
1:C:345:PRO:HD2	1:C:367:LEU:HD23	1.77	0.66
1:D:250:MET:CG	1:D:250:MET:CE	2.73	0.66
1:D:60:LYS:O	1:D:60:LYS:HG2	1.93	0.66
1:A:120:LEU:O	1:A:294:THR:CG2	2.38	0.66
1:A:249:VAL:HG23	1:A:249:VAL:O	1.94	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:CG	1:B:234:MET:CE	2.73	0.66
1:C:182:ILE:HG22	1:C:183:ASP:N	2.08	0.66
1:C:250:MET:CG	1:C:250:MET:CE	2.73	0.66
1:C:365:LYS:N	1:C:365:LYS:HD3	2.06	0.66
1:B:154:LEU:HB2	1:B:368:VAL:HG13	1.77	0.66
1:B:216:GLU:C	1:B:216:GLU:N	2.45	0.66
1:B:250:MET:CG	1:B:250:MET:CE	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:146:PHE:CD2	1:B:147:MET:HG2	2.30	0.66
1:B:160:LYS:H	1:B:376:MET:CE	2.07	0.66
1:B:60:LYS:O	1:B:60:LYS:HG2	1.93	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:D:160:LYS:H	1:D:376:MET:CE	2.07	0.66
1:A:117:ASN:HB3	1:A:290:ARG:O	1.96	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:C:160:LYS:H	1:C:376:MET:CE	2.07	0.66
1:A:323:TYR:CG	1:A:323:TYR:O	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
1:B:257:GLY:HA3	1:C:257:GLY:HA3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:315:ALA:C	1:A:316:VAL:HG23	2.16	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:D:194:PHE:O	1:D:195:PRO:C	2.28	0.66
1:D:134:LYS:HZ1	1:D:266:GLU:CG	2.09	0.66
1:A:234:MET:CE	1:A:234:MET:CG	2.73	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:CG	1:B:323:TYR:O	2.48	0.66
1:D:231:VAL:CG1	1:D:234:MET:HE3	2.26	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:C:134:LYS:HZ1	1:C:266:GLU:CG	2.09	0.65
1:D:154:LEU:HB2	1:D:368:VAL:HG13	1.77	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:B:60:LYS:HZ1	1:C:169:GLU:HG2	1.60	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:D:117:ASN:HB3	1:D:290:ARG:O	1.96	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:353:PRO:O	1:D:392:ALA:HB1	1.97	0.65
1:D:9:GLU:N	1:D:56:THR:HG1	1.95	0.65
1:A:119:ARG:HB3	1:A:121:LEU:HD11	1.78	0.65
1:C:231:VAL:CG1	1:C:234:MET:HE3	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:D:315:ALA:C	1:D:316:VAL:HG23	2.16	0.65
1:A:154:LEU:HB2	1:A:368:VAL:HG13	1.77	0.65
1:C:315:ALA:C	1:C:316:VAL:HG23	2.17	0.65
1:D:323:TYR:O	1:D:323:TYR:CG	2.48	0.65
1:C:278:HIS:CD2	1:C:280:ALA:HB2	2.32	0.65
1:C:136:PRO:HB3	1:C:308:ASP:OD1	1.97	0.65
1:D:136:PRO:HB3	1:D:308:ASP:OD1	1.97	0.65
1:A:46:ILE:HG12	1:A:112:MET:HE1	1.77	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:B:12:LEU:HD21	1:B:41:GLU:HG3	1.79	0.64
1:A:346:VAL:HG22	1:A:368:VAL:HG21	1.76	0.64
1:B:134:LYS:HZ1	1:B:266:GLU:CG	2.10	0.64
1:B:74:TYR:C	1:B:74:TYR:HD2	2.01	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:C:160:LYS:HZ1	1:C:373:GLY:N	1.94	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:D:74:TYR:HD2	1:D:74:TYR:C	2.01	0.64
1:A:160:LYS:NZ	1:A:373:GLY:H	1.96	0.64
1:B:147:MET:CG	1:B:147:MET:CE	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:CG	1:C:323:TYR:O	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:A:74:TYR:HD2	1:A:74:TYR:C	2.01	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:N	1:D:113:LYS:HD2	2.07	0.64
1:D:138:PHE:CD1	1:D:146:PHE:HE1	2.15	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:B:76:GLU:HG2	1:B:77:LYS:O	1.98	0.64
1:D:184:LEU:HD12	1:D:224:LEU:HD11	1.80	0.64
1:A:147:MET:CG	1:A:147:MET:CE	2.76	0.63
1:B:110:PHE:C	1:C:283:ALA:HB1	2.18	0.63
1:B:136:PRO:HB3	1:B:308:ASP:OD1	1.97	0.63
1:C:346:VAL:CG2	1:C:368:VAL:HG23	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:76:GLU:HG2	1:D:77:LYS:O	1.98	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
1:C:12:LEU:HD21	1:C:41:GLU:HG3	1.79	0.63
1:D:134:LYS:NZ	1:D:266:GLU:HG3	2.13	0.63
1:D:55:TRP:CH2	1:D:58:LEU:CB	2.76	0.63
1:A:10:TRP:C	1:A:12:LEU:H	2.02	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:169:GLU:HG2	1:C:60:LYS:HZ1	1.62	0.63
1:B:353:PRO:O	1:B:392:ALA:HB1	1.97	0.63
1:C:341:ARG:CB	1:C:342:PRO:HD2	2.28	0.63
1:C:15:VAL:HA	1:C:72:VAL:HG23	1.81	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:B:315:ALA:C	1:B:316:VAL:HG23	2.16	0.63
1:C:76:GLU:HG2	1:C:77:LYS:O	1.98	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:113:LYS:HD2	1:C:113:LYS:N	2.07	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:D:10:TRP:C	1:D:12:LEU:H	2.02	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:224:LEU:HD22	1:B:276:HIS:CG	2.34	0.63
1:B:11:TYR:CD2	1:B:45:ARG:CG	2.82	0.63
1:C:224:LEU:HD22	1:C:276:HIS:CG	2.34	0.63
1:D:341:ARG:CB	1:D:342:PRO:HD2	2.28	0.63
1:D:160:LYS:NZ	1:D:373:GLY:H	1.96	0.63
1:A:76:GLU:HG2	1:A:77:LYS:O	1.98	0.63
1:B:346:VAL:CG2	1:B:368:VAL:HG23	2.28	0.63
1:B:160:LYS:NZ	1:B:373:GLY:H	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:CG	1:D:147:MET:CE	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:C:137:GLN:HG2	1:C:137:GLN:O	1.99	0.62
1:C:184:LEU:HD12	1:C:224:LEU:HD11	1.80	0.62
1:B:208:ARG:NH2	1:D:145:GLU:OE2	2.28	0.62
1:B:184:LEU:HD12	1:B:224:LEU:HD11	1.80	0.62
1:C:10:TRP:C	1:C:12:LEU:H	2.02	0.62
1:C:300:LYS:HD3	1:C:332:PHE:CZ	2.35	0.62
1:C:46:ILE:HG22	1:C:86:ILE:HD12	1.81	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:300:LYS:HD3	1:B:332:PHE:CZ	2.35	0.62
1:C:74:TYR:HD2	1:C:74:TYR:C	2.01	0.62
1:D:217:THR:HG21	1:D:221:LYS:HE3	1.82	0.62
1:A:134:LYS:HZ1	1:A:266:GLU:CG	2.13	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:C:134:LYS:NZ	1:C:266:GLU:HG2	2.15	0.62
1:A:113:LYS:N	1:A:113:LYS:HD2	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:137:GLN:HG2	1:D:137:GLN:O	1.99	0.62
1:D:15:VAL:HA	1:D:72:VAL:HG23	1.81	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: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
1:B:10:TRP:C	1:B:12:LEU:H	2.02	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:ARG:HG3	1:B:152:ARG:NH1	2.14	0.61
1:B:231:VAL:CG1	1:B:234:MET:HE3	2.30	0.61
1:B:46:ILE:HG22	1:B:86:ILE:HD12	1.81	0.61
1:D:224:LEU:HD22	1:D:276:HIS:CG	2.34	0.61
1:B:11:TYR:N	1:B:11:TYR:CD1	2.60	0.61
1:B:55:TRP:CH2	1:B:58:LEU:CB	2.76	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:229:GLY:O	1:B:234:MET:HG3	1.99	0.61
1:B:15:VAL:HA	1:B:72:VAL:HG23	1.81	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:46:ILE:HG22	1:D:86:ILE:HD12	1.81	0.61
1:D:27:ILE:CG2	1:D:86:ILE:O	2.48	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:O	1:D:419:VAL:HG12	2.01	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:D:12:LEU:CD2	1:D:41:GLU:HG3	2.31	0.61
1:B:310:ILE:O	1:B:346:VAL:HB	2.00	0.61
1:B:60:LYS:HE2	1:C:169:GLU:OE2	2.01	0.61
1:D:112:MET:CE	1:D:115:LEU:HD11	2.31	0.61
1:D:152:ARG:HG3	1:D:152:ARG:NH1	2.14	0.61
1:D:389:LEU:O	1:D:393:ILE:HG13	2.00	0.61
1:D:47:ALA:HB2	1:D:86:ILE:HD13	1.82	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:217:THR:HG21	1:C:221:LYS:HE3	1.82	0.61
1:C:417:ARG:HD3	2:C:481:HOH:O	1.59	0.61
1:C:12:LEU:CD2	1:C:41:GLU:HG3	2.31	0.61
1:D:134:LYS:NZ	1:D:266:GLU:HG2	2.15	0.61
1:A:152:ARG:NH1	1:A:152:ARG:HG3	2.14	0.60
1:A:47:ALA:HB2	1:A:86:ILE:HD13	1.82	0.60
1:C:263:TYR:CE2	1:C:267:VAL:HG23	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:TYR:CE2	1:A:267:VAL:HG23	2.36	0.60
1:C:152:ARG:HG3	1:C:152:ARG:NH1	2.14	0.60
1:D:131:ARG:HG2	1:D:132:HIS:HD1	1.65	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:373:GLY:O	1:B:375:VAL:N	2.34	0.60
1:C:112:MET:CE	1:C:115:LEU:HD11	2.31	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:HG12	1:B:419:VAL:O	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:112:MET:CE	1:A:115:LEU:HD11	2.31	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: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:A:27:ILE:CG2	1:A:86:ILE:O	2.48	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:373:GLY:O	1:D:375:VAL:N	2.34	0.60
1:A:296:LEU:HD12	1:A:329:ILE:HA	1.83	0.59
1:A:55:TRP:CZ3	1:A:58:LEU:N	2.70	0.59
