



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:03 AM UTC

PDB ID : 4GPD / pdb_00004gpd
Title : THE STRUCTURE OF LOBSTER APO-D-GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE AT 3.0 ANGSTROMS RESOLUTION
Authors : Griffith, J.P.; Song, S.; Rossmann, M.G.
Deposited on : 1988-01-04
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

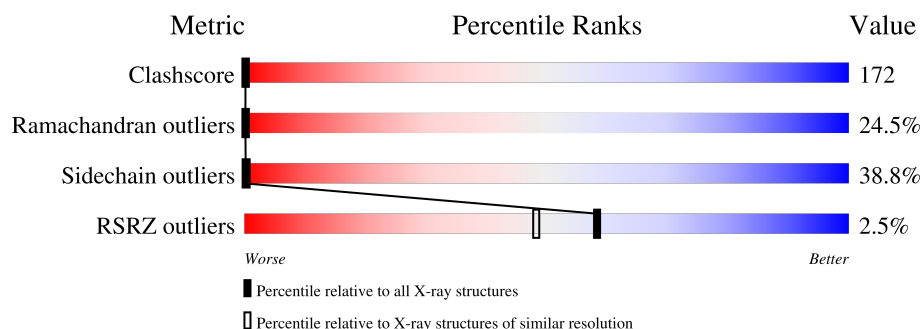
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	1	333	2% 5% 19% 41% 35%
1	2	333	2% 5% 21% 40% 35%
1	3	333	2% 5% 19% 42% 36%
1	4	333	3% 5% 20% 43% 33%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10150 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 APO-D-GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	333	Total	C	N	O	S	0	0	0
			2507	1591	419	482	15			
1	2	333	Total	C	N	O	S	0	0	0
			2507	1591	419	482	15			
1	3	333	Total	C	N	O	S	0	0	0
			2507	1591	419	482	15			
1	4	333	Total	C	N	O	S	0	0	0
			2507	1591	419	482	15			

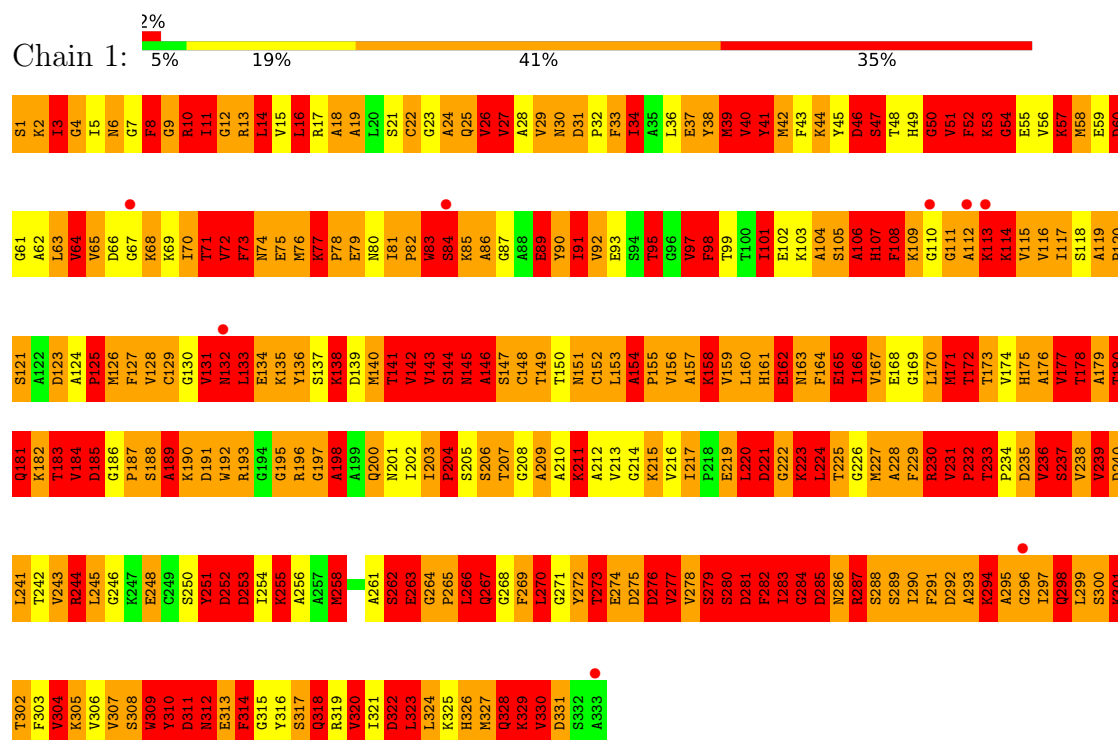
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	1	23	Total	O	0	0
			23	23		
2	2	28	Total	O	0	0
			28	28		
2	3	27	Total	O	0	0
			27	27		
2	4	44	Total	O	0	0
			44	44		

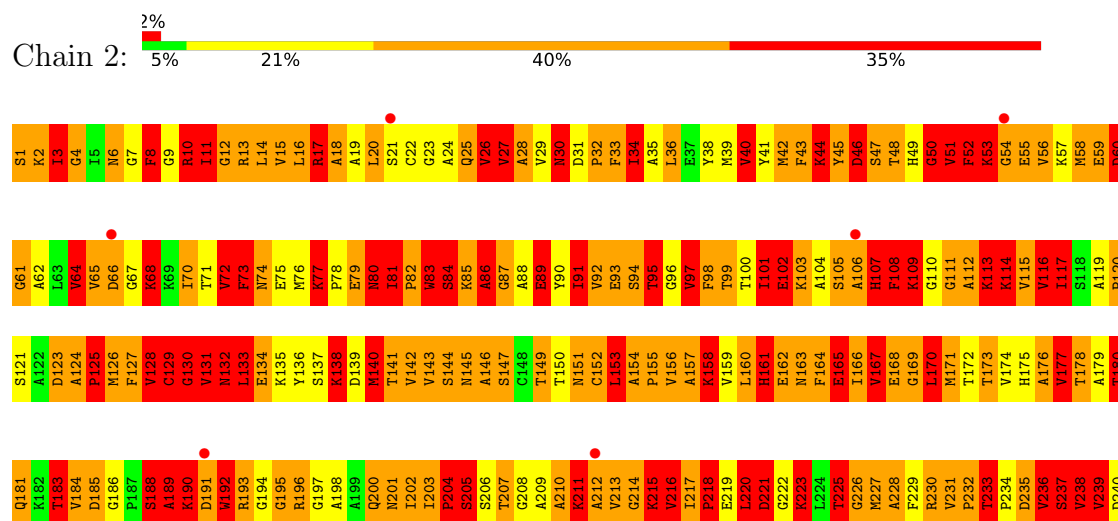
3 Residue-property plots

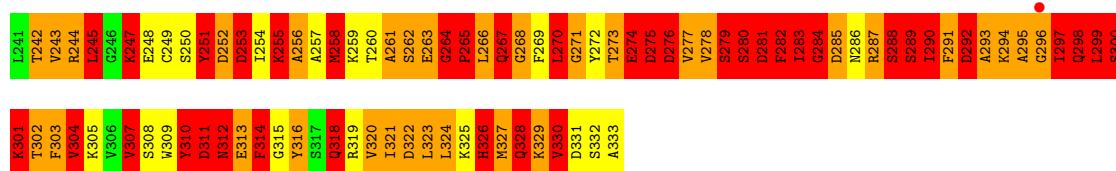
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: APO-D-GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE

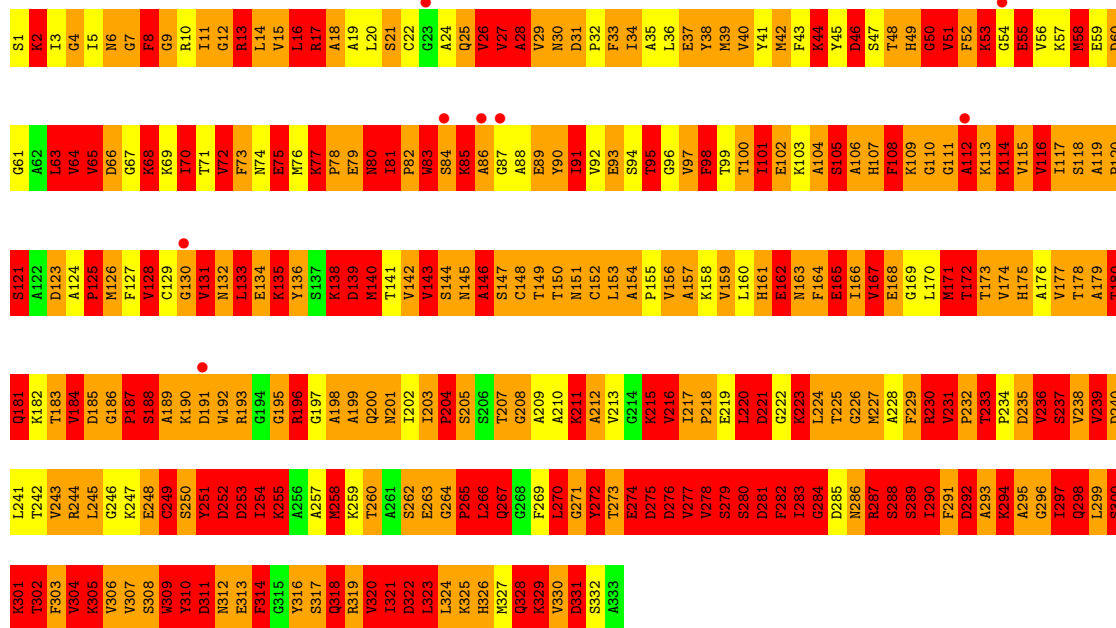
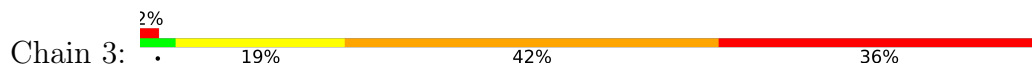


• Molecule 1: APO-D-GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE

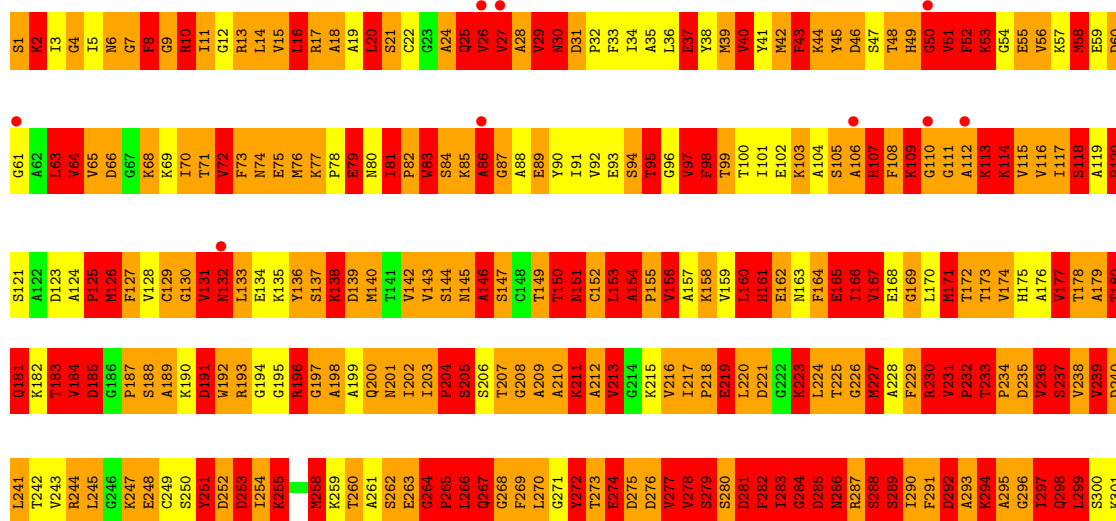
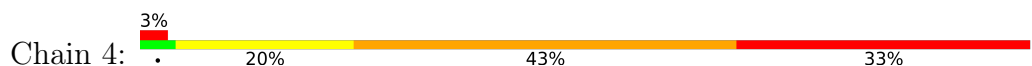




• Molecule 1: APO-D-GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE



• Molecule 1: APO-D-GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE



I302	F303	V304	K305	V306	V307	S308	W309	Y310	D311	N312	E313	F314	G315	Y316	S317	Q318	R319	V320	I321	D322	L323	L324	K325	H326	M327	Q328	K329	V330	D331	S332	A333
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	83.02Å 80.96Å 82.55Å 110.85° 71.47° 116.86°	Depositor
Resolution (Å)	6.00 – 2.80 6.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (6.00-2.80) 62.9 (6.00-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.54 (at 2.51Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.218 , (Not available) 0.230 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	28.2	Xtriage
Anisotropy	0.280	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.94 , 212.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.025 for k,h,-l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	10150	wwPDB-VP
Average B, all atoms (Å ²)	10.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.83% 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	1	2.00	64/2553 (2.5%)	3.36	430/3451 (12.5%)
1	2	2.04	61/2553 (2.4%)	3.42	412/3451 (11.9%)
1	3	2.13	76/2553 (3.0%)	3.54	447/3451 (13.0%)
1	4	2.04	72/2553 (2.8%)	3.57	451/3451 (13.1%)
All	All	2.06	273/10212 (2.7%)	3.48	1740/13804 (12.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	3	0	2

All (273) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	3	203	ILE	CA-CB	14.55	1.65	1.54
1	2	296	GLY	N-CA	11.43	1.61	1.44
1	3	235	ASP	C-O	10.98	1.32	1.23
1	2	235	ASP	C-O	10.38	1.36	1.24
1	3	236	VAL	N-CA	10.36	1.59	1.46
1	2	236	VAL	N-CA	9.85	1.58	1.46
1	3	201	ASN	CA-CB	9.33	1.68	1.53
1	4	300	SER	CA-CB	-9.19	1.46	1.53
1	3	85	LYS	N-CA	8.90	1.57	1.46
1	3	223	LYS	C-O	8.65	1.35	1.24
1	3	322	ASP	C-O	8.64	1.34	1.24
1	1	114	LYS	N-CA	8.63	1.56	1.46
1	2	303	PHE	C-O	8.62	1.34	1.24
1	1	201	ASN	N-CA	-8.27	1.36	1.45
1	2	178	THR	CA-CB	8.18	1.65	1.53
1	3	203	ILE	CA-C	-8.16	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	3	226	GLY	N-CA	8.12	1.53	1.45
1	1	203	ILE	CA-CB	8.10	1.64	1.54
1	2	287	ARG	NE-CZ	-8.09	1.24	1.33
1	3	63	LEU	CA-CB	-8.08	1.41	1.53
1	4	184	VAL	C-N	-8.06	1.22	1.33
1	4	227	MET	CA-CB	-7.96	1.43	1.53
1	3	138	LYS	C-O	7.94	1.33	1.24
1	1	224	LEU	N-CA	7.87	1.55	1.45
1	4	136	TYR	CA-CB	7.81	1.65	1.53
1	4	263	GLU	C-O	7.80	1.32	1.24
1	4	299	LEU	N-CA	7.79	1.55	1.45
1	1	296	GLY	N-CA	7.73	1.56	1.45
1	3	73	PHE	N-CA	7.70	1.55	1.45
1	2	203	ILE	CA-CB	7.69	1.64	1.54
1	4	286	ASN	C-O	7.67	1.33	1.24
1	4	244	ARG	CD-NE	-7.66	1.35	1.46
1	3	136	TYR	CA-CB	7.66	1.64	1.53
1	1	162	GLU	C-N	-7.64	1.23	1.34
1	3	267	GLN	C-O	7.57	1.33	1.24
1	2	114	LYS	N-CA	7.56	1.55	1.46
1	1	226	GLY	N-CA	7.48	1.52	1.45
1	2	245	LEU	C-O	7.47	1.32	1.24
1	3	50	GLY	N-CA	-7.47	1.34	1.45
1	4	232	PRO	C-O	7.47	1.33	1.24
1	3	84	SER	C-O	7.39	1.33	1.24
1	3	287	ARG	C-O	7.37	1.33	1.24
1	1	300	SER	CA-C	7.33	1.60	1.53
1	4	223	LYS	C-O	7.33	1.34	1.23
1	2	231	VAL	CA-CB	-7.32	1.48	1.55
1	3	246	GLY	N-CA	7.32	1.55	1.45
1	2	284	GLY	CA-C	7.31	1.62	1.51
1	4	50	GLY	N-CA	-7.26	1.34	1.45
1	3	300	SER	N-CA	7.25	1.55	1.46
1	3	201	ASN	N-CA	-7.22	1.37	1.45
1	2	315	GLY	N-CA	7.20	1.54	1.45
1	1	224	LEU	C-O	7.17	1.32	1.23
1	1	236	VAL	C-O	7.16	1.32	1.24
1	3	233	THR	N-CA	7.11	1.56	1.46
1	2	209	ALA	C-O	-7.11	1.15	1.24
1	4	236	VAL	N-CA	7.10	1.55	1.46
1	2	279	SER	C-N	-7.09	1.23	1.33
1	1	141	THR	CA-CB	7.08	1.64	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	4	254	ILE	N-CA	7.07	1.54	1.46
1	3	83	TRP	CA-CB	-7.05	1.41	1.53
1	2	29	VAL	C-O	7.04	1.30	1.24
1	4	235	ASP	C-O	7.04	1.32	1.23
1	2	50	GLY	N-CA	-7.01	1.35	1.45
1	4	150	THR	C-O	-7.00	1.15	1.24
1	4	233	THR	CB-OG1	6.98	1.54	1.43
1	4	114	LYS	N-CA	6.97	1.54	1.46
1	4	234	PRO	N-CD	6.96	1.57	1.47
1	4	284	GLY	N-CA	6.95	1.55	1.45
1	3	286	ASN	N-CA	6.91	1.55	1.46
1	1	26	VAL	C-O	6.90	1.32	1.24
1	1	149	THR	CB-OG1	6.89	1.54	1.43
1	3	276	ASP	N-CA	-6.82	1.37	1.46
1	3	234	PRO	N-CD	6.81	1.57	1.47
1	4	226	GLY	N-CA	6.80	1.52	1.45
1	1	322	ASP	N-CA	6.79	1.54	1.46
1	3	233	THR	CB-OG1	6.77	1.54	1.43
1	3	17	ARG	CD-NE	-6.75	1.36	1.46
1	4	233	THR	N-CA	6.74	1.55	1.46
1	1	279	SER	C-N	-6.70	1.24	1.33
1	4	113	LYS	C-O	6.68	1.32	1.24
1	3	247	LYS	N-CA	6.64	1.54	1.46
1	1	50	GLY	N-CA	-6.59	1.35	1.45
1	3	82	PRO	C-N	-6.59	1.24	1.33
1	3	196	ARG	N-CA	6.58	1.54	1.45
1	1	196	ARG	CD-NE	6.57	1.55	1.46
1	2	232	PRO	C-O	6.56	1.32	1.24
1	2	320	VAL	N-CA	6.53	1.54	1.46
1	3	209	ALA	C-O	-6.52	1.16	1.24
1	3	165	GLU	C-O	6.49	1.32	1.24
1	4	193	ARG	CD-NE	-6.48	1.37	1.46
1	2	239	VAL	N-CA	6.47	1.54	1.46
1	2	276	ASP	CA-CB	6.47	1.64	1.53
1	4	166	ILE	C-N	-6.45	1.26	1.33
1	2	300	SER	CA-C	6.44	1.61	1.52
1	4	2	LYS	N-CA	6.43	1.53	1.46
1	4	245	LEU	C-O	6.37	1.32	1.23
1	1	323	LEU	N-CA	6.34	1.53	1.46
1	4	281	ASP	N-CA	6.31	1.54	1.46
1	1	275	ASP	N-CA	6.29	1.54	1.46
1	4	168	GLU	N-CA	6.28	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	201	ASN	CA-CB	6.27	1.63	1.53
1	3	139	ASP	N-CA	6.23	1.54	1.46
1	3	120	PRO	C-O	6.23	1.31	1.23
1	1	184	VAL	N-CA	6.22	1.54	1.46
1	1	284	GLY	N-CA	6.22	1.54	1.45
1	3	114	LYS	N-CA	6.21	1.53	1.46
1	4	180	THR	CB-OG1	6.20	1.53	1.43
1	2	165	GLU	C-O	6.19	1.31	1.24
1	1	229	PHE	CA-C	6.18	1.59	1.52
1	2	233	THR	CB-OG1	6.18	1.53	1.43
1	1	237	SER	N-CA	6.15	1.54	1.46
1	1	276	ASP	CA-CB	6.14	1.63	1.53
1	4	268	GLY	C-O	6.13	1.30	1.24
1	1	300	SER	CA-CB	-6.10	1.42	1.52
1	3	84	SER	N-CA	6.09	1.54	1.46
1	3	287	ARG	CD-NE	-6.09	1.37	1.46
1	3	262	SER	C-O	6.08	1.31	1.24
1	2	194	GLY	CA-C	6.05	1.60	1.51
1	4	225	THR	C-O	6.04	1.30	1.23
1	4	279	SER	C-N	-6.04	1.25	1.33
1	3	157	ALA	N-CA	6.03	1.53	1.46
1	3	171	MET	C-O	-6.03	1.16	1.23
1	1	273	THR	CB-OG1	6.03	1.53	1.43
1	3	244	ARG	N-CA	6.03	1.53	1.46
1	4	260	THR	C-N	-6.03	1.25	1.33
1	4	95	THR	CA-CB	6.02	1.63	1.53
1	2	183	THR	CA-CB	6.00	1.64	1.53
1	2	179	ALA	CA-CB	-6.00	1.44	1.53
1	3	306	VAL	N-CA	6.00	1.53	1.46
1	3	323	LEU	N-CA	5.98	1.53	1.46
1	4	300	SER	CA-C	5.98	1.59	1.53
1	4	315	GLY	N-CA	5.98	1.54	1.45
1	4	125	PRO	CA-CB	-5.98	1.45	1.53
1	1	95	THR	CA-CB	5.96	1.63	1.53
1	4	205	SER	C-N	-5.95	1.25	1.33
1	2	256	ALA	C-O	5.94	1.31	1.24
1	3	198	ALA	CA-CB	5.94	1.63	1.53
1	3	178	THR	CA-CB	5.93	1.67	1.53
1	4	27	VAL	N-CA	5.91	1.53	1.46
1	3	265	PRO	C-O	5.90	1.31	1.24
1	4	298	GLN	N-CA	5.90	1.53	1.46
1	2	196	ARG	CD-NE	5.88	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	3	49	HIS	CA-CB	5.86	1.63	1.53
1	2	234	PRO	N-CD	5.86	1.55	1.47
1	3	159	VAL	C-O	-5.86	1.17	1.24
1	1	222	GLY	C-O	5.83	1.31	1.23
1	3	18	ALA	N-CA	5.82	1.53	1.46
1	1	281	ASP	N-CA	5.82	1.53	1.46
1	4	227	MET	CB-CG	-5.81	1.35	1.52
1	3	199	ALA	N-CA	5.79	1.54	1.46
1	1	314	PHE	C-N	-5.78	1.27	1.33
1	4	282	PHE	CA-CB	5.78	1.63	1.53
1	2	27	VAL	CA-CB	5.78	1.62	1.54
1	1	128	VAL	CA-C	5.77	1.59	1.52
1	1	159	VAL	N-CA	5.76	1.53	1.46
1	4	248	GLU	N-CA	5.76	1.53	1.46
1	2	97	VAL	C-N	-5.76	1.25	1.33
1	4	202	ILE	C-O	5.76	1.30	1.24
1	4	293	ALA	C-O	5.76	1.31	1.24
1	2	155	PRO	C-N	-5.75	1.27	1.34
1	3	163	ASN	C-O	5.73	1.31	1.24
1	4	313	GLU	CA-CB	-5.73	1.44	1.53
1	2	300	SER	CA-CB	-5.70	1.43	1.53
1	1	158	LYS	C-O	5.70	1.31	1.24
1	1	265	PRO	C-O	5.70	1.31	1.24
1	1	138	LYS	C-N	-5.70	1.26	1.34
1	1	225	THR	N-CA	5.69	1.54	1.46
1	2	191	ASP	C-N	-5.68	1.25	1.33
1	2	287	ARG	CD-NE	-5.68	1.38	1.46
1	1	71	THR	C-N	-5.67	1.26	1.33
1	3	162	GLU	C-N	-5.66	1.26	1.33
1	3	248	GLU	N-CA	5.65	1.53	1.45
1	1	178	THR	CA-CB	5.64	1.62	1.53
1	3	231	VAL	C-O	5.62	1.30	1.24
1	3	180	THR	CB-OG1	5.61	1.52	1.43
1	2	151	ASN	C-O	-5.61	1.17	1.24
1	3	225	THR	C-O	5.61	1.29	1.24
1	1	42	MET	N-CA	5.60	1.53	1.46
1	3	296	GLY	C-N	-5.60	1.24	1.33
1	1	136	TYR	CA-CB	5.59	1.61	1.53
1	2	94	SER	C-O	5.59	1.31	1.23
1	1	223	LYS	C-O	5.59	1.31	1.24
1	4	196	ARG	CD-NE	5.57	1.54	1.46
1	2	113	LYS	C-O	5.56	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	4	213	VAL	N-CA	5.55	1.53	1.46
1	1	230	ARG	CA-CB	-5.54	1.45	1.53
1	2	214	GLY	N-CA	5.54	1.53	1.45
1	3	187	PRO	N-CD	5.54	1.55	1.47
1	4	25	GLN	C-O	-5.53	1.17	1.23
1	3	149	THR	C-O	-5.53	1.17	1.24
1	3	237	SER	N-CA	5.53	1.53	1.46
1	1	230	ARG	CD-NE	5.53	1.53	1.46
1	4	144	SER	C-N	-5.52	1.27	1.33
1	3	50	GLY	CA-C	-5.51	1.44	1.51
1	2	192	TRP	CA-CB	5.50	1.62	1.53
1	4	50	GLY	CA-C	-5.50	1.44	1.51
1	4	294	LYS	N-CA	5.49	1.53	1.46
1	3	63	LEU	CB-CG	-5.49	1.42	1.53
1	3	298	GLN	C-O	5.47	1.31	1.23
1	4	183	THR	CA-CB	5.46	1.62	1.53
1	1	26	VAL	N-CA	5.46	1.53	1.46
1	1	52	PHE	N-CA	5.46	1.53	1.46
1	2	220	LEU	C-N	-5.45	1.26	1.33
1	1	231	VAL	N-CA	-5.45	1.41	1.46
1	2	316	TYR	C-N	-5.44	1.26	1.33
1	4	137	SER	N-CA	5.44	1.53	1.46
1	1	180	THR	CB-OG1	5.43	1.52	1.43
1	4	73	PHE	N-CA	5.43	1.53	1.46
1	4	225	THR	N-CA	5.42	1.54	1.46
1	1	165	GLU	C-O	5.42	1.30	1.24
1	2	11	ILE	C-N	-5.41	1.26	1.33
1	1	178	THR	CB-OG1	5.40	1.52	1.43
1	4	201	ASN	CA-CB	5.39	1.63	1.53
1	1	40	VAL	N-CA	5.39	1.52	1.46
1	3	244	ARG	CZ-NH2	5.36	1.40	1.33
1	1	82	PRO	C-N	-5.36	1.26	1.33
1	3	245	LEU	C-O	5.36	1.30	1.24
1	1	133	LEU	C-O	5.36	1.30	1.24
1	3	72	VAL	N-CA	5.35	1.51	1.46
1	1	251	TYR	N-CA	5.33	1.53	1.46
1	2	261	ALA	C-O	5.33	1.30	1.24
1	2	276	ASP	N-CA	-5.33	1.39	1.46
1	2	21	SER	N-CA	5.30	1.53	1.46
1	3	133	LEU	C-O	5.30	1.30	1.24
1	1	11	ILE	C-O	5.30	1.30	1.24
1	2	179	ALA	C-O	5.29	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	244	ARG	NE-CZ	5.29	1.38	1.33
1	1	308	SER	C-O	5.27	1.29	1.24
1	3	317	SER	C-N	-5.27	1.27	1.33
1	2	205	SER	CB-OG	5.26	1.52	1.42
1	3	254	ILE	N-CA	5.25	1.52	1.46
1	1	245	LEU	C-O	5.25	1.29	1.23
1	4	313	GLU	N-CA	5.25	1.52	1.46
1	1	294	LYS	N-CA	5.25	1.52	1.46
1	1	246	GLY	N-CA	5.23	1.52	1.45
1	4	242	THR	CA-CB	5.23	1.61	1.53
1	1	154	ALA	C-O	-5.22	1.17	1.24
1	2	74	ASN	C-N	-5.22	1.27	1.33
1	3	205	SER	N-CA	-5.22	1.40	1.46
1	2	161	HIS	CG-CD2	5.21	1.41	1.35
1	3	38	TYR	N-CA	5.20	1.52	1.46
1	2	82	PRO	C-N	-5.19	1.26	1.33
1	4	193	ARG	CG-CD	-5.19	1.36	1.52
1	3	164	PHE	CA-CB	-5.18	1.44	1.53
1	4	310	TYR	CA-C	5.18	1.55	1.52
1	1	262	SER	C-O	5.17	1.30	1.24
1	4	178	THR	CA-CB	5.16	1.62	1.53
1	2	323	LEU	N-CA	5.15	1.52	1.46
1	3	65	VAL	N-CA	5.14	1.52	1.46
1	4	224	LEU	N-CA	5.13	1.52	1.45
1	2	274	GLU	C-N	-5.13	1.27	1.33
1	4	315	GLY	CA-C	5.13	1.59	1.51
1	4	26	VAL	C-O	5.13	1.30	1.24
1	4	288	SER	CA-CB	-5.12	1.44	1.53
1	2	48	THR	CA-CB	5.09	1.61	1.53
1	4	165	GLU	C-O	5.09	1.30	1.24
1	1	291	PHE	C-N	-5.08	1.27	1.33
1	2	167	VAL	C-N	-5.08	1.27	1.33
1	3	175	HIS	CE1-NE2	5.08	1.37	1.32
1	4	139	ASP	C-O	5.08	1.30	1.24
1	4	152	CYS	C-N	-5.07	1.26	1.33
1	1	147	SER	N-CA	-5.07	1.39	1.46
1	2	72	VAL	N-CA	5.07	1.52	1.46
1	3	49	HIS	CG-CD2	-5.06	1.30	1.35
1	1	195	GLY	CA-C	5.06	1.59	1.51
1	2	195	GLY	CA-C	5.05	1.59	1.51
1	2	126	MET	CA-CB	-5.05	1.46	1.52
1	4	302	THR	N-CA	5.04	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	4	272	TYR	CA-CB	5.03	1.61	1.53
1	4	296	GLY	N-CA	5.02	1.52	1.45
1	3	27	VAL	CA-CB	5.01	1.61	1.54
1	2	65	VAL	N-CA	5.01	1.52	1.46
1	1	195	GLY	C-N	-5.00	1.26	1.33