1:B:12:LEU:CD2	1:B:41:GLU:HG3	2.31	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:A:231:VAL:CG1	1:A:234:MET:HE3	2.32	0.59
1:B:112:MET:CE	1:B:115:LEU:HD11	2.31	0.59
1:A:195:PRO:CG	1:B:131:ARG:HB2	2.32	0.59
1:C:204:ARG:O	1:C:208:ARG:CD	2.50	0.59
1:C:27:ILE:CG2	1:C:86:ILE:O	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:122:ASP:OD1	1:D:300:LYS:HE2	2.03	0.59
1:B:122:ASP:OD1	1:B:300:LYS:HE2	2.03	0.59
1:B:151:ASP:CA	1:B:151:ASP:CG	2.69	0.59
1:B:15:VAL:HG13	1:B:72:VAL:HB	1.85	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:C:353:PRO:HG3	1:C:415:SER:HG	1.66	0.59
1:D:162:LYS:O	1:D:163:MET:HG2	2.03	0.59
1:D:419:VAL:HB	1:D:419:VAL:CG2	2.16	0.59
1:B:308:ASP:O	1:B:309:GLN:HG3	2.03	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:CG2	1:B:249:VAL:O	2.50	0.59
1:B:283:ALA:HB1	1:C:110:PHE:C	2.22	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: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
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:A:359:LEU:O	1:A:363:PHE:HD1	1.86	0.58
1:B:359:LEU:O	1:B:363:PHE:HD1	1.86	0.58
1:C:98:LEU:HD23	1:C:98:LEU:C	2.24	0.58
1:A:188:ASP:OD1	1:A:190:ASN:HB2	2.03	0.58
1:A:11:TYR:CD2	1:A:45:ARG:CG	2.82	0.58
1:A:98:LEU:C	1:A:98:LEU:HD23	2.24	0.58
1:B:199:PHE:CD2	1:B:237:ARG:HD3	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:122:ASP:OD1	1:C:300:LYS:HE2	2.03	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: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:131:ARG:HG3	1:D:132:HIS:HD1	1.68	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: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: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: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:C:225:ILE:O	1:C:250:MET:HB3	2.04	0.58
1:B:195:PRO:CG	1:D:131:ARG:HB2	2.33	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:C:231:VAL:HG13	1:C:234:MET:HE3	1.85	0.58
1:C:55:TRP:CZ3	1:C:58:LEU:N	2.70	0.58
1:D:158:VAL:HG11	1:D:188:ASP:HB2	1.86	0.58
1:D:98:LEU:HD23	1:D:98:LEU:C	2.24	0.58
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:375:VAL:HG13	1:C:385:GLY:O	2.03	0.57
1:D:160:LYS:HE3	1:D:160:LYS:CD	2.18	0.57
1:D:231:VAL:HG13	1:D:234:MET:HE3	1.85	0.57
1:B:204:ARG:O	1:B:208:ARG:CD	2.50	0.57
1:B:55:TRP:CZ3	1:B:58:LEU:N	2.70	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:A:155:THR:O	1:A:183:ASP:HB2	2.03	0.57
1:A:279:ARG:HD3	1:A:295:MET:HE2	1.86	0.57
1:B:375:VAL:HG13	1:B:385:GLY:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:ARG:HG3	1:C:132:HIS:ND1	2.19	0.57
1:C:160:LYS:NZ	1:C:373:GLY:N	2.53	0.57
1:C:155:THR:O	1:C:183:ASP:HB2	2.03	0.57
1:D:346:VAL:CG2	1:D:368:VAL:HG21	2.34	0.57
1:D:55:TRP:CZ3	1:D:58:LEU:N	2.70	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: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:D:21:PRO:HA	1:D:25:GLU:OE2	2.05	0.57
1:B:98:LEU:C	1:B:98:LEU:HD23	2.24	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: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
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:A:160:LYS:NZ	1:A:373:GLY:N	2.53	0.57
1:C:58:LEU:HD13	1:C:58:LEU:O	2.05	0.57
1:B:336:LYS:HD3	1:B:337:TRP:N	2.19	0.57
1:B:77:LYS:HA	1:B:82:TYR:CD1	2.40	0.57
1:D:253:ILE:CD1	1:D:277:ALA:CB	2.74	0.57
1:A:263:TYR:HE2	1:A:267:VAL:HG23	1.69	0.57
1:A:58:LEU:O	1:A:58:LEU:HD13	2.05	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:A:112:MET:HA	1:A:113:LYS:HD2	1.87	0.56
1:A:55:TRP:CG	1:A:57:THR:HG23	2.39	0.56
1:B:160:LYS:NZ	1:B:373:GLY:N	2.53	0.56
1:C:152:ARG:HG3	1:C:152:ARG:HH11	1.68	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:A:16:ASP:OD2	1:A:16:ASP:C	2.44	0.56
1:A:112:MET:HE2	1:A:115:LEU:HD11	1.87	0.56
1:A:134:LYS:HZ2	1:A:266:GLU:HG3	1.69	0.56
1:A:77:LYS:HA	1:A:82:TYR:CD1	2.40	0.56
1:B:112:MET:HA	1:B:113:LYS:HD2	1.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:311:HIS:CD2	1:C:346:VAL:CG1	2.79	0.56
1:D:336:LYS:HD3	1:D:337:TRP:N	2.19	0.56
1:A:336:LYS:HD3	1:A:337:TRP:N	2.19	0.56
1:A:303:ARG:NH2	1:A:342:PRO:CA	2.46	0.56
1:B:152:ARG:HG3	1:B:152:ARG:HH11	1.68	0.56
1:B:16:ASP:OD2	1:B:16:ASP:C	2.44	0.56
1:C:144:ARG:CG	1:C:149:VAL:O	2.53	0.56
1:D:58:LEU:HD13	1:D:58:LEU:O	2.05	0.56
1:B:55:TRP:CG	1:B:57:THR:HG23	2.39	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:D:160:LYS:HZ1	1:D:373:GLY:N	1.97	0.56
1:A:21:PRO:HA	1:A:25:GLU:OE2	2.05	0.56
1:A:249:VAL:CG2	1:A:249:VAL:O	2.50	0.56
1:A:308:ASP:C	1:A:309:GLN:HG3	2.26	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:D:308:ASP:C	1:D:309:GLN:HG3	2.26	0.56
1:B:206:LEU:HA	1:B:209:VAL:CG2	2.36	0.56
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:C:231:VAL:CG1	1:C:234:MET:CE	2.84	0.56
1:D:225:ILE:O	1:D:250:MET:HB3	2.04	0.56
1:D:160:LYS:NZ	1:D:373:GLY:N	2.53	0.56
1:B:123:PHE:CZ	1:B:300:LYS:CG	2.79	0.56
1:C:151:ASP:CG	1:C:151:ASP:CA	2.69	0.56
1:D:202:ARG:NE	1:D:223:TYR:OH	2.26	0.56
1:D:263:TYR:C	1:D:263:TYR:HD2	2.09	0.56
1:D:77:LYS:HA	1:D:82:TYR:CD1	2.40	0.56
1:A:151:ASP:CA	1:A:151:ASP:CG	2.69	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:206:LEU:HA	1:A:209:VAL:CG2	2.36	0.56
1:A:74:TYR:CE2	1:A:76:GLU:N	2.74	0.56
1:B:254:VAL:O	1:B:281:MET:HE2	2.06	0.56
1:B:323:TYR:C	1:B:323:TYR:CD1	2.79	0.56
1:D:72:VAL:HG13	1:D:86:ILE:HG12	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ARG:CG	1:A:149:VAL:O	2.53	0.55
1:A:231:VAL:CG1	1:A:234:MET:CE	2.84	0.55
1:C:15:VAL:CG1	1:C:72:VAL:HB	2.36	0.55
1:D:23:ARG:N	1:D:23:ARG:HE	2.00	0.55
1:A:156:ALA:O	1:A:370:GLN:HA	2.05	0.55
1:B:263:TYR:C	1:B:263:TYR:HD2	2.10	0.55
1:C:263:TYR:HD2	1:C:263:TYR:C	2.10	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:323:TYR:C	1:C:323:TYR:CD1	2.79	0.55
1:D:74:TYR:CE2	1:D:76:GLU:N	2.74	0.55
1:D:9:GLU:O	1:D:9:GLU:HG2	2.05	0.55
1:B:231:VAL:CG1	1:B:234:MET:CE	2.84	0.55
1:B:58:LEU:O	1:B:58:LEU:HD13	2.05	0.55
1:D:226:ASN:ND2	1:D:228:THR:OG1	2.32	0.55
1:D:323:TYR:C	1:D:323:TYR:CD1	2.79	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
1:A:78:HIS:HB3	1:A:83:ILE:HG12	1.89	0.55
1:B:300:LYS:O	1:B:301:ALA:C	2.45	0.55
1:B:352:HIS:HB2	1:B:353:PRO:CD	2.32	0.55
1:B:9:GLU:O	1:B:9:GLU:HG2	2.05	0.55
1:D:78:HIS:HB3	1:D:83:ILE:HG12	1.89	0.55
1:A:323:TYR:CD1	1:A:323:TYR:C	2.79	0.55
1:B:271:LEU:HD12	1:B:273:LEU:HD12	1.89	0.55
1:B:64:MET:CE	1:B:64:MET:SD	2.95	0.55
1:C:23:ARG:HD2	2:D:449:HOH:O	2.05	0.55
1:C:308:ASP:C	1:C:309:GLN:HG3	2.26	0.55
1:D:102:PHE:N	1:D:102:PHE:CD1	2.73	0.55
1:D:300:LYS:O	1:D:301:ALA:C	2.45	0.55
1:D:112:MET:HA	1:D:113:LYS:HD2	1.87	0.55
1:D:43:ALA:CB	1:D:75:LEU:HD22	2.37	0.55
1:A:300:LYS:O	1:A:301:ALA:C	2.45	0.55
1:B:308:ASP:C	1:B:309:GLN:HG3	2.26	0.55
1:C:74:TYR:CE2	1:C:76:GLU:N	2.74	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:112:MET:HE2	1:C:115:LEU:HD11	1.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:37:VAL:HG12	1:A:41:GLU:OE2	2.07	0.55
1:A:15:VAL:CG1	1:A:72:VAL:HB	2.36	0.55
1:B:384:ALA:HB1	1:B:411:GLU:HB3	1.88	0.55
1:C:102:PHE:CD1	1:C:102:PHE:N	2.73	0.55
1:D:151:ASP:CA	1:D:151:ASP:CG	2.69	0.55
1:D:16:ASP:C	1:D:16:ASP:OD2	2.44	0.55
1:A:162:LYS:HD2	1:A:188:ASP:OD2	2.07	0.54
1:C:128:GLU:OE2	1:D:95:GLU:OE2	2.24	0.54
1:C:384:ALA:HB1	1:C:411:GLU:HB3	1.88	0.54
1:C:64:MET:CE	1:C:64:MET:SD	2.95	0.54
1:A:30:TYR:CE1	1:A:120:LEU:CD2	2.90	0.54
1:A:315:ALA:O	1:A:316:VAL:CG2	2.55	0.54
1:A:43:ALA:CB	1:A:75:LEU:HD22	2.37	0.54
1:C:72:VAL:HG13	1:C:86:ILE:HG12	1.88	0.54
1:D:315:ALA:O	1:D:316:VAL:CG2	2.55	0.54
1:D:37:VAL:HG12	1:D:41:GLU:OE2	2.08	0.54
1:A:419:VAL:HB	1:A:419:VAL:CG2	2.16	0.54
1:B:98:LEU:O	1:B:101:LEU:HB3	2.08	0.54
1:C:315:ALA:O	1:C:316:VAL:CG2	2.55	0.54
1:C:37:VAL:HG12	1:C:41:GLU:OE2	2.07	0.54
1:D:327:LYS:HD3	1:D:331:ASP:OD1	2.08	0.54