All (1740) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	227	MET	CA-CB-CG	32.95	179.99	114.10
1	2	287	ARG	CD-NE-CZ	32.43	169.80	124.40
1	4	244	ARG	CD-NE-CZ	30.02	166.43	124.40
1	4	73	PHE	CA-CB-CG	28.37	142.17	113.80
1	2	314	PHE	CA-CB-CG	22.01	135.81	113.80
1	3	274	GLU	CB-CG-CD	21.58	149.29	112.60
1	1	300	SER	CA-CB-OG	21.16	153.43	111.10
1	3	73	PHE	CA-CB-CG	21.14	134.94	113.80
1	4	300	SER	CA-CB-OG	20.30	151.71	111.10
1	2	300	SER	CA-CB-OG	20.01	151.13	111.10
1	1	310	TYR	CA-CB-CG	18.93	147.98	113.90
1	3	287	ARG	CD-NE-CZ	18.92	150.88	124.40
1	3	17	ARG	CD-NE-CZ	17.97	149.56	124.40
1	1	287	ARG	CD-NE-CZ	16.88	148.03	124.40
1	4	322	ASP	CA-CB-CG	16.74	129.34	112.60
1	3	212	ALA	CA-C-O	-16.64	102.78	120.42
1	4	132	ASN	CA-CB-CG	16.22	128.82	112.60
1	3	231	VAL	N-CA-CB	-16.06	100.75	111.83
1	3	49	HIS	CA-CB-CG	-16.00	97.80	113.80
1	2	10	ARG	NE-CZ-NH2	-15.97	104.83	119.20
1	4	312	ASN	CA-CB-CG	15.91	128.51	112.60
1	1	252	ASP	CA-CB-CG	-15.85	96.75	112.60
1	1	108	PHE	CA-CB-CG	15.77	129.57	113.80
1	1	185	ASP	CA-CB-CG	-15.70	96.90	112.60
1	2	8	PHE	CA-CB-CG	15.59	129.39	113.80
1	4	49	HIS	CA-C-N	15.55	151.90	121.41
1	4	49	HIS	C-N-CA	15.55	151.90	121.41
1	4	26	VAL	CA-C-O	-15.26	101.71	120.78
1	4	267	GLN	OE1-CD-NE2	15.21	137.81	122.60
1	2	200	GLN	CB-CG-CD	15.17	138.38	112.60
1	4	252	ASP	CA-CB-CG	-15.11	97.49	112.60
1	2	10	ARG	NE-CZ-NH1	15.05	136.55	121.50
1	4	163	ASN	CA-CB-CG	15.01	127.61	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	167	VAL	CB-CA-C	15.01	124.40	111.05
1	3	139	ASP	CA-CB-CG	14.97	127.57	112.60
1	4	46	ASP	CA-CB-CG	-14.85	97.75	112.60
1	3	17	ARG	CA-CB-CG	14.84	143.77	114.10
1	1	191	ASP	CA-CB-CG	14.77	127.37	112.60
1	4	281	ASP	CA-CB-CG	14.64	127.24	112.60
1	1	275	ASP	CA-CB-CG	14.51	127.11	112.60
1	4	193	ARG	CG-CD-NE	14.37	143.61	112.00
1	1	73	PHE	CA-CB-CG	14.34	128.14	113.80
1	3	203	ILE	CA-C-O	-14.23	112.54	119.94
1	3	98	PHE	CA-CB-CG	14.17	127.97	113.80
1	3	310	TYR	CA-CB-CG	13.93	138.98	113.90
1	2	52	PHE	CA-CB-CG	13.87	127.67	113.80
1	2	44	LYS	CA-CB-CG	13.81	141.73	114.10
1	3	300	SER	CA-C-N	13.67	147.65	121.54
1	3	300	SER	C-N-CA	13.67	147.65	121.54
1	3	201	ASN	N-CA-C	13.67	132.17	110.17
1	3	151	ASN	CA-CB-CG	13.66	126.26	112.60
1	1	300	SER	CA-C-O	13.61	134.92	120.63
1	1	276	ASP	CA-CB-CG	-13.60	99.00	112.60
1	2	29	VAL	CA-C-O	-13.31	105.84	121.28
1	2	296	GLY	N-CA-C	-13.19	94.38	116.01
1	1	132	ASN	CA-CB-CG	13.13	125.73	112.60
1	4	132	ASN	OD1-CG-ND2	-13.06	109.54	122.60
1	2	196	ARG	CB-CG-CD	13.03	141.27	111.30
1	4	155	PRO	CA-C-N	13.02	138.89	120.53
1	4	155	PRO	C-N-CA	13.02	138.89	120.53
1	2	293	ALA	CA-C-O	-12.96	106.98	120.98
1	4	225	THR	CA-C-O	-12.93	107.82	121.14
1	2	328	GLN	OE1-CD-NE2	12.73	135.33	122.60
1	2	303	PHE	CA-C-O	-12.72	106.33	120.32
1	3	236	VAL	CA-C-O	-12.71	104.89	120.78
1	3	49	HIS	CA-C-N	12.70	146.31	121.41
1	3	49	HIS	C-N-CA	12.70	146.31	121.41
1	1	49	HIS	CA-C-N	12.63	146.16	121.41
1	1	49	HIS	C-N-CA	12.63	146.16	121.41
1	2	231	VAL	N-CA-CB	-12.59	103.14	111.83
1	3	230	ARG	CA-C-N	12.48	140.59	122.24
1	3	230	ARG	C-N-CA	12.48	140.59	122.24
1	1	286	ASN	CA-C-O	-12.46	102.69	120.51
1	4	191	ASP	CA-CB-CG	12.38	124.98	112.60
1	3	319	ARG	NE-CZ-NH2	12.37	130.33	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3	83	TRP	CA-CB-CG	12.34	137.04	113.60
1	3	63	LEU	CA-CB-CG	12.30	159.35	116.30
1	1	200	GLN	CA-C-N	12.29	144.56	122.92
1	1	200	GLN	C-N-CA	12.29	144.56	122.92
1	1	50	GLY	N-CA-C	12.23	142.16	113.18
1	4	8	PHE	CA-CB-CG	12.23	126.03	113.80
1	3	196	ARG	CD-NE-CZ	-12.13	107.42	124.40
1	3	177	VAL	CA-C-N	12.13	141.85	122.81
1	3	177	VAL	C-N-CA	12.13	141.85	122.81
1	4	319	ARG	NE-CZ-NH1	-12.12	109.39	121.50
1	3	293	ALA	CA-C-O	-12.10	108.02	121.58
1	2	83	TRP	CA-CB-CG	12.06	136.51	113.60
1	3	302	THR	CA-C-N	12.04	139.96	122.86
1	3	302	THR	C-N-CA	12.04	139.96	122.86
1	1	267	GLN	OE1-CD-NE2	11.97	134.57	122.60
1	2	236	VAL	CB-CA-C	11.91	130.83	111.29
1	3	164	PHE	CA-CB-CG	11.88	125.68	113.80
1	4	109	LYS	N-CA-CB	11.84	130.50	110.49
1	4	126	MET	O-C-N	11.78	134.34	123.50
1	4	314	PHE	N-CA-C	11.77	125.94	110.88
1	2	73	PHE	CA-CB-CG	11.75	125.55	113.80
1	2	267	GLN	OE1-CD-NE2	11.73	134.33	122.60
1	4	39	MET	CA-CB-CG	11.70	137.50	114.10
1	1	163	ASN	OD1-CG-ND2	11.64	134.24	122.60
1	2	209	ALA	CA-C-N	11.56	135.91	120.65
1	2	209	ALA	C-N-CA	11.56	135.91	120.65
1	1	175	HIS	CA-CB-CG	11.55	125.35	113.80
1	1	323	LEU	N-CA-C	-11.53	96.95	111.02
1	4	233	THR	CA-CB-OG1	-11.46	92.41	109.60
1	2	56	VAL	N-CA-C	11.42	118.43	106.21
1	1	329	LYS	N-CA-CB	11.35	129.68	110.49
1	4	311	ASP	N-CA-CB	11.31	129.60	110.49
1	2	201	ASN	N-CA-C	11.30	128.37	110.17
1	3	252	ASP	CA-CB-CG	-11.30	101.30	112.60
1	4	111	GLY	O-C-N	11.30	137.39	122.70
1	3	50	GLY	N-CA-C	11.30	139.96	113.18
1	2	235	ASP	CA-C-O	-11.26	106.60	118.65
1	3	201	ASN	CA-CB-CG	-11.24	101.36	112.60
1	3	168	GLU	CA-CB-CG	11.22	136.54	114.10
1	3	233	THR	CA-C-N	11.22	131.50	119.05
1	3	233	THR	C-N-CA	11.22	131.50	119.05
1	4	224	LEU	O-C-N	11.18	136.24	123.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3	210	ALA	O-C-N	11.15	133.56	122.07
1	3	163	ASN	N-CA-C	11.14	126.13	112.54
1	3	278	VAL	CB-CA-C	11.09	129.48	111.29
1	1	323	LEU	CB-CA-C	11.03	128.46	110.92
1	1	282	PHE	CA-CB-CG	-10.99	102.81	113.80
1	1	263	GLU	CB-CG-CD	10.98	131.27	112.60
1	2	236	VAL	CA-C-O	-10.98	107.05	120.78
1	3	177	VAL	CA-C-O	10.96	134.48	120.78
1	1	1	SER	CA-CB-OG	10.96	133.01	111.10
1	3	133	LEU	N-CA-CB	-10.95	91.98	110.49
1	4	258	MET	O-C-N	10.94	136.99	122.33
1	4	196	ARG	CD-NE-CZ	-10.93	109.10	124.40
1	1	177	VAL	CA-C-O	10.92	134.43	120.78
1	4	265	PRO	CB-CA-C	10.87	129.50	111.56
1	3	120	PRO	CB-CA-C	10.85	125.17	110.95
1	1	200	GLN	OE1-CD-NE2	-10.83	111.77	122.60
1	4	185	ASP	CA-CB-CG	-10.82	101.78	112.60
1	2	185	ASP	CA-CB-CG	-10.77	101.83	112.60
1	3	168	GLU	CB-CG-CD	10.74	130.86	112.60
1	4	237	SER	CA-CB-OG	10.71	132.52	111.10
1	2	66	ASP	CA-CB-CG	-10.67	101.93	112.60
1	1	178	THR	CA-CB-OG1	-10.65	93.62	109.60
1	4	17	ARG	CD-NE-CZ	10.65	139.31	124.40
1	4	283	ILE	CB-CG1-CD1	10.62	136.10	113.80
1	1	296	GLY	N-CA-C	-10.62	99.60	115.32
1	2	310	TYR	CA-CB-CG	10.62	133.02	113.90
1	3	236	VAL	CB-CA-C	10.59	128.66	111.29
1	4	16	LEU	O-C-N	10.52	133.39	122.03
1	2	296	GLY	O-C-N	10.48	133.41	122.51
1	4	151	ASN	CA-CB-CG	10.47	123.07	112.60
1	3	134	GLU	N-CA-CB	10.45	125.71	109.82
1	1	163	ASN	CA-CB-CG	-10.43	102.17	112.60
1	1	83	TRP	CA-CB-CG	10.41	133.38	113.60
1	2	201	ASN	N-CA-CB	-10.41	93.67	110.63
1	4	120	PRO	CA-C-O	-10.40	109.17	121.86
1	2	17	ARG	O-C-N	10.34	136.34	122.59
1	2	27	VAL	N-CA-CB	-10.33	94.18	111.23
1	2	162	GLU	CA-CB-CG	10.33	134.76	114.10
1	3	46	ASP	CA-CB-CG	-10.31	102.29	112.60
1	1	146	ALA	CA-C-N	10.30	141.22	121.54
1	1	146	ALA	C-N-CA	10.30	141.22	121.54
1	2	252	ASP	CA-CB-CG	-10.29	102.31	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	163	ASN	OD1-CG-ND2	-10.29	112.31	122.60
1	1	300	SER	CB-CA-C	10.28	125.69	111.51
1	4	169	GLY	O-C-N	-10.28	115.46	123.27
1	4	43	PHE	CA-CB-CG	10.27	124.07	113.80
1	2	286	ASN	CA-C-O	-10.26	105.84	120.51
1	4	98	PHE	CA-CB-CG	10.24	124.04	113.80
1	2	303	PHE	O-C-N	10.24	135.35	123.27
1	3	163	ASN	OD1-CG-ND2	10.24	132.84	122.60
1	4	252	ASP	OD1-CG-OD2	10.23	147.45	122.90
1	2	303	PHE	CA-CB-CG	10.23	124.03	113.80
1	2	163	ASN	CA-CB-CG	-10.21	102.39	112.60
1	4	51	VAL	CB-CA-C	10.18	127.99	111.29
1	2	192	TRP	N-CA-C	10.17	132.47	110.80
1	4	43	PHE	O-C-N	10.11	133.46	122.34
1	2	245	LEU	N-CA-C	10.10	124.26	111.24
1	1	314	PHE	CA-CB-CG	10.09	123.89	113.80
1	3	157	ALA	CB-CA-C	10.06	126.45	110.96
1	1	120	PRO	CA-C-O	-10.05	109.91	121.56
1	2	211	LYS	CA-CB-CG	10.04	134.17	114.10
1	3	188	SER	CA-C-O	10.02	134.84	120.51
1	2	190	LYS	N-CA-CB	10.00	123.89	110.59
1	4	230	ARG	O-C-N	10.00	135.07	123.27
1	2	114	LYS	N-CA-CB	-9.97	94.16	110.71
1	3	2	LYS	CA-C-O	-9.97	106.75	120.21
1	3	291	PHE	CA-CB-CG	9.96	123.77	113.80
1	3	254	ILE	CB-CA-C	9.94	125.06	112.04
1	3	253	ASP	CA-CB-CG	9.93	122.53	112.60
1	2	97	VAL	CA-C-O	-9.88	108.43	120.78
1	4	263	GLU	CB-CG-CD	9.88	129.40	112.60
1	2	128	VAL	CA-C-O	-9.86	110.35	120.90
1	2	196	ARG	CD-NE-CZ	-9.85	110.61	124.40
1	4	200	GLN	CA-C-O	9.82	129.66	118.77
1	3	212	ALA	O-C-N	9.80	133.32	122.15
1	4	244	ARG	CA-C-O	-9.79	109.47	120.43
1	3	300	SER	O-C-N	-9.78	109.58	122.59
1	4	233	THR	N-CA-CB	-9.78	92.96	110.37
1	4	103	LYS	CA-C-O	-9.78	110.06	120.42
1	1	135	LYS	CG-CD-CE	9.77	133.76	111.30
1	1	154	ALA	O-C-N	9.76	132.55	121.32
1	2	196	ARG	NE-CZ-NH2	9.76	127.99	119.20
1	3	280	SER	N-CA-CB	-9.76	93.99	110.49
1	4	66	ASP	CA-CB-CG	9.76	122.36	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	259	LYS	O-C-N	9.75	133.96	122.17
1	3	300	SER	CA-C-O	9.73	134.43	120.51
1	1	207	THR	CA-CB-OG1	-9.73	95.00	109.60
1	1	207	THR	CA-CB-CG2	9.70	126.98	110.50
1	1	300	SER	O-C-N	-9.68	114.60	123.50
1	3	178	THR	N-CA-C	9.67	125.19	109.72
1	2	66	ASP	N-CA-CB	-9.65	97.23	111.91
1	2	132	ASN	CA-CB-CG	9.65	122.25	112.60
1	2	238	VAL	CA-C-N	-9.65	110.77	122.93
1	2	238	VAL	C-N-CA	-9.65	110.77	122.93
1	1	115	VAL	N-CA-C	9.64	122.20	108.42
1	2	56	VAL	N-CA-CB	-9.64	102.64	112.28
1	4	74	ASN	CA-CB-CG	-9.62	102.97	112.60
1	4	245	LEU	N-CA-C	9.60	125.12	113.12
1	3	233	THR	CA-CB-OG1	-9.60	95.20	109.60
1	2	313	GLU	N-CA-CB	9.59	124.23	109.94
1	4	298	GLN	CB-CG-CD	9.59	128.90	112.60
1	2	163	ASN	OD1-CG-ND2	9.58	132.18	122.60
1	3	200	GLN	CA-C-N	9.56	138.88	122.64
1	3	200	GLN	C-N-CA	9.56	138.88	122.64
1	4	254	ILE	CB-CA-C	9.55	124.56	112.04
1	1	142	VAL	N-CA-CB	-9.55	95.47	111.23
1	3	108	PHE	CA-CB-CG	9.55	123.35	113.80
1	2	163	ASN	N-CA-C	9.54	124.72	112.89
1	2	295	ALA	CA-C-N	-9.54	109.47	122.63
1	2	295	ALA	C-N-CA	-9.54	109.47	122.63
1	2	74	ASN	OD1-CG-ND2	9.53	132.13	122.60
1	1	286	ASN	O-C-N	9.52	135.26	122.59
1	3	65	VAL	CB-CA-C	9.51	125.00	110.83
1	1	48	THR	CA-C-O	-9.50	110.39	120.55
1	1	244	ARG	N-CA-C	-9.49	93.70	109.46
1	2	114	LYS	CB-CA-C	9.49	125.94	109.80
1	4	296	GLY	N-CA-C	-9.49	101.27	115.32
1	3	176	ALA	CA-C-O	-9.49	110.39	121.11
1	4	44	LYS	CA-CB-CG	9.48	133.05	114.10
1	4	81	ILE	CB-CA-C	9.47	120.28	111.00
1	4	187	PRO	CB-CA-C	-9.46	99.54	111.56
1	1	196	ARG	CD-NE-CZ	-9.46	111.16	124.40
1	3	331	ASP	CA-CB-CG	-9.45	103.15	112.60
1	3	301	LYS	CA-C-O	-9.43	107.02	120.51
1	3	286	ASN	OD1-CG-ND2	9.43	132.03	122.60
1	2	314	PHE	N-CA-C	9.42	125.11	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	163	ASN	N-CA-C	9.39	122.71	111.82
1	3	286	ASN	CA-C-O	-9.39	107.08	120.51
1	1	72	VAL	CB-CA-C	9.39	128.07	111.18
1	4	251	TYR	CA-CB-CG	-9.37	97.04	113.90
1	3	300	SER	CB-CA-C	9.34	129.00	110.42
1	4	209	ALA	N-CA-C	-9.34	99.47	112.45
1	4	127	PHE	CA-C-N	9.33	138.77	121.97
1	4	127	PHE	C-N-CA	9.33	138.77	121.97
1	4	230	ARG	CA-C-O	-9.33	110.05	120.32
1	3	267	GLN	CA-C-O	-9.32	107.18	120.51
1	3	192	TRP	N-CA-C	9.32	126.74	111.37
1	4	295	ALA	CA-C-O	9.31	130.17	120.40
1	3	183	THR	CA-CB-OG1	-9.30	95.65	109.60
1	3	233	THR	N-CA-CB	-9.30	93.81	110.37
1	1	237	SER	CA-CB-OG	9.28	129.67	111.10
1	1	201	ASN	N-CA-C	9.28	124.53	110.14
1	1	183	THR	N-CA-CB	9.27	123.91	110.47
1	2	126	MET	CB-CA-C	9.25	123.54	111.42
1	2	281	ASP	CA-CB-CG	9.25	121.85	112.60
1	1	298	GLN	OE1-CD-NE2	-9.24	113.36	122.60
1	3	191	ASP	CA-C-N	9.22	134.65	120.82
1	3	191	ASP	C-N-CA	9.22	134.65	120.82
1	4	253	ASP	CA-CB-CG	-9.21	103.39	112.60
1	1	198	ALA	CA-C-O	-9.19	107.37	120.51
1	3	191	ASP	N-CA-CB	-9.17	97.86	110.42
1	4	212	ALA	O-C-N	9.17	132.65	122.20
1	4	42	MET	CA-C-O	-9.16	107.38	119.11
1	4	282	PHE	CA-CB-CG	-9.16	104.64	113.80
1	3	287	ARG	NE-CZ-NH2	9.16	127.44	119.20
1	1	188	SER	CA-C-O	9.14	129.02	119.51
1	2	203	ILE	CA-C-O	-9.14	107.70	119.95
1	2	239	VAL	CB-CA-C	9.14	123.27	110.84
1	3	314	PHE	N-CA-C	9.12	124.15	111.56
1	1	286	ASN	OD1-CG-ND2	9.12	131.72	122.60
1	3	13	ARG	NE-CZ-NH2	-9.12	110.99	119.20
1	3	247	LYS	CB-CA-C	9.12	124.70	109.84
1	1	230	ARG	CD-NE-CZ	-9.09	111.67	124.40
1	4	263	GLU	N-CA-CB	9.08	124.31	110.14
1	1	83	TRP	CA-C-O	9.08	133.49	120.51
1	2	212	ALA	O-C-N	9.08	132.55	122.20
1	4	310	TYR	CA-CB-CG	9.08	130.24	113.90
1	2	227	MET	O-C-N	9.07	132.70	122.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	162	GLU	O-C-N	9.07	132.54	122.11
1	1	263	GLU	CA-CB-CG	9.07	132.23	114.10
1	3	151	ASN	OD1-CG-ND2	-9.05	113.55	122.60
1	4	192	TRP	CA-CB-CG	9.05	130.79	113.60
1	2	207	THR	CA-CB-OG1	-9.05	96.03	109.60
1	4	293	ALA	CA-C-O	-9.03	107.59	120.51
1	1	167	VAL	N-CA-C	-9.03	104.49	111.62
1	3	195	GLY	N-CA-C	-9.03	100.32	113.86
1	3	323	LEU	N-CA-C	-9.02	100.02	111.02
1	3	149	THR	O-C-N	9.01	131.72	122.08
1	3	168	GLU	CA-C-N	8.98	132.34	121.38
1	3	168	GLU	C-N-CA	8.98	132.34	121.38
1	4	275	ASP	N-CA-C	-8.98	100.51	112.72
1	2	68	LYS	N-CA-CB	8.97	123.47	110.37
1	2	191	ASP	N-CA-C	8.97	122.70	112.57
1	1	101	ILE	N-CA-CB	8.96	121.67	110.47
1	1	313	GLU	CA-C-O	-8.93	107.74	120.51
1	3	209	ALA	CA-C-N	8.91	132.02	120.44
1	3	209	ALA	C-N-CA	8.91	132.02	120.44
1	1	275	ASP	CA-C-N	8.91	138.55	121.54
1	1	275	ASP	C-N-CA	8.91	138.55	121.54
1	2	200	GLN	CA-C-O	8.90	130.19	119.06
1	1	147	SER	CA-C-O	8.89	133.23	120.51
1	2	27	VAL	N-CA-C	8.88	127.81	109.34
1	4	201	ASN	N-CA-C	8.88	124.07	109.95
1	1	314	PHE	N-CA-C	8.87	123.94	112.41
1	2	20	LEU	N-CA-C	8.87	121.91	111.71
1	4	2	LYS	CA-C-O	-8.87	109.32	120.14
1	1	221	ASP	CA-CB-CG	8.87	121.47	112.60
1	4	161	HIS	CA-CB-CG	8.85	122.65	113.80
1	3	151	ASN	N-CA-C	-8.84	101.64	111.28
1	4	299	LEU	CB-CA-C	8.83	127.90	109.79
1	3	257	ALA	CA-C-O	8.82	129.90	120.55
1	2	120	PRO	CA-C-O	-8.80	111.10	122.19
1	2	143	VAL	CA-C-O	-8.78	112.55	121.59
1	4	152	CYS	CA-C-O	-8.75	109.46	119.79
1	3	313	GLU	CB-CG-CD	8.73	127.45	112.60
1	3	46	ASP	O-C-N	8.73	134.17	123.44
1	1	38	TYR	CA-C-N	8.72	132.17	120.65
1	1	38	TYR	C-N-CA	8.72	132.17	120.65
1	2	233	THR	CA-CB-OG1	-8.72	96.52	109.60
1	2	210	ALA	CB-CA-C	-8.71	97.55	110.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	297	ILE	CB-CA-C	8.69	123.55	111.38
1	2	244	ARG	N-CA-C	-8.68	95.15	108.96
1	3	181	GLN	OE1-CD-NE2	8.68	131.28	122.60
1	2	164	PHE	CA-C-O	8.68	127.94	118.65
1	4	178	THR	CA-CB-OG1	-8.67	96.60	109.60
1	3	16	LEU	N-CA-C	-8.66	100.07	111.24
1	2	323	LEU	N-CA-C	-8.66	100.45	111.02
1	3	134	GLU	CB-CG-CD	8.66	127.32	112.60
1	4	208	GLY	N-CA-C	8.64	133.66	113.18
1	2	226	GLY	CA-C-O	8.63	129.50	121.38
1	4	244	ARG	N-CA-C	-8.63	95.23	108.96
1	1	188	SER	N-CA-C	-8.63	99.51	112.54
1	3	267	GLN	OE1-CD-NE2	8.63	131.23	122.60
1	4	292	ASP	CA-C-O	8.62	131.04	121.39
1	1	191	ASP	CA-C-N	8.62	138.00	121.54
1	1	191	ASP	C-N-CA	8.62	138.00	121.54
1	3	84	SER	CB-CA-C	8.62	127.56	110.42
1	3	282	PHE	CA-CB-CG	-8.62	105.18	113.80
1	2	311	ASP	N-CA-CB	8.61	125.03	110.49
1	1	307	VAL	CA-CB-CG2	8.60	125.01	110.40
1	4	28	ALA	CA-C-O	-8.59	110.29	120.43
1	3	7	GLY	CA-C-O	-8.59	109.40	122.71
1	3	133	LEU	CB-CA-C	8.59	127.51	110.42
1	1	231	VAL	N-CA-CB	-8.58	105.91	111.83
1	2	151	ASN	N-CA-C	-8.57	100.77	111.75
1	2	291	PHE	CA-CB-CG	8.57	122.37	113.80
1	4	188	SER	N-CA-CB	8.56	124.96	110.49
1	3	8	PHE	CA-CB-CG	8.56	122.36	113.80
1	1	306	VAL	CA-C-O	-8.55	111.66	121.75
1	3	280	SER	CB-CA-C	8.55	127.43	110.42
1	3	149	THR	CA-CB-OG1	-8.54	96.80	109.60
1	3	79	GLU	CB-CG-CD	8.53	127.10	112.60
1	4	92	VAL	CA-C-O	-8.53	111.44	120.48
1	3	296	GLY	CA-C-N	8.52	136.99	122.67
1	3	296	GLY	C-N-CA	8.52	136.99	122.67
1	4	269	PHE	CB-CA-C	8.51	124.46	110.24
1	2	60	ASP	CA-C-N	8.51	138.09	121.41
1	2	60	ASP	C-N-CA	8.51	138.09	121.41
1	4	207	THR	CA-CB-OG1	-8.49	96.87	109.60
1	3	307	VAL	N-CA-CB	-8.48	100.77	111.46
1	4	262	SER	CA-CB-OG	8.48	128.07	111.10
1	4	201	ASN	N-CA-CB	-8.48	97.28	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	164	PHE	CA-C-O	8.47	128.36	118.79
1	3	183	THR	CA-C-O	-8.47	108.40	120.51
1	2	84	SER	O-C-N	8.46	133.84	122.59
1	1	51	VAL	CB-CA-C	8.45	125.15	111.29
1	4	114	LYS	CB-CA-C	8.44	126.06	109.35
1	4	147	SER	CA-C-N	8.44	131.41	120.44
1	4	147	SER	C-N-CA	8.44	131.41	120.44
1	1	258	MET	CA-C-O	-8.44	110.27	119.97
1	4	25	GLN	N-CA-CB	8.39	122.30	109.97
1	2	13	ARG	CD-NE-CZ	-8.37	112.68	124.40
1	1	127	PHE	CA-C-N	8.37	134.57	122.94
1	1	127	PHE	C-N-CA	8.37	134.57	122.94
1	2	247	LYS	N-CA-CB	8.35	124.04	110.42
1	2	115	VAL	N-CA-C	8.35	122.34	108.81
1	2	253	ASP	N-CA-CB	8.35	123.08	110.22
1	4	37	GLU	CB-CG-CD	-8.34	98.42	112.60
1	4	218	PRO	CB-CA-C	8.34	124.28	112.11
1	1	201	ASN	N-CA-CB	-8.33	98.02	110.85
1	4	111	GLY	N-CA-C	-8.33	93.43	113.18
1	1	114	LYS	N-CA-CB	-8.32	97.71	110.77
1	4	235	ASP	CA-C-O	-8.32	109.37	118.52
1	4	313	GLU	CA-CB-CG	8.30	130.69	114.10
1	3	183	THR	CB-CA-C	-8.29	93.92	110.42
1	3	319	ARG	CD-NE-CZ	-8.29	112.80	124.40
1	4	29	VAL	CA-C-O	-8.28	110.39	121.32
1	2	25	GLN	O-C-N	8.27	132.65	123.22
1	2	164	PHE	CA-CB-CG	8.27	122.07	113.80
1	1	192	TRP	N-CA-C	8.26	128.40	110.80
1	1	172	THR	O-C-N	8.26	132.85	123.27
1	3	85	LYS	N-CA-C	-8.26	97.92	110.30
1	4	319	ARG	NE-CZ-NH2	8.26	126.63	119.20
1	3	248	GLU	N-CA-CB	8.24	121.67	110.38
1	3	210	ALA	CB-CA-C	-8.24	97.94	110.88
1	3	17	ARG	NE-CZ-NH1	8.24	129.74	121.50
1	4	328	GLN	OE1-CD-NE2	-8.24	114.36	122.60
1	2	152	CYS	O-C-N	8.22	131.52	122.15
1	1	233	THR	CA-CB-OG1	-8.21	97.29	109.60
1	3	149	THR	CA-C-O	-8.20	112.05	121.07
1	3	196	ARG	CA-C-O	-8.16	112.69	121.99
1	4	183	THR	CB-CA-C	-8.15	94.46	110.27
1	1	27	VAL	N-CA-C	8.14	126.27	109.34
1	4	181	GLN	CG-CD-NE2	8.14	128.61	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	212	ALA	CA-C-O	-8.14	111.09	120.20
1	1	240	ASP	CB-CA-C	8.13	123.52	110.19
1	4	6	ASN	CA-CB-CG	-8.12	104.48	112.60
1	4	223	LYS	CA-C-O	-8.10	109.88	119.35
1	4	260	THR	CA-C-O	-8.09	110.07	119.61
1	3	275	ASP	CA-C-N	8.08	136.97	121.54
1	3	275	ASP	C-N-CA	8.08	136.97	121.54
1	4	193	ARG	CB-CG-CD	8.07	129.87	111.30
1	3	6	ASN	CA-CB-CG	-8.06	104.54	112.60
1	3	199	ALA	N-CA-CB	-8.06	100.28	111.00
1	4	233	THR	CB-CA-C	8.06	126.05	110.17
1	2	217	ILE	CA-C-N	8.05	129.90	119.84
1	2	217	ILE	C-N-CA	8.05	129.90	119.84
1	1	134	GLU	CA-C-O	-8.04	112.37	120.82
1	3	275	ASP	N-CA-C	-8.04	100.54	111.55
1	3	191	ASP	N-CA-C	8.03	122.56	111.55
1	4	162	GLU	CA-C-O	-8.03	111.93	120.92
1	2	26	VAL	CA-C-O	-8.03	110.75	120.78