1:D:300:LYS:HD3	1:D:332:PHE:CE1	2.42	0.54
1:D:15:VAL:CG1	1:D:72:VAL:HB	2.36	0.54
1:A:49:GLU:HB3	1:A:109:VAL:HG23	1.90	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:16:ASP:OD2	1:C:16:ASP:C	2.44	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:300:LYS:HD3	1:B:332:PHE:CE1	2.42	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:C:300:LYS:O	1:C:301:ALA:C	2.45	0.54
1:C:28:VAL:HG23	1:C:88:TYR:CE2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:76:GLU:CG	1:C:77:LYS:H	2.21	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:A:72:VAL:HG13	1:A:86:ILE:HG12	1.88	0.54
1:B:10:TRP:C	1:B:12:LEU:N	2.60	0.54
1:B:162:LYS:HD2	1:B:188:ASP:OD2	2.07	0.54
1:B:37:VAL:HG12	1:B:41:GLU:OE2	2.07	0.54
1:C:49:GLU:HB3	1:C:109:VAL:HG23	1.90	0.54
1:B:62:PRO:HG3	1:C:165:TRP:CE3	2.41	0.54
1:C:23:ARG:HE	1:C:23:ARG:N	2.00	0.54
1:D:160:LYS:HE2	1:D:160:LYS:CD	2.18	0.54
1:D:321:GLY:O	1:D:322:ASN:C	2.46	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:D:10:TRP:C	1:D:12:LEU:N	2.60	0.54
1:D:204:ARG:O	1:D:208:ARG:CD	2.50	0.54
1:D:351:LEU:CD2	1:D:359:LEU:HD21	2.37	0.54
1:A:311:HIS:CD2	1:A:346:VAL:CG1	2.79	0.54
1:A:76:GLU:CG	1:A:77:LYS:H	2.21	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:HE2	1:A:160:LYS:CD	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:232:ASN:O	1:D:236:LYS:HG3	2.08	0.54
1:D:281:MET:CG	1:D:281:MET:O	2.54	0.54
1:D:336:LYS:HD3	1:D:338:GLU:H	1.73	0.54
1:D:49:GLU:HB3	1:D:109:VAL:HG23	1.90	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:327:LYS:HD3	1:B:331:ASP:OD1	2.08	0.53
1:B:318:LYS:NZ	1:C:113:LYS:NZ	2.57	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:A:162:LYS:C	1:A:163:MET:HG2	2.29	0.53
1:B:37:VAL:HG21	1:B:114:ALA:HB1	1.90	0.53
1:B:141:GLN:CD	1:B:141:GLN:HA	2.29	0.53
1:B:162:LYS:C	1:B:163:MET:HG2	2.29	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:119:ARG:HB3	1:C:121:LEU:CD1	2.38	0.53
1:C:162:LYS:C	1:C:163:MET:HG2	2.29	0.53
1:C:232:ASN:O	1:C:236:LYS:HG3	2.08	0.53
1:C:78:HIS:HB3	1:C:83:ILE:HG12	1.89	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:321:GLY:O	1:A:322:ASN:C	2.46	0.53
1:A:413:LYS:O	1:A:416:LEU:HB2	2.08	0.53
1:B:321:GLY:O	1:B:322:ASN:C	2.46	0.53
1:C:141:GLN:CD	1:C:141:GLN:HA	2.29	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:336:LYS:O	1:B:337:TRP:HB2	2.08	0.53
1:C:147:MET:CE	1:C:220:THR:HG22	2.39	0.53
1:D:37:VAL:HG21	1:D:114:ALA:HB1	1.90	0.53
1:D:11:TYR:N	1:D:11:TYR:CD1	2.60	0.53
1:A:9:GLU:HG2	1:A:9:GLU:O	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:HE3	1:C:160:LYS:CD	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:281:MET:CG	1:A:281:MET:O	2.54	0.53
1:A:32:PHE:CD2	1:A:34:PRO:HD3	2.44	0.53
1:B:286:THR:HG21	1:B:295:MET:HA	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:LEU:CD2	1:B:359:LEU:HD21	2.37	0.53
1:C:102:PHE:HD1	1:C:102:PHE:N	2.07	0.53
1:B:60:LYS:HZ3	1:C:169:GLU:HG2	1.74	0.53
1:B:113:LYS:HD3	1:C:318:LYS:HE3	1.91	0.53
1:C:98:LEU:HD11	1:C:301:ALA:CB	2.36	0.53
1:A:147:MET:CE	1:A:220:THR:HG22	2.39	0.53
1:A:231:VAL:HG13	1:A:234:MET:HE2	1.91	0.53
1:B:74:TYR:CE2	1:B:76:GLU:N	2.74	0.53
1:C:233:ILE:O	1:C:233:ILE:HG22	2.07	0.53
1:D:278:HIS:CG	1:D:311:HIS:HE1	2.26	0.53
1:A:141:GLN:HA	1:A:141:GLN:CD	2.29	0.53
1:A:336:LYS:O	1:A:337:TRP:HB2	2.08	0.53
1:A:37:VAL:HG21	1:A:114:ALA:HB1	1.90	0.53
1:B:302:ALA:O	1:B:307:VAL:HG22	2.09	0.53
1:B:153:PRO:HB2	1:B:369:ILE:HD11	1.91	0.53
1:C:69:MET:O	1:C:89:PRO:HG3	2.08	0.53
1:D:141:GLN:HA	1:D:141:GLN:CD	2.29	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:A:119:ARG:HB3	1:A:121:LEU:CD1	2.38	0.52
1:A:233:ILE:HG22	1:A:233:ILE:O	2.07	0.52
1:A:263:TYR:HD2	1:A:263:TYR:C	2.10	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: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:147:MET:CE	1:B:220:THR:HG22	2.39	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: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: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:131:ARG:CG	1:C:132:HIS:ND1	2.72	0.52
1:C:302:ALA:O	1:C:307:VAL:HG22	2.09	0.52
1:D:147:MET:CE	1:D:220:THR:HG22	2.39	0.52
1:D:233:ILE:O	1:D:237:ARG:N	2.39	0.52
1:D:315:ALA:O	1:D:316:VAL:HG23	2.09	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:D:162:LYS:C	1:D:163:MET:HG2	2.29	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:134:LYS:HZ2	1:B:266:GLU:HG3	1.75	0.52
1:B:345:PRO:HB2	1:B:367:LEU:CD2	2.40	0.52
1:D:302:ALA:O	1:D:307:VAL:HG22	2.09	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:C:279:ARG:CD	1:C:295:MET:HE1	2.40	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:HG13	1:A:227:ILE:O	2.07	0.52
1:C:279:ARG:HD3	1:C:295:MET:HE2	1.92	0.52
1:C:389:LEU:HD12	1:C:389:LEU:O	2.10	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:298:LEU:C	1:D:300:LYS:N	2.63	0.52
1:D:153:PRO:HB2	1:D:369:ILE:HD11	1.91	0.52
1:A:102:PHE:HD1	1:A:102:PHE:N	2.07	0.51
1:A:254:VAL:O	1:A:281:MET:HE2	2.11	0.51
1:A:315:ALA:O	1:A:316:VAL:HG23	2.09	0.51
1:B:279:ARG:CD	1:B:295:MET:HE1	2.40	0.51
1:B:298:LEU:C	1:B:300:LYS:N	2.63	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:112:MET:HE2	1:B:115:LEU:HD11	1.93	0.51
1:B:233:ILE:O	1:B:237:ARG:N	2.39	0.51
1:C:321:GLY:O	1:C:322:ASN:C	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:LEU:HD12	1:A:389:LEU:O	2.10	0.51
1:A:60:LYS:O	1:A:61:LEU:C	2.49	0.51
1:D:134:LYS:HZ2	1:D:266:GLU:HG3	1.76	0.51
1:D:215:ALA:O	1:D:216:GLU:O	2.28	0.51
1:D:279:ARG:CD	1:D:295:MET:HE1	2.38	0.51
1:A:160:LYS:HZ2	1:A:373:GLY:CA	2.23	0.51
1:A:172:GLU:CB	1:A:172:GLU:CD	2.72	0.51
1:A:23:ARG:N	1:A:23:ARG:HE	2.00	0.51
1:A:345:PRO:HB2	1:A:367:LEU:CD2	2.40	0.51
1:B:120:LEU:C	1:B:120:LEU:HD13	2.31	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:B:51:SER:OG	1:B:52:ILE:N	2.41	0.51
1:B:98:LEU:HD11	1:B:301:ALA:CB	2.36	0.51
1:C:286:THR:HG21	1:C:295:MET:HA	1.91	0.51
1:D:254:VAL:O	1:D:281:MET:HE2	2.11	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:59:TRP:CG	1:C:60:LYS:N	2.79	0.51
1:A:120:LEU:C	1:A:120:LEU:HD13	2.31	0.51
1:A:192:THR:OG1	1:A:193:SER:N	2.41	0.51
1:A:59:TRP:CG	1:A:60:LYS:N	2.79	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:102:PHE:O	1:D:103:SER:C	2.49	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: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:B:231:VAL:HG13	1:B:234:MET:HE2	1.93	0.51
1:B:384:ALA:HB1	1:B:411:GLU:CB	2.41	0.51
1:B:59:TRP:CG	1:B:60:LYS:N	2.79	0.51
1:C:141:GLN:CA	1:C:141:GLN:CD	2.79	0.51
1:C:60:LYS:O	1:C:61:LEU:C	2.49	0.51
1:A:151:ASP:O	1:A:152:ARG:O	2.28	0.51
1:A:325:GLU:O	1:A:326:ILE:C	2.49	0.51
1:B:60:LYS:O	1:B:61:LEU:C	2.49	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151:ASP:O	1:C:152:ARG:O	2.28	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:B:102:PHE:O	1:B:103:SER:C	2.49	0.51
1:B:141:GLN:CA	1:B:141:GLN:CD	2.79	0.51
1:B:151:ASP:O	1:B:152:ARG:O	2.28	0.51
1:C:254:VAL:O	1:C:281:MET:HE2	2.11	0.51
1:D:141:GLN:CA	1:D:141:GLN:CD	2.79	0.51
1:D:178:TRP:CD1	1:D:221:LYS:HB3	2.46	0.51
1:D:60:LYS:O	1:D:61:LEU:C	2.49	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
1:C:95:GLU:OE1	1:C:132:HIS:CE1	2.64	0.50
1:C:227:ILE:HG13	1:C:227:ILE:O	2.07	0.50
1:D:117:ASN:ND2	1:D:290:ARG:CB	2.63	0.50
1:D:95:GLU:OE1	1:D:132:HIS:CE1	2.64	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:A:141:GLN:CD	1:A:141:GLN:CA	2.79	0.50
1:B:28:VAL:HG11	1:B:30:TYR:CZ	2.47	0.50
1:C:120:LEU:C	1:C:120:LEU:HD13	2.31	0.50
1:C:233:ILE:O	1:C:237:ARG:N	2.39	0.50
1:D:112:MET:HE2	1:D:115:LEU:HD11	1.91	0.50
1:D:231:VAL:CG1	1:D:234:MET:CE	2.84	0.50
1:A:157:THR:HG21	1:A:177:LEU:CD2	2.41	0.50
1:A:56:THR:CG2	1:A:56:THR:CA	2.87	0.50
1:B:281:MET:O	1:B:281:MET:CG	2.54	0.50
1:B:34:PRO:HB3	1:B:37:VAL:HG23	1.93	0.50
1:C:10:TRP:CE3	1:C:10:TRP:CA	2.91	0.50
1:C:278:HIS:CG	1:C:311:HIS:CE1	2.98	0.50
1:C:281:MET:CG	1:C:281:MET:O	2.54	0.50
1:C:28:VAL:HG11	1:C:30:TYR:CZ	2.46	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:CG	1:A:137:GLN:O	2.60	0.50
1:A:298:LEU:C	1:A:300:LYS:N	2.63	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:347:ALA:HB3	1:B:369:ILE:HA	1.93	0.50
1:C:325:GLU:O	1:C:326:ILE:C	2.49	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:157:THR:HG21	1:D:177:LEU:CD2	2.41	0.50
1:D:98:LEU:HD11	1:D:301:ALA:CB	2.36	0.50
1:A:212:ARG:O	1:A:216:GLU:HB2	2.12	0.50
1:A:147:MET:HE3	1:A:220:THR:HG22	1.94	0.50
1:A:286:THR:HG22	1:A:295:MET:N	2.27	0.50
1:C:102:PHE:O	1:C:103:SER:C	2.49	0.50
1:B:55:TRP:CH2	1:C:376:MET:O	2.65	0.50
1:D:81:GLY:C	1:D:82:TYR:CD2	2.85	0.50
1:A:231:VAL:HG13	1:A:234:MET:HE3	1.89	0.50
1:A:231:VAL:HA	1:A:234:MET:HE2	1.92	0.50
1:B:389:LEU:HD12	1:B:389:LEU:O	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:D:120:LEU:HD13	1:D:120:LEU:C	2.31	0.50
1:A:183:ASP:C	1:A:184:LEU:HD23	2.32	0.50
1:A:81:GLY:C	1:A:82:TYR:CD2	2.85	0.50
1:B:279:ARG:HD3	1:B:295:MET:HE2	1.92	0.50
1:C:298:LEU:C	1:C:300:LYS:N	2.63	0.50
1:C:347:ALA:HB3	1:C:369:ILE:HA	1.93	0.50
1:C:47:ALA:HB1	1:C:70:ALA:HB3	1.93	0.50
1:D:315:ALA:C	1:D:316:VAL:CG2	2.80	0.50
1:D:384:ALA:HB1	1:D:411:GLU:CB	2.41	0.50
1:A:95:GLU:OE1	1:A:132:HIS:CE1	2.64	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
1:B:157:THR:HG21	1:B:177:LEU:CD2	2.41	0.50
1:B:15:VAL:HG13	1:B:72:VAL:HG23	1.92	0.50
1:B:183:ASP:C	1:B:184:LEU:HD23	2.32	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:137:GLN:HB2	1:C:265:ARG:CZ	2.42	0.50
1:C:315:ALA:C	1:C:316:VAL:CG2	2.80	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:B:176:GLU:HG3	1:C:59:TRP:CH2	2.46	0.50
1:D:28:VAL:HG11	1:D:30:TYR:CZ	2.47	0.50
1:A:315:ALA:C	1:A:316:VAL:CG2	2.80	0.50
1:A:343:VAL:HG12	1:A:344:PHE:H	1.76	0.50
1:A:64:MET:HG3	1:A:64:MET:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:ARG:O	1:B:216:GLU:HB2	2.12	0.50
1:B:315:ALA:C	1:B:316:VAL:CG2	2.80	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:279:ARG:HH11	1:A:295:MET:HE2	1.77	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:183:ASP:C	1:D:184:LEU:HD23	2.32	0.49
1:A:174:ALA:O	1:A:175:TYR:C	2.49	0.49
1:A:51:SER:OG	1:A:52:ILE:N	2.41	0.49
1:C:81:GLY:C	1:C:82:TYR:CD2	2.85	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:160:LYS:CD	1:B:160:LYS:HE3	2.18	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:HG2	1:D:21:PRO:O	2.13	0.49
1:A:225:ILE:HG13	1:A:226:ASN:H	1.74	0.49
1:A:38:SER:HB2	1:A:40:GLU:H	1.77	0.49
1:B:130:LEU:HG	1:B:130:LEU:O	2.13	0.49
1:B:268:THR:HB	1:B:273:LEU:O	2.12	0.49
1:B:47:ALA:HB1	1:B:70:ALA:HB3	1.93	0.49
1:C:183:ASP:C	1:C:184:LEU:HD23	2.32	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:B:353:PRO:HG3	1:B:415:SER:HG	1.77	0.49
1:B:81:GLY:C	1:B:82:TYR:CD2	2.85	0.49
1:D:55:TRP:CH2	1:D:58:LEU:N	2.76	0.49
1:A:130:LEU:HG	1:A:130:LEU:O	2.13	0.49
1:A:15:VAL:HG13	1:A:72:VAL:HG23	1.91	0.49
1:A:268:THR:HB	1:A:273:LEU:O	2.12	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: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:325:GLU:O	1:D:326:ILE:C	2.49	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:311:HIS:CD2	1:D:346:VAL:CG1	2.79	0.49
1:D:51:SER:OG	1:D:52:ILE:N	2.41	0.49
1:A:186:LYS:HZ1	1:A:278:HIS:CE1	2.31	0.49
1:A:19:TYR:HD1	1:A:21:PRO:HD3	1.78	0.49
1:A:377:GLY:O	1:A:378:HIS:C	2.49	0.49
1:B:112:MET:HE3	1:B:115:LEU:HD11	1.94	0.49
1:B:138:PHE:CD1	1:B:146:PHE:CE1	2.99	0.49
1:B:19:TYR:HD1	1:B:21:PRO:HD3	1.78	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:D:19:TYR:HD1	1:D:21:PRO:HD3	1.78	0.49
1:D:279:ARG:HD3	1:D:295:MET:HE2	1.94	0.49
1:A:293:ILE:CG2	1:A:297:ALA:HB3	2.43	0.49
1:A:98:LEU:HD11	1:A:301:ALA:CB	2.36	0.49
1:B:343:VAL:CG1	1:B:344:PHE:N	2.75	0.49
1:B:45:ARG:HA	1:B:48:SER:HB3	1.95	0.49
1:C:130:LEU:HG	1:C:130:LEU:O	2.13	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: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:A:137:GLN:HB2	1:A:265:ARG:CZ	2.42	0.49
1:B:21:PRO:O	1:B:21:PRO:HG2	2.13	0.49
1:B:300:LYS:HD2	1:B:337:TRP:CH2	2.47	0.49
1:B:32:PHE:HE2	1:B:42:ALA:HB3	1.78	0.49
1:B:336:LYS:HD3	1:B:336:LYS:CE	2.20	0.49
1:C:205:LYS:O	1:C:209:VAL:CG2	2.61	0.49
1:A:254:VAL:HG23	1:A:279:ARG:HA	1.95	0.49
1:A:319:MET:C	1:A:321:GLY:H	2.16	0.49
1:A:32:PHE:HE2	1:A:42:ALA:HB3	1.78	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:C:298:LEU:C	1:C:300:LYS:H	2.16	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:HG13	1:B:227:ILE:O	2.07	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:C:134:LYS:HZ2	1:C:266:GLU:HG3	1.76	0.48
1:D:118:LEU:HD12	1:D:119:ARG:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:220:THR:CG2	1:D:221:LYS:N	2.76	0.48
1:D:64:MET:O	1:D:64:MET:HG3	2.12	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:B:231:VAL:HA	1:B:234:MET:HE2	1.94	0.48
1:B:325:GLU:O	1:B:326:ILE:C	2.49	0.48
1:C:174:ALA:O	1:C:175:TYR:C	2.49	0.48
1:C:231:VAL:HG13	1:C:234:MET:HE2	1.95	0.48
1:C:56:THR:CA	1:C:56:THR:CG2	2.87	0.48
1:C:64:MET:HG3	1:C:64:MET:O	2.12	0.48
1:D:254:VAL:HG23	1:D:279:ARG:HA	1.95	0.48
1:A:178:TRP:CZ2	1:A:185:LEU:HB2	2.48	0.48
1:A:21:PRO:HG2	1:A:21:PRO:O	2.13	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:206:LEU:HA	1:C:209:VAL:HG23	1.94	0.48
1:C:52:ILE:HD13	1:C:69:MET:HG2	1.96	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:102:PHE:O	1:A:103:SER:C	2.49	0.48
1:A:206:LEU:N	1:A:206:LEU:HD22	2.29	0.48
1:A:45:ARG:HA	1:A:48:SER:HB3	1.95	0.48
1:B:178:TRP:CZ2	1:B:185:LEU:HB2	2.48	0.48
1:B:83:ILE:HG22	1:B:83:ILE:O	2.14	0.48
1:C:189:GLU:HA	1:C:250:MET:CE	2.44	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:55:TRP:HZ2	1:C:377:GLY:HA2	1.78	0.48
1:B:27:ILE:HG23	1:B:87:ALA:HA	1.96	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:119:ARG:O	1:C:121:LEU:HD13	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:10:TRP:CA	1:D:10:TRP:CE3	2.91	0.48
1:D:296:LEU:HB2	1:D:329:ILE:HG12	1.95	0.48
1:D:45:ARG:HA	1:D:48:SER:HB3	1.95	0.48
1:A:296:LEU:HB2	1:A:329:ILE:HG12	1.96	0.48
1:B:377:GLY:O	1:B:378:HIS:C	2.49	0.48
1:B:64:MET:O	1:B:64:MET:HG3	2.12	0.48
1:C:189:GLU:HB3	1:C:278:HIS:CE1	2.49	0.48
1:C:9:GLU:HG2	1:C:9:GLU:O	2.05	0.48
1:D:27:ILE:HG23	1:D:87:ALA:HA	1.96	0.48
1:D:298:LEU:C	1:D:300:LYS:H	2.16	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:C:319:MET:C	1:C:321:GLY:H	2.17	0.48
1:D:166:SER:OG	1:D:169:GLU:HG3	2.14	0.48
1:D:193:SER:OG	1:D:199:PHE:N	2.46	0.48
1:D:189:GLU:HA	1:D:250:MET:CE	2.44	0.48
1:D:254:VAL:HG12	1:D:281:MET:HE3	1.96	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
1:C:186:LYS:HZ1	1:C:278:HIS:CE1	2.32	0.48
1:A:189:GLU:HB3	1:A:278:HIS:CE1	2.49	0.48
1:A:83:ILE:O	1:A:83:ILE:HG22	2.14	0.48
1:B:57:THR:CA	1:B:57:THR:CG2	2.87	0.48
1:C:293:ILE:CG2	1:C:297:ALA:HB3	2.43	0.48
1:C:332:PHE:O	1:C:332:PHE:CG	2.63	0.48
1:D:206:LEU:N	1:D:206:LEU:HD22	2.29	0.48
1:D:343:VAL:CG1	1:D:344:PHE:N	2.76	0.48
1:B:273:LEU:HD23	1:B:273:LEU:HA	1.66	0.47
1:B:319:MET:C	1:B:321:GLY:H	2.16	0.47
1:C:254:VAL:HG12	1:C:281:MET:HE3	1.96	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: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:298:LEU:C	1:B:300:LYS:H	2.16	0.47
1:B:296:LEU:HB2	1:B:329:ILE:HG12	1.95	0.47
1:C:193:SER:OG	1:C:199:PHE:N	2.46	0.47
1:D:112:MET:HE3	1:D:115:LEU:HD11	1.95	0.47
1:D:138:PHE:CD1	1:D:146:PHE:CE1	2.99	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:225:ILE:HG13	1:D:226:ASN:H	1.74	0.47
1:A:166:SER:OG	1:A:169:GLU:HG3	2.14	0.47
1:A:88:TYR:HA	1:A:89:PRO:HD3	1.69	0.47
1:B:108:ASN:N	1:B:108:ASN:OD1	2.48	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:C:57:THR:CA	1:C:57:THR:CG2	2.87	0.47