1	3	79	GLU	CA-CB-CG	8.02	130.15	114.10
1	2	46	ASP	OD1-CG-OD2	-8.02	103.65	122.90
1	3	212	ALA	N-CA-CB	8.02	122.03	110.16
1	2	315	GLY	N-CA-C	-8.02	102.79	112.49
1	2	304	VAL	N-CA-CB	-8.01	100.41	112.35
1	1	145	ASN	CA-CB-CG	8.01	120.61	112.60
1	4	234	PRO	N-CA-C	8.01	124.06	113.57
1	1	91	ILE	CA-C-N	8.00	133.11	123.19
1	1	91	ILE	C-N-CA	8.00	133.11	123.19
1	4	10	ARG	NE-CZ-NH1	8.00	129.50	121.50
1	3	116	VAL	CA-C-N	8.00	131.38	122.59
1	3	116	VAL	C-N-CA	8.00	131.38	122.59
1	4	150	THR	O-C-N	7.98	130.58	122.12
1	3	9	GLY	O-C-N	7.97	133.07	122.70
1	2	230	ARG	CD-NE-CZ	7.97	135.56	124.40
1	2	95	THR	CA-CB-OG1	-7.97	97.65	109.60
1	2	147	SER	CA-C-O	7.96	131.89	120.51
1	4	242	THR	OG1-CB-CG2	7.96	125.22	109.30
1	1	315	GLY	N-CA-C	-7.95	102.87	112.49
1	3	152	CYS	CA-C-O	-7.94	111.12	120.10
1	2	140	MET	CB-CA-C	7.93	122.81	109.80
1	4	244	ARG	NE-CZ-NH1	7.93	129.43	121.50
1	2	183	THR	CB-CA-C	-7.92	94.01	110.17
1	2	290	ILE	CA-C-O	-7.92	111.40	120.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	133	LEU	N-CA-CB	-7.92	97.10	110.49
1	2	320	VAL	CB-CA-C	7.92	124.28	111.29
1	3	230	ARG	CB-CA-C	7.92	122.79	109.48
1	2	191	ASP	CA-C-N	7.92	136.66	121.54
1	2	191	ASP	C-N-CA	7.92	136.66	121.54
1	3	81	ILE	O-C-N	7.91	129.68	121.14
1	4	288	SER	CA-CB-OG	7.90	126.90	111.10
1	1	275	ASP	CB-CA-C	7.90	123.97	112.12
1	2	240	ASP	CB-CA-C	7.90	123.38	109.72
1	1	236	VAL	CA-C-O	-7.89	110.91	120.78
1	4	204	PRO	CB-CA-C	7.89	124.59	111.56
1	4	240	ASP	CA-CB-CG	-7.89	104.71	112.60
1	1	51	VAL	CA-C-O	-7.89	110.92	120.78
1	3	244	ARG	N-CA-C	-7.89	95.71	108.41
1	2	83	TRP	CA-C-O	7.88	131.79	120.51
1	2	165	GLU	N-CA-CB	-7.88	97.17	110.49
1	4	151	ASN	N-CA-C	-7.88	102.68	111.82
1	2	47	SER	CA-C-N	7.88	130.68	120.44
1	2	47	SER	C-N-CA	7.88	130.68	120.44
1	1	178	THR	N-CA-C	7.87	120.35	109.18
1	4	191	ASP	CA-C-N	7.85	136.54	121.54
1	4	191	ASP	C-N-CA	7.85	136.54	121.54
1	2	282	PHE	CA-CB-CG	-7.85	105.95	113.80
1	2	176	ALA	N-CA-CB	-7.85	98.40	110.65
1	2	231	VAL	CB-CA-C	7.85	124.53	111.89
1	1	27	VAL	CA-C-O	7.83	130.57	120.78
1	3	244	ARG	CA-C-O	-7.82	112.21	120.58
1	1	304	VAL	N-CA-CB	-7.82	99.55	112.06
1	4	97	VAL	CA-C-O	-7.82	111.22	120.75
1	3	175	HIS	CA-C-N	7.79	135.05	122.81
1	3	175	HIS	C-N-CA	7.79	135.05	122.81
1	4	162	GLU	CB-CG-CD	-7.79	99.35	112.60
1	2	183	THR	CA-CB-OG1	-7.78	97.92	109.60
1	1	40	VAL	CB-CA-C	7.78	121.84	111.88
1	1	138	LYS	CA-C-N	7.78	131.48	120.28
1	1	138	LYS	C-N-CA	7.78	131.48	120.28
1	1	196	ARG	NE-CZ-NH2	7.78	126.20	119.20
1	4	123	ASP	CB-CA-C	7.77	122.28	110.08
1	4	196	ARG	NE-CZ-NH1	-7.77	113.73	121.50
1	1	162	GLU	CA-CB-CG	7.75	129.61	114.10
1	4	115	VAL	N-CA-C	7.74	121.48	108.86
1	1	34	ILE	CA-C-O	-7.74	113.34	120.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	63	LEU	O-C-N	7.73	132.09	123.04
1	3	197	GLY	CA-C-N	7.73	136.31	121.54
1	3	197	GLY	C-N-CA	7.73	136.31	121.54
1	2	170	LEU	N-CA-CB	-7.72	98.25	111.69
1	4	13	ARG	NE-CZ-NH2	-7.72	112.25	119.20
1	4	309	TRP	CA-C-O	-7.71	112.39	121.11
1	3	115	VAL	N-CA-C	7.70	119.43	108.42
1	3	317	SER	CA-C-O	-7.68	112.93	121.00
1	1	201	ASN	CA-C-N	7.68	133.10	123.12
1	1	201	ASN	C-N-CA	7.68	133.10	123.12
1	1	287	ARG	NE-CZ-NH2	7.68	126.11	119.20
1	2	64	VAL	CA-C-O	-7.66	112.34	120.53
1	2	109	LYS	N-CA-CB	7.65	123.42	110.49
1	2	93	GLU	CB-CG-CD	7.64	125.60	112.60
1	3	134	GLU	CA-C-O	-7.64	112.66	121.07
1	3	244	ARG	CD-NE-CZ	7.64	135.09	124.40
1	2	328	GLN	CA-CB-CG	7.63	129.37	114.10
1	1	306	VAL	CB-CA-C	7.63	121.89	110.90
1	2	163	ASN	CB-CG-OD1	-7.62	105.55	120.80
1	3	72	VAL	N-CA-CB	-7.62	99.64	112.44
1	3	142	VAL	CB-CA-C	7.62	123.78	111.29
1	4	15	VAL	N-CA-C	-7.61	102.86	110.62
1	2	190	LYS	N-CA-C	-7.60	104.53	113.88
1	3	251	TYR	CA-CB-CG	-7.60	100.22	113.90
1	2	25	GLN	OE1-CD-NE2	7.59	130.19	122.60
1	1	287	ARG	N-CA-CB	7.59	123.31	110.49
1	2	298	GLN	OE1-CD-NE2	-7.59	115.01	122.60
1	1	98	PHE	CA-CB-CG	7.58	121.38	113.80
1	3	329	LYS	N-CA-CB	7.57	123.28	110.49
1	4	267	GLN	CB-CG-CD	-7.56	99.75	112.60
1	1	232	PRO	CB-CA-C	7.55	124.02	111.56
1	4	196	ARG	NE-CZ-NH2	7.55	126.00	119.20
1	4	40	VAL	N-CA-CB	7.55	118.54	110.62
1	1	181	GLN	N-CA-CB	-7.54	97.74	110.49
1	2	49	HIS	CA-C-N	7.54	136.18	121.41
1	2	49	HIS	C-N-CA	7.54	136.18	121.41
1	4	200	GLN	N-CA-C	-7.53	104.60	114.31
1	4	232	PRO	CB-CA-C	7.53	123.98	111.56
1	2	21	SER	N-CA-C	-7.52	104.08	113.18
1	4	50	GLY	N-CA-C	7.52	131.00	113.18
1	2	216	VAL	CA-CB-CG2	7.51	123.17	110.40
1	4	296	GLY	CA-C-N	-7.50	111.91	122.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	296	GLY	C-N-CA	-7.50	111.91	122.34
1	3	92	VAL	CA-C-O	-7.50	112.18	120.72
1	2	275	ASP	CA-C-N	7.49	135.84	121.54
1	2	275	ASP	C-N-CA	7.49	135.84	121.54
1	2	10	ARG	CA-C-O	-7.48	109.81	120.51
1	4	255	LYS	CA-C-N	7.48	135.82	121.54
1	4	255	LYS	C-N-CA	7.48	135.82	121.54
1	1	236	VAL	CB-CA-C	7.47	123.54	111.29
1	1	167	VAL	CA-C-O	-7.46	114.16	120.80
1	4	239	VAL	N-CA-CB	7.45	118.84	110.72
1	4	302	THR	CA-C-O	7.45	126.62	118.65
1	2	178	THR	N-CA-C	7.45	119.76	109.18
1	3	72	VAL	CA-C-O	-7.45	113.85	121.67
1	3	209	ALA	N-CA-C	-7.45	102.53	111.69
1	2	80	ASN	CA-CB-CG	-7.45	105.15	112.60
1	3	272	TYR	CA-C-N	7.45	134.08	121.87
1	3	272	TYR	C-N-CA	7.45	134.08	121.87
1	1	328	GLN	CA-C-O	-7.44	113.19	121.00
1	1	126	MET	O-C-N	7.44	132.49	122.59
1	3	132	ASN	OD1-CG-ND2	-7.44	115.16	122.60
1	1	241	LEU	CA-C-N	7.43	133.71	122.93
1	1	241	LEU	C-N-CA	7.43	133.71	122.93
1	2	287	ARG	NE-CZ-NH2	7.43	125.89	119.20
1	4	28	ALA	O-C-N	7.43	131.95	123.48
1	4	51	VAL	CA-CB-CG1	7.43	123.04	110.40
1	1	2	LYS	CA-C-O	-7.43	111.69	120.60
1	2	141	THR	CB-CA-C	-7.42	97.31	109.56
1	4	126	MET	CA-C-O	-7.42	112.83	120.63
1	1	180	THR	CA-CB-CG2	7.42	123.12	110.50
1	1	189	ALA	CA-C-O	-7.42	109.91	120.51
1	2	191	ASP	CA-CB-CG	7.42	120.02	112.60
1	3	221	ASP	CA-C-O	-7.41	109.91	120.51
1	1	274	GLU	CB-CG-CD	7.40	125.18	112.60
1	3	253	ASP	N-CA-CB	7.40	123.00	110.49
1	2	300	SER	CA-C-O	7.40	131.09	120.51
1	2	300	SER	N-CA-CB	7.40	122.99	110.49
1	3	302	THR	CA-CB-CG2	7.40	123.08	110.50
1	4	326	HIS	CA-CB-CG	-7.39	106.41	113.80
1	3	112	ALA	CA-C-O	-7.39	109.94	120.51
1	3	298	GLN	CA-C-O	-7.39	111.96	120.31
1	2	132	ASN	OD1-CG-ND2	-7.39	115.21	122.60
1	3	163	ASN	N-CA-CB	-7.39	98.13	110.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	131	VAL	N-CA-CB	-7.38	101.78	110.64
1	4	317	SER	CA-C-N	7.38	130.77	120.29
1	4	317	SER	C-N-CA	7.38	130.77	120.29
1	1	46	ASP	CA-CB-CG	-7.38	105.22	112.60
1	1	138	LYS	CA-C-O	-7.37	109.97	120.51
1	2	23	GLY	O-C-N	7.37	132.28	122.70
1	2	202	ILE	N-CA-C	-7.37	96.54	107.51
1	2	50	GLY	N-CA-C	7.36	130.63	113.18
1	4	298	GLN	CA-C-O	-7.36	112.50	120.75
1	1	311	ASP	N-CA-CB	7.35	122.92	110.49
1	4	289	SER	CA-C-O	-7.35	110.00	120.51
1	4	302	THR	CA-C-N	7.35	134.02	123.14
1	4	302	THR	C-N-CA	7.35	134.02	123.14
1	3	289	SER	CA-CB-OG	7.35	125.80	111.10
1	2	103	LYS	CA-C-O	-7.35	112.63	120.42
1	3	275	ASP	CB-CA-C	7.34	120.87	111.40
1	1	84	SER	N-CA-C	-7.34	95.17	110.80
1	4	274	GLU	CA-C-O	7.33	131.00	120.51
1	3	328	GLN	CA-C-O	-7.33	113.06	120.90
1	4	248	GLU	CA-C-O	-7.33	113.62	120.95
1	1	223	LYS	CA-C-O	-7.32	110.61	119.32
1	3	139	ASP	N-CA-C	-7.32	104.35	113.20
1	3	254	ILE	CA-C-O	7.32	128.66	121.05
1	4	43	PHE	CA-C-O	-7.32	110.65	118.77
1	3	314	PHE	CA-CB-CG	7.31	121.11	113.80
1	4	42	MET	O-C-N	7.31	133.11	122.43
1	3	235	ASP	CA-C-O	-7.31	108.44	118.38
1	4	79	GLU	CA-CB-CG	7.30	128.71	114.10
1	4	233	THR	CA-CB-CG2	7.29	122.90	110.50
1	4	198	ALA	CA-C-O	-7.29	110.08	120.51
1	3	281	ASP	O-C-N	7.28	132.27	122.59
1	1	63	LEU	CA-C-O	-7.26	112.42	120.69
1	1	244	ARG	CB-CA-C	7.26	121.70	109.80
1	4	302	THR	CA-CB-CG2	7.25	122.82	110.50
1	2	74	ASN	CA-CB-CG	-7.24	105.36	112.60
1	2	202	ILE	N-CA-CB	7.24	120.46	111.41
1	4	180	THR	CA-CB-OG1	-7.24	98.75	109.60
1	1	134	GLU	CB-CG-CD	7.23	124.89	112.60
1	1	27	VAL	N-CA-CB	-7.23	99.31	111.23
1	2	323	LEU	CB-CA-C	7.22	122.41	110.92
1	2	280	SER	N-CA-CB	-7.22	98.28	110.49
1	1	46	ASP	O-C-N	7.22	132.52	123.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	89	GLU	N-CA-C	7.22	121.32	112.23
1	1	132	ASN	CA-C-N	7.21	135.32	121.54
1	1	132	ASN	C-N-CA	7.21	135.32	121.54
1	1	287	ARG	CA-C-O	-7.21	110.20	120.51
1	1	180	THR	CA-CB-OG1	-7.21	98.79	109.60
1	4	296	GLY	O-C-N	7.21	130.96	122.38
1	1	211	LYS	CA-CB-CG	7.21	128.51	114.10
1	3	77	LYS	CA-C-O	7.20	130.02	120.16
1	2	183	THR	OG1-CB-CG2	7.18	123.67	109.30
1	3	134	GLU	CB-CA-C	-7.18	99.50	110.92
1	3	84	SER	CA-C-O	-7.18	110.24	120.51
1	4	322	ASP	CA-C-O	-7.18	113.51	120.90
1	3	186	GLY	O-C-N	7.17	128.94	121.77
1	4	181	GLN	CA-C-N	7.17	135.23	121.54
1	4	181	GLN	C-N-CA	7.17	135.23	121.54
1	1	111	GLY	O-C-N	7.16	132.01	122.70
1	1	111	GLY	N-CA-C	-7.16	96.22	113.18
1	4	286	ASN	CA-C-O	-7.16	110.28	120.51
1	2	279	SER	N-CA-C	-7.15	95.57	110.80
1	4	285	ASP	N-CA-CB	7.15	122.57	110.49
1	3	217	ILE	CA-C-N	7.14	128.76	119.84
1	3	217	ILE	C-N-CA	7.14	128.76	119.84
1	4	275	ASP	CA-C-N	7.13	135.16	121.54
1	4	275	ASP	C-N-CA	7.13	135.16	121.54
1	4	198	ALA	O-C-N	7.13	132.07	122.59
1	1	72	VAL	N-CA-C	-7.12	98.24	108.42
1	4	236	VAL	CB-CA-C	7.12	122.96	111.29
1	2	64	VAL	N-CA-CB	7.12	120.43	111.46
1	2	316	TYR	CA-C-N	7.11	130.12	120.38
1	2	316	TYR	C-N-CA	7.11	130.12	120.38
1	3	146	ALA	CA-C-N	7.11	135.12	121.54
1	3	146	ALA	C-N-CA	7.11	135.12	121.54
1	2	116	VAL	CA-C-N	7.11	131.76	122.95
1	2	116	VAL	C-N-CA	7.11	131.76	122.95
1	1	106	ALA	CA-C-O	-7.10	110.35	120.51
1	1	162	GLU	CA-C-N	7.10	131.10	120.31
1	1	162	GLU	C-N-CA	7.10	131.10	120.31
1	2	134	GLU	CB-CG-CD	7.10	124.67	112.60
1	4	284	GLY	N-CA-C	-7.10	96.36	113.18
1	2	164	PHE	N-CA-C	-7.09	101.80	113.50
1	3	102	GLU	CB-CA-C	-7.09	99.46	110.81
1	4	111	GLY	CA-C-O	-7.09	108.23	120.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	301	LYS	CA-CB-CG	-7.09	99.92	114.10
1	2	176	ALA	CB-CA-C	7.09	121.92	110.16
1	3	27	VAL	CA-C-O	7.09	129.64	120.78
1	4	258	MET	CA-C-O	-7.08	111.43	119.79
1	1	29	VAL	CA-C-O	-7.08	113.39	121.75
1	3	46	ASP	CA-C-O	-7.08	110.65	120.21
1	4	313	GLU	CA-C-O	-7.07	113.39	120.82
1	2	162	GLU	CA-C-N	7.07	133.51	121.14
1	2	162	GLU	C-N-CA	7.07	133.51	121.14
1	1	193	ARG	CD-NE-CZ	-7.07	114.50	124.40
1	2	83	TRP	N-CA-C	-7.06	95.76	110.80
1	2	310	TYR	CA-C-N	7.06	135.02	121.54
1	2	310	TYR	C-N-CA	7.06	135.02	121.54
1	4	266	LEU	CA-C-O	7.06	128.37	119.12
1	3	225	THR	CA-C-N	-7.06	111.17	120.91
1	3	225	THR	C-N-CA	-7.06	111.17	120.91
1	1	182	LYS	CA-C-O	-7.05	113.45	121.07
1	4	266	LEU	N-CA-C	-7.05	104.67	113.20
1	3	181	GLN	CA-CB-CG	-7.05	100.00	114.10
1	3	310	TYR	N-CA-C	7.05	119.32	108.12
1	2	46	ASP	N-CA-CB	7.04	121.94	110.32
1	2	289	SER	CA-CB-OG	7.04	125.19	111.10
1	2	11	ILE	N-CA-C	7.04	117.80	110.62
1	4	240	ASP	CA-C-O	-7.03	112.69	120.70
1	1	181	GLN	O-C-N	-7.03	113.25	122.59
1	2	85	LYS	N-CA-C	-7.03	95.83	110.80
1	2	177	VAL	CA-C-O	7.03	129.56	120.78
1	1	162	GLU	CG-CD-OE1	7.02	134.56	118.40
1	2	46	ASP	O-C-N	7.02	131.97	123.26
1	2	163	ASN	N-CA-CB	-7.02	98.96	110.40
1	2	133	LEU	N-CA-CB	-7.02	98.63	110.49
1	3	128	VAL	CA-C-O	-7.02	112.06	121.32
1	2	210	ALA	O-C-N	7.02	129.33	122.03
1	2	280	SER	CB-CA-C	7.01	124.38	110.42
1	3	64	VAL	CA-C-N	-7.01	114.49	123.19
1	3	64	VAL	C-N-CA	-7.01	114.49	123.19
1	1	231	VAL	O-C-N	7.01	127.22	121.40
1	1	243	VAL	O-C-N	7.00	130.99	123.00
1	4	225	THR	N-CA-C	-7.00	99.62	108.45
1	3	29	VAL	CA-C-O	-6.99	112.04	120.78
1	1	37	GLU	CA-CB-CG	6.99	128.08	114.10
1	4	241	LEU	CA-C-N	6.98	132.63	123.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	241	LEU	C-N-CA	6.98	132.63	123.00
1	2	141	THR	CA-CB-CG2	6.98	122.36	110.50
1	3	201	ASN	N-CA-CB	-6.98	99.26	110.63
1	1	147	SER	N-CA-C	6.97	125.64	110.80
1	1	172	THR	N-CA-CB	6.96	121.51	110.65
1	2	259	LYS	N-CA-C	-6.96	102.91	111.40
1	3	26	VAL	CA-C-O	-6.96	112.08	120.78
1	4	285	ASP	O-C-N	6.94	131.82	122.59
1	3	80	ASN	CB-CG-OD1	-6.94	106.93	120.80
1	4	181	GLN	CA-C-O	6.93	130.43	120.51
1	3	144	SER	CA-C-O	-6.93	113.28	121.11
1	3	297	ILE	N-CA-CB	-6.93	97.57	111.91
1	1	120	PRO	CB-CA-C	6.92	120.09	111.23
1	1	229	PHE	N-CA-CB	6.92	122.43	110.81
1	4	43	PHE	N-CA-CB	6.92	120.10	110.90
1	4	114	LYS	CA-C-N	6.92	133.69	122.69
1	4	114	LYS	C-N-CA	6.92	133.69	122.69
1	2	231	VAL	O-C-N	6.92	127.14	121.40
1	2	267	GLN	CB-CG-CD	-6.92	100.84	112.60
1	3	313	GLU	CG-CD-OE1	6.91	134.30	118.40
1	3	139	ASP	CB-CA-C	6.91	123.24	110.11
1	2	313	GLU	CA-CB-CG	6.90	127.91	114.10
1	1	9	GLY	N-CA-C	-6.90	96.82	113.18
1	4	307	VAL	N-CA-CB	-6.90	101.87	111.25
1	2	228	ALA	CA-C-O	6.90	128.72	120.99
1	3	266	LEU	O-C-N	6.89	131.75	122.59
1	4	39	MET	N-CA-C	-6.88	103.47	110.97
1	2	279	SER	CA-C-O	-6.88	110.67	120.51
1	4	309	TRP	CA-CB-CG	6.88	126.67	113.60
1	2	178	THR	OG1-CB-CG2	6.87	123.05	109.30
1	1	235	ASP	CA-CB-CG	-6.87	105.73	112.60
1	4	262	SER	CA-C-O	-6.87	110.69	120.51
1	3	248	GLU	N-CA-C	-6.86	101.97	110.41
1	2	235	ASP	OD1-CG-OD2	-6.86	106.43	122.90
1	2	230	ARG	NE-CZ-NH1	6.86	128.36	121.50
1	3	280	SER	CA-CB-OG	-6.86	97.38	111.10
1	4	267	GLN	CG-CD-NE2	-6.84	106.14	116.40
1	4	309	TRP	O-C-N	6.83	132.07	123.19
1	1	40	VAL	CA-CB-CG2	6.83	122.00	110.40
1	4	165	GLU	N-CA-C	6.83	125.34	110.80
1	3	215	LYS	CA-CB-CG	6.82	127.74	114.10
1	3	233	THR	CA-CB-CG2	6.82	122.10	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	212	ALA	CA-C-O	-6.81	112.57	120.20
1	4	30	ASN	O-C-N	6.81	131.10	123.40
1	4	224	LEU	CA-C-O	-6.81	113.16	121.06
1	2	43	PHE	CA-C-O	-6.81	111.69	120.00
1	2	130	GLY	CA-C-N	6.81	129.19	120.88
1	2	130	GLY	C-N-CA	6.81	129.19	120.88
1	4	168	GLU	CB-CG-CD	6.80	124.16	112.60
1	4	219	GLU	CB-CG-CD	6.80	124.16	112.60
1	4	163	ASN	N-CA-C	6.80	120.83	112.54
1	3	178	THR	CB-CA-C	-6.79	95.96	109.33
1	3	164	PHE	O-C-N	6.78	131.61	122.59
1	1	329	LYS	CA-C-O	-6.78	110.81	120.51
1	4	300	SER	CA-C-N	6.78	134.49	121.54
1	4	300	SER	C-N-CA	6.78	134.49	121.54
1	1	310	TYR	CA-C-O	6.78	130.20	120.51
1	2	51	VAL	CA-C-O	-6.78	112.31	120.78
1	1	24	ALA	CB-CA-C	6.78	121.69	109.83
1	1	317	SER	CA-C-N	6.78	130.27	120.38
1	1	317	SER	C-N-CA	6.78	130.27	120.38
1	3	312	ASN	CA-CB-CG	6.77	119.37	112.60
1	4	291	PHE	CA-CB-CG	6.77	120.57	113.80
1	2	213	VAL	N-CA-CB	6.77	118.30	110.65
1	1	26	VAL	CA-C-O	-6.76	112.33	120.78
1	4	171	MET	CG-SD-CE	6.76	115.77	100.90
1	1	244	ARG	NE-CZ-NH1	6.76	128.26	121.50
1	2	33	PHE	N-CA-CB	-6.76	103.19	114.27
1	2	59	GLU	CB-CA-C	-6.75	99.08	110.43
1	1	307	VAL	CA-CB-CG1	-6.75	98.92	110.40
1	3	192	TRP	CB-CA-C	-6.75	99.53	110.74
1	3	147	SER	CB-CA-C	-6.75	96.99	110.42
1	2	284	GLY	N-CA-C	-6.75	97.19	113.18
1	4	313	GLU	CB-CA-C	6.75	121.47	110.88
1	1	104	ALA	CA-C-O	6.74	127.88	120.80
1	2	312	ASN	CA-C-O	-6.74	110.87	120.51
1	4	318	GLN	CA-C-O	6.74	127.56	120.42
1	4	260	THR	N-CA-CB	6.73	122.30	110.18
1	2	167	VAL	CB-CA-C	6.73	122.32	111.29
1	3	55	GLU	N-CA-C	-6.73	96.34	108.58
1	4	109	LYS	O-C-N	6.72	131.53	122.59
1	1	295	ALA	CA-C-N	-6.72	111.29	121.51
1	1	295	ALA	C-N-CA	-6.72	111.29	121.51
1	1	120	PRO	N-CA-C	-6.72	100.53	111.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3	308	SER	O-C-N	6.72	131.55	123.36
1	1	179	ALA	O-C-N	6.71	129.83	122.11
1	3	306	VAL	CB-CA-C	6.71	121.01	110.81
1	4	183	THR	O-C-N	6.71	133.15	122.41
1	3	220	LEU	CA-CB-CG	6.71	139.78	116.30
1	1	296	GLY	O-C-N	6.70	130.36	122.38
1	3	258	MET	CA-CB-CG	-6.69	100.72	114.10
1	4	281	ASP	N-CA-C	-6.69	96.55	110.80
1	3	121	SER	CA-CB-OG	6.69	124.48	111.10
1	1	41	TYR	N-CA-C	-6.69	104.38	112.54
1	3	157	ALA	N-CA-C	-6.68	103.68	110.97
1	3	176	ALA	N-CA-CB	-6.68	99.65	111.08
1	2	279	SER	CB-CA-C	6.68	123.72	110.42
1	2	141	THR	CA-CB-OG1	-6.68	99.58	109.60
1	3	179	ALA	CA-C-O	-6.68	113.44	120.92
1	3	202	ILE	CA-C-O	-6.68	112.84	120.65
1	3	281	ASP	CB-CG-OD1	6.68	133.76	118.40
1	2	56	VAL	CA-C-O	-6.68	116.82	122.63
1	4	31	ASP	N-CA-C	6.68	122.41	108.39
1	4	238	VAL	CB-CA-C	6.68	120.71	110.96
1	1	163	ASN	CB-CG-OD1	-6.67	107.45	120.80
1	4	114	LYS	N-CA-CB	-6.67	98.93	111.00
1	4	132	ASN	CB-CG-ND2	6.67	126.41	116.40
1	3	117	ILE	N-CA-CB	-6.67	104.96	111.89
1	1	41	TYR	N-CA-CB	6.66	121.45	110.39
1	1	183	THR	CA-CB-CG2	6.66	121.82	110.50
1	4	181	GLN	O-C-N	-6.66	113.74	122.59
1	1	281	ASP	N-CA-C	-6.66	96.62	110.80
1	4	125	PRO	CB-CA-C	6.65	122.54	111.56
1	1	320	VAL	O-C-N	6.65	130.88	122.57
1	3	279	SER	N-CA-C	-6.64	96.64	110.80
1	3	307	VAL	CA-CB-CG1	-6.64	99.11	110.40
1	4	137	SER	CB-CA-C	6.64	121.59	110.43
1	2	18	ALA	O-C-N	6.64	129.81	122.11
1	1	52	PHE	CA-CB-CG	6.64	120.44	113.80
1	2	274	GLU	CB-CA-C	-6.64	98.33	109.75
1	4	168	GLU	CA-CB-CG	6.63	127.36	114.10
1	1	21	SER	N-CA-C	-6.62	105.17	113.18
1	2	12	GLY	CA-C-O	6.62	127.29	120.80
1	3	225	THR	CA-C-O	-6.62	114.10	121.05
1	2	292	ASP	CA-CB-CG	6.62	119.22	112.60
1	3	80	ASN	CB-CG-ND2	6.62	126.33	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3	328	GLN	CG-CD-NE2	6.62	126.33	116.40
1	4	293	ALA	O-C-N	6.62	131.39	122.59
1	4	149	THR	CA-C-N	6.61	129.44	120.38
1	4	149	THR	C-N-CA	6.61	129.44	120.38
1	4	245	LEU	CA-C-O	-6.61	111.78	119.78
1	3	273	THR	CA-CB-OG1	-6.61	99.69	109.60
1	4	127	PHE	CB-CA-C	6.61	120.81	109.51
1	2	64	VAL	CA-CB-CG1	6.61	121.63	110.40
1	3	173	THR	CB-CA-C	6.60	121.14	109.72
1	3	177	VAL	O-C-N	-6.59	114.33	122.57
1	4	137	SER	CA-C-N	6.59	134.13	121.54
1	4	137	SER	C-N-CA	6.59	134.13	121.54
1	4	313	GLU	CG-CD-OE2	6.59	133.57	118.40
1	1	178	THR	CB-CA-C	-6.59	97.27	111.11
1	2	207	THR	CA-CB-CG2	6.59	121.70	110.50
1	3	254	ILE	N-CA-CB	-6.59	102.24	110.47
1	3	328	GLN	CB-CG-CD	6.58	123.79	112.60
1	4	231	VAL	N-CA-CB	-6.58	106.08	111.67
1	4	322	ASP	CB-CG-OD1	6.58	133.53	118.40
1	4	114	LYS	CB-CG-CD	6.58	126.42	111.30
1	1	6	ASN	CA-C-O	6.57	129.91	120.51
1	3	225	THR	CA-CB-OG1	-6.57	99.75	109.60
1	1	217	ILE	CA-C-N	6.56	128.04	119.84
1	1	217	ILE	C-N-CA	6.56	128.04	119.84
1	2	52	PHE	CB-CA-C	6.56	123.47	110.42
1	4	323	LEU	N-CA-C	-6.56	100.61	111.37
1	2	270	LEU	CA-C-N	6.56	134.26	121.41
1	2	270	LEU	C-N-CA	6.56	134.26	121.41
1	2	142	VAL	CA-CB-CG1	6.55	121.54	110.40
1	3	303	PHE	CA-C-O	-6.55	113.25	120.33
1	4	319	ARG	CD-NE-CZ	-6.55	115.22	124.40
1	2	113	LYS	N-CA-C	6.55	124.75	110.80
1	2	196	ARG	CA-CB-CG	6.55	127.20	114.10
1	4	27	VAL	N-CA-CB	-6.55	100.42	111.23
1	2	230	ARG	NH1-CZ-NH2	-6.55	110.79	119.30
1	2	167	VAL	CA-CB-CG2	6.54	121.53	110.40
1	2	147	SER	CA-C-N	6.54	131.76	120.58
1	2	147	SER	C-N-CA	6.54	131.76	120.58
1	3	85	LYS	CA-CB-CG	6.54	127.18	114.10
1	3	180	THR	CA-CB-OG1	-6.54	99.79	109.60
1	2	223	LYS	CA-C-O	-6.54	111.54	119.32
1	4	103	LYS	N-CA-CB	6.54	119.83	110.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3	138	LYS	N-CA-C	6.53	124.72	110.80
1	4	253	ASP	CB-CG-OD2	-6.53	103.37	118.40
1	3	216	VAL	CA-C-O	6.53	128.94	120.78
1	3	83	TRP	N-CA-C	-6.52	96.92	110.80
1	1	107	HIS	CA-CB-CG	6.52	120.32	113.80
1	2	304	VAL	O-C-N	-6.52	115.72	122.95
1	2	111	GLY	O-C-N	6.51	131.17	122.70
1	1	323	LEU	CA-CB-CG	6.51	139.07	116.30
1	4	178	THR	CB-CA-C	-6.51	98.01	110.24
1	2	15	VAL	O-C-N	6.50	128.53	121.83
1	4	231	VAL	O-C-N	6.50	127.36	121.57
1	3	203	ILE	N-CA-CB	-6.50	103.43	112.27
1	1	196	ARG	NE-CZ-NH1	-6.50	115.00	121.50
1	4	26	VAL	CB-CA-C	6.49	121.93	111.29
1	4	169	GLY	CA-C-O	6.49	126.90	121.06
1	3	97	VAL	N-CA-CB	-6.49	103.62	110.82
1	4	151	ASN	CA-C-O	-6.49	112.51	119.97
1	2	176	ALA	CA-C-O	-6.48	113.37	120.30
1	4	161	HIS	O-C-N	6.48	131.21	122.59
1	1	133	LEU	CB-CA-C	6.48	123.31	110.42
1	3	274	GLU	CB-CA-C	-6.47	97.54	110.42
1	2	165	GLU	CB-CG-CD	-6.47	101.60	112.60
1	1	41	TYR	O-C-N	6.47	131.09	122.43
1	3	111	GLY	CA-C-O	-6.47	109.32	120.57
1	2	245	LEU	CA-C-O	-6.46	114.02	120.80
1	3	262	SER	N-CA-C	-6.46	104.24	111.28
1	4	84	SER	O-C-N	6.46	131.18	122.59
1	1	47	SER	CA-C-O	-6.46	114.04	120.82
1	2	313	GLU	CA-C-O	-6.46	113.99	120.90
1	4	181	GLN	OE1-CD-NE2	-6.45	116.15	122.60
1	2	101	ILE	CA-C-O	6.45	128.84	120.78
1	4	193	ARG	CD-NE-CZ	6.44	133.42	124.40
1	2	188	SER	CA-C-O	6.44	126.02	119.97
1	4	184	VAL	CA-C-N	6.44	133.83	121.54
1	4	184	VAL	C-N-CA	6.44	133.83	121.54
1	2	155	PRO	CA-C-N	6.44	130.64	120.47
1	2	155	PRO	C-N-CA	6.44	130.64	120.47
1	2	177	VAL	CA-CB-CG1	6.44	121.34	110.40
1	1	175	HIS	CB-CA-C	6.43	121.09	109.83
1	1	147	SER	CA-C-N	6.43	129.22	120.54
1	1	147	SER	C-N-CA	6.43	129.22	120.54
1	3	281	ASP	N-CA-C	-6.43	97.10	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	188	SER	CA-C-O	6.43	129.70	120.51
1	4	7	GLY	O-C-N	6.42	128.87	122.77
1	4	31	ASP	CA-CB-CG	-6.42	106.18	112.60
1	2	11	ILE	CA-C-O	-6.42	114.27	120.95
1	4	303	PHE	CA-C-O	-6.42	113.38	120.70
1	4	142	VAL	O-C-N	-6.42	114.55	122.57
1	4	177	VAL	CB-CA-C	6.41	121.81	111.29
1	3	258	MET	CA-C-O	-6.41	113.12	120.24
1	2	235	ASP	CA-C-N	-6.41	110.44	121.97
1	2	235	ASP	C-N-CA	-6.41	110.44	121.97
1	4	235	ASP	CA-C-N	-6.41	110.44	121.97
1	4	235	ASP	C-N-CA	-6.41	110.44	121.97
1	4	314	PHE	CA-CB-CG	6.41	120.21	113.80
1	3	271	GLY	CA-C-O	-6.40	109.44	120.57
1	2	153	LEU	CA-C-O	-6.39	112.19	119.41
1	3	181	GLN	CA-C-O	6.39	129.65	120.51
1	1	223	LYS	CA-C-N	-6.39	112.65	122.62
1	1	223	LYS	C-N-CA	-6.39	112.65	122.62
1	3	250	SER	O-C-N	6.39	130.89	123.41
1	4	229	PHE	N-CA-CB	6.39	120.98	110.69
1	4	37	GLU	OE1-CD-OE2	6.39	138.23	122.90
1	4	24	ALA	CA-C-O	6.39	127.89	120.80
1	4	203	ILE	N-CA-CB	-6.39	102.27	111.21
1	3	305	LYS	CG-CD-CE	6.38	125.98	111.30
1	1	10	ARG	NE-CZ-NH1	6.38	127.88	121.50
1	1	280	SER	N-CA-CB	-6.38	99.71	110.49
1	1	10	ARG	NE-CZ-NH2	-6.38	113.46	119.20
1	3	279	SER	O-C-N	6.38	131.07	122.59
1	3	295	ALA	CA-C-O	6.37	128.60	120.57
1	2	128	VAL	N-CA-C	-6.37	99.94	108.35
1	1	4	GLY	O-C-N	6.37	130.97	122.70
1	3	123	ASP	CA-C-O	-6.37	111.10	119.06
1	4	126	MET	CB-CA-C	-6.37	102.72	111.51
1	3	151	ASN	CB-CA-C	6.36	121.35	110.79
1	3	68	LYS	CA-CB-CG	6.36	126.82	114.10
1	2	45	TYR	N-CA-CB	-6.36	100.45	110.69
1	2	298	GLN	CB-CG-CD	6.36	123.41	112.60
1	1	67	GLY	O-C-N	6.36	130.96	122.70
1	1	256	ALA	CA-C-O	-6.35	113.82	120.55
1	2	107	HIS	N-CA-CB	6.35	121.22	110.49
1	3	231	VAL	CA-CB-CG1	6.34	121.18	110.40
1	4	37	GLU	CG-CD-OE1	-6.34	103.83	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	93	GLU	CG-CD-OE1	6.33	132.96	118.40
1	3	234	PRO	N-CA-C	6.33	122.32	113.53
1	2	314	PHE	N-CA-CB	-6.31	101.01	111.49
1	3	239	VAL	N-CA-CB	6.31	117.60	110.72
1	4	17	ARG	CA-CB-CG	6.31	126.73	114.10
1	2	168	GLU	CA-C-N	6.31	128.17	121.48
1	2	168	GLU	C-N-CA	6.31	128.17	121.48
1	3	263	GLU	O-C-N	6.31	129.56	122.11
1	1	207	THR	N-CA-CB	6.31	121.84	111.62
1	4	127	PHE	CA-CB-CG	-6.31	107.49	113.80
1	1	270	LEU	CA-C-O	-6.30	113.86	121.05
1	2	273	THR	CA-CB-CG2	6.30	121.20	110.50
1	1	139	ASP	O-C-N	6.29	129.59	122.22
1	3	234	PRO	CA-N-CD	-6.29	103.19	112.00
1	1	192	TRP	CB-CA-C	-6.29	97.91	110.42
1	2	49	HIS	CA-CB-CG	-6.29	107.52	113.80
1	3	85	LYS	N-CA-CB	6.28	119.58	109.28
1	1	209	ALA	N-CA-C	-6.28	103.00	112.04
1	1	211	LYS	CA-C-O	6.27	129.48	120.51
1	1	239	VAL	CB-CA-C	6.27	119.37	110.84
1	2	30	ASN	OD1-CG-ND2	-6.26	116.34	122.60
1	3	7	GLY	O-C-N	6.26	129.12	122.86
1	1	322	ASP	CA-C-N	-6.25	112.10	120.79
1	1	322	ASP	C-N-CA	-6.25	112.10	120.79
1	2	91	ILE	O-C-N	6.25	129.81	122.69
1	2	30	ASN	CA-CB-CG	6.24	118.84	112.60
1	4	304	VAL	N-CA-CB	-6.24	104.55	112.60
1	3	35	ALA	N-CA-CB	-6.24	101.19	110.17
1	1	183	THR	CB-CA-C	-6.24	99.27	110.37
1	3	47	SER	CB-CA-C	6.23	120.67	110.88
1	1	240	ASP	N-CA-CB	-6.23	100.77	110.55
1	1	279	SER	CA-C-N	6.23	133.43	121.54
1	1	279	SER	C-N-CA	6.23	133.43	121.54
1	1	230	ARG	CA-C-N	6.22	131.39	122.24
1	1	230	ARG	C-N-CA	6.22	131.39	122.24
1	1	331	ASP	O-C-N	6.22	129.29	122.20
1	3	140	MET	CA-C-O	6.22	127.12	120.46
1	3	320	VAL	N-CA-CB	6.22	121.50	111.23
1	3	277	VAL	N-CA-CB	-6.22	100.97	111.23
1	3	287	ARG	CA-C-O	-6.21	111.62	120.51
1	3	235	ASP	CA-CB-CG	-6.21	106.39	112.60
1	2	251	TYR	CA-CB-CG	-6.21	102.72	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3	45	TYR	N-CA-CB	-6.21	100.06	110.80
1	4	299	LEU	N-CA-CB	-6.21	100.75	111.55
1	2	315	GLY	CA-C-O	6.20	127.84	120.90
1	3	313	GLU	CA-CB-CG	6.20	126.50	114.10
1	1	144	SER	CB-CA-C	-6.20	99.58	109.80
1	2	84	SER	N-CA-C	-6.19	97.61	110.80
1	4	298	GLN	CB-CA-C	6.19	119.96	109.99
1	1	298	GLN	CB-CG-CD	6.19	123.13	112.60
1	1	37	GLU	N-CA-CB	6.19	120.81	110.41
1	1	115	VAL	CB-CA-C	-6.19	100.04	111.18
1	1	167	VAL	CA-CB-CG2	6.19	120.92	110.40
1	2	34	ILE	N-CA-CB	-6.19	101.01	111.23
1	3	91	ILE	CA-C-O	-6.19	113.71	120.71
1	1	18	ALA	CA-C-O	6.19	129.36	120.51
1	4	10	ARG	CB-CA-C	6.19	122.73	110.42
1	3	27	VAL	N-CA-CB	-6.18	101.03	111.23
1	1	139	ASP	N-CA-CB	6.18	119.74	110.22
1	3	258	MET	O-C-N	6.18	130.27	122.23
1	2	68	LYS	O-C-N	6.18	130.78	123.36
1	4	197	GLY	CA-C-N	6.18	133.34	121.54
1	4	197	GLY	C-N-CA	6.18	133.34	121.54
1	4	266	LEU	CB-CA-C	6.18	121.85	110.11
1	1	309	TRP	CA-C-N	6.17	133.33	121.54
1	1	309	TRP	C-N-CA	6.17	133.33	121.54
1	2	138	LYS	CG-CD-CE	6.17	125.50	111.30
1	4	253	ASP	OD1-CG-OD2	6.17	137.71	122.90
1	2	225	THR	N-CA-CB	6.17	121.12	111.56
1	3	292	ASP	O-C-N	6.17	130.33	122.93
1	4	166	ILE	CA-C-O	-6.16	113.08	120.78
1	3	183	THR	OG1-CB-CG2	6.16	121.62	109.30
1	4	84	SER	N-CA-C	-6.16	97.68	110.80
1	4	63	LEU	CB-CA-C	6.16	119.90	109.80
1	1	286	ASN	CB-CG-ND2	-6.16	107.17	116.40
1	2	303	PHE	N-CA-CB	6.16	120.22	110.55
1	4	45	TYR	N-CA-C	6.16	118.94	108.90
1	2	50	GLY	CA-C-N	6.15	133.04	121.97
1	2	50	GLY	C-N-CA	6.15	133.04	121.97
1	4	187	PRO	CA-C-O	-6.15	114.41	121.36
1	1	55	GLU	CA-C-N	-6.15	115.83	122.59
1	1	55	GLU	C-N-CA	-6.15	115.83	122.59
1	4	140	MET	CA-C-O	-6.15	113.68	120.69
1	1	209	ALA	CA-C-N	-6.15	111.43	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	209	ALA	C-N-CA	-6.15	111.43	120.28
1	3	328	GLN	OE1-CD-NE2	-6.14	116.46	122.60
1	3	66	ASP	N-CA-CB	-6.14	102.86	112.13
1	1	144	SER	CA-CB-OG	-6.13	98.83	111.10
1	1	188	SER	CA-CB-OG	6.13	123.36	111.10
1	3	25	GLN	CG-CD-NE2	-6.13	107.20	116.40
1	2	48	THR	CA-C-O	-6.13	114.39	120.82
1	4	162	GLU	CG-CD-OE2	-6.13	104.31	118.40
1	4	185	ASP	CB-CA-C	6.12	122.60	110.42
1	3	70	ILE	CB-CA-C	6.12	119.88	111.31
1	3	244	ARG	NE-CZ-NH1	6.12	127.62	121.50
1	3	157	ALA	CA-C-N	6.11	129.99	120.82
1	3	157	ALA	C-N-CA	6.11	129.99	120.82
1	4	258	MET	N-CA-CB	6.11	119.72	110.30
1	1	287	ARG	NH1-CZ-NH2	-6.11	111.36	119.30
1	1	196	ARG	CB-CG-CD	6.10	125.34	111.30
1	3	205	SER	CB-CA-C	-6.10	103.13	110.94
1	3	187	PRO	CA-C-O	-6.10	114.60	121.43
1	1	295	ALA	N-CA-C	6.10	120.67	107.49
1	2	149	THR	CA-CB-OG1	-6.10	100.45	109.60
1	3	304	VAL	N-CA-CB	-6.09	101.18	111.23
1	4	72	VAL	CA-C-O	-6.09	113.85	120.67
1	4	258	MET	CB-CG-SD	-6.09	94.44	112.70
1	3	199	ALA	CA-C-O	6.08	125.48	118.55
1	3	318	GLN	CA-CB-CG	6.08	126.26	114.10
1	2	28	ALA	CA-C-O	-6.08	113.94	120.75
1	2	124	ALA	CA-C-O	-6.08	114.08	120.70
1	3	33	PHE	O-C-N	6.07	130.66	122.59
1	3	83	TRP	N-CA-CB	6.07	120.75	110.49
1	1	176	ALA	O-C-N	-6.07	116.13	123.29
1	2	301	LYS	N-CA-C	6.07	123.72	110.80
1	1	287	ARG	O-C-N	6.07	130.66	122.59
1	3	322	ASP	CA-C-N	-6.07	112.36	120.79
1	3	322	ASP	C-N-CA	-6.07	112.36	120.79
1	4	107	HIS	N-CA-CB	6.07	120.74	110.49
1	1	97	VAL	CA-C-O	-6.06	113.20	120.78
1	4	55	GLU	N-CA-C	-6.06	98.94	108.63
1	4	235	ASP	CB-CG-OD1	6.06	132.33	118.40
1	4	298	GLN	OE1-CD-NE2	-6.06	116.54	122.60
1	3	301	LYS	O-C-N	6.05	130.64	122.59
1	1	26	VAL	CB-CA-C	6.05	121.22	111.29
1	3	248	GLU	CA-C-O	-6.05	115.09	121.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3	318	GLN	CG-CD-NE2	6.05	125.48	116.40
1	2	173	THR	CA-C-O	6.05	127.02	120.43
1	4	192	TRP	N-CA-C	6.05	123.68	110.80
1	1	289	SER	CA-C-O	-6.05	111.86	120.51
1	2	308	SER	CA-C-O	-6.04	113.83	120.36
1	3	179	ALA	N-CA-CB	6.04	119.63	109.78
1	1	166	ILE	N-CA-CB	6.04	121.19	111.23
1	1	253	ASP	N-CA-CB	6.04	120.69	110.49
1	4	323	LEU	CA-CB-CG	6.03	137.41	116.30
1	3	235	ASP	CA-C-N	-6.03	111.11	121.97
1	3	235	ASP	C-N-CA	-6.03	111.11	121.97
1	3	273	THR	CA-C-N	6.03	133.05	121.54
1	3	273	THR	C-N-CA	6.03	133.05	121.54
1	3	290	ILE	CB-CA-C	6.03	119.55	110.63
1	2	65	VAL	CA-C-N	-6.02	113.97	122.34
1	2	65	VAL	C-N-CA	-6.02	113.97	122.34
1	2	183	THR	CA-C-O	-6.02	111.22	119.05
1	3	82	PRO	CA-C-O	-6.02	113.82	122.31
1	4	79	GLU	O-C-N	6.02	130.60	122.59
1	2	259	LYS	N-CA-CB	6.01	119.03	110.13
1	2	204	PRO	O-C-N	-6.01	114.53	122.64
1	2	274	GLU	CA-CB-CG	6.01	126.12	114.10
1	3	147	SER	N-CA-CB	-6.01	100.34	110.49
1	4	2	LYS	CA-CB-CG	6.01	126.11	114.10
1	3	121	SER	N-CA-CB	6.00	120.98	111.43
1	1	234	PRO	N-CD-CG	-6.00	94.20	103.20
1	4	144	SER	CA-C-O	-6.00	113.76	120.66
1	1	2	LYS	N-CA-C	-6.00	98.87	109.06
1	4	187	PRO	N-CA-C	6.00	120.62	111.15
1	3	311	ASP	N-CA-CB	5.99	120.62	110.49
1	2	79	GLU	N-CA-C	-5.99	106.06	113.19
1	4	31	ASP	N-CA-CB	-5.99	102.41	111.21
1	1	228	ALA	CA-C-N	5.99	132.39	122.33
1	1	228	ALA	C-N-CA	5.99	132.39	122.33
1	1	141	THR	N-CA-C	5.99	120.71	113.41
1	3	302	THR	CA-CB-OG1	-5.99	100.62	109.60
1	2	45	TYR	CA-C-O	-5.98	114.37	120.71
1	4	317	SER	CA-C-O	-5.98	111.95	120.51
1	4	147	SER	CA-C-O	5.98	129.06	120.51
1	3	204	PRO	O-C-N	-5.98	114.57	122.64
1	3	148	CYS	CA-C-N	5.98	129.10	120.79
1	3	148	CYS	C-N-CA	5.98	129.10	120.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3	187	PRO	N-CA-CB	-5.98	98.30	103.32
1	3	116	VAL	N-CA-CB	5.97	121.25	111.45
1	4	247	LYS	CB-CG-CD	5.97	125.03	111.30
1	3	72	VAL	CB-CA-C	5.97	119.62	110.55
1	3	162	GLU	CA-CB-CG	5.97	126.03	114.10
1	4	162	GLU	N-CA-C	-5.97	101.53	111.37
1	2	258	MET	CA-C-O	-5.96	113.11	119.97
1	2	303	PHE	N-CA-C	-5.96	98.80	108.52
1	1	300	SER	CA-C-N	5.96	132.93	121.54
1	1	300	SER	C-N-CA	5.96	132.93	121.54
1	1	155	PRO	CB-CA-C	5.96	121.39	111.56
1	1	248	GLU	N-CA-C	-5.96	102.62	110.43
1	1	162	GLU	CG-CD-OE2	-5.96	104.70	118.40
1	3	21	SER	CA-C-O	5.95	126.79	119.05
1	4	310	TYR	N-CA-C	5.95	117.58	108.12
1	4	85	LYS	O-C-N	5.94	130.50	122.59
1	1	322	ASP	CB-CG-OD2	-5.94	104.73	118.40
1	1	64	VAL	CB-CA-C	5.94	119.20	110.77
1	2	79	GLU	CB-CG-CD	5.94	122.69	112.60
1	3	244	ARG	CA-CB-CG	5.94	125.97	114.10
1	1	149	THR	N-CA-C	-5.93	104.73	111.14
1	3	278	VAL	N-CA-CB	-5.93	101.44	111.23
1	4	25	GLN	O-C-N	5.93	130.13	122.89
1	3	91	ILE	CB-CA-C	-5.93	103.56	110.91
1	3	48	THR	O-C-N	-5.93	115.00	122.17
1	4	235	ASP	OD1-CG-OD2	-5.92	108.68	122.90
1	4	83	TRP	N-CA-CB	5.92	120.50	110.49
1	1	25	GLN	O-C-N	5.92	130.03	123.16
1	2	298	GLN	CA-CB-CG	5.92	125.94	114.10
1	1	184	VAL	CB-CA-C	5.91	120.99	111.29
1	2	92	VAL	CA-C-O	-5.91	113.89	121.40
1	4	95	THR	CA-CB-OG1	-5.91	100.73	109.60
1	4	187	PRO	N-CD-CG	-5.91	94.33	103.20
1	2	189	ALA	O-C-N	5.91	130.45	122.59
1	2	153	LEU	CB-CA-C	5.91	119.58	109.24
1	2	260	THR	O-C-N	5.91	128.93	122.20
1	3	311	ASP	OD1-CG-OD2	-5.90	108.73	122.90
1	2	244	ARG	CA-C-O	-5.90	113.82	120.43
1	3	93	GLU	N-CA-C	5.90	118.43	107.99
1	3	151	ASN	CB-CG-OD1	5.90	132.59	120.80
1	3	321	ILE	CA-CB-CG2	5.90	120.53	110.50
1	4	129	CYS	N-CA-CB	5.90	120.45	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3	79	GLU	N-CA-C	-5.89	106.17	113.19
1	1	131	VAL	CB-CA-C	5.89	119.64	111.92
1	2	275	ASP	N-CA-C	-5.88	103.49	111.55
1	1	69	LYS	CA-C-O	5.88	127.15	120.80
1	2	330	VAL	CA-CB-CG1	5.88	120.40	110.40
1	3	31	ASP	CB-CG-OD1	5.88	131.93	118.40
1	4	327	MET	CB-CA-C	5.88	120.02	110.96
1	2	127	PHE	CA-C-O	-5.88	114.31	121.36
1	4	162	GLU	N-CA-CB	5.88	119.36	109.78
1	3	165	GLU	CG-CD-OE1	5.88	131.91	118.40
1	3	196	ARG	CA-CB-CG	5.88	125.85	114.10
1	1	48	THR	N-CA-C	5.87	118.56	111.40
1	1	181	GLN	CA-C-O	5.87	128.90	120.51
1	2	79	GLU	CA-CB-CG	5.87	125.83	114.10
1	3	4	GLY	N-CA-C	-5.87	99.28	113.18
1	1	224	LEU	N-CA-CB	-5.87	100.69	111.37
1	4	142	VAL	CA-CB-CG1	5.86	120.36	110.40
1	2	83	TRP	CB-CA-C	5.86	122.07	110.42
1	3	120	PRO	CA-C-O	-5.86	114.58	122.08
1	2	328	GLN	CG-CD-NE2	-5.85	107.62	116.40
1	1	176	ALA	N-CA-CB	-5.85	101.39	110.57
1	3	25	GLN	CB-CG-CD	-5.84	102.67	112.60
1	4	240	ASP	CA-C-N	5.84	131.22	122.99
1	4	240	ASP	C-N-CA	5.84	131.22	122.99
1	2	259	LYS	CA-CB-CG	5.83	125.77	114.10
1	4	157	ALA	CA-C-N	5.83	132.68	121.54
1	4	157	ALA	C-N-CA	5.83	132.68	121.54
1	1	191	ASP	N-CA-CB	-5.83	100.64	110.49
1	2	117	ILE	CB-CG1-CD1	5.83	126.04	113.80
1	2	326	HIS	CA-CB-CG	5.83	119.62	113.80
1	3	303	PHE	O-C-N	5.82	130.81	123.12
1	2	44	LYS	CA-C-O	-5.82	111.66	119.11
1	3	136	TYR	N-CA-C	5.82	118.73	109.24
1	4	181	GLN	CB-CA-C	5.82	122.00	110.42
1	1	89	GLU	N-CA-CB	-5.81	100.67	110.49
1	1	152	CYS	O-C-N	5.81	130.12	122.33
1	4	286	ASN	N-CA-CB	-5.81	100.67	110.49
1	1	52	PHE	CB-CA-C	5.81	121.97	110.42
1	3	18	ALA	N-CA-C	-5.81	102.68	111.56
1	4	4	GLY	O-C-N	5.80	130.25	122.70
1	1	267	GLN	CB-CG-CD	-5.80	102.74	112.60
1	3	208	GLY	CA-C-O	5.80	130.66	120.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	300	SER	N-CA-CB	5.79	120.81	110.79
1	4	188	SER	N-CA-C	-5.79	98.48	110.80
1	2	273	THR	CA-CB-OG1	-5.78	100.92	109.60
1	1	244	ARG	CA-C-O	-5.78	114.01	120.54
1	1	209	ALA	N-CA-CB	5.78	119.15	110.19
1	3	114	LYS	N-CA-CB	-5.78	100.77	110.83
1	3	114	LYS	CB-CA-C	5.78	120.41	109.37
1	4	149	THR	CA-C-O	5.78	126.89	120.82
1	2	213	VAL	O-C-N	5.78	128.12	121.94
1	3	132	ASN	CA-CB-CG	5.78	118.38	112.60
1	3	208	GLY	CA-C-N	5.77	130.45	120.58
1	3	208	GLY	C-N-CA	5.77	130.45	120.58
1	4	86	ALA	CA-C-O	5.76	128.75	120.51
1	3	167	VAL	O-C-N	5.76	129.77	122.57
1	1	127	PHE	CA-CB-CG	-5.76	108.04	113.80
1	3	181	GLN	N-CA-CB	-5.75	100.77	110.49
1	1	176	ALA	CA-C-O	-5.75	114.12	120.38
1	4	52	PHE	CA-C-O	-5.75	112.29	120.51
1	1	258	MET	N-CA-CB	5.74	119.18	110.28
1	3	65	VAL	N-CA-C	-5.74	100.13	108.17
1	4	278	VAL	CA-C-O	5.74	127.96	120.78
1	2	299	LEU	CA-C-N	5.74	132.51	121.54
1	2	299	LEU	C-N-CA	5.74	132.51	121.54
1	4	295	ALA	N-CA-C	5.74	118.07	108.02
1	1	95	THR	CA-C-O	5.74	128.72	120.51
1	1	195	GLY	N-CA-C	-5.74	99.58	113.18
1	1	304	VAL	CA-CB-CG1	-5.74	100.65	110.40
1	1	313	GLU	N-CA-CB	5.74	120.18	110.49
1	1	314	PHE	CA-C-O	-5.74	113.01	119.95
1	1	143	VAL	CA-CB-CG2	-5.73	100.65	110.40
1	1	279	SER	CB-CA-C	5.73	121.83	110.42
1	2	40	VAL	CA-C-O	5.73	127.94	120.78
1	4	313	GLU	CB-CG-CD	-5.73	102.86	112.60
1	1	115	VAL	CA-C-N	5.73	131.05	122.75
1	1	115	VAL	C-N-CA	5.73	131.05	122.75
1	1	235	ASP	CA-C-O	-5.73	113.18	119.08
1	1	191	ASP	CB-CA-C	5.72	121.81	110.42
1	1	279	SER	O-C-N	-5.72	114.98	122.59
1	2	132	ASN	CA-C-N	5.72	132.47	121.54
1	2	132	ASN	C-N-CA	5.72	132.47	121.54
1	3	79	GLU	CG-CD-OE1	5.72	131.56	118.40
1	4	254	ILE	O-C-N	-5.72	116.29	121.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3	318	GLN	CG-CD-OE1	-5.72	109.37	120.80
1	2	239	VAL	O-C-N	5.71	129.37	123.03
1	2	264	GLY	O-C-N	5.71	127.48	121.77
1	1	237	SER	CA-C-O	5.71	128.68	120.51
1	3	238	VAL	CA-C-O	5.71	125.90	120.25
1	3	131	VAL	CA-C-O	-5.70	113.93	119.92
1	3	157	ALA	CA-C-O	-5.70	115.01	121.00
1	1	40	VAL	N-CA-C	-5.70	104.38	110.36
1	3	270	LEU	O-C-N	5.70	129.44	123.06
1	2	46	ASP	CB-CG-OD1	5.69	131.48	118.40
1	4	183	THR	N-CA-CB	5.69	120.43	110.42
1	1	293	ALA	CA-C-O	-5.68	112.38	120.51
1	4	265	PRO	N-CA-CB	-5.68	97.28	103.25
1	1	55	GLU	CB-CG-CD	5.68	122.25	112.60
1	1	69	LYS	CA-CB-CG	5.68	125.46	114.10
1	2	17	ARG	CD-NE-CZ	5.68	132.35	124.40
1	3	84	SER	N-CA-C	-5.68	98.71	110.80
1	3	247	LYS	N-CA-C	-5.68	100.73	109.76
1	3	319	ARG	NE-CZ-NH1	-5.68	115.82	121.50
1	4	81	ILE	O-C-N	5.68	127.27	121.14
1	4	264	GLY	CA-C-N	-5.67	112.75	119.84
1	4	264	GLY	C-N-CA	-5.67	112.75	119.84
1	3	220	LEU	N-CA-CB	5.67	118.86	110.53
1	1	63	LEU	CA-C-N	-5.67	115.56	123.10
1	1	63	LEU	C-N-CA	-5.67	115.56	123.10
1	3	4	GLY	O-C-N	5.67	130.07	122.70
1	2	65	VAL	CA-CB-CG2	5.67	120.03	110.40
1	3	281	ASP	N-CA-CB	5.67	120.07	110.49
1	3	175	HIS	O-C-N	-5.67	116.33	122.79
1	4	107	HIS	CA-CB-CG	-5.66	108.14	113.80
1	1	233	THR	CA-CB-CG2	5.66	120.13	110.50
1	2	3	ILE	N-CA-CB	5.66	120.57	111.23
1	2	207	THR	CA-C-N	5.66	132.50	121.41
1	2	207	THR	C-N-CA	5.66	132.50	121.41
1	1	193	ARG	CA-C-N	5.66	132.50	121.41
1	1	193	ARG	C-N-CA	5.66	132.50	121.41
1	2	193	ARG	CA-CB-CG	5.66	125.42	114.10
1	1	143	VAL	CA-CB-CG1	5.65	120.01	110.40
1	3	93	GLU	CA-C-N	5.65	132.34	121.54
1	3	93	GLU	C-N-CA	5.65	132.34	121.54
1	4	216	VAL	N-CA-C	5.65	116.09	111.62
1	1	239	VAL	CA-C-O	5.65	126.61	120.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	4	GLY	N-CA-C	-5.65	99.80	113.18
1	4	279	SER	N-CA-C	-5.65	98.77	110.80
1	3	307	VAL	CA-CB-CG2	5.65	120.00	110.40
1	1	148	CYS	O-C-N	5.64	127.96	122.09
1	4	94	SER	N-CA-CB	-5.64	101.33	110.14
1	1	60	ASP	CB-CA-C	5.64	121.64	110.42
1	1	171	MET	CA-C-O	5.64	127.48	120.54
1	4	180	THR	O-C-N	5.63	130.08	122.59
1	2	279	SER	CA-CB-OG	5.63	122.36	111.10
1	4	132	ASN	CA-C-N	5.63	132.29	121.54