1:D:172:GLU:CD	1:D:172:GLU:CB	2.72	0.47
1:A:108:ASN:N	1:A:108:ASN:OD1	2.48	0.47
1:A:263:TYR:HE2	1:A:267:VAL:CG2	2.27	0.47
1:A:56:THR:C	1:A:56:THR:CB	2.81	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:N	1:C:206:LEU:HD22	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:A:55:TRP:CH2	1:A:58:LEU:N	2.76	0.47
1:B:206:LEU:HD22	1:B:206:LEU:N	2.29	0.47
1:C:167:VAL:HG23	1:C:196:PHE:O	2.15	0.47
1:C:211:ASP:O	1:C:212:ARG:C	2.52	0.47
1:D:147:MET:HE3	1:D:220:THR:HG22	1.95	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:A:211:ASP:O	1:A:212:ARG:C	2.53	0.47
1:B:30:TYR:CE1	1:B:120:LEU:HD22	2.50	0.47
1:B:351:LEU:N	1:B:351:LEU:HD12	2.28	0.47
1:C:192:THR:OG1	1:C:193:SER:N	2.41	0.47
1:D:319:MET:C	1:D:321:GLY:H	2.17	0.47
1:D:400:VAL:H	1:D:400:VAL:HG23	1.42	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:294:THR:C	1:C:296:LEU:N	2.68	0.47
1:D:263:TYR:HE2	1:D:267:VAL:CG2	2.28	0.47
1:D:189:GLU:HB3	1:D:278:HIS:CE1	2.49	0.47
1:A:294:THR:C	1:A:296:LEU:N	2.68	0.47
1:A:195:PRO:HG2	1:B:131:ARG:HE	1.80	0.47
1:B:174:ALA:O	1:B:175:TYR:C	2.49	0.47
1:C:147:MET:HE3	1:C:220:THR:HG22	1.97	0.47
1:C:253:ILE:HG21	1:C:253:ILE:HD12	1.62	0.47
1:D:170:TYR:CE1	1:D:191:PHE:HE1	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:LEU:HA	1:A:154:LEU:HD23	1.40	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:A:189:GLU:HA	1:A:250:MET:CE	2.44	0.47
1:A:57:THR:CG2	1:A:57:THR:CA	2.87	0.47
1:B:172:GLU:CB	1:B:172:GLU:CD	2.72	0.47
1:B:332:PHE:O	1:B:332:PHE:CG	2.63	0.47
1:B:56:THR:CB	1:B:56:THR:C	2.81	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:C:377:GLY:O	1:C:378:HIS:C	2.49	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: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:56:THR:CA	1:B:56:THR:CG2	2.87	0.47
1:B:52:ILE:HD13	1:B:69:MET:HG2	1.96	0.47
1:C:108:ASN:N	1:C:108:ASN:OD1	2.48	0.47
1:C:383:ARG:HG2	1:C:383:ARG:O	2.15	0.47
1:D:174:ALA:O	1:D:175:TYR:C	2.49	0.47
1:A:30:TYR:CE1	1:A:120:LEU:HD22	2.50	0.46
1:A:332:PHE:O	1:A:332:PHE:CG	2.63	0.46
1:B:58:LEU:O	1:B:58:LEU:CD1	2.63	0.46
1:C:172:GLU:CB	1:C:172:GLU:CD	2.72	0.46
1:C:225:ILE:HG13	1:C:226:ASN:H	1.74	0.46
1:D:167:VAL:HG23	1:D:196:PHE:O	2.15	0.46
1:C:30:TYR:CE1	1:C:120:LEU:HD22	2.50	0.46
1:D:378:HIS:HE1	1:D:380:ASP:CB	2.14	0.46
1:D:58:LEU:O	1:D:58:LEU:CD1	2.63	0.46
1:A:279:ARG:O	1:A:281:MET:N	2.48	0.46
1:A:11:TYR:CE2	1:A:45:ARG:HG2	2.51	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:C:268:THR:HG23	1:C:268:THR:H	1.42	0.46
1:C:27:ILE:HG23	1:C:87:ALA:HA	1.96	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:298:LEU:C	1:A:300:LYS:H	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:47:ALA:HB2	1:D:86:ILE:HG21	1.97	0.46
1:A:254:VAL:HG12	1:A:281:MET:HE3	1.96	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:279:ARG:O	1:C:281:MET:N	2.48	0.46
1:C:47:ALA:HB2	1:C:86:ILE:HG21	1.97	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:B:352:HIS:O	1:B:353:PRO:C	2.54	0.46
1:C:352:HIS:O	1:C:353:PRO:C	2.54	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:401:ASP:CB	1:A:404:GLU:HG2	2.36	0.46
1:B:383:ARG:O	1:B:383:ARG:HG2	2.15	0.46
1:D:279:ARG:O	1:D:281:MET:N	2.48	0.46
1:D:387:LYS:HE3	2:D:465:HOH:O	2.16	0.46
1:A:352:HIS:O	1:A:353:PRO:C	2.54	0.46
1:A:409:SER:HB3	1:A:412:LEU:HB3	1.98	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:B:47:ALA:HB2	1:B:86:ILE:HG21	1.97	0.46
1:C:187:ASP:OD1	1:C:223:TYR:HE1	1.99	0.46
1:C:154:LEU:CB	1:C:368:VAL:HG13	2.44	0.46
1:B:55:TRP:CZ2	1:C:376:MET:O	2.69	0.46
1:C:32:PHE:CE2	1:C:42:ALA:HB3	2.51	0.46
1:D:56:THR:CA	1:D:56:THR:CG2	2.87	0.46
1:A:126:PRO:O	1:A:127:TYR:O	2.34	0.46
1:A:210:ARG:HD3	1:A:221:LYS:O	2.16	0.46
1:A:189:GLU:CB	1:A:278:HIS:CE1	2.99	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:210:ARG:HD3	1:C:221:LYS:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:189:GLU:CB	1:C:278:HIS:CE1	2.99	0.46
1:D:160:LYS:HZ2	1:D:373:GLY:CA	2.28	0.46
1:D:177:LEU:HA	1:D:177:LEU:HD23	1.75	0.46
1:A:187:ASP:OD1	1:A:223:TYR:HE1	1.99	0.46
1:A:58:LEU:O	1:A:58:LEU:CD1	2.63	0.46
1:B:189:GLU:CB	1:B:278:HIS:CE1	2.99	0.46
1:B:182:ILE:HG12	1:B:386:ALA:HB1	1.98	0.46
1:D:175:TYR:CE2	1:D:213:VAL:CG2	2.99	0.46
1:B:126:PRO:O	1:B:127:TYR:O	2.34	0.45
1:B:282:HIS:CG	1:B:283:ALA:N	2.84	0.45
1:B:294:THR:C	1:B:296:LEU:N	2.68	0.45
1:B:296:LEU:N	1:B:329:ILE:HD11	2.31	0.45
1:B:55:TRP:CE2	1:B:57:THR:HG21	2.51	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:282:HIS:CG	1:D:283:ALA:N	2.84	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:HG22	1:D:83:ILE:O	2.14	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: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:231:VAL:HA	1:D:234:MET:HE2	1.99	0.45
1:D:341:ARG:HB2	1:D:342:PRO:HD2	1.98	0.45
1:D:182:ILE:HG12	1:D:386:ALA:HB1	1.98	0.45
1:A:144:ARG:NH1	1:A:150:LYS:O	2.49	0.45
1:B:110:PHE:C	1:C:283:ALA:CB	2.83	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:B:279:ARG:HH11	1:B:295:MET:HE2	1.81	0.45
1:C:279:ARG:HH11	1:C:295:MET:HE2	1.81	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:D:294:THR:C	1:D:296:LEU:N	2.68	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:282:HIS:CG	1:A:283:ALA:N	2.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:ARG:HG2	1:A:383:ARG:O	2.15	0.45
1:A:75:LEU:HD12	1:A:75:LEU:C	2.37	0.45
1:B:32:PHE:C	1:B:33:GLU:HG3	2.37	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:CG	1:C:283:ALA:N	2.84	0.45
1:D:108:ASN:N	1:D:108:ASN:OD1	2.48	0.45
1:D:126:PRO:O	1:D:127:TYR:O	2.34	0.45
1:D:279:ARG:HH11	1:D:295:MET:HE2	1.82	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: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:B:11:TYR:HD2	1:B:45:ARG:HA	1.82	0.45
1:B:154:LEU:CB	1:B:368:VAL:HG13	2.44	0.45
1:B:404:GLU:O	1:B:407:LYS:HB2	2.16	0.45
1:B:32:PHE:CE2	1:B:42:ALA:HB3	2.51	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:B:192:THR:OG1	1:C:94:GLU:OE1	2.19	0.45
1:A:138:PHE:CE1	1:A:146:PHE:HE1	2.34	0.45
1:A:160:LYS:HZ1	1:A:373:GLY:N	2.04	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:A:17:LEU:CD2	1:A:74:TYR:N	2.80	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:HA	1:B:269:GLU:OE1	2.16	0.45
1:B:271:LEU:H	1:B:271:LEU:HG	1.47	0.45
1:B:153:PRO:HB2	1:B:369:ILE:CD1	2.46	0.45
1:B:98:LEU:HD23	1:B:99:VAL:N	2.32	0.45
1:C:322:ASN:O	1:C:324:GLU:N	2.50	0.45
1:C:32:PHE:C	1:C:33:GLU:HG3	2.37	0.45
1:C:404:GLU:O	1:C:407:LYS:HB2	2.16	0.45
1:C:98:LEU:HD23	1:C:99:VAL:N	2.32	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:D:43:ALA:HB1	1:D:72:VAL:HG11	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:185:LEU:HA	1:D:185:LEU:HD12	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:117:ASN:ND2	1:A:290:ARG:CB	2.63	0.45
1:A:11:TYR:HD2	1:A:45:ARG:HA	1.82	0.45
1:A:205:LYS:O	1:A:209:VAL:CG2	2.61	0.45
1:A:387:LYS:HE3	2:A:466:HOH:O	2.16	0.45
1:C:125:PRO:HA	1:C:126:PRO:HD2	1.69	0.45
1:C:231:VAL:HA	1:C:234:MET:HE2	1.98	0.45
1:B:263:TYR:HD1	1:C:232:ASN:ND2	2.14	0.45
1:C:341:ARG:HB2	1:C:342:PRO:HD2	1.98	0.45
1:D:187:ASP:OD1	1:D:223:TYR:HE1	1.99	0.45
1:D:130:LEU:O	1:D:339:HIS:CE1	2.70	0.45
1:D:409:SER:HB3	1:D:412:LEU:HB3	1.98	0.45
1:D:98:LEU:HD23	1:D:99:VAL:N	2.32	0.45
1:A:176:GLU:OE1	1:A:383:ARG:NH1	2.50	0.45
1:A:177:LEU:HA	1:A:177:LEU:HD23	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:387:LYS:HE3	2:C:466:HOH:O	2.16	0.45
1:D:168:GLU:O	1:D:170:TYR:N	2.50	0.45
1:D:206:LEU:CA	1:D:209:VAL:HG23	2.47	0.45
1:D:189:GLU:CB	1:D:278:HIS:CE1	2.99	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:43:ALA:HB1	1:A:72:VAL:HG11	1.99	0.45
1:B:211:ASP:O	1:B:212:ARG:C	2.52	0.45
1:B:186:LYS:NZ	1:B:278:HIS:CE1	2.85	0.45
1:B:419:VAL:CA	1:B:419:VAL:CG2	2.89	0.45
1:B:11:TYR:CE2	1:B:45:ARG:HG2	2.51	0.45