1	4	132	ASN	C-N-CA	5.63	132.29	121.54
1	2	6	ASN	CA-C-O	5.62	127.31	120.62
1	1	46	ASP	CA-C-O	-5.62	113.34	120.20
1	1	79	GLU	CB-CG-CD	5.62	122.15	112.60
1	1	72	VAL	CA-C-O	-5.62	115.41	121.19
1	1	279	SER	N-CA-C	-5.61	98.84	110.80
1	2	141	THR	O-C-N	5.61	130.40	122.20
1	1	45	TYR	N-CA-C	5.61	118.11	109.07
1	1	74	ASN	CA-C-N	5.61	132.26	121.54
1	1	74	ASN	C-N-CA	5.61	132.26	121.54
1	3	297	ILE	N-CA-C	-5.61	100.21	108.85
1	1	225	THR	CA-C-O	-5.61	115.36	121.14
1	3	99	THR	CA-C-N	-5.61	114.00	122.81
1	3	99	THR	C-N-CA	-5.61	114.00	122.81
1	4	180	THR	CA-CB-CG2	5.61	120.03	110.50
1	1	258	MET	CB-CG-SD	-5.61	95.88	112.70
1	3	58	MET	O-C-N	5.60	129.34	123.06
1	1	163	ASN	N-CA-CB	-5.60	101.60	110.28
1	3	110	GLY	O-C-N	5.60	127.56	122.19
1	4	216	VAL	N-CA-CB	-5.59	107.05	111.64
1	3	224	LEU	CA-CB-CG	5.59	135.88	116.30
1	4	103	LYS	O-C-N	5.59	128.52	122.15
1	3	252	ASP	CB-CG-OD2	-5.59	105.54	118.40
1	1	308	SER	CA-C-O	-5.59	114.12	120.32
1	1	200	GLN	O-C-N	-5.59	114.87	122.36
1	2	196	ARG	NE-CZ-NH1	-5.58	115.92	121.50
1	1	273	THR	CA-CB-CG2	5.58	119.99	110.50
1	2	127	PHE	CA-CB-CG	-5.58	108.22	113.80
1	3	107	HIS	CA-CB-CG	5.58	119.38	113.80
1	2	180	THR	CA-C-O	5.58	128.49	120.51
1	1	40	VAL	CA-C-O	5.58	127.07	121.27
1	2	111	GLY	CA-C-O	-5.57	110.88	120.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	281	ASP	O-C-N	5.57	130.00	122.59
1	1	3	ILE	CB-CG1-CD1	-5.57	102.11	113.80
1	1	313	GLU	CA-C-N	-5.56	113.75	122.49
1	1	313	GLU	C-N-CA	-5.56	113.75	122.49
1	2	44	LYS	N-CA-CB	5.56	119.76	110.41
1	1	327	MET	CA-CB-CG	-5.56	102.98	114.10
1	3	281	ASP	CA-C-O	-5.56	112.56	120.51
1	4	320	VAL	CB-CA-C	5.56	120.41	111.29
1	3	78	PRO	CA-N-CD	-5.55	104.22	112.00
1	2	25	GLN	CA-C-O	-5.55	114.27	120.54
1	4	167	VAL	CA-C-O	-5.54	114.87	120.69
1	4	16	LEU	N-CA-C	-5.54	104.88	111.03
1	4	58	MET	O-C-N	5.54	129.46	122.65
1	4	239	VAL	O-C-N	5.53	129.26	122.95
1	2	230	ARG	CB-CG-CD	5.53	124.02	111.30
1	1	84	SER	O-C-N	5.53	129.94	122.59
1	1	141	THR	OG1-CB-CG2	5.53	120.35	109.30
1	3	18	ALA	CB-CA-C	5.53	121.36	111.03
1	2	255	LYS	CA-C-O	-5.52	112.61	120.51
1	3	75	GLU	N-CA-CB	5.52	119.82	110.49
1	2	268	GLY	CA-C-O	-5.52	111.83	119.01
1	4	252	ASP	CB-CG-OD2	-5.52	105.70	118.40
1	2	316	TYR	CA-CB-CG	-5.52	103.97	113.90
1	4	260	THR	O-C-N	5.52	129.50	122.33
1	3	204	PRO	CA-C-N	5.51	129.78	121.40
1	3	204	PRO	C-N-CA	5.51	129.78	121.40
1	1	27	VAL	CA-C-N	5.51	132.07	121.54
1	1	27	VAL	C-N-CA	5.51	132.07	121.54
1	3	192	TRP	CA-CB-CG	5.51	124.06	113.60
1	2	240	ASP	CA-CB-CG	5.49	118.09	112.60
1	4	115	VAL	O-C-N	-5.49	117.12	123.00
1	2	152	CYS	N-CA-CB	5.49	118.29	110.16
1	3	181	GLN	O-C-N	-5.49	115.29	122.59
1	3	287	ARG	O-C-N	5.49	129.89	122.59
1	1	149	THR	CA-CB-CG2	5.49	119.83	110.50
1	3	85	LYS	CA-C-O	-5.49	114.87	120.80
1	3	180	THR	CA-CB-CG2	5.49	119.83	110.50
1	4	196	ARG	CG-CD-NE	-5.49	99.92	112.00
1	2	81	ILE	N-CA-CB	-5.49	104.08	110.17
1	4	178	THR	OG1-CB-CG2	5.49	120.27	109.30
1	1	107	HIS	N-CA-CB	5.48	119.76	110.49
1	3	73	PHE	CA-C-N	5.48	130.96	121.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3	73	PHE	C-N-CA	5.48	130.96	121.64
1	1	139	ASP	N-CA-C	-5.48	105.41	111.71
1	4	21	SER	O-C-N	5.48	129.77	122.43
1	3	270	LEU	CA-C-O	-5.48	114.79	121.36
1	1	178	THR	CA-CB-CG2	5.48	119.81	110.50
1	3	249	CYS	O-C-N	5.47	129.87	122.59
1	4	269	PHE	O-C-N	-5.47	115.02	122.19
1	4	156	VAL	N-CA-CB	-5.47	103.63	110.47
1	4	200	GLN	CB-CG-CD	5.47	121.90	112.60
1	1	266	LEU	CA-C-O	5.47	126.32	119.59
1	1	223	LYS	CA-CB-CG	5.47	125.03	114.10
1	3	290	ILE	CA-CB-CG2	5.46	119.79	110.50
1	4	238	VAL	N-CA-CB	-5.46	104.58	111.46
1	3	48	THR	CA-CB-CG2	5.46	119.78	110.50
1	2	161	HIS	CA-CB-CG	5.46	119.26	113.80
1	1	277	VAL	CA-CB-CG2	-5.46	101.13	110.40
1	3	301	LYS	CA-CB-CG	5.46	125.01	114.10
1	4	13	ARG	CA-C-O	-5.46	112.71	120.51
1	4	79	GLU	N-CA-CB	5.45	119.70	110.49
1	4	273	THR	CA-CB-OG1	-5.45	101.42	109.60
1	3	229	PHE	CA-C-N	-5.45	114.53	122.65
1	3	229	PHE	C-N-CA	-5.45	114.53	122.65
1	2	142	VAL	CA-C-N	5.45	128.71	120.75
1	2	142	VAL	C-N-CA	5.45	128.71	120.75
1	4	26	VAL	CA-CB-CG2	5.45	119.66	110.40
1	2	61	GLY	CA-C-N	5.45	130.77	122.11
1	2	61	GLY	C-N-CA	5.45	130.77	122.11
1	3	224	LEU	O-C-N	5.45	129.76	123.17
1	2	45	TYR	O-C-N	-5.44	116.30	123.21
1	1	49	HIS	CA-C-O	5.44	125.13	119.14
1	1	97	VAL	O-C-N	5.44	129.37	122.57
1	2	265	PRO	N-CD-CG	-5.44	95.04	103.20
1	2	221	ASP	OD1-CG-OD2	5.44	135.95	122.90
1	1	136	TYR	N-CA-C	5.44	118.48	109.46
1	3	65	VAL	CA-CB-CG2	5.43	119.64	110.40
1	3	73	PHE	CB-CA-C	5.43	123.43	111.09
1	4	153	LEU	CA-CB-CG	5.43	135.31	116.30
1	1	11	ILE	CA-C-O	-5.43	113.99	120.78
1	2	281	ASP	CB-CG-OD1	5.43	130.89	118.40
1	1	134	GLU	CA-CB-CG	5.43	124.95	114.10
1	1	198	ALA	O-C-N	5.43	129.81	122.59
1	3	9	GLY	N-CA-C	-5.43	100.32	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	4	GLY	N-CA-C	-5.42	100.32	113.18
1	3	322	ASP	CA-C-O	-5.42	113.73	119.97
1	4	219	GLU	CA-CB-CG	5.42	124.94	114.10
1	1	175	HIS	N-CA-C	-5.42	102.50	110.52
1	3	193	ARG	CB-CG-CD	5.41	123.75	111.30
1	4	139	ASP	N-CA-C	-5.41	105.54	111.82
1	4	310	TYR	CA-C-N	5.41	131.87	121.54
1	4	310	TYR	C-N-CA	5.41	131.87	121.54
1	1	138	LYS	N-CA-C	5.40	122.31	110.80
1	4	66	ASP	N-CA-CB	-5.40	103.98	112.13
1	1	200	GLN	CG-CD-OE1	5.40	131.59	120.80
1	2	72	VAL	CB-CA-C	5.40	118.81	110.50
1	3	196	ARG	CB-CA-C	5.39	121.95	110.19
1	1	184	VAL	N-CA-C	-5.39	98.12	109.34
1	3	143	VAL	CA-C-O	-5.39	116.19	121.58
1	1	201	ASN	OD1-CG-ND2	-5.39	117.21	122.60
1	1	192	TRP	CA-C-O	-5.39	112.81	120.51
1	2	225	THR	CB-CA-C	-5.39	100.60	110.62
1	3	120	PRO	N-CD-CG	-5.39	95.12	103.20
1	4	85	LYS	CA-CB-CG	5.38	124.87	114.10
1	2	312	ASN	CA-CB-CG	5.38	117.98	112.60
1	2	286	ASN	O-C-N	5.38	129.75	122.59
1	2	310	TYR	N-CA-C	5.37	122.25	110.80
1	4	113	LYS	N-CA-C	5.37	122.24	110.80
1	4	123	ASP	CA-CB-CG	5.37	117.97	112.60
1	1	266	LEU	CB-CA-C	5.37	120.10	110.81
1	1	243	VAL	CA-C-O	-5.37	115.59	121.28
1	2	15	VAL	N-CA-C	-5.37	105.30	110.72
1	2	284	GLY	O-C-N	5.37	129.68	122.70
1	4	315	GLY	N-CA-C	-5.37	100.45	113.18
1	2	89	GLU	CA-C-O	-5.37	113.46	119.79
1	1	196	ARG	CA-CB-CG	5.36	124.83	114.10
1	4	138	LYS	N-CA-C	5.36	122.22	110.80
1	2	276	ASP	CA-C-O	5.36	128.18	120.51
1	1	263	GLU	N-CA-CB	5.36	118.64	110.39
1	3	159	VAL	CB-CA-C	-5.35	102.51	111.29
1	2	207	THR	CA-C-O	5.35	127.05	121.38
1	2	113	LYS	CB-CG-CD	5.35	123.60	111.30
1	3	44	LYS	CB-CA-C	-5.35	99.78	110.42
1	1	119	ALA	CA-C-O	5.35	127.48	120.16
1	1	281	ASP	CA-CB-CG	5.35	117.95	112.60
1	4	265	PRO	CA-C-O	-5.34	110.87	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3	120	PRO	N-CA-C	-5.34	103.39	111.41
1	2	170	LEU	CB-CA-C	5.34	121.82	110.07
1	2	259	LYS	CA-C-O	-5.34	114.83	120.55
1	3	102	GLU	CA-C-N	5.34	127.43	120.28
1	3	102	GLU	C-N-CA	5.34	127.43	120.28
1	2	307	VAL	CA-CB-CG2	5.33	119.47	110.40
1	4	178	THR	N-CA-CB	5.33	119.05	111.05
1	2	125	PRO	CA-C-O	-5.33	110.90	120.60
1	4	281	ASP	CB-CA-C	5.33	121.03	110.42
1	3	179	ALA	O-C-N	5.33	128.24	122.11
1	1	57	LYS	CA-C-N	5.33	129.30	120.94
1	1	57	LYS	C-N-CA	5.33	129.30	120.94
1	1	148	CYS	N-CA-C	5.33	117.50	111.11
1	2	55	GLU	N-CA-C	-5.33	99.46	110.80
1	3	104	ALA	N-CA-CB	5.32	118.44	110.19
1	4	8	PHE	O-C-N	5.32	129.67	122.59
1	3	147	SER	N-CA-C	5.32	122.13	110.80
1	3	229	PHE	N-CA-CB	5.32	118.95	110.65
1	1	172	THR	CA-C-N	-5.32	115.66	123.00
1	1	172	THR	C-N-CA	-5.32	115.66	123.00
1	1	222	GLY	N-CA-C	5.32	125.78	113.18
1	3	304	VAL	CA-CB-CG2	5.32	119.44	110.40
1	4	10	ARG	CD-NE-CZ	5.32	131.84	124.40
1	4	9	GLY	N-CA-C	-5.31	100.59	113.18
1	2	42	MET	CA-CB-CG	-5.31	103.47	114.10
1	2	252	ASP	CA-C-N	-5.31	112.63	120.28
1	2	252	ASP	C-N-CA	-5.31	112.63	120.28
1	1	131	VAL	N-CA-CB	-5.31	101.82	110.31
1	1	180	THR	N-CA-C	5.31	122.11	110.80
1	4	210	ALA	CA-C-O	5.31	127.23	121.02
1	3	205	SER	CA-C-O	-5.30	113.77	119.98
1	4	46	ASP	CB-CG-OD1	-5.30	106.20	118.40
1	2	82	PRO	CA-N-CD	-5.30	104.58	112.00
1	2	178	THR	CA-CB-OG1	-5.30	101.65	109.60
1	4	48	THR	CA-C-O	-5.30	113.53	120.00
1	4	26	VAL	CA-C-N	-5.29	112.44	121.97
1	4	26	VAL	C-N-CA	-5.29	112.44	121.97
1	4	165	GLU	CB-CA-C	-5.29	99.89	110.42
1	1	255	LYS	CA-C-N	5.29	127.37	120.28
1	1	255	LYS	C-N-CA	5.29	127.37	120.28
1	2	280	SER	CA-CB-OG	-5.29	100.52	111.10
1	2	26	VAL	CA-C-N	-5.29	112.45	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	26	VAL	C-N-CA	-5.29	112.45	121.97
1	3	28	ALA	CB-CA-C	5.29	120.94	110.42
1	3	247	LYS	CA-C-O	-5.29	114.67	120.69
1	2	86	ALA	CA-C-O	5.28	128.07	120.51
1	2	107	HIS	CA-C-O	-5.28	112.95	120.51
1	3	230	ARG	CG-CD-NE	-5.28	100.38	112.00
1	3	310	TYR	CB-CG-CD1	5.28	128.72	120.80
1	3	291	PHE	N-CA-CB	5.28	119.04	110.17
1	3	81	ILE	CB-CA-C	5.28	116.17	111.00
1	3	101	ILE	CA-C-N	5.28	127.67	120.54
1	3	101	ILE	C-N-CA	5.28	127.67	120.54
1	2	323	LEU	CA-C-N	5.27	128.08	120.38
1	2	323	LEU	C-N-CA	5.27	128.08	120.38
1	3	49	HIS	N-CA-C	5.27	119.63	112.04
1	4	109	LYS	CB-CG-CD	5.27	123.42	111.30
1	1	158	LYS	CA-C-O	-5.27	112.97	120.51
1	1	266	LEU	N-CA-CB	-5.27	103.29	110.56
1	1	283	ILE	N-CA-CB	-5.27	102.54	111.23
1	2	32	PRO	CA-C-N	-5.27	115.92	125.66
1	2	32	PRO	C-N-CA	-5.27	115.92	125.66
1	3	119	ALA	O-C-N	5.26	126.02	121.54
1	4	201	ASN	CA-CB-CG	-5.26	107.33	112.60
1	4	333	ALA	N-CA-CB	-5.26	102.50	110.40
1	1	233	THR	N-CA-CB	-5.26	101.01	110.37
1	3	260	THR	OG1-CB-CG2	5.26	119.82	109.30
1	2	162	GLU	CG-CD-OE2	-5.26	106.31	118.40
1	3	44	LYS	N-CA-C	5.26	122.00	110.80
1	2	253	ASP	N-CA-C	-5.25	105.67	111.71
1	2	236	VAL	CA-CB-CG1	5.25	119.33	110.40
1	2	129	CYS	CA-C-O	-5.25	113.01	120.51
1	2	188	SER	CA-C-N	5.25	131.57	121.54
1	2	188	SER	C-N-CA	5.25	131.57	121.54
1	3	141	THR	O-C-N	5.25	129.86	122.20
1	2	284	GLY	CA-C-N	5.25	131.56	121.54
1	2	284	GLY	C-N-CA	5.25	131.56	121.54
1	4	55	GLU	N-CA-CB	5.25	118.17	109.88
1	4	201	ASN	CB-CG-ND2	5.25	124.27	116.40
1	4	187	PRO	CA-CB-CG	-5.24	94.54	104.50
1	4	64	VAL	CA-CB-CG1	5.24	119.31	110.40
1	1	284	GLY	N-CA-C	-5.23	100.78	113.18
1	2	68	LYS	CA-CB-CG	5.23	124.57	114.10
1	2	218	PRO	CA-N-CD	-5.23	104.67	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	199	ALA	CB-CA-C	-5.23	100.89	109.99
1	3	243	VAL	O-C-N	5.23	128.75	123.00
1	3	81	ILE	CA-C-O	-5.23	114.92	119.62
1	1	60	ASP	CA-C-N	5.23	131.65	121.41
1	1	60	ASP	C-N-CA	5.23	131.65	121.41
1	3	159	VAL	CA-C-O	-5.23	114.25	120.78
1	3	89	GLU	CB-CG-CD	5.22	121.48	112.60
1	1	23	GLY	N-CA-C	-5.22	100.80	113.18
1	4	109	LYS	CA-CB-CG	-5.22	103.66	114.10
1	1	230	ARG	CG-CD-NE	-5.22	100.52	112.00
1	3	105	SER	N-CA-C	-5.22	99.68	110.80
1	4	267	GLN	CA-CB-CG	-5.22	103.66	114.10
1	1	285	ASP	CA-C-O	-5.22	113.05	120.51
1	2	189	ALA	CA-C-O	-5.22	113.05	120.51
1	3	178	THR	CA-CB-OG1	-5.21	101.78	109.60
1	2	133	LEU	CB-CA-C	5.21	120.79	110.42
1	3	284	GLY	N-CA-C	-5.21	100.83	113.18
1	4	82	PRO	CB-CA-C	5.21	117.78	110.95
1	1	54	GLY	O-C-N	5.21	129.47	122.70
1	3	78	PRO	CA-C-O	-5.21	111.67	118.86
1	2	97	VAL	CB-CA-C	-5.21	102.75	111.29
1	4	208	GLY	CA-C-O	5.21	129.63	120.57
1	4	263	GLU	CG-CD-OE2	-5.21	106.42	118.40
1	3	141	THR	CA-CB-OG1	-5.20	101.79	109.60
1	1	16	LEU	CB-CA-C	5.20	120.77	110.42
1	1	193	ARG	CA-CB-CG	5.20	124.50	114.10
1	4	287	ARG	N-CA-CB	5.20	119.28	110.49
1	3	309	TRP	CB-CA-C	-5.20	100.73	109.83
1	4	89	GLU	CA-C-O	-5.20	114.99	120.55
1	4	206	SER	N-CA-C	-5.20	102.59	110.28
1	1	233	THR	CA-C-N	5.19	124.69	119.19
1	1	233	THR	C-N-CA	5.19	124.69	119.19
1	1	138	LYS	CB-CA-C	-5.19	100.09	110.42
1	4	180	THR	N-CA-CB	5.19	119.26	110.49
1	3	231	VAL	CA-C-O	5.19	127.49	120.90
1	1	201	ASN	CA-C-O	5.18	127.83	121.56
1	3	5	ILE	N-CA-CB	-5.18	102.68	111.23
1	3	240	ASP	CA-C-O	-5.18	114.92	120.46
1	4	146	ALA	CA-C-O	-5.18	113.10	120.51
1	4	160	LEU	CA-C-N	5.18	131.44	121.54
1	4	160	LEU	C-N-CA	5.18	131.44	121.54
1	4	174	VAL	CB-CA-C	5.18	119.78	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	154	ALA	CA-C-N	5.18	126.31	119.84
1	4	154	ALA	C-N-CA	5.18	126.31	119.84
1	2	311	ASP	OD1-CG-OD2	-5.17	110.48	122.90
1	1	269	PHE	CA-C-N	5.17	128.82	121.42
1	1	269	PHE	C-N-CA	5.17	128.82	121.42
1	3	207	THR	CA-CB-OG1	-5.17	101.84	109.60
1	4	69	LYS	N-CA-C	5.17	116.90	108.63
1	4	87	GLY	O-C-N	5.17	129.42	122.70
1	2	240	ASP	N-CA-C	-5.17	100.75	109.07
1	4	287	ARG	NE-CZ-NH1	5.17	126.67	121.50
1	1	200	GLN	CA-C-O	5.17	125.08	119.24
1	3	221	ASP	CA-CB-CG	5.17	117.77	112.60
1	1	320	VAL	N-CA-CB	5.17	119.76	111.23
1	4	272	TYR	CA-CB-CG	-5.17	104.60	113.90
1	1	112	ALA	O-C-N	5.17	129.46	122.59
1	4	212	ALA	N-CA-CB	5.17	118.30	110.14
1	4	115	VAL	CB-CA-C	-5.16	102.43	110.69
1	4	219	GLU	CA-C-N	5.16	128.89	121.71
1	4	219	GLU	C-N-CA	5.16	128.89	121.71
1	1	177	VAL	CA-C-N	5.16	132.19	123.01
1	1	177	VAL	C-N-CA	5.16	132.19	123.01
1	1	318	GLN	CA-CB-CG	5.16	124.42	114.10
1	4	147	SER	N-CA-C	5.16	121.79	110.80
1	3	84	SER	CA-C-N	-5.16	113.06	121.26
1	3	84	SER	C-N-CA	-5.16	113.06	121.26
1	1	173	THR	CA-CB-OG1	-5.16	101.87	109.60
1	4	185	ASP	N-CA-CB	-5.15	101.78	110.49
1	3	142	VAL	CA-C-N	5.15	127.51	120.35
1	3	142	VAL	C-N-CA	5.15	127.51	120.35
1	1	220	LEU	N-CA-CB	5.15	118.30	110.42
1	4	166	ILE	O-C-N	5.15	129.00	122.57
1	2	151	ASN	CB-CA-C	5.14	120.44	110.46
1	2	227	MET	CA-C-O	-5.14	115.81	121.31
1	3	172	THR	N-CA-CB	5.14	118.68	110.65
1	1	301	LYS	CD-CE-NZ	5.14	128.35	111.90
1	4	204	PRO	O-C-N	-5.14	115.70	122.64
1	1	310	TYR	CA-C-N	5.14	131.35	121.54
1	1	310	TYR	C-N-CA	5.14	131.35	121.54
1	1	329	LYS	CG-CD-CE	5.14	123.11	111.30
1	3	141	THR	CA-C-O	-5.14	113.56	119.78
1	2	160	LEU	CA-C-N	5.13	131.35	121.54
1	2	160	LEU	C-N-CA	5.13	131.35	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	310	TYR	CB-CA-C	-5.13	104.96	115.28
1	4	181	GLN	N-CA-CB	-5.13	101.82	110.49
1	1	291	PHE	N-CA-C	-5.13	102.69	110.28
1	2	271	GLY	CA-C-O	-5.12	111.66	120.57
1	3	321	ILE	CB-CA-C	5.12	119.69	111.29
1	1	121	SER	CA-CB-OG	5.12	121.34	111.10
1	1	75	GLU	CB-CA-C	-5.11	100.25	110.42
1	1	147	SER	N-CA-CB	-5.11	101.85	110.49
1	1	31	ASP	N-CA-C	5.11	119.77	108.27
1	4	164	PHE	N-CA-CB	5.11	119.13	110.49
1	1	14	LEU	CA-CB-CG	5.11	134.19	116.30
1	1	75	GLU	N-CA-CB	5.11	119.12	110.49
1	4	260	THR	N-CA-C	-5.11	105.70	112.34
1	1	31	ASP	CB-CG-OD1	5.10	130.14	118.40
1	1	262	SER	N-CA-CB	-5.10	101.87	110.49
1	1	277	VAL	CA-C-N	-5.10	112.78	121.97
1	1	277	VAL	C-N-CA	-5.10	112.78	121.97
1	2	85	LYS	O-C-N	5.10	129.38	122.59
1	2	153	LEU	N-CA-CB	-5.10	103.02	110.47
1	1	114	LYS	CB-CA-C	5.10	118.30	110.14
1	3	116	VAL	CA-CB-CG1	5.10	119.07	110.40
1	2	117	ILE	CA-CB-CG2	5.10	119.17	110.50
1	4	73	PHE	CB-CA-C	5.10	123.88	111.65
1	4	163	ASN	CA-C-N	5.10	131.28	121.54
1	4	163	ASN	C-N-CA	5.10	131.28	121.54
1	1	120	PRO	O-C-N	5.09	129.33	123.01
1	2	304	VAL	CA-C-O	5.09	126.63	121.64
1	3	42	MET	CA-C-O	5.09	125.63	119.11
1	1	180	THR	CA-C-O	5.09	127.79	120.51
1	4	46	ASP	OD1-CG-OD2	5.09	135.12	122.90
1	4	163	ASN	N-CA-CB	-5.09	101.94	110.39
1	3	302	THR	CA-C-O	5.08	124.80	119.51
1	1	330	VAL	N-CA-CB	-5.08	102.85	111.23
1	2	57	LYS	CA-C-O	-5.08	116.00	121.38
1	4	120	PRO	O-C-N	5.07	129.52	123.13
1	2	111	GLY	N-CA-C	-5.07	101.17	113.18
1	2	157	ALA	CA-C-N	5.07	131.23	121.54
1	2	157	ALA	C-N-CA	5.07	131.23	121.54
1	4	166	ILE	CA-C-N	5.07	128.66	122.63
1	4	166	ILE	C-N-CA	5.07	128.66	122.63
1	1	24	ALA	CA-C-N	5.07	129.59	122.09
1	1	24	ALA	C-N-CA	5.07	129.59	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	52	PHE	N-CA-C	-5.07	100.01	110.80
1	4	194	GLY	N-CA-C	-5.07	101.17	113.18
1	4	191	ASP	CA-C-O	-5.06	113.64	119.56
1	4	307	VAL	CA-CB-CG1	-5.06	101.80	110.40
1	1	267	GLN	CA-CB-CG	-5.06	103.98	114.10
1	4	263	GLU	CA-CB-CG	5.06	124.22	114.10
1	1	10	ARG	CA-C-O	-5.06	113.28	120.51
1	1	275	ASP	N-CA-C	-5.06	102.03	109.62
1	3	317	SER	CA-C-N	5.06	127.82	120.79
1	3	317	SER	C-N-CA	5.06	127.82	120.79
1	4	35	ALA	O-C-N	5.06	128.67	122.96
1	4	252	ASP	CB-CG-OD1	-5.06	106.77	118.40
1	2	239	VAL	CA-C-N	-5.06	116.02	123.00
1	2	239	VAL	C-N-CA	-5.06	116.02	123.00
1	3	301	LYS	N-CA-CB	5.06	119.03	110.49
1	4	18	ALA	O-C-N	5.05	129.12	122.30
1	4	20	LEU	N-CA-CB	-5.05	102.53	109.91
1	3	276	ASP	N-CA-C	5.05	121.56	110.80
1	1	301	LYS	N-CA-C	5.05	121.56	110.80
1	1	224	LEU	CA-CB-CG	5.05	133.97	116.30
1	2	200	GLN	N-CA-C	-5.05	107.78	114.04
1	4	179	ALA	N-CA-C	-5.05	104.86	111.02
1	4	233	THR	CA-C-O	5.05	127.07	120.16
1	4	20	LEU	N-CA-C	5.04	116.47	110.97
1	3	80	ASN	N-CA-CB	-5.04	103.23	110.65
1	2	103	LYS	O-C-N	5.04	127.90	122.15
1	2	55	GLU	CG-CD-OE2	-5.04	106.81	118.40
1	3	316	TYR	CB-CG-CD2	5.04	128.36	120.80
1	1	113	LYS	N-CA-C	5.04	121.53	110.80
1	2	242	THR	CA-C-O	5.04	126.05	120.71
1	4	184	VAL	N-CA-CB	-5.04	102.92	111.23
1	4	312	ASN	CA-C-N	-5.04	113.89	120.44
1	4	312	ASN	C-N-CA	-5.04	113.89	120.44
1	2	102	GLU	CG-CD-OE2	-5.04	106.81	118.40
1	1	151	ASN	CA-CB-CG	5.04	117.64	112.60
1	2	203	ILE	CB-CA-C	-5.04	102.19	111.36
1	4	258	MET	CA-CB-CG	-5.04	104.03	114.10
1	1	82	PRO	CA-C-O	-5.03	115.06	122.31
1	2	307	VAL	N-CA-CB	-5.03	104.98	111.82
1	3	249	CYS	CA-C-N	-5.03	113.09	121.94
1	3	249	CYS	C-N-CA	-5.03	113.09	121.94
1	2	169	GLY	O-C-N	-5.03	119.03	123.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3	266	LEU	N-CA-CB	5.03	118.99	110.49
1	1	47	SER	O-C-N	5.03	127.25	122.07
1	1	245	LEU	CA-C-O	-5.03	115.61	120.89
1	2	240	ASP	CA-C-N	5.03	129.83	122.39
1	2	240	ASP	C-N-CA	5.03	129.83	122.39
1	3	272	TYR	CA-C-O	5.03	127.69	120.51
1	2	318	GLN	CG-CD-NE2	5.02	123.94	116.40
1	1	125	PRO	N-CA-C	-5.02	102.12	112.47
1	4	131	VAL	N-CA-C	5.02	118.17	111.44
1	1	89	GLU	N-CA-C	5.02	121.49	110.80
1	2	196	ARG	CB-CA-C	5.02	120.00	110.51
1	4	95	THR	N-CA-CB	-5.02	102.01	110.49
1	1	39	MET	N-CA-CB	5.02	117.23	109.91
1	2	297	ILE	CB-CG1-CD1	-5.01	103.27	113.80
1	3	320	VAL	O-C-N	5.01	128.84	122.57
1	2	281	ASP	N-CA-C	-5.01	100.12	110.80
1	4	71	THR	CA-CB-CG2	5.01	119.02	110.50
1	1	279	SER	CA-CB-OG	5.01	121.12	111.10
1	2	34	ILE	CA-C-O	5.01	127.04	120.78
1	2	46	ASP	CA-C-O	-5.01	113.87	119.98
1	1	308	SER	CA-C-N	-5.01	115.19	122.65
1	1	308	SER	C-N-CA	-5.01	115.19	122.65
1	1	239	VAL	N-CA-CB	5.00	116.99	110.99
1	3	132	ASN	CA-C-O	5.00	127.66	120.51
1	3	235	ASP	O-C-N	-5.00	117.20	121.85
1	4	277	VAL	CA-C-N	-5.00	112.97	121.97
1	4	277	VAL	C-N-CA	-5.00	112.97	121.97

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	3	13	ARG	Sidechain
1	3	196	ARG	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	1	2507	0	2524	941	2
1	2	2507	0	2524	893	25
1	3	2507	0	2524	930	13
1	4	2507	0	2523	921	13
2	1	23	0	0	13	0
2	2	28	0	0	26	4
2	3	27	0	0	28	2
2	4	44	0	0	32	3
All	All	10150	0	10095	3454	31

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 172.

All (3454) 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)
1:4:32:PRO:HA	1:4:74:ASN:ND2	1.32	1.40
1:2:277:VAL:HG21	1:4:41:TYR:CE1	1.58	1.39
1:2:32:PRO:HA	1:2:74:ASN:ND2	1.38	1.34
1:1:220:LEU:HA	1:1:223:LYS:NZ	1.43	1.32
1:1:126:MET:HB2	1:1:215:LYS:NZ	1.45	1.30
1:3:138:LYS:NZ	1:3:330:VAL:HG13	1.42	1.30
1:2:97:VAL:O	1:2:98:PHE:CD1	1.82	1.30
1:4:75:GLU:N	2:4:347:HOH:O	1.62	1.30
1:1:292:ASP:OD1	1:1:295:ALA:HB3	1.32	1.28
1:4:32:PRO:CA	1:4:74:ASN:HD21	1.51	1.24
1:1:188:SER:O	1:1:190:LYS:N	1.70	1.23
1:4:270:LEU:HD23	1:4:271:GLY:N	1.50	1.23
1:1:128:VAL:O	1:1:132:ASN:HB3	1.38	1.23
1:1:292:ASP:CG	1:1:295:ALA:HB3	1.63	1.22
1:3:52:PHE:N	2:3:370:HOH:O	1.70	1.22
1:1:276:ASP:O	1:1:278:VAL:HG13	1.38	1.22
1:1:169:GLY:O	1:1:170:LEU:HD23	1.38	1.22
1:2:52:PHE:N	2:2:400:HOH:O	1.67	1.22
1:3:113:LYS:HB3	1:3:114:LYS:CD	1.69	1.22
1:2:251:TYR:N	1:2:299:LEU:HD12	1.53	1.21
1:4:119:ALA:HB1	1:4:120:PRO:CD	1.70	1.21
1:2:41:TYR:CE1	1:4:277:VAL:HG21	1.75	1.21
1:1:127:PHE:CB	1:1:132:ASN:HB2	1.72	1.20
1:2:236:VAL:O	1:2:237:SER:HB2	1.39	1.19
1:1:127:PHE:CE2	1:1:136:TYR:HB2	1.76	1.19
1:4:74:ASN:O	1:4:75:GLU:HG2	1.42	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:17:ARG:HG2	1:3:43:PHE:HE2	1.09	1.17
1:3:65:VAL:HG22	1:3:66:ASP:OD2	1.40	1.17
1:1:295:ALA:HB2	1:4:193:ARG:HH22	1.08	1.17
1:3:127:PHE:HB3	1:3:132:ASN:CB	1.75	1.17
1:3:270:LEU:HD23	1:3:271:GLY:N	1.58	1.16
1:3:276:ASP:OD1	1:3:277:VAL:HG13	1.45	1.16
1:4:220:LEU:HA	1:4:223:LYS:HZ3	1.10	1.15
1:1:1:SER:OG	1:1:25:GLN:HB2	1.44	1.15
1:1:299:LEU:HD23	1:1:304:VAL:HG23	1.23	1.15
1:2:295:ALA:CB	1:3:193:ARG:HH12	1.60	1.15
1:2:183:THR:HG22	2:2:413:HOH:O	1.47	1.15
1:4:181:GLN:HE21	1:4:203:ILE:HD12	1.06	1.15
1:1:17:ARG:HG2	1:1:43:PHE:HE2	1.09	1.14
1:2:225:THR:HG21	1:3:298:GLN:NE2	1.59	1.14
1:2:11:ILE:H	1:2:11:ILE:HD12	1.04	1.14
1:2:297:ILE:HD13	1:2:297:ILE:H	1.07	1.14
1:3:131:VAL:HG12	1:3:158:LYS:NZ	1.61	1.14
1:4:113:LYS:HD3	1:4:114:LYS:HZ2	0.99	1.14
1:1:208:GLY:HA3	1:1:211:LYS:HG2	1.17	1.14
1:2:26:VAL:O	1:2:27:VAL:HB	1.40	1.14
1:2:77:LYS:N	2:2:408:HOH:O	1.78	1.14
1:3:211:LYS:HA	1:3:211:LYS:CE	1.77	1.14
1:4:26:VAL:C	1:4:27:VAL:HG12	1.71	1.14
1:1:90:TYR:CE2	1:1:328:GLN:NE2	2.16	1.13
1:1:8:PHE:CD2	1:1:8:PHE:O	2.02	1.13
1:1:41:TYR:CE1	1:3:277:VAL:HG21	1.83	1.13
1:3:4:GLY:HA2	1:3:27:VAL:CG2	1.78	1.13
1:2:128:VAL:O	1:2:132:ASN:HB3	1.48	1.12
1:1:52:PHE:C	1:1:53:LYS:HE2	1.72	1.12
1:1:113:LYS:HB3	1:1:114:LYS:HD2	1.29	1.12
1:2:75:GLU:C	2:2:408:HOH:O	1.93	1.12
1:2:212:ALA:O	1:2:216:VAL:HB	1.48	1.12
1:1:193:ARG:HH22	1:4:295:ALA:HB2	0.99	1.12
1:1:71:THR:HG21	1:1:73:PHE:CE1	1.84	1.11
1:1:8:PHE:O	1:1:8:PHE:HD2	1.29	1.11
1:2:41:TYR:CZ	1:4:277:VAL:HG21	1.84	1.11
1:3:30:ASN:OD1	1:3:81:ILE:HG13	1.50	1.11
1:3:113:LYS:CB	1:3:114:LYS:HD2	1.80	1.11
1:1:277:VAL:HG21	1:3:41:TYR:CE1	1.85	1.11
1:1:297:ILE:CD1	1:1:297:ILE:H	1.64	1.11
1:2:27:VAL:HG13	1:2:28:ALA:H	1.14	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:161:HIS:ND1	1:3:165:GLU:O	1.84	1.10
1:2:30:ASN:OD1	1:2:81:ILE:HG13	1.51	1.10
1:4:73:PHE:O	2:4:335:HOH:O	1.68	1.10
1:3:113:LYS:C	1:3:114:LYS:HE3	1.75	1.10
1:2:193:ARG:HH22	1:3:295:ALA:HB2	0.96	1.10
1:3:101:ILE:HB	1:3:123:ASP:OD1	1.50	1.10
1:3:127:PHE:CB	1:3:132:ASN:HB2	1.81	1.10
1:1:4:GLY:HA2	1:1:27:VAL:HG21	1.29	1.09
1:4:28:ALA:HB3	1:4:83:TRP:HZ3	1.15	1.09
1:4:154:ALA:HB3	1:4:155:PRO:CD	1.82	1.09
1:1:113:LYS:C	1:1:114:LYS:HE3	1.77	1.09
1:2:297:ILE:H	1:2:297:ILE:CD1	1.64	1.09
1:4:58:MET:CE	1:4:58:MET:H	1.64	1.09
1:4:78:PRO:HG3	1:4:98:PHE:CE2	1.87	1.09
1:4:216:VAL:HG13	1:4:217:ILE:HG22	1.17	1.09
1:1:127:PHE:HB3	1:1:132:ASN:CB	1.81	1.09
1:3:27:VAL:HG22	1:3:28:ALA:H	1.03	1.09
1:1:220:LEU:CA	1:1:223:LYS:HZ2	1.66	1.09
1:4:113:LYS:HD3	1:4:114:LYS:NZ	1.67	1.08
1:4:125:PRO:HG2	1:4:140:MET:CE	1.83	1.08
1:3:154:ALA:HB3	1:3:155:PRO:CD	1.82	1.08
1:3:211:LYS:HA	1:3:211:LYS:HE2	1.22	1.08
1:3:307:VAL:O	1:3:307:VAL:HG13	1.41	1.08
1:1:202:ILE:CD1	1:4:233:THR:HG21	1.83	1.08
1:1:270:LEU:HD23	1:1:271:GLY:N	1.68	1.08
1:2:33:PHE:HZ	1:2:76:MET:HE1	1.04	1.08
1:1:44:LYS:NZ	1:1:44:LYS:HB3	1.67	1.08
1:1:6:ASN:HA	1:1:30:ASN:HD21	1.16	1.07
1:1:277:VAL:HA	1:4:193:ARG:HG3	1.29	1.07
1:3:78:PRO:HG3	1:3:98:PHE:CE2	1.89	1.07
1:1:154:ALA:HB3	1:1:155:PRO:CD	1.85	1.07
1:2:1:SER:O	1:2:2:LYS:HG2	1.54	1.07
1:4:27:VAL:HG22	1:4:28:ALA:H	0.98	1.07
1:4:44:LYS:HG3	1:4:56:VAL:HG21	1.30	1.07
1:4:161:HIS:ND1	1:4:165:GLU:O	1.85	1.07
1:1:113:LYS:HB3	1:1:114:LYS:CD	1.85	1.07
1:2:17:ARG:HG3	1:2:43:PHE:CE2	1.90	1.07
1:4:113:LYS:HB3	1:4:114:LYS:HD2	1.36	1.07
1:4:161:HIS:O	1:4:165:GLU:N	1.88	1.07
1:1:208:GLY:CA	1:1:211:LYS:HG2	1.85	1.06
1:2:91:ILE:HD13	1:2:115:VAL:HG22	1.33	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:51:VAL:C	2:4:340:HOH:O	1.97	1.06
1:1:27:VAL:HG13	1:1:28:ALA:H	1.19	1.06
1:1:307:VAL:O	1:1:307:VAL:HG13	1.53	1.06
1:1:169:GLY:C	1:1:170:LEU:HD23	1.79	1.06
1:4:154:ALA:HB3	1:4:155:PRO:HD2	1.08	1.06
1:2:248:GLU:HA	1:2:302:THR:CG2	1.85	1.06
1:1:211:LYS:HA	1:1:211:LYS:HZ3	1.18	1.05
1:4:258:MET:HG2	1:4:270:LEU:HD11	1.37	1.05
1:2:11:ILE:H	1:2:11:ILE:CD1	1.67	1.05
1:3:81:ILE:HD13	1:3:82:PRO:HD2	1.38	1.05
1:2:27:VAL:HG13	1:2:28:ALA:N	1.65	1.05
1:1:297:ILE:H	1:1:297:ILE:HD13	1.20	1.05
1:3:85:LYS:O	1:3:86:ALA:HB2	1.52	1.05
1:1:32:PRO:HA	1:1:74:ASN:ND2	1.71	1.05
1:2:3:ILE:HG22	1:2:4:GLY:H	1.19	1.05
1:1:208:GLY:HA3	1:1:211:LYS:CG	1.86	1.04
1:2:78:PRO:HG3	1:2:98:PHE:CE2	1.92	1.04
1:3:46:ASP:HB3	1:3:50:GLY:H	1.22	1.04
1:4:125:PRO:HG2	1:4:140:MET:HE3	1.39	1.04
1:1:17:ARG:HG2	1:1:43:PHE:CE2	1.92	1.04
1:2:251:TYR:H	1:2:299:LEU:CD1	1.68	1.04
1:1:202:ILE:HD11	1:4:233:THR:HG21	1.32	1.04
1:2:220:LEU:O	1:2:222:GLY:N	1.91	1.04
1:3:276:ASP:CG	1:3:277:VAL:HG22	1.82	1.04
1:2:255:LYS:HE2	1:2:293:ALA:HB1	1.36	1.03
1:3:27:VAL:HG22	1:3:28:ALA:N	1.69	1.03
1:4:77:LYS:C	2:4:348:HOH:O	2.01	1.03
1:3:11:ILE:H	1:3:11:ILE:HD13	1.18	1.03
1:3:138:LYS:HZ2	1:3:330:VAL:CG1	1.69	1.03
1:4:27:VAL:CG2	1:4:28:ALA:H	1.70	1.03
1:2:11:ILE:HD12	1:2:11:ILE:N	1.73	1.03
1:3:251:TYR:H	1:3:299:LEU:HD12	1.13	1.03
1:2:281:ASP:O	1:2:283:ILE:N	1.92	1.03
1:3:138:LYS:NZ	1:3:330:VAL:CG1	2.22	1.03
1:1:277:VAL:HA	1:4:193:ARG:CD	1.88	1.03
1:4:1:SER:HB3	1:4:25:GLN:HE21	1.19	1.03
1:4:53:LYS:HB3	1:4:53:LYS:HZ3	1.22	1.03
1:1:225:THR:OG1	1:4:298:GLN:OE1	1.76	1.02
1:2:295:ALA:HB1	1:3:193:ARG:HH12	1.21	1.02
1:4:58:MET:H	1:4:58:MET:HE2	1.24	1.02
1:4:8:PHE:O	1:4:8:PHE:HD2	1.42	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:131:VAL:HG12	1:2:158:LYS:NZ	1.75	1.02
1:3:127:PHE:HB3	1:3:132:ASN:HB2	1.04	1.02
1:1:31:ASP:O	1:1:34:ILE:HG23	1.59	1.02
1:1:101:ILE:HG23	1:1:142:VAL:HG11	1.38	1.02
1:1:193:ARG:HH12	1:4:295:ALA:HB1	1.20	1.02
1:4:284:GLY:HA2	1:4:314:PHE:CE1	1.95	1.02
1:1:270:LEU:HD23	1:1:271:GLY:H	1.25	1.01
1:2:277:VAL:HG23	1:2:278:VAL:H	1.23	1.01
1:4:32:PRO:CA	1:4:74:ASN:ND2	2.16	1.01
1:4:108:PHE:O	1:4:109:LYS:C	2.03	1.01
1:4:113:LYS:HB3	1:4:114:LYS:CD	1.89	1.01
1:1:211:LYS:HA	1:1:211:LYS:NZ	1.73	1.01
1:3:32:PRO:HA	1:3:74:ASN:ND2	1.75	1.01
1:4:129:CYS:HA	1:4:132:ASN:HD22	1.22	1.01
1:4:138:LYS:HE2	1:4:330:VAL:HG13	1.42	1.01
1:2:113:LYS:HG2	1:2:114:LYS:HE3	1.42	1.01
1:1:27:VAL:HG22	1:1:28:ALA:N	1.72	1.00
1:4:119:ALA:CB	1:4:120:PRO:HD2	1.88	1.00
1:1:252:ASP:O	1:1:255:LYS:N	1.94	1.00
1:1:277:VAL:HA	1:4:193:ARG:CG	1.89	1.00
1:2:135:LYS:NZ	1:2:140:MET:HE1	1.77	1.00
1:4:284:GLY:HA2	1:4:314:PHE:HE1	1.22	1.00
1:1:2:LYS:CG	1:1:89:GLU:HG3	1.90	1.00
1:1:193:ARG:NH2	1:4:295:ALA:HB2	1.77	1.00
1:1:243:VAL:HG22	1:1:304:VAL:HG12	1.44	1.00
1:3:4:GLY:HA2	1:3:27:VAL:HG21	1.43	1.00
1:1:154:ALA:HB3	1:1:155:PRO:HD3	1.39	0.99
1:2:225:THR:HG23	1:2:226:GLY:N	1.75	0.99
1:3:196:ARG:NH1	1:3:196:ARG:HG2	1.75	0.99
1:1:7:GLY:O	1:1:8:PHE:HB3	1.59	0.99
1:1:30:ASN:OD1	1:1:81:ILE:HG13	1.60	0.99
1:1:236:VAL:O	1:1:237:SER:HB3	1.60	0.99
1:2:10:ARG:NH1	1:2:46:ASP:OD1	1.96	0.99
1:1:171:MET:SD	1:1:209:ALA:HB2	2.02	0.99
1:4:280:SER:O	2:4:357:HOH:O	1.79	0.99
1:3:17:ARG:HG2	1:3:43:PHE:CE2	1.97	0.99
1:1:127:PHE:HB3	1:1:132:ASN:HB2	1.02	0.98
1:1:2:LYS:HG3	1:1:89:GLU:HG3	0.99	0.98
1:2:33:PHE:CZ	1:2:76:MET:HE1	1.97	0.98
1:3:295:ALA:C	1:3:297:ILE:HG23	1.88	0.98
1:2:175:HIS:CD2	1:2:230:ARG:NH2	2.30	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:193:ARG:HB2	1:3:277:VAL:HG12	1.45	0.98
1:2:328:GLN:HA	1:2:328:GLN:HE21	1.27	0.98
1:3:201:ASN:HD22	1:3:201:ASN:N	1.53	0.98
1:4:89:GLU:HG3	1:4:90:TYR:CD1	1.97	0.98
1:4:311:ASP:O	1:4:313:GLU:N	1.96	0.98
1:3:138:LYS:HZ2	1:3:330:VAL:HG13	1.21	0.98
1:1:188:SER:O	1:1:191:ASP:N	1.96	0.98
1:3:131:VAL:CG1	1:3:158:LYS:NZ	2.26	0.98
1:1:6:ASN:HA	1:1:30:ASN:ND2	1.76	0.98
1:2:17:ARG:HG3	1:2:43:PHE:HE2	1.22	0.98
1:2:203:ILE:HG22	1:2:203:ILE:O	1.61	0.98
1:3:2:LYS:HG3	1:3:89:GLU:HG3	1.46	0.98
1:3:28:ALA:HA	1:3:71:THR:O	1.64	0.98
1:4:251:TYR:HH	1:4:291:PHE:HZ	1.04	0.98
1:1:17:ARG:CG	1:1:43:PHE:HE2	1.77	0.98
1:1:44:LYS:HB3	1:1:44:LYS:HZ2	1.20	0.98
1:3:32:PRO:HD3	2:3:377:HOH:O	1.63	0.97
1:3:243:VAL:HG22	1:3:304:VAL:HG12	1.42	0.97
1:1:2:LYS:HG3	1:1:89:GLU:CG	1.93	0.97
1:1:113:LYS:O	1:1:114:LYS:HE3	1.64	0.97
1:4:113:LYS:HB3	1:4:114:LYS:CE	1.92	0.97
1:4:119:ALA:HB1	1:4:120:PRO:HD2	0.99	0.97
1:1:126:MET:HB2	1:1:215:LYS:HZ2	1.19	0.97
1:2:161:HIS:ND1	1:2:165:GLU:O	1.95	0.97
1:3:121:SER:OG	1:3:124:ALA:HB3	1.63	0.97
1:1:292:ASP:OD2	1:1:295:ALA:HB3	1.64	0.97
1:3:297:ILE:H	1:3:297:ILE:HD13	1.26	0.97
1:4:270:LEU:HD23	1:4:270:LEU:C	1.89	0.97
1:4:283:ILE:HD11	2:4:358:HOH:O	1.63	0.97
1:2:145:ASN:O	1:2:145:ASN:ND2	1.98	0.97
1:2:188:SER:HB3	1:2:192:TRP:N	1.78	0.97
1:2:244:ARG:HG3	1:3:244:ARG:HH12	1.28	0.97
1:3:76:MET:O	1:3:77:LYS:HD2	1.65	0.97
1:1:236:VAL:O	1:1:237:SER:CB	2.09	0.97
1:2:127:PHE:CE2	1:2:136:TYR:HB2	2.00	0.97
1:3:127:PHE:CZ	1:3:140:MET:HE1	1.99	0.96
1:1:53:LYS:HD2	1:1:54:GLY:H	1.30	0.96
1:1:4:GLY:CA	1:1:27:VAL:HG21	1.94	0.96
1:2:232:PRO:O	1:2:233:THR:O	1.83	0.96
1:3:8:PHE:CD1	1:3:29:VAL:HG11	2.01	0.96
1:3:175:HIS:CD2	1:3:230:ARG:NH2	2.34	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:8:PHE:HD2	1:2:8:PHE:O	1.46	0.96
1:1:95:THR:HG22	1:1:97:VAL:H	1.30	0.96
1:3:11:ILE:N	1:3:11:ILE:CD1	2.28	0.96
1:3:307:VAL:O	1:3:307:VAL:CG1	2.14	0.96
1:1:26:VAL:CG1	1:1:70:ILE:HG21	1.95	0.96
1:2:276:ASP:O	1:2:278:VAL:HG13	1.64	0.96
1:4:188:SER:O	1:4:190:LYS:N	1.98	0.96
1:4:8:PHE:O	1:4:8:PHE:CD2	2.18	0.96
1:1:244:ARG:HH12	1:4:244:ARG:HG3	1.31	0.95
1:2:32:PRO:CA	1:2:74:ASN:ND2	2.29	0.95
1:2:65:VAL:HG22	1:2:66:ASP:OD2	1.66	0.95
1:4:52:PHE:N	2:4:340:HOH:O	1.97	0.95
1:4:52:PHE:O	1:4:53:LYS:HB3	1.64	0.95
1:3:104:ALA:O	1:3:107:HIS:N	1.99	0.95
1:3:113:LYS:O	1:3:114:LYS:HE3	1.63	0.95
1:2:41:TYR:OH	1:4:277:VAL:HG11	1.66	0.95
1:2:52:PHE:O	1:2:53:LYS:NZ	1.99	0.95
1:1:71:THR:HG22	1:1:72:VAL:N	1.78	0.95
1:3:26:VAL:C	1:3:27:VAL:HG12	1.90	0.95
1:3:129:CYS:HA	1:3:132:ASN:ND2	1.81	0.95
1:1:97:VAL:O	1:1:98:PHE:CD1	2.19	0.95
1:1:193:ARG:HH12	1:4:295:ALA:CB	1.79	0.95
1:1:295:ALA:HB2	1:4:193:ARG:NH2	1.81	0.95
1:2:188:SER:O	1:2:191:ASP:N	1.99	0.95
1:2:248:GLU:HA	1:2:302:THR:HG22	1.46	0.95
1:1:121:SER:CB	1:1:124:ALA:HB3	1.97	0.94
1:1:293:ALA:O	1:1:294:LYS:HB3	1.67	0.94
1:1:299:LEU:CD2	1:1:304:VAL:HG23	1.96	0.94
1:4:2:LYS:NZ	1:4:88:ALA:HA	1.82	0.94
1:3:90:TYR:CE2	1:3:328:GLN:NE2	2.35	0.94
1:2:193:ARG:NH2	1:3:295:ALA:HB2	1.80	0.94
1:3:101:ILE:O	1:3:105:SER:OG	1.84	0.94
1:3:294:LYS:C	1:3:297:ILE:HD12	1.93	0.94
1:1:298:GLN:NE2	1:4:225:THR:CG2	2.31	0.94
1:2:1:SER:HB3	1:2:25:GLN:HB2	1.49	0.94
1:1:190:LYS:HD2	2:1:397:HOH:O	1.66	0.94
1:1:298:GLN:HE22	1:4:225:THR:CG2	1.81	0.94
1:2:59:GLU:O	1:2:60:ASP:C	2.11	0.94
1:2:295:ALA:HB1	1:3:193:ARG:NH1	1.83	0.94
1:4:132:ASN:ND2	1:4:133:LEU:CD2	2.31	0.94
1:2:113:LYS:HE2	1:2:114:LYS:HZ1	1.32	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:181:GLN:NE2	1:4:203:ILE:HD12	1.83	0.93
1:2:135:LYS:HZ3	1:2:140:MET:HE1	1.31	0.93
1:2:95:THR:HG22	1:2:97:VAL:H	1.34	0.93
1:2:277:VAL:O	1:2:278:VAL:O	1.86	0.93
1:1:130:GLY:O	1:1:133:LEU:HD12	1.69	0.93
1:2:127:PHE:HD1	1:2:143:VAL:CG2	1.82	0.93
1:3:6:ASN:HA	1:3:30:ASN:ND2	1.81	0.93
1:4:276:ASP:OD1	1:4:277:VAL:HG22	1.69	0.93
1:4:28:ALA:HB3	1:4:83:TRP:CZ3	2.04	0.93
1:1:292:ASP:OD1	1:1:295:ALA:CB	2.16	0.93
1:3:3:ILE:O	1:3:88:ALA:HB1	1.67	0.93
1:3:294:LYS:C	1:3:297:ILE:CD1	2.42	0.93
1:4:279:SER:O	1:4:281:ASP:N	2.02	0.93
1:1:132:ASN:HD21	1:1:133:LEU:HD21	1.34	0.92
1:3:19:ALA:O	1:3:22:CYS:HB2	1.69	0.92
1:4:17:ARG:NH2	2:4:339:HOH:O	2.01	0.92
1:4:31:ASP:O	1:4:34:ILE:HG22	1.69	0.92
1:3:252:ASP:O	1:3:255:LYS:HG2	1.69	0.92
1:3:236:VAL:O	1:3:237:SER:HB2	1.65	0.92
1:1:101:ILE:HG22	1:1:105:SER:OG	1.70	0.92
1:1:183:THR:O	1:1:184:VAL:HB	1.67	0.92
1:2:113:LYS:CG	1:2:114:LYS:HE3	1.99	0.92