1:C:126:PRO:O	1:C:127:TYR:O	2.34	0.45
1:C:159:PRO:HB3	1:C:173:ILE:HD12	1.99	0.45
1:C:160:LYS:HE2	1:C:160:LYS:CD	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:210:ARG:HD3	1:D:221:LYS:O	2.16	0.45
1:D:186:LYS:NZ	1:D:278:HIS:CE1	2.85	0.45
1:D:322:ASN:O	1:D:324:GLU:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:336:LYS:O	1:D:337:TRP:CB	2.62	0.45
1:A:32:PHE:C	1:A:33:GLU:HG3	2.37	0.44
1:A:404:GLU:O	1:A:407:LYS:HB2	2.16	0.44
1:B:160:LYS:HE2	1:B:160:LYS:CD	2.18	0.44
1:B:130:LEU:O	1:B:339:HIS:CE1	2.70	0.44
1:C:112:MET:HE3	1:C:115:LEU:HD11	1.98	0.44
1:C:186:LYS:NZ	1:C:278:HIS:CE1	2.85	0.44
1:B:232:ASN:ND2	1:C:263:TYR:HD1	2.15	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:C:43:ALA:HB1	1:C:72:VAL:HG11	1.99	0.44
1:C:75:LEU:HD12	1:C:75:LEU:C	2.37	0.44
1:D:296:LEU:N	1:D:329:ILE:HD11	2.31	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:263:TYR:O	1:B:263:TYR:CD2	2.70	0.44
1:B:176:GLU:OE1	1:B:383:ARG:NH1	2.50	0.44
1:B:409:SER:HA	1:B:410:PRO:HD2	1.63	0.44
1:B:283:ALA:CB	1:C:110:PHE:C	2.86	0.44
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:D:377:GLY:O	1:D:378:HIS:C	2.49	0.44
1:D:75:LEU:HD12	1:D:75:LEU:C	2.37	0.44
1:A:263:TYR:O	1:A:263:TYR:CD2	2.70	0.44
1:A:341:ARG:HB2	1:A:342:PRO:HD2	1.98	0.44
1:A:98:LEU:HD23	1:A:99:VAL:N	2.32	0.44
1:B:175:TYR:O	1:B:179:SER:HB2	2.18	0.44
1:B:293:ILE:HG22	1:B:294:THR:N	2.28	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:A:297:ALA:O	1:A:300:LYS:HB3	2.17	0.44
1:B:121:LEU:N	1:B:121:LEU:CD1	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:269:GLU:HA	1:C:269:GLU:OE1	2.16	0.44
1:C:176:GLU:OE1	1:C:383:ARG:NH1	2.50	0.44
1:D:211:ASP:O	1:D:212:ARG:C	2.53	0.44
1:D:32:PHE:C	1:D:33:GLU:HG3	2.37	0.44
1:D:94:GLU:HG2	1:D:97:SER:CB	2.40	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:GLN:O	1:A:103:SER:N	2.51	0.44
1:A:340:ILE:HG12	1:A:340:ILE:H	1.50	0.44
1:B:278:HIS:CD2	1:B:280:ALA:CB	2.99	0.44
1:B:43:ALA:HB1	1:B:72:VAL:HG11	1.99	0.44
1:C:378:HIS:HA	1:C:379:PRO:HD2	1.61	0.44
1:C:390:ARG:HA	1:C:390:ARG:HD2	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:341:ARG:CB	1:B:342:PRO:CD	2.96	0.44
1:B:419:VAL:CG1	1:B:419:VAL:O	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:10:TRP:C	1:A:12:LEU:N	2.60	0.44
1:A:251:ILE:HG21	1:A:251:ILE:HD13	1.19	0.44
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: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:D:45:ARG:O	1:D:46:ILE:C	2.56	0.44
1:A:189:GLU:HA	1:A:250:MET:HE2	1.99	0.44
1:A:224:LEU:CD2	1:A:276:HIS:CD2	3.01	0.44
1:A:154:LEU:CB	1:A:368:VAL:HG13	2.44	0.44
1:B:17:LEU:CD2	1:B:74:TYR:N	2.79	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:A:268:THR:HG23	1:A:268:THR:H	1.42	0.44
1:B:261:LEU:O	1:B:261:LEU:CD2	2.66	0.44
1:B:75:LEU:C	1:B:75:LEU:HD12	2.37	0.44
1:B:78:HIS:CB	1:B:83:ILE:HG12	2.48	0.44
1:C:175:TYR:O	1:C:179:SER:HB2	2.17	0.44
1:C:263:TYR:O	1:C:263:TYR:CD2	2.71	0.44
1:C:56:THR:CB	1:C:56:THR:C	2.81	0.44
1:C:78:HIS:CB	1:C:83:ILE:HG12	2.48	0.44
1:D:127:TYR:HB3	1:D:128:GLU:H	1.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:189:GLU:HA	1:D:250:MET:HE2	2.00	0.44
1:D:392:ALA:HB2	1:D:412:LEU:HD13	1.99	0.44
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:55:TRP:CE3	1:A:57:THR:HG23	2.48	0.43
1:B:46:ILE:HA	1:B:112:MET:HE1	2.00	0.43
1:B:143:ILE:HD11	1:B:308:ASP:HB2	2.00	0.43
1:B:147:MET:HE3	1:B:220:THR:HG22	1.98	0.43
1:B:23:ARG:N	1:B:23:ARG:HE	2.00	0.43
1:B:297:ALA:O	1:B:300:LYS:HB3	2.17	0.43
1:C:367:LEU:HD23	1:C:367:LEU:HA	1.63	0.43
1:D:231:VAL:HG13	1:D:234:MET:HE2	1.96	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:A:120:LEU:HD13	1:A:121:LEU:N	2.33	0.43
1:A:121:LEU:N	1:A:121:LEU:CD1	2.81	0.43
1:A:269:GLU:HA	1:A:269:GLU:OE1	2.16	0.43
1:B:100:GLN:O	1:B:103:SER:N	2.51	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:B:55:TRP:NE1	1:B:57:THR:HG21	2.33	0.43
1:C:168:GLU:O	1:C:170:TYR:N	2.50	0.43
1:B:288:ASN:ND2	1:C:288:ASN:HD21	2.14	0.43
1:C:311:HIS:CD2	1:C:346:VAL:HG12	2.50	0.43
1:D:199:PHE:CE1	1:D:203:VAL:HG11	2.53	0.43
1:A:191:PHE:CD2	1:A:194:PHE:CE1	3.06	0.43
1:B:200:GLU:O	1:B:204:ARG:HG3	2.18	0.43
1:B:199:PHE:CE1	1:B:203:VAL:HG11	2.53	0.43
1:B:261:LEU:HD22	1:B:261:LEU:O	2.19	0.43
1:C:199:PHE:CE1	1:C:203:VAL:HG11	2.53	0.43
1:C:182:ILE:HG12	1:C:386:ALA:HB1	1.98	0.43
1:C:11:TYR:HD2	1:C:45:ARG:HA	1.82	0.43
1:D:261:LEU:CD2	1:D:261:LEU:O	2.66	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:A:185:LEU:HA	1:A:185:LEU:HD12	1.68	0.43
1:A:45:ARG:O	1:A:46:ILE:C	2.56	0.43
1:A:79:GLY:O	1:A:81:GLY:N	2.51	0.43
1:B:231:VAL:HG13	1:B:234:MET:HE3	1.88	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:121:LEU:CD1	1:C:121:LEU:N	2.81	0.43
1:C:160:LYS:HZ2	1:C:373:GLY:CA	2.31	0.43
1:C:191:PHE:HD2	1:C:194:PHE:CE1	2.36	0.43
1:C:189:GLU:HA	1:C:250:MET:HE2	1.99	0.43
1:C:224:LEU:CD2	1:C:276:HIS:CD2	3.01	0.43
1:C:30:TYR:CE1	1:C:120:LEU:HD23	2.53	0.43
1:D:175:TYR:O	1:D:179:SER:HB2	2.18	0.43
1:D:231:VAL:HG12	1:D:234:MET:HE3	2.00	0.43
1:D:261:LEU:O	1:D:261:LEU:HD22	2.19	0.43
1:D:224:LEU:CD2	1:D:276:HIS:CD2	3.01	0.43
1:D:31:TYR:O	1:D:119:ARG:N	2.44	0.43
1:D:352:HIS:O	1:D:353:PRO:C	2.54	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:298:LEU:HD23	1:C:299:ALA:N	2.33	0.43
1:C:341:ARG:CB	1:C:342:PRO:CD	2.96	0.43
1:C:55:TRP:CH2	1:C:58:LEU:N	2.76	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: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:56:THR:C	1:D:56:THR:CB	2.81	0.43
1:B:189:GLU:HA	1:B:250:MET:HE2	2.01	0.43
1:B:191:PHE:CD2	1:B:194:PHE:CE1	3.06	0.43
1:B:94:GLU:HG2	1:B:97:SER:CB	2.40	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: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: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:130:LEU:C	1:C:132:HIS:H	2.22	0.43
1:C:261:LEU:O	1:C:261:LEU:HD22	2.19	0.43
1:C:27:ILE:O	1:C:123:PHE:HA	2.19	0.43
1:C:294:THR:O	1:C:295:MET:C	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:PRO:HB2	1:C:65:ALA:HB2	2.01	0.43
1:D:55:TRP:NE1	1:D:57:THR:HG21	2.33	0.43
1:A:130:LEU:C	1:A:132:HIS:H	2.22	0.43
1:A:160:LYS:HE3	1:A:160:LYS:CD	2.18	0.43
1:B:120:LEU:HD13	1:B:121:LEU:N	2.33	0.43
1:B:130:LEU:C	1:B:132:HIS:H	2.22	0.43
1:B:252:ASP:CB	1:B:255:VAL:CG2	2.89	0.43
1:B:62:PRO:HB2	1:B:65:ALA:HB2	2.01	0.43
1:A:112:MET:HE3	1:A:115:LEU:HD11	2.00	0.43
1:A:261:LEU:HD22	1:A:261:LEU:O	2.19	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:419:VAL:O	1:A:419:VAL:CG1	2.65	0.43
1:A:55:TRP:NE1	1:A:57:THR:HG21	2.33	0.43
1:B:386:ALA:O	1:B:387:LYS:C	2.57	0.43
1:D:294:THR:O	1:D:295:MET:C	2.57	0.43
1:D:17:LEU:CD2	1:D:74:TYR:N	2.79	0.43
1:A:294:THR:O	1:A:295:MET:C	2.57	0.43
1:A:363:PHE:CD1	1:A:363:PHE:N	2.85	0.43
1:B:213:VAL:HG13	1:B:217:THR:CG2	2.49	0.43
1:B:27:ILE:O	1:B:123:PHE:HA	2.19	0.43
1:B:294:THR:O	1:B:295:MET:C	2.57	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:A:298:LEU:HD23	1:A:299:ALA:N	2.33	0.42
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: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:401:ASP:OD1	1:C:403:ASP:HB2	2.20	0.42
1:D:213:VAL:HG13	1:D:217:THR:CG2	2.49	0.42
1:D:253:ILE:HG23	1:D:253:ILE:H	1.64	0.42
1:D:266:GLU:O	1:D:269:GLU:HB2	2.19	0.42
1:D:298:LEU:HD23	1:D:299:ALA:N	2.33	0.42
1:D:341:ARG:CB	1:D:342:PRO:CD	2.96	0.42
1:D:55:TRP:CE2	1:D:57:THR:HG21	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:HIS:CD2	1:A:280:ALA:CB	2.99	0.42
1:A:62:PRO:HB2	1:A:65:ALA:HB2	2.01	0.42
1:B:378:HIS:HE1	1:B:380:ASP:CB	2.14	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:270:ASP:OD1	1:C:270:ASP:N	2.51	0.42