1:3:252:ASP:O	1:3:255:LYS:N	2.01	0.92
1:4:211:LYS:N	1:4:211:LYS:HE2	1.84	0.92
1:2:244:ARG:CB	1:3:244:ARG:HH22	1.81	0.92
1:1:251:TYR:HB2	1:1:299:LEU:HG	1.51	0.92
1:2:277:VAL:HG21	1:4:41:TYR:HE1	1.10	0.92
1:3:32:PRO:HA	1:3:74:ASN:HD21	1.35	0.92
1:1:126:MET:SD	1:1:146:ALA:HB2	2.10	0.92
1:2:297:ILE:HD13	1:2:297:ILE:N	1.75	0.92
1:3:138:LYS:HZ1	1:3:330:VAL:HG13	1.32	0.92
1:3:161:HIS:O	1:3:162:GLU:C	2.12	0.92
1:3:277:VAL:HG23	1:3:278:VAL:H	1.34	0.92
1:4:74:ASN:OD1	1:4:75:GLU:N	2.02	0.92
1:4:208:GLY:HA3	1:4:211:LYS:HG2	1.52	0.92
1:2:6:ASN:ND2	1:2:93:GLU:OE1	2.01	0.92
1:4:4:GLY:HA2	1:4:27:VAL:CG2	2.00	0.92
1:1:119:ALA:HB1	1:1:120:PRO:CD	2.00	0.91
1:2:33:PHE:HZ	1:2:76:MET:CE	1.83	0.91
1:2:266:LEU:HD23	1:2:270:LEU:HD12	1.49	0.91
1:4:97:VAL:O	1:4:98:PHE:CD1	2.24	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:126:MET:HE3	1:1:212:ALA:HA	1.51	0.91
1:2:66:ASP:O	1:2:68:LYS:HD3	1.70	0.91
1:2:294:LYS:C	1:2:297:ILE:CD1	2.43	0.91
1:4:173:THR:HG23	1:4:228:ALA:HB2	1.51	0.91
1:4:292:ASP:OD2	1:4:295:ALA:HB3	1.70	0.91
1:1:32:PRO:HA	1:1:74:ASN:HD21	1.35	0.91
1:2:293:ALA:O	1:2:294:LYS:HB3	1.70	0.91
1:4:136:TYR:O	1:4:137:SER:OG	1.88	0.91
1:1:276:ASP:OD1	1:1:277:VAL:N	2.03	0.91
1:3:276:ASP:OD1	1:3:277:VAL:CG1	2.17	0.91
1:1:136:TYR:OH	1:1:331:ASP:OD2	1.88	0.91
1:1:220:LEU:O	1:1:221:ASP:C	2.13	0.91
1:3:251:TYR:O	1:3:254:ILE:HB	1.71	0.91
1:1:158:LYS:O	1:1:162:GLU:HG2	1.68	0.91
1:1:298:GLN:NE2	1:4:225:THR:OG1	2.04	0.91
1:3:127:PHE:HZ	1:3:140:MET:HE1	1.30	0.91
1:3:131:VAL:HG12	1:3:158:LYS:HZ2	1.21	0.91
1:2:17:ARG:NE	2:2:399:HOH:O	1.62	0.91
1:3:292:ASP:CG	1:3:295:ALA:HB3	1.96	0.91
1:4:27:VAL:HG22	1:4:28:ALA:N	1.83	0.91
1:4:216:VAL:HG13	1:4:217:ILE:CG2	2.00	0.91
1:1:266:LEU:O	1:1:267:GLN:O	1.89	0.91
1:1:273:THR:HG22	1:1:290:ILE:HD11	1.51	0.91
1:4:211:LYS:HA	1:4:211:LYS:NZ	1.85	0.91
1:3:319:ARG:O	1:3:320:VAL:C	2.13	0.90
1:1:193:ARG:NE	1:4:277:VAL:HA	1.85	0.90
1:2:34:ILE:HD11	1:2:39:MET:HG2	1.53	0.90
1:2:152:CYS:SG	1:2:239:VAL:HG11	2.11	0.90
1:3:65:VAL:CG2	1:3:66:ASP:OD2	2.20	0.90
1:3:299:LEU:HD22	1:3:300:SER:H	1.37	0.90
1:4:208:GLY:HA3	1:4:211:LYS:CG	2.01	0.90
1:4:278:VAL:HA	1:4:281:ASP:OD2	1.71	0.90
1:1:216:VAL:HG13	1:1:217:ILE:HG22	1.50	0.90
1:4:26:VAL:C	1:4:27:VAL:CG1	2.39	0.90
1:4:129:CYS:HA	1:4:132:ASN:ND2	1.86	0.90
1:1:101:ILE:CG2	1:1:142:VAL:HG11	2.01	0.90
1:2:3:ILE:C	1:2:27:VAL:HG23	1.96	0.90
1:4:43:PHE:HA	2:4:452:HOH:O	1.72	0.90
1:4:53:LYS:HD2	1:4:54:GLY:N	1.86	0.90
1:4:243:VAL:HG23	1:4:304:VAL:HG12	1.53	0.90
1:3:8:PHE:CD2	1:3:8:PHE:O	2.24	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:251:TYR:H	1:2:299:LEU:HD12	0.76	0.90
1:1:126:MET:HB2	1:1:215:LYS:HZ3	1.20	0.90
1:3:83:TRP:HD1	1:3:112:ALA:HB2	1.37	0.90
1:4:30:ASN:O	1:4:30:ASN:ND2	2.05	0.90
1:2:26:VAL:O	1:2:27:VAL:CB	2.19	0.89
1:2:99:THR:O	1:2:121:SER:OG	1.91	0.89
1:3:4:GLY:CA	1:3:27:VAL:HG21	2.02	0.89
1:3:156:VAL:HG22	1:3:258:MET:HE2	1.52	0.89
1:1:54:GLY:HA3	1:1:66:ASP:OD2	1.72	0.89
1:1:66:ASP:O	1:1:68:LYS:HD3	1.71	0.89
1:2:298:GLN:NE2	1:3:225:THR:HG21	1.87	0.89
1:4:6:ASN:HA	1:4:30:ASN:HD21	1.34	0.89
1:1:121:SER:HB2	1:1:124:ALA:HB3	1.54	0.89
1:1:286:ASN:OD1	1:1:318:GLN:NE2	2.06	0.89
1:3:8:PHE:O	1:3:8:PHE:HD2	1.53	0.89
1:2:1:SER:C	1:2:2:LYS:HG2	1.95	0.89
1:2:170:LEU:HD22	1:2:225:THR:HG22	1.54	0.89
1:4:17:ARG:CZ	2:4:339:HOH:O	2.21	0.89
1:1:145:ASN:HB2	1:1:323:LEU:CD2	2.03	0.89
1:2:34:ILE:HD11	1:2:39:MET:CG	2.01	0.89
1:3:211:LYS:HE2	1:3:211:LYS:CA	2.01	0.89
1:1:258:MET:HG2	1:1:270:LEU:HD11	1.53	0.89
1:1:273:THR:HG22	1:1:290:ILE:CD1	2.02	0.89
1:2:283:ILE:O	1:2:284:GLY:O	1.90	0.89
1:2:328:GLN:HE21	1:2:328:GLN:CA	1.81	0.89
1:3:83:TRP:CD1	1:3:112:ALA:HB2	2.08	0.89
1:3:220:LEU:O	1:3:222:GLY:N	2.06	0.89
1:3:318:GLN:O	1:3:321:ILE:HB	1.72	0.89
1:4:154:ALA:CB	1:4:155:PRO:HD2	1.98	0.89
1:1:216:VAL:CG1	1:1:217:ILE:HG22	2.03	0.89
1:1:219:GLU:O	1:1:223:LYS:NZ	2.06	0.89
1:2:188:SER:HB3	1:2:191:ASP:C	1.96	0.89
1:1:298:GLN:HE22	1:4:225:THR:CB	1.86	0.88
1:3:6:ASN:HA	1:3:30:ASN:HD21	1.35	0.88
1:3:154:ALA:CB	1:3:155:PRO:CD	2.48	0.88
1:2:152:CYS:SG	1:2:239:VAL:CG1	2.60	0.88
1:2:295:ALA:CB	1:3:193:ARG:NH1	2.36	0.88
1:4:112:ALA:O	1:4:113:LYS:HB2	1.71	0.88
1:2:6:ASN:HA	1:2:30:ASN:ND2	1.87	0.88
1:2:8:PHE:CZ	1:2:39:MET:HG2	2.08	0.88
1:3:154:ALA:CB	1:3:155:PRO:HD3	2.02	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:295:ALA:N	1:3:297:ILE:HD12	1.89	0.88
1:4:44:LYS:O	1:4:51:VAL:HA	1.72	0.88
1:1:277:VAL:HG23	1:1:278:VAL:H	1.37	0.88
1:2:108:PHE:O	1:2:111:GLY:N	2.05	0.88
1:3:201:ASN:N	1:3:201:ASN:ND2	2.12	0.88
1:4:329:LYS:NZ	1:4:329:LYS:C	2.31	0.88
1:2:132:ASN:ND2	1:2:133:LEU:CD2	2.36	0.88
1:2:193:ARG:HH22	1:3:295:ALA:CB	1.83	0.88
1:3:81:ILE:CD1	1:3:82:PRO:HD2	2.02	0.88
1:4:220:LEU:HA	1:4:223:LYS:NZ	1.88	0.88
1:1:113:LYS:HB3	1:1:114:LYS:CE	2.04	0.88
1:2:91:ILE:HD12	1:2:114:LYS:O	1.73	0.88
1:1:161:HIS:O	1:1:162:GLU:C	2.17	0.88
1:2:32:PRO:HA	1:2:74:ASN:HD21	1.08	0.88
1:2:299:LEU:CD2	1:2:304:VAL:HG23	2.04	0.88
1:2:329:LYS:C	1:2:329:LYS:HZ3	1.81	0.88
1:3:11:ILE:HD13	1:3:11:ILE:N	1.84	0.88
1:4:131:VAL:HG12	1:4:158:LYS:NZ	1.89	0.88
1:1:63:LEU:HB2	1:1:72:VAL:HG11	1.55	0.88
1:3:200:GLN:OE1	1:4:48:THR:HG22	1.72	0.88
1:4:164:PHE:O	1:4:165:GLU:HB2	1.74	0.88
1:2:127:PHE:CD1	1:2:143:VAL:CG2	2.57	0.88
1:2:210:ALA:O	1:2:211:LYS:O	1.91	0.88
1:2:244:ARG:NH2	1:3:244:ARG:HG3	1.89	0.88
1:4:211:LYS:HA	1:4:211:LYS:CE	2.04	0.88
1:2:3:ILE:C	1:2:27:VAL:CG2	2.47	0.88
1:1:176:ALA:HB1	1:1:233:THR:O	1.73	0.87
1:2:319:ARG:HA	1:2:322:ASP:OD2	1.73	0.87
1:4:255:LYS:HD3	1:4:293:ALA:HB1	1.56	0.87
1:1:14:LEU:HA	1:1:17:ARG:HG3	1.55	0.87
1:1:220:LEU:HA	1:1:223:LYS:HZ2	0.74	0.87
1:2:51:VAL:C	2:2:400:HOH:O	2.03	0.87
1:2:217:ILE:HG12	1:2:220:LEU:HD22	1.57	0.87
1:4:297:ILE:C	1:4:297:ILE:HD13	1.98	0.87
1:1:297:ILE:CD1	1:1:297:ILE:N	2.36	0.87
1:2:318:GLN:OE1	1:2:318:GLN:HA	1.71	0.87
1:3:145:ASN:O	1:3:146:ALA:O	1.91	0.87
1:4:276:ASP:CG	1:4:277:VAL:HG22	1.99	0.87
1:1:27:VAL:HG13	1:1:28:ALA:N	1.87	0.87
1:1:298:GLN:NE2	1:4:225:THR:HG21	1.88	0.87
1:3:131:VAL:CG1	1:3:158:LYS:HZ3	1.85	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:294:LYS:C	1:2:297:ILE:HD11	2.00	0.87
1:3:175:HIS:CG	1:3:230:ARG:HH21	1.92	0.87
1:2:66:ASP:O	1:2:68:LYS:CD	2.23	0.87
1:2:311:ASP:O	1:2:312:ASN:C	2.18	0.87
1:3:104:ALA:O	1:3:105:SER:C	2.17	0.87
1:1:27:VAL:CG1	1:1:28:ALA:H	1.74	0.87
1:1:212:ALA:O	1:1:216:VAL:HB	1.74	0.87
1:2:225:THR:HG21	1:3:298:GLN:CD	1.98	0.87
1:4:25:GLN:O	1:4:26:VAL:O	1.92	0.87
1:1:66:ASP:HB3	2:1:432:HOH:O	1.74	0.87
1:1:8:PHE:HA	1:1:12:GLY:HA3	1.57	0.87
1:1:145:ASN:ND2	1:1:145:ASN:O	2.08	0.86
1:2:296:GLY:O	1:2:307:VAL:HG23	1.74	0.86
1:3:85:LYS:O	1:3:86:ALA:CB	2.20	0.86
1:4:132:ASN:ND2	1:4:133:LEU:HD21	1.90	0.86
1:1:53:LYS:HB3	1:1:53:LYS:HZ3	1.39	0.86
1:1:298:GLN:OE1	1:4:226:GLY:N	2.09	0.86
1:3:154:ALA:HB3	1:3:155:PRO:HD2	1.55	0.86
1:1:3:ILE:HG22	1:1:4:GLY:H	1.38	0.86
1:1:243:VAL:HG22	1:1:304:VAL:CG1	2.04	0.86
1:4:154:ALA:CB	1:4:155:PRO:CD	2.52	0.86
1:4:321:ILE:O	1:4:325:LYS:HG2	1.74	0.86
1:1:126:MET:CB	1:1:215:LYS:NZ	2.35	0.86
1:1:220:LEU:O	1:1:222:GLY:N	2.08	0.86
1:2:216:VAL:CG1	1:2:217:ILE:HG22	2.05	0.86
1:3:3:ILE:HG22	1:3:4:GLY:H	1.38	0.86
1:3:276:ASP:O	1:3:278:VAL:HG13	1.75	0.86
1:1:83:TRP:HA	1:1:86:ALA:HB3	1.58	0.86
1:1:243:VAL:CG2	1:1:304:VAL:HG12	2.03	0.86
1:3:55:GLU:O	1:3:65:VAL:HA	1.76	0.86
1:2:277:VAL:C	1:2:278:VAL:O	2.18	0.86
1:3:66:ASP:O	1:3:68:LYS:HD3	1.73	0.86
1:3:75:GLU:O	2:3:378:HOH:O	1.92	0.86
1:1:251:TYR:H	1:1:299:LEU:HD12	1.40	0.86
1:3:291:PHE:HA	1:3:308:SER:OG	1.75	0.86
1:1:282:PHE:CZ	1:1:290:ILE:HD13	2.11	0.86
1:2:294:LYS:O	1:2:297:ILE:HD11	1.75	0.86
1:3:71:THR:HG21	1:3:73:PHE:CZ	2.10	0.86
1:1:75:GLU:N	2:1:437:HOH:O	2.09	0.85
1:1:244:ARG:HH22	1:4:244:ARG:HB2	1.40	0.85
1:3:208:GLY:HA3	1:3:211:LYS:HG2	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:277:VAL:O	1:4:278:VAL:O	1.93	0.85
1:1:220:LEU:CA	1:1:223:LYS:NZ	2.33	0.85
1:2:113:LYS:HE2	1:2:114:LYS:NZ	1.90	0.85
1:3:291:PHE:HA	1:3:308:SER:HG	1.41	0.85
1:4:2:LYS:HB3	1:4:2:LYS:HZ3	1.41	0.85
1:3:84:SER:OG	1:3:111:GLY:HA3	1.76	0.85
1:2:153:LEU:O	1:2:153:LEU:HD23	1.75	0.85
1:4:276:ASP:O	1:4:278:VAL:HG13	1.76	0.85
1:1:297:ILE:HD13	1:1:297:ILE:N	1.84	0.85
1:1:11:ILE:HG22	1:1:15:VAL:HG21	1.57	0.85
1:1:101:ILE:O	1:1:105:SER:OG	1.95	0.85
1:2:243:VAL:HG23	1:2:245:LEU:HD23	1.58	0.85
1:4:52:PHE:C	1:4:53:LYS:HZ3	1.85	0.85
1:4:53:LYS:HB3	1:4:53:LYS:NZ	1.91	0.85
1:2:3:ILE:CG2	1:2:4:GLY:H	1.87	0.85
1:1:219:GLU:C	1:1:223:LYS:HZ1	1.85	0.85
1:3:17:ARG:NE	2:3:369:HOH:O	1.91	0.85
1:3:53:LYS:NZ	1:3:53:LYS:HB3	1.91	0.85
1:3:292:ASP:OD2	1:3:295:ALA:HB3	1.76	0.85
1:4:8:PHE:HZ	1:4:39:MET:HB2	1.41	0.85
1:2:32:PRO:O	1:2:33:PHE:HB2	1.74	0.85
1:2:296:GLY:HA3	1:2:307:VAL:HG21	1.59	0.85
1:3:2:LYS:NZ	1:3:87:GLY:O	2.08	0.85
1:4:1:SER:HB3	1:4:25:GLN:HB2	1.58	0.85
1:4:183:THR:O	1:4:184:VAL:HB	1.76	0.85
1:1:53:LYS:HB3	1:1:53:LYS:NZ	1.92	0.85
1:1:129:CYS:O	1:1:133:LEU:HD11	1.77	0.85
1:2:27:VAL:CG1	1:2:28:ALA:N	2.34	0.85
1:2:74:ASN:C	1:2:74:ASN:OD1	2.20	0.85
1:2:170:LEU:CD2	1:2:225:THR:HG22	2.07	0.85
1:2:244:ARG:HH22	1:3:244:ARG:HG3	1.41	0.85
1:3:53:LYS:HB3	1:3:53:LYS:HZ3	1.42	0.85
1:4:252:ASP:C	1:4:252:ASP:OD1	2.14	0.85
1:2:298:GLN:HE22	1:3:225:THR:HG21	1.39	0.84
1:2:91:ILE:HD12	1:2:91:ILE:H	1.41	0.84
1:2:127:PHE:CD1	1:2:143:VAL:HG21	2.11	0.84
1:3:56:VAL:O	1:3:56:VAL:HG13	1.78	0.84
1:4:239:VAL:CG1	1:4:310:TYR:HE1	1.90	0.84
1:1:1:SER:HG	1:1:25:GLN:HB2	1.41	0.84
1:1:251:TYR:H	1:1:299:LEU:CD1	1.90	0.84
1:3:50:GLY:O	1:3:51:VAL:HG23	1.76	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:105:SER:O	1:3:107:HIS:N	2.10	0.84
1:4:25:GLN:C	1:4:26:VAL:O	2.15	0.84
1:1:207:THR:OG1	1:1:208:GLY:N	2.02	0.84
1:2:3:ILE:O	1:2:88:ALA:HB1	1.78	0.84
1:2:175:HIS:CD2	1:2:230:ARG:HH21	1.93	0.84
1:2:196:ARG:NH1	1:2:196:ARG:HG2	1.90	0.84
1:2:244:ARG:CG	1:3:244:ARG:HH22	1.89	0.84
1:3:8:PHE:CZ	1:3:39:MET:HG2	2.12	0.84
1:3:251:TYR:H	1:3:299:LEU:CD1	1.89	0.84
1:4:6:ASN:HA	1:4:30:ASN:ND2	1.92	0.84
1:1:193:ARG:NH1	1:1:204:PRO:HG2	1.91	0.84
1:2:113:LYS:HB3	1:2:114:LYS:CD	2.08	0.84
1:3:154:ALA:HB3	1:3:155:PRO:HD3	1.55	0.84
1:4:251:TYR:HB2	1:4:299:LEU:CB	2.06	0.84
1:1:168:GLU:CG	1:1:244:ARG:HD2	2.06	0.84
1:2:10:ARG:O	1:2:14:LEU:HD22	1.77	0.84
1:3:27:VAL:CG2	1:3:28:ALA:N	2.36	0.84
1:3:134:GLU:O	1:3:136:TYR:N	2.10	0.84
1:4:173:THR:HG23	1:4:228:ALA:CB	2.08	0.84
1:4:273:THR:HG22	1:4:290:ILE:HD11	1.60	0.84
1:1:161:HIS:ND1	1:1:165:GLU:O	2.09	0.84
1:1:307:VAL:O	1:1:307:VAL:CG1	2.25	0.84
1:2:15:VAL:O	1:2:18:ALA:HB3	1.77	0.84
1:2:185:ASP:C	1:2:195:GLY:O	2.21	0.84
1:3:75:GLU:N	2:3:377:HOH:O	2.02	0.84
1:3:128:VAL:O	1:3:132:ASN:ND2	2.10	0.84
1:3:161:HIS:HB2	1:3:166:ILE:HD12	1.60	0.84
1:3:207:THR:OG1	1:3:208:GLY:N	2.08	0.84
1:3:297:ILE:H	1:3:297:ILE:CD1	1.91	0.84
1:4:89:GLU:HG3	1:4:90:TYR:HD1	1.38	0.84
1:1:205:SER:HB3	1:1:228:ALA:HB3	1.60	0.84
1:4:78:PRO:CG	1:4:98:PHE:CE2	2.61	0.84
1:4:183:THR:HB	1:4:184:VAL:HG12	1.59	0.84
1:1:188:SER:HB3	1:1:191:ASP:C	2.03	0.83
1:4:11:ILE:CD1	1:4:11:ILE:H	1.91	0.83
1:1:53:LYS:HD2	1:1:54:GLY:N	1.92	0.83
1:4:251:TYR:CZ	1:4:297:ILE:HG12	2.13	0.83
1:1:95:THR:CG2	1:1:97:VAL:HG23	2.07	0.83
1:1:193:ARG:HH22	1:4:295:ALA:CB	1.87	0.83
1:2:8:PHE:HA	1:2:12:GLY:HA3	1.59	0.83
1:3:270:LEU:HD23	1:3:270:LEU:C	2.03	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:104:ALA:O	1:4:107:HIS:N	2.12	0.83
1:1:95:THR:HG22	1:1:97:VAL:N	1.93	0.83
1:3:27:VAL:HG22	1:3:28:ALA:O	1.78	0.83
1:3:188:SER:HB3	1:3:191:ASP:C	2.03	0.83
1:4:58:MET:SD	1:4:58:MET:N	2.50	0.83
1:2:11:ILE:HG22	1:2:15:VAL:CG2	2.08	0.83
1:3:205:SER:HB3	1:3:228:ALA:HB3	1.59	0.83
1:1:34:ILE:HG12	1:1:39:MET:HE2	1.60	0.83
1:1:51:VAL:C	2:1:430:HOH:O	2.22	0.83
1:1:65:VAL:O	1:1:68:LYS:HG2	1.78	0.83
1:1:277:VAL:HG11	1:3:41:TYR:OH	1.77	0.83
1:2:299:LEU:HD23	1:2:304:VAL:HG23	1.60	0.83
1:3:10:ARG:O	1:3:14:LEU:HD22	1.78	0.83
1:1:244:ARG:HH22	1:4:244:ARG:CB	1.90	0.83
1:2:188:SER:O	1:2:190:LYS:N	2.12	0.83
1:3:50:GLY:C	1:3:51:VAL:HG23	2.03	0.83
1:4:30:ASN:OD1	1:4:81:ILE:HG13	1.77	0.83
1:1:137:SER:O	1:1:140:MET:HG3	1.79	0.83
1:2:244:ARG:HB2	1:3:244:ARG:NH2	1.94	0.83
1:3:11:ILE:H	1:3:11:ILE:CD1	1.86	0.83
1:3:167:VAL:HG13	1:3:245:LEU:O	1.78	0.83
1:4:2:LYS:NZ	1:4:87:GLY:O	2.12	0.83
1:1:9:GLY:O	1:1:13:ARG:HG3	1.78	0.83
1:1:277:VAL:O	1:1:278:VAL:HG22	1.79	0.83
1:2:54:GLY:HA2	1:2:66:ASP:OD1	1.77	0.83
1:4:40:VAL:HG11	1:4:58:MET:SD	2.18	0.83
1:1:59:GLU:O	1:1:60:ASP:C	2.21	0.82
1:1:202:ILE:HD11	1:4:233:THR:CG2	2.08	0.82
1:1:227:MET:HE3	1:4:296:GLY:HA2	1.58	0.82
1:3:4:GLY:CA	1:3:27:VAL:CG2	2.55	0.82
1:1:11:ILE:H	1:1:11:ILE:HD12	1.45	0.82
1:2:64:VAL:O	1:2:64:VAL:HG22	1.77	0.82
1:4:219:GLU:O	1:4:223:LYS:NZ	2.12	0.82
1:4:293:ALA:O	1:4:294:LYS:HB3	1.78	0.82
1:1:128:VAL:O	1:1:132:ASN:CB	2.26	0.82
1:1:277:VAL:HG21	1:3:41:TYR:HE1	1.41	0.82
1:2:293:ALA:O	1:2:294:LYS:CB	2.26	0.82
1:4:196:ARG:HG3	1:4:197:GLY:H	1.43	0.82
1:1:6:ASN:CA	1:1:30:ASN:HD21	1.92	0.82
1:2:27:VAL:CG1	1:2:28:ALA:H	1.74	0.82
1:2:277:VAL:HG21	1:4:41:TYR:CZ	2.15	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:173:THR:CG2	1:2:228:ALA:HB2	2.10	0.82