1:C:45:ARG:O	1:C:46:ILE:C	2.56	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: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: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:D:311:HIS:CD2	1:D:346:VAL:HG12	2.50	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: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:C:177:LEU:HD23	1:C:177:LEU:HA	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: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:253:ILE:HG23	1:C:253:ILE:H	1.64	0.42
1:C:143:ILE:HD11	1:C:308:ASP:HB2	2.00	0.42
1:A:393:ILE:HD13	1:A:393:ILE:HG21	1.81	0.42
1:B:185:LEU:HD12	1:B:185:LEU:HA	1.68	0.42
1:C:266:GLU:O	1:C:269:GLU:HB2	2.18	0.42
1:C:322:ASN:OD1	1:C:324:GLU:HG2	2.20	0.42
1:D:130:LEU:C	1:D:132:HIS:H	2.22	0.42
1:D:328:ARG:HB3	1:D:329:ILE:H	1.71	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:A:110:PHE:HZ	1:A:293:ILE:HD13	1.85	0.42
1:A:112:MET:HE2	1:A:115:LEU:CD1	2.50	0.42
1:A:279:ARG:CD	1:A:295:MET:HE1	2.47	0.42
1:B:298:LEU:HD23	1:B:299:ALA:N	2.33	0.42
1:B:314:THR:CG2	1:B:348:SER:O	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:HIS:CD2	1:B:346:VAL:HG12	2.50	0.42
1:B:316:VAL:HG22	1:B:355:LEU:HD13	2.02	0.42
1:B:79:GLY:O	1:B:81:GLY:N	2.51	0.42
1:C:187:ASP:OD1	1:C:223:TYR:CE1	2.73	0.42
1:D:187:ASP:OD1	1:D:223:TYR:CE1	2.73	0.42
1:D:143:ILE:HD11	1:D:308:ASP:HB2	2.00	0.42
1:D:316:VAL:HG22	1:D:355:LEU:HD13	2.02	0.42
1:D:314:THR:CG2	1:D:348:SER:O	2.68	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: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:D:191:PHE:CD2	1:D:194:PHE:HE1	2.38	0.42
1:D:252:ASP:O	1:D:256:ALA:CB	2.68	0.42
1:A:105:VAL:HG13	1:A:105:VAL:H	1.51	0.42
1:A:270:ASP:OD1	1:A:270:ASP:N	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:C:163:MET:SD	1:C:190:ASN:HB3	2.60	0.42
1:C:252:ASP:O	1:C:256:ALA:CB	2.68	0.42
1:C:110:PHE:HZ	1:C:293:ILE:HD13	1.85	0.42
1:C:55:TRP:NE1	1:C:57:THR:HG21	2.33	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:D:19:TYR:HE1	1:D:21:PRO:CA	2.33	0.42
1:D:282:HIS:C	1:D:284:ALA:H	2.24	0.42
1:D:110:PHE:HZ	1:D:293:ILE:HD13	1.85	0.42
1:D:44:GLY:O	1:D:45:ARG:C	2.57	0.42
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:191:PHE:CD2	1:B:194:PHE:HE1	2.38	0.41
1:B:110:PHE:HZ	1:B:293:ILE:HD13	1.85	0.41
1:B:90:LEU:HD21	1:B:126:PRO:CG	2.46	0.41
1:C:206:LEU:HA	1:C:209:VAL:HG21	2.01	0.41
1:C:30:TYR:HE1	1:C:120:LEU:HD23	1.85	0.41
1:D:252:ASP:CB	1:D:255:VAL:CG2	2.89	0.41
1:D:30:TYR:HE1	1:D:120:LEU:HD23	1.85	0.41
1:A:206:LEU:HA	1:A:209:VAL:HG21	2.01	0.41
1:A:300:LYS:O	1:A:303:ARG:N	2.49	0.41
1:A:78:HIS:CB	1:A:83:ILE:HG12	2.48	0.41
1:B:206:LEU:HA	1:B:209:VAL:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:VAL:CG1	1:B:344:PHE:H	2.34	0.41
1:C:231:VAL:HG12	1:C:234:MET:HE3	2.01	0.41
1:C:237:ARG:HH21	1:C:237:ARG:HD2	1.56	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:HD3	1:D:336:LYS:CE	2.20	0.41
1:D:373:GLY:O	1:D:374:GLY:C	2.59	0.41
1:D:90:LEU:HD21	1:D:126:PRO:CG	2.45	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:73:PHE:N	1:A:73:PHE:CD2	2.88	0.41
1:B:117:ASN:ND2	1:B:290:ARG:CB	2.63	0.41
1:B:186:LYS:HZ1	1:B:278:HIS:CE1	2.38	0.41
1:C:393:ILE:HD13	1:C:393:ILE:HG21	1.81	0.41
1:D:37:VAL:CG2	1:D:114:ALA:HB1	2.49	0.41
1:A:163:MET:SD	1:A:190:ASN:HB3	2.60	0.41
1:A:140:VAL:HG23	1:A:342:PRO:O	2.21	0.41
1:A:46:ILE:HG12	1:A:112:MET:HE3	2.01	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:B:282:HIS:C	1:B:284:ALA:H	2.24	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:A:132:HIS:O	1:A:133:PHE:CD1	2.74	0.41
1:A:293:ILE:HG22	1:A:294:THR:N	2.28	0.41
1:A:386:ALA:O	1:A:387:LYS:C	2.57	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:HG22	1:B:225:ILE:H	1.43	0.41
1:B:253:ILE:HG21	1:B:253:ILE:HD12	1.63	0.41
1:B:388:ALA:C	1:B:390:ARG:N	2.74	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:188:ASP:C	1:C:190:ASN:H	2.19	0.41
1:C:336:LYS:O	1:C:337:TRP:CB	2.62	0.41
1:C:44:GLY:O	1:C:45:ARG:C	2.57	0.41
1:D:141:GLN:OE1	1:D:141:GLN:HA	2.20	0.41
1:D:166:SER:O	1:D:170:TYR:HB2	2.20	0.41
1:D:286:THR:CG2	1:D:293:ILE:O	2.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:140:VAL:HG23	1:B:342:PRO:O	2.21	0.41
1:B:30:TYR:HE1	1:B:120:LEU:HD23	1.85	0.41
1:C:169:GLU:O	1:C:173:ILE:HG22	2.21	0.41
1:C:388:ALA:C	1:C:390:ARG:N	2.74	0.41
1:C:32:PHE:CZ	1:C:43:ALA:HB2	2.56	0.41
1:D:378:HIS:HA	1:D:379:PRO:HD2	1.61	0.41
1:A:141:GLN:OE1	1:A:141:GLN:HA	2.20	0.41
1:A:400:VAL:H	1:A:400:VAL:HG23	1.42	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:367:LEU:HA	1:D:367:LEU:HD23	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:282:HIS:C	1:A:284:ALA:H	2.24	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:B:45:ARG:O	1:B:46:ILE:C	2.56	0.41
1:D:132:HIS:O	1:D:133:PHE:CD1	2.73	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:D:110:PHE:CE1	1:D:293:ILE:HD11	2.56	0.41
1:D:140:VAL:HG23	1:D:342:PRO:O	2.21	0.41
1:A:255:VAL:CG2	1:A:280:ALA:O	2.69	0.41
1:B:373:GLY:O	1:B:374:GLY:C	2.59	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: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:32:PHE:CZ	1:D:43:ALA:HB2	2.56	0.41
1:A:199:PHE:O	1:A:203:VAL:HG13	2.21	0.41
1:A:55:TRP:CE2	1:A:57:THR:HG21	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:GLU:O	1:B:383:ARG:HG3	2.21	0.41
1:C:150:LYS:HG3	1:C:151:ASP:N	2.36	0.41
1:C:31:TYR:O	1:C:119:ARG:N	2.44	0.41
1:C:73:PHE:N	1:C:73:PHE:CD2	2.88	0.41
1:D:46:ILE:HA	1:D:112:MET:HE1	2.01	0.41
1:D:128:GLU:OE1	1:D:128:GLU:HA	2.21	0.41
1:D:295:MET:HG3	1:D:329:ILE:CD1	2.51	0.41
1:D:332:PHE:CG	1:D:332:PHE:O	2.63	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:A:268:THR:HB	1:A:273:LEU:HB2	2.03	0.41
1:A:39:PRO:HG3	1:A:82:TYR:OH	2.21	0.41
1:B:111:GLY:O	1:B:112:MET:C	2.60	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: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:HA	1:A:367:LEU:HD23	1.63	0.40
1:A:378:HIS:HA	1:A:379:PRO:HD2	1.61	0.40
1:A:388:ALA:C	1:A:390:ARG:N	2.74	0.40
1:A:44:GLY:O	1:A:45:ARG:C	2.57	0.40
1:B:37:VAL:CG2	1:B:114:ALA:HB1	2.49	0.40
1:B:160:LYS:HZ2	1:B:373:GLY:CA	2.34	0.40
1:B:58:LEU:HA	1:B:58:LEU:HD22	1.87	0.40
1:C:282:HIS:C	1:C:284:ALA:H	2.24	0.40
1:C:316:VAL:HG22	1:C:355:LEU:HD13	2.02	0.40
1:C:336:LYS:HD2	1:C:336:LYS:CE	2.20	0.40
1:D:212:ARG:O	1:D:215:ALA:HB3	2.22	0.40
1:A:110:PHE:CE1	1:A:293:ILE:HD11	2.56	0.40
1:B:105:VAL:HG13	1:B:105:VAL:H	1.51	0.40
1:B:113:LYS:HZ1	1:C:318:LYS:NZ	2.19	0.40
1:B:150:LYS:HG3	1:B:151:ASP:N	2.36	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: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:B:295:MET:HG3	1:B:329:ILE:HD13	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:PRO:HG3	1:B:82:TYR:OH	2.21	0.40
1:C:154:LEU:HD23	1:C:154:LEU:HA	1.40	0.40
1:C:168:GLU:O	1:C:169:GLU:C	2.60	0.40
1:C:182:ILE:HG22	1:C:184:LEU:N	2.36	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:D:141:GLN:CG	1:D:141:GLN:NE2	2.75	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:D:386:ALA:O	1:D:387:LYS:C	2.57	0.40
1:D:43:ALA:HB3	1:D:75:LEU:CD2	2.51	0.40
1:A:252:ASP:CB	1:A:255:VAL:HG21	2.48	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:252:ASP:CB	1:C:255:VAL:HG21	2.48	0.40
1:C:340:ILE:HG12	1:C:340:ILE:H	1.50	0.40
1:C:39:PRO:HG3	1:C:82:TYR:OH	2.21	0.40
1:D:150:LYS:HG3	1:D:151:ASP:N	2.36	0.40
1:D:168:GLU:O	1:D:169:GLU:C	2.60	0.40
1:D:169:GLU:O	1:D:173:ILE:HG22	2.21	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: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:A:160:LYS:N	1:A:376:MET:CE	2.82	0.40
1:A:52:ILE:HD13	1:A:69:MET:CG	2.51	0.40
1:A:43:ALA:HB3	1:A:75:LEU:CD2	2.51	0.40
1:C:110:PHE:CE1	1:C:293:ILE:HD11	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:94:GLU:OE1	1:D:192:THR:OG1[2_555]	2.09	0.11
2:A:469:HOH:O	2:A:469:HOH:O[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

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	2
1	B	414/430 (96%)	298 (72%)	71 (17%)	45 (11%)	0	2
1	C	414/430 (96%)	298 (72%)	71 (17%)	45 (11%)	0	2
1	D	414/430 (96%)	298 (72%)	71 (17%)	45 (11%)	0	2
All	All	1656/1720 (96%)	1192 (72%)	284 (17%)	180 (11%)	0	2

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

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Mol	Chain	Res	Type
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
1	A	414	LYS
1	B	43	ALA
1	B	51	SER

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Mol	Chain	Res	Type
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
1	A	169	GLU
1	A	283	ALA
1	B	23	ARG

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Mol	Chain	Res	Type
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
1	C	349	GLY
1	C	350	GLY
1	C	373	GLY

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

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Mol	Chain	Res	Type
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%)	247 (73%)	91 (27%)	0	2
1	B	338/351 (96%)	247 (73%)	91 (27%)	0	2
1	C	338/351 (96%)	247 (73%)	91 (27%)	0	2
1	D	338/351 (96%)	247 (73%)	91 (27%)	0	2
All	All	1352/1404 (96%)	988 (73%)	364 (27%)	0	2

All (364) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	GLU
1	A	10	TRP
1	A	13	ASP
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
1	A	38	SER
1	A	39	PRO

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Mol	Chain	Res	Type
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	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	118	LEU
1	A	121	LEU
1	A	124	HIS
1	A	127	TYR
1	A	128	GLU
1	A	147	MET
1	A	152	ARG
1	A	163	MET
1	A	168	GLU
1	A	173	ILE
1	A	189	GLU
1	A	193	SER
1	A	195	PRO
1	A	198	ARG
1	A	203	VAL
1	A	205	LYS
1	A	216	GLU

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Mol	Chain	Res	Type
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	253	ILE
1	A	259	SER
1	A	262	GLN
1	A	263	TYR
1	A	271	LEU
1	A	282	HIS
1	A	285	PHE
1	A	286	THR
1	A	289	PRO
1	A	290	ARG
1	A	294	THR
1	A	298	LEU
1	A	300	LYS
1	A	303	ARG
1	A	304	MET
1	A	318	LYS
1	A	327	LYS
1	A	330	ASN
1	A	335	SER
1	A	341	ARG
1	A	342	PRO
1	A	344	PHE
1	A	351	LEU
1	A	359	LEU
1	A	360	ILE
1	A	365	LYS
1	A	368	VAL
1	A	370	GLN
1	B	9	GLU
1	B	10	TRP
1	B	13	ASP
1	B	15	VAL
1	B	16	ASP
1	B	18	ASN

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Mol	Chain	Res	Type
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	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
1	B	109	VAL
1	B	113	LYS
1	B	118	LEU
1	B	121	LEU
1	B	124	HIS
1	B	127	TYR
1	B	128	GLU
1	B	147	MET
1	B	152	ARG
1	B	163	MET
1	B	168	GLU
1	B	173	ILE

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Mol	Chain	Res	Type
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	216	GLU
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	253	ILE
1	B	259	SER
1	B	262	GLN
1	B	263	TYR
1	B	271	LEU
1	B	282	HIS
1	B	285	PHE
1	B	286	THR
1	B	289	PRO
1	B	290	ARG
1	B	294	THR
1	B	298	LEU
1	B	300	LYS
1	B	303	ARG
1	B	304	MET
1	B	318	LYS
1	B	327	LYS
1	B	330	ASN
1	B	335	SER
1	B	341	ARG
1	B	342	PRO
1	B	344	PHE
1	B	351	LEU
1	B	359	LEU
1	B	360	ILE
1	B	365	LYS
1	B	368	VAL

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Mol	Chain	Res	Type
1	B	370	GLN
1	C	9	GLU
1	C	10	TRP
1	C	13	ASP
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
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	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	118	LEU
1	C	121	LEU
1	C	124	HIS

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Mol	Chain	Res	Type
1	C	127	TYR
1	C	128	GLU
1	C	147	MET
1	C	152	ARG
1	C	163	MET
1	C	168	GLU
1	C	173	ILE
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	216	GLU
1	C	225	ILE
1	C	231	VAL
1	C	232	ASN
1	C	234	MET
1	C	240	MET
1	C	244	GLU
1	C	249	VAL
1	C	250	MET
1	C	253	ILE
1	C	259	SER
1	C	262	GLN
1	C	263	TYR
1	C	271	LEU
1	C	282	HIS
1	C	285	PHE
1	C	286	THR
1	C	289	PRO
1	C	290	ARG
1	C	294	THR
1	C	298	LEU
1	C	300	LYS
1	C	303	ARG
1	C	304	MET
1	C	318	LYS
1	C	327	LYS
1	C	330	ASN
1	C	335	SER
1	C	341	ARG

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Mol	Chain	Res	Type
1	C	342	PRO
1	C	344	PHE
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	D	9	GLU
1	D	10	TRP
1	D	13	ASP
1	D	15	VAL
1	D	16	ASP
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	91	THR
1	D	94	GLU
1	D	95	GLU
1	D	98	LEU
1	D	100	GLN

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Mol	Chain	Res	Type
1	D	103	SER
1	D	105	VAL
1	D	109	VAL
1	D	113	LYS
1	D	118	LEU
1	D	121	LEU
1	D	124	HIS
1	D	127	TYR
1	D	128	GLU
1	D	147	MET
1	D	152	ARG
1	D	163	MET
1	D	168	GLU
1	D	173	ILE
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	216	GLU
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	253	ILE
1	D	259	SER
1	D	262	GLN
1	D	263	TYR
1	D	271	LEU
1	D	282	HIS
1	D	285	PHE
1	D	286	THR
1	D	289	PRO
1	D	290	ARG
1	D	294	THR
1	D	298	LEU
1	D	300	LYS

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Mol	Chain	Res	Type
1	D	303	ARG
1	D	304	MET
1	D	318	LYS
1	D	327	LYS
1	D	330	ASN
1	D	335	SER
1	D	341	ARG
1	D	342	PRO
1	D	344	PHE
1	D	351	LEU
1	D	359	LEU
1	D	360	ILE
1	D	365	LYS
1	D	368	VAL
1	D	370	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	100	GLN
1	A	117	ASN
1	A	137	GLN
1	A	226	ASN
1	A	276	HIS
1	A	282	HIS
1	A	291	HIS
1	A	311	HIS
1	A	330	ASN
1	A	339	HIS
1	A	370	GLN
1	B	35	ASN
1	B	100	GLN
1	B	117	ASN
1	B	137	GLN
1	B	226	ASN
1	B	276	HIS
1	B	282	HIS
1	B	291	HIS
1	B	311	HIS
1	B	330	ASN
1	B	339	HIS

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Mol	Chain	Res	Type
1	B	370	GLN
1	C	35	ASN
1	C	100	GLN
1	C	117	ASN
1	C	137	GLN
1	C	226	ASN
1	C	276	HIS
1	C	282	HIS
1	C	288	ASN
1	C	291	HIS
1	C	311	HIS
1	C	330	ASN
1	C	339	HIS
1	C	370	GLN
1	D	35	ASN
1	D	100	GLN
1	D	117	ASN
1	D	137	GLN
1	D	226	ASN
1	D	276	HIS
1	D	282	HIS
1	D	291	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 carbohydrates 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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	416/430 (96%)	-0.01	11 (2%) 56 27	61, 89, 123, 154	0
1	B	416/430 (96%)	0.10	10 (2%) 59 30	61, 89, 123, 154	0
1	C	416/430 (96%)	0.22	31 (7%) 14 4	61, 89, 123, 154	0
1	D	416/430 (96%)	0.24	23 (5%) 25 9	61, 89, 123, 154	0
All	All	1664/1720 (96%)	0.14	75 (4%) 33 12	61, 89, 123, 154	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	422	SER	13.2
1	D	424	ALA	12.2
1	D	57	THR	10.5
1	C	424	ALA	6.9
1	D	420	GLY	6.7
1	D	423	LYS	6.0
1	D	418	GLU	5.9
1	D	421	LEU	5.3
1	C	423	LYS	4.4
1	D	280	ALA	4.4
1	C	278	HIS	4.3
1	C	421	LEU	4.0
1	B	278	HIS	4.0
1	C	422	SER	3.9
1	D	257	GLY	3.8
1	C	420	GLY	3.7
1	A	419	VAL	3.7
1	C	402	LEU	3.7
1	D	278	HIS	3.7
1	C	257	GLY	3.5
1	A	107	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	108	ASN	3.4
1	A	278	HIS	3.3
1	C	419	VAL	3.2
1	D	107	GLY	3.2
1	C	311	HIS	3.0
1	D	395	ALA	3.0
1	D	19	TYR	3.0
1	B	107	GLY	2.9
1	D	255	VAL	2.9
1	B	280	ALA	2.9
1	B	419	VAL	2.8
1	C	82	TYR	2.8
1	A	87	ALA	2.8
1	A	108	ASN	2.7
1	A	405	LYS	2.6
1	C	315	ALA	2.6
1	B	9	GLU	2.6
1	C	59	TRP	2.6
1	C	397	ILE	2.6
1	B	257	GLY	2.5
1	B	277	ALA	2.5
1	D	254	VAL	2.5
1	B	279	ARG	2.5
1	C	60	LYS	2.5
1	C	108	ASN	2.5
1	C	416	LEU	2.5
1	C	258	TRP	2.5
1	C	406	ALA	2.4
1	D	11	TYR	2.4
1	D	108	ASN	2.4
1	C	348	SER	2.4
1	A	103	SER	2.4
1	D	283	ALA	2.4
1	C	418	GLU	2.4
1	A	279	ARG	2.3
1	D	252	ASP	2.3
1	C	280	ALA	2.3
1	B	252	ASP	2.3
1	A	281	MET	2.2
1	D	400	VAL	2.2
1	C	365	LYS	2.2
1	D	282	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	255	VAL	2.2
1	C	11	TYR	2.2
1	C	320	ALA	2.1
1	D	20	GLU	2.1
1	C	281	MET	2.1
1	A	68	SER	2.1
1	C	75	LEU	2.1
1	C	107	GLY	2.1
1	C	254	VAL	2.1
1	D	419	VAL	2.0
1	C	36	GLY	2.0
1	A	282	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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.