1:4:188:SER:O	1:4:191:ASP:N	2.12	0.82
1:1:71:THR:O	1:1:72:VAL:HG12	1.79	0.82
1:1:276:ASP:OD1	1:1:277:VAL:HG22	1.80	0.82
1:2:97:VAL:O	1:2:98:PHE:CG	2.32	0.82
1:3:97:VAL:O	1:3:98:PHE:CB	2.25	0.82
1:1:243:VAL:CG2	1:1:304:VAL:CG1	2.57	0.82
1:2:105:SER:O	1:2:108:PHE:CD1	2.32	0.82
1:2:244:ARG:HG3	1:3:244:ARG:NH1	1.93	0.82
1:2:251:TYR:HB2	1:2:299:LEU:HB2	1.60	0.82
1:1:129:CYS:SG	1:1:269:PHE:HE1	2.02	0.82
1:1:261:ALA:O	1:1:262:SER:C	2.21	0.82
1:1:276:ASP:CG	1:1:277:VAL:N	2.28	0.82
1:2:225:THR:CG2	1:3:298:GLN:NE2	2.43	0.82
1:1:8:PHE:HD2	1:1:8:PHE:C	1.88	0.82
1:1:22:CYS:SG	1:1:321:ILE:HG21	2.19	0.82
1:1:244:ARG:NH2	1:4:244:ARG:HB2	1.94	0.82
1:2:137:SER:HB3	1:2:138:LYS:NZ	1.95	0.82
1:3:284:GLY:HA2	1:3:314:PHE:HE1	1.45	0.81
1:2:212:ALA:O	1:2:216:VAL:CB	2.29	0.81
1:2:217:ILE:HG12	1:2:220:LEU:CD2	2.11	0.81
1:3:40:VAL:O	1:3:44:LYS:HG3	1.80	0.81
1:1:127:PHE:CE2	1:1:136:TYR:CB	2.61	0.81
1:1:169:GLY:O	1:1:170:LEU:CD2	2.25	0.81
1:1:193:ARG:NH1	1:4:295:ALA:HB1	1.94	0.81
1:1:272:TYR:OH	1:1:274:GLU:CD	2.24	0.81
1:1:124:ALA:O	1:1:125:PRO:O	1.97	0.81
1:1:284:GLY:HA2	1:1:314:PHE:CE1	2.15	0.81
1:2:296:GLY:H	1:2:297:ILE:CD1	1.94	0.81
1:2:13:ARG:O	1:2:16:LEU:N	2.13	0.81
1:4:3:ILE:HG22	1:4:4:GLY:H	1.43	0.81
1:4:58:MET:HE2	1:4:58:MET:N	1.95	0.81
1:1:281:ASP:O	1:1:283:ILE:N	2.14	0.81
1:1:4:GLY:HA2	1:1:27:VAL:CG2	2.08	0.81
1:1:41:TYR:HE1	1:3:277:VAL:HG21	1.41	0.81
1:3:284:GLY:HA2	1:3:314:PHE:CE1	2.15	0.81
1:1:1:SER:O	1:1:25:GLN:HG2	1.80	0.81
1:1:132:ASN:ND2	1:1:133:LEU:CD2	2.44	0.81
1:3:71:THR:HG21	1:3:73:PHE:CE1	2.15	0.81
1:3:286:ASN:ND2	1:3:314:PHE:CZ	2.48	0.81
1:4:8:PHE:HA	1:4:12:GLY:HA3	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:129:CYS:HA	1:3:132:ASN:HD21	1.43	0.81
1:2:137:SER:HB3	1:2:138:LYS:HZ2	1.46	0.81
1:2:276:ASP:OD1	1:2:277:VAL:HG13	1.81	0.81
1:4:3:ILE:O	1:4:27:VAL:HG23	1.81	0.81
1:4:287:ARG:O	1:4:288:SER:HB2	1.81	0.81
1:2:26:VAL:HG23	1:2:27:VAL:H	1.44	0.80
1:3:97:VAL:O	1:3:98:PHE:CG	2.34	0.80
1:1:66:ASP:CB	2:1:432:HOH:O	2.29	0.80
1:1:231:VAL:HG11	1:4:231:VAL:HG11	1.63	0.80
1:3:44:LYS:O	1:3:51:VAL:HA	1.80	0.80
1:2:14:LEU:O	1:2:18:ALA:HB2	1.81	0.80
1:3:277:VAL:O	1:3:278:VAL:C	2.24	0.80
1:2:105:SER:O	1:2:108:PHE:HD1	1.63	0.80
1:2:297:ILE:CD1	1:2:297:ILE:N	2.35	0.80
1:3:173:THR:HG23	1:3:228:ALA:HB2	1.63	0.80
1:4:270:LEU:C	1:4:270:LEU:CD2	2.53	0.80
1:2:3:ILE:HG22	1:2:4:GLY:N	1.97	0.80
1:2:232:PRO:O	1:2:233:THR:C	2.23	0.80
1:3:91:ILE:HG21	1:3:107:HIS:NE2	1.97	0.80
1:3:113:LYS:HB3	1:3:114:LYS:HD2	0.86	0.80
1:3:180:THR:OG1	1:3:181:GLN:N	2.14	0.80
1:4:85:LYS:O	1:4:86:ALA:HB2	1.79	0.80
1:4:321:ILE:HG22	1:4:325:LYS:HE3	1.63	0.80
1:2:244:ARG:CG	1:3:244:ARG:HH12	1.93	0.80
1:4:26:VAL:O	1:4:27:VAL:HB	1.80	0.80
1:4:78:PRO:C	1:4:80:ASN:H	1.87	0.80
1:4:127:PHE:HE1	1:4:140:MET:HE1	1.46	0.80
1:4:150:THR:CG2	1:4:212:ALA:HB3	2.11	0.80
1:1:17:ARG:HB3	1:1:43:PHE:CZ	2.16	0.80
1:3:97:VAL:O	1:3:98:PHE:HB2	1.82	0.80
1:4:138:LYS:CE	1:4:330:VAL:HG13	2.11	0.80
1:4:307:VAL:HG13	1:4:307:VAL:O	1.79	0.80
1:1:161:HIS:CD2	1:1:162:GLU:N	2.49	0.80
1:2:8:PHE:O	1:2:8:PHE:CD2	2.33	0.80
1:2:10:ARG:HH12	1:2:46:ASP:CG	1.88	0.80
1:4:187:PRO:O	1:4:187:PRO:HG2	1.79	0.80
1:4:208:GLY:CA	1:4:211:LYS:HG2	2.11	0.80
1:4:273:THR:OG1	1:4:274:GLU:N	2.13	0.80
1:3:138:LYS:CE	1:3:330:VAL:HG13	2.11	0.79
1:2:76:MET:O	1:2:77:LYS:HD3	1.81	0.79
1:2:277:VAL:HA	1:3:193:ARG:CD	2.12	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:281:ASP:C	1:2:283:ILE:H	1.90	0.79
1:2:329:LYS:C	1:2:329:LYS:NZ	2.40	0.79
1:4:26:VAL:O	1:4:27:VAL:CB	2.30	0.79
1:4:180:THR:HG23	1:4:181:GLN:H	1.47	0.79
1:1:58:MET:SD	1:1:58:MET:N	2.55	0.79
1:1:250:SER:O	1:1:252:ASP:N	2.15	0.79
1:1:276:ASP:OD1	1:1:277:VAL:HG13	1.81	0.79
1:1:323:LEU:HD12	1:1:327:MET:SD	2.22	0.79
1:2:78:PRO:CG	1:2:98:PHE:CE2	2.65	0.79
1:3:4:GLY:HA2	1:3:27:VAL:HG23	1.62	0.79
1:3:81:ILE:HD13	1:3:82:PRO:O	1.81	0.79
1:3:216:VAL:CG1	1:3:217:ILE:N	2.45	0.79
1:3:251:TYR:N	1:3:299:LEU:HD12	1.96	0.79
1:1:126:MET:HE2	1:1:215:LYS:HD2	1.63	0.79
1:1:129:CYS:O	1:1:133:LEU:CD1	2.30	0.79
1:1:277:VAL:HA	1:4:193:ARG:HD3	1.63	0.79
1:4:83:TRP:CA	1:4:86:ALA:HB3	2.12	0.79
1:1:40:VAL:O	1:1:44:LYS:HG3	1.82	0.79
1:1:117:ILE:HD13	1:1:121:SER:OG	1.82	0.79
1:3:8:PHE:HA	1:3:12:GLY:HA3	1.64	0.79
1:4:132:ASN:ND2	1:4:133:LEU:HD23	1.97	0.79
1:4:188:SER:C	1:4:190:LYS:H	1.91	0.79
1:4:105:SER:O	1:4:108:PHE:HD1	1.65	0.79
1:1:26:VAL:HG12	1:1:70:ILE:HG21	1.62	0.79
1:1:270:LEU:CD2	1:1:271:GLY:N	2.46	0.79
1:3:277:VAL:C	1:3:278:VAL:O	2.22	0.79
1:4:319:ARG:O	1:4:320:VAL:C	2.25	0.79
1:1:132:ASN:ND2	1:1:133:LEU:HD21	1.96	0.79
1:1:295:ALA:CB	1:4:193:ARG:HH12	1.96	0.79
1:4:11:ILE:HD12	1:4:11:ILE:N	1.96	0.79
1:2:318:GLN:O	1:2:321:ILE:HB	1.82	0.79
1:3:175:HIS:CD2	1:3:230:ARG:HH21	1.98	0.79
1:4:265:PRO:N	2:4:453:HOH:O	2.16	0.79
1:1:318:GLN:HA	1:1:318:GLN:OE1	1.81	0.79
1:4:329:LYS:C	1:4:329:LYS:HZ3	1.89	0.79
1:1:104:ALA:O	1:1:107:HIS:N	2.16	0.78
1:3:212:ALA:O	1:3:216:VAL:HB	1.82	0.78
1:3:232:PRO:O	1:3:233:THR:C	2.25	0.78
1:4:52:PHE:CE1	1:4:53:LYS:HE3	2.17	0.78
1:2:220:LEU:O	1:2:221:ASP:C	2.25	0.78
1:4:89:GLU:OE1	1:4:90:TYR:HE1	1.67	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:295:ALA:HB2	1:3:193:ARG:HH22	1.46	0.78
1:2:320:VAL:O	1:2:324:LEU:HB2	1.84	0.78
1:3:277:VAL:O	1:3:278:VAL:O	2.02	0.78
1:1:124:ALA:C	1:1:125:PRO:O	2.24	0.78
1:2:232:PRO:HG2	1:3:232:PRO:HB2	1.63	0.78
1:4:74:ASN:O	1:4:75:GLU:CG	2.27	0.78
1:1:8:PHE:CD2	1:1:8:PHE:C	2.60	0.78
1:2:132:ASN:ND2	1:2:133:LEU:HD21	1.98	0.78
1:2:203:ILE:O	1:2:203:ILE:CG2	2.27	0.78
1:3:117:ILE:HB	1:3:144:SER:HA	1.63	0.78
1:1:126:MET:CB	1:1:215:LYS:HZ3	1.94	0.78
1:1:225:THR:CG2	1:4:298:GLN:OE1	2.31	0.78
1:1:273:THR:OG1	1:1:274:GLU:N	2.17	0.78
1:2:181:GLN:HG2	1:2:198:ALA:CB	2.14	0.78
1:3:100:THR:H	1:3:103:LYS:HB2	1.49	0.78
1:4:3:ILE:O	1:4:88:ALA:HB1	1.83	0.78
1:1:213:VAL:O	1:1:216:VAL:HG12	1.82	0.78
1:2:277:VAL:O	1:3:193:ARG:HD3	1.84	0.78
1:4:44:LYS:HZ2	1:4:44:LYS:HB3	1.47	0.78
1:1:131:VAL:HG12	1:1:158:LYS:HE2	1.66	0.78
1:2:4:GLY:N	1:2:27:VAL:HG21	1.99	0.78
1:2:113:LYS:CB	1:2:114:LYS:HE3	2.14	0.78
1:2:251:TYR:N	1:2:299:LEU:CD1	2.35	0.78
1:2:292:ASP:OD2	1:2:295:ALA:HB3	1.84	0.78
1:4:38:TYR:O	1:4:42:MET:N	2.17	0.78
1:1:8:PHE:N	1:1:31:ASP:OD2	2.17	0.77
1:1:127:PHE:CD1	1:1:143:VAL:HG21	2.19	0.77
1:1:168:GLU:HG2	1:1:244:ARG:HD2	1.64	0.77
1:3:8:PHE:N	1:3:31:ASP:OD2	2.16	0.77
1:3:294:LYS:O	1:3:297:ILE:HD11	1.84	0.77
1:4:26:VAL:O	1:4:27:VAL:HG12	1.84	0.77
1:4:51:VAL:HB	2:4:340:HOH:O	1.83	0.77
1:1:160:LEU:HD21	1:1:254:ILE:HD12	1.65	0.77
1:1:276:ASP:O	1:1:278:VAL:N	2.17	0.77
1:2:41:TYR:CE1	1:4:277:VAL:CG2	2.63	0.77
1:2:81:ILE:HD12	1:2:83:TRP:CE2	2.19	0.77
1:2:276:ASP:O	1:2:278:VAL:N	2.17	0.77
1:3:131:VAL:HG13	1:3:158:LYS:HZ3	1.48	0.77
1:3:276:ASP:O	1:3:278:VAL:HG22	1.83	0.77
1:1:320:VAL:O	1:1:324:LEU:N	2.16	0.77
1:2:235:ASP:CG	1:2:235:ASP:O	2.25	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:244:ARG:HG3	1:3:244:ARG:HH22	1.47	0.77
1:3:13:ARG:O	1:3:16:LEU:N	2.15	0.77
1:3:252:ASP:O	1:3:254:ILE:N	2.17	0.77
1:2:3:ILE:HD13	1:2:324:LEU:CD1	2.15	0.77
1:2:112:ALA:O	1:2:113:LYS:HB2	1.83	0.77
1:2:261:ALA:HB1	1:2:266:LEU:HD22	1.67	0.77
1:3:258:MET:HG2	1:3:270:LEU:HD11	1.65	0.77
1:3:216:VAL:CG1	1:3:217:ILE:H	1.97	0.77
1:3:330:VAL:HG12	1:3:331:ASP:N	1.99	0.77
1:1:145:ASN:CG	1:1:323:LEU:HD23	2.08	0.77
1:2:46:ASP:HB3	1:2:50:GLY:H	1.49	0.77
1:2:141:THR:OG1	1:2:142:VAL:N	2.18	0.77
1:2:250:SER:O	1:2:252:ASP:N	2.18	0.77
1:3:200:GLN:C	1:3:201:ASN:HD22	1.93	0.77
1:4:44:LYS:HE3	1:4:45:TYR:CE2	2.20	0.77
1:2:78:PRO:HG3	1:2:98:PHE:HE2	1.43	0.77
1:3:78:PRO:HG3	1:3:98:PHE:HE2	1.46	0.77
1:2:75:GLU:N	2:2:407:HOH:O	1.76	0.77
1:3:145:ASN:O	1:3:145:ASN:ND2	2.18	0.77
1:4:210:ALA:O	1:4:211:LYS:O	2.03	0.77
1:1:277:VAL:O	1:1:278:VAL:O	2.03	0.77
1:2:138:LYS:HE3	1:2:330:VAL:HG13	1.67	0.77
1:1:175:HIS:N	1:1:229:PHE:O	2.17	0.76
1:1:258:MET:CG	1:1:270:LEU:HD11	2.15	0.76
1:3:180:THR:O	1:3:181:GLN:C	2.26	0.76
1:4:32:PRO:HA	1:4:74:ASN:HD21	0.67	0.76
1:2:129:CYS:O	1:2:133:LEU:HD11	1.85	0.76
1:3:131:VAL:CG1	1:3:158:LYS:HZ2	1.96	0.76
1:3:216:VAL:HG12	1:3:217:ILE:H	1.50	0.76
1:4:75:GLU:CA	2:4:347:HOH:O	2.14	0.76
1:1:46:ASP:HB3	1:1:50:GLY:H	1.50	0.76
1:2:52:PHE:CA	2:2:400:HOH:O	2.21	0.76
1:2:85:LYS:O	1:2:86:ALA:HB2	1.85	0.76
1:2:101:ILE:O	1:2:105:SER:OG	2.03	0.76
1:2:106:ALA:O	1:2:107:HIS:C	2.27	0.76
1:4:97:VAL:O	1:4:98:PHE:CG	2.38	0.76
1:4:113:LYS:CB	1:4:114:LYS:HE3	2.15	0.76
1:1:90:TYR:CZ	1:1:328:GLN:NE2	2.52	0.76
1:3:129:CYS:O	1:3:132:ASN:ND2	2.18	0.76
1:3:272:TYR:CE2	1:3:293:ALA:HB2	2.21	0.76
1:1:284:GLY:HA2	1:1:314:PHE:HE1	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:161:HIS:HA	1:2:166:ILE:HG13	1.67	0.76
1:2:292:ASP:CG	1:2:295:ALA:HB3	2.11	0.76
1:2:295:ALA:N	1:2:297:ILE:HD12	2.00	0.76
1:3:292:ASP:OD1	1:3:295:ALA:HB3	1.84	0.76
1:4:27:VAL:HG22	1:4:28:ALA:O	1.85	0.76
1:4:104:ALA:O	1:4:105:SER:C	2.29	0.76
1:1:83:TRP:CA	1:1:86:ALA:HB3	2.15	0.76
1:1:298:GLN:HE22	1:4:225:THR:HG21	1.49	0.76
1:2:6:ASN:OD1	1:2:30:ASN:ND2	2.18	0.76
1:2:175:HIS:CG	1:2:230:ARG:HH21	2.03	0.76
1:2:244:ARG:CB	1:3:244:ARG:NH2	2.47	0.76
1:3:16:LEU:HD21	1:3:70:ILE:CD1	2.16	0.76
1:1:126:MET:HE2	1:1:215:LYS:HZ2	1.51	0.76
1:2:278:VAL:HA	1:2:281:ASP:OD2	1.84	0.76
1:4:74:ASN:C	2:4:347:HOH:O	2.12	0.76
1:4:76:MET:O	1:4:77:LYS:HD3	1.85	0.76
1:1:217:ILE:HG12	1:1:220:LEU:CD2	2.16	0.76
1:3:66:ASP:O	1:3:68:LYS:CD	2.34	0.76
1:4:55:GLU:O	1:4:65:VAL:HA	1.85	0.76
1:2:116:VAL:HG11	1:2:324:LEU:HD23	1.68	0.76
1:2:129:CYS:O	1:2:133:LEU:CD1	2.34	0.76
1:2:277:VAL:HA	1:3:193:ARG:NE	2.00	0.76
1:3:330:VAL:O	1:3:332:SER:N	2.18	0.76
1:2:65:VAL:CG2	1:2:66:ASP:OD2	2.33	0.75
1:3:281:ASP:O	1:3:283:ILE:N	2.18	0.75
1:4:258:MET:CG	1:4:270:LEU:HD11	2.15	0.75
1:1:244:ARG:NH1	1:4:244:ARG:HG3	2.01	0.75
1:2:117:ILE:HD11	1:2:142:VAL:O	1.85	0.75
1:2:124:ALA:O	1:2:125:PRO:O	2.04	0.75
1:4:264:GLY:C	2:4:453:HOH:O	2.29	0.75
1:4:329:LYS:HZ2	1:4:330:VAL:N	1.83	0.75
1:2:76:MET:N	2:2:408:HOH:O	2.05	0.75
1:2:113:LYS:C	1:2:114:LYS:HG2	2.02	0.75
1:3:91:ILE:HG21	1:3:107:HIS:CE1	2.21	0.75
1:1:71:THR:CG2	1:1:72:VAL:N	2.46	0.75
1:2:299:LEU:HD22	1:2:300:SER:H	1.51	0.75
1:3:329:LYS:C	1:3:329:LYS:HZ3	1.94	0.75
1:4:156:VAL:HG22	1:4:258:MET:HE2	1.67	0.75
1:1:44:LYS:HG2	1:1:56:VAL:HG11	1.69	0.75
1:1:296:GLY:HA3	1:4:227:MET:HE3	1.69	0.75
1:2:58:MET:N	1:2:58:MET:SD	2.55	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:251:TYR:HB2	1:3:299:LEU:HB2	1.66	0.75
1:4:182:LYS:HE3	1:4:187:PRO:HG2	1.69	0.75
1:2:145:ASN:HD22	1:2:145:ASN:C	1.93	0.75
1:3:94:SER:O	1:3:95:THR:C	2.29	0.75
1:4:113:LYS:CD	1:4:114:LYS:NZ	2.47	0.75
1:2:193:ARG:NE	1:3:277:VAL:HA	2.01	0.75
1:4:182:LYS:HE3	1:4:187:PRO:CG	2.17	0.75
1:1:27:VAL:CG2	1:1:28:ALA:H	1.98	0.75
1:1:277:VAL:C	1:1:278:VAL:O	2.30	0.75
1:3:129:CYS:O	1:3:133:LEU:HG	1.87	0.75
1:4:34:ILE:CD1	1:4:42:MET:SD	2.74	0.75
1:1:277:VAL:HG12	1:4:193:ARG:HA	1.68	0.75
1:4:14:LEU:HA	1:4:17:ARG:HB2	1.69	0.75
1:4:136:TYR:OH	1:4:331:ASP:OD2	2.05	0.75
1:1:129:CYS:SG	1:1:269:PHE:CE1	2.79	0.74
1:1:174:VAL:CG1	1:1:231:VAL:HG21	2.17	0.74
1:1:311:ASP:O	1:1:312:ASN:C	2.30	0.74
1:4:253:ASP:HB2	2:4:355:HOH:O	1.86	0.74
1:2:269:PHE:O	1:2:288:SER:HB3	1.87	0.74
1:2:277:VAL:HG23	1:2:278:VAL:N	1.98	0.74
1:3:76:MET:O	1:3:77:LYS:CD	2.34	0.74
1:3:252:ASP:HA	1:3:255:LYS:HG3	1.69	0.74
1:4:118:SER:O	1:4:316:TYR:OH	2.03	0.74
1:4:277:VAL:C	1:4:278:VAL:O	2.29	0.74
1:1:27:VAL:HG22	1:1:28:ALA:H	1.52	0.74
1:4:53:LYS:HZ3	1:4:53:LYS:CB	1.99	0.74
1:4:272:TYR:CE2	1:4:293:ALA:HB2	2.22	0.74
1:1:236:VAL:O	1:1:237:SER:HB2	1.87	0.74
1:1:325:LYS:O	1:1:326:HIS:C	2.30	0.74
1:3:279:SER:C	1:3:281:ASP:H	1.96	0.74
1:4:203:ILE:O	1:4:204:PRO:O	2.06	0.74
1:3:113:LYS:C	1:3:114:LYS:CE	2.60	0.74
1:3:283:ILE:O	1:3:284:GLY:O	2.05	0.74
1:1:101:ILE:HG23	1:1:142:VAL:CG1	2.17	0.74
1:3:59:GLU:O	1:3:60:ASP:C	2.30	0.74
1:4:262:SER:O	1:4:267:GLN:HA	1.86	0.74
1:1:174:VAL:O	1:1:237:SER:HA	1.88	0.74
1:2:32:PRO:O	1:2:33:PHE:CB	2.35	0.74
1:2:142:VAL:O	1:2:142:VAL:HG22	1.86	0.74
1:2:319:ARG:NH2	2:2:419:HOH:O	2.20	0.74
1:3:159:VAL:O	1:3:163:ASN:HB2	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:106:ALA:O	1:4:107:HIS:O	2.06	0.74
1:2:52:PHE:C	1:2:53:LYS:HZ3	1.95	0.74
1:4:113:LYS:HB3	1:4:114:LYS:HE3	1.69	0.74
1:2:278:VAL:O	1:2:279:SER:OG	2.06	0.74
1:4:182:LYS:CE	1:4:187:PRO:HG2	2.18	0.74
1:1:152:CYS:SG	1:1:239:VAL:CG1	2.76	0.73
1:4:4:GLY:HA2	1:4:27:VAL:HG23	1.68	0.73
1:1:11:ILE:HG22	1:1:15:VAL:CG2	2.17	0.73
1:1:34:ILE:HD11	1:1:39:MET:HG2	1.68	0.73
1:1:131:VAL:HG12	1:1:158:LYS:CE	2.18	0.73
1:1:251:TYR:CB	1:1:299:LEU:HG	2.18	0.73
1:2:156:VAL:HA	1:2:258:MET:HE3	1.70	0.73
1:2:287:ARG:O	1:2:319:ARG:NH1	2.22	0.73
1:3:161:HIS:HA	1:3:166:ILE:HG13	1.68	0.73
1:3:175:HIS:O	1:3:231:VAL:HG23	1.87	0.73
1:3:248:GLU:HG2	1:3:302:THR:HG22	1.70	0.73
1:3:265:PRO:C	1:3:267:GLN:H	1.93	0.73
1:1:329:LYS:NZ	1:1:330:VAL:N	2.36	0.73
1:2:175:HIS:N	1:2:229:PHE:O	2.21	0.73
1:3:294:LYS:HA	1:3:297:ILE:HG13	1.70	0.73
1:4:4:GLY:CA	1:4:27:VAL:CG2	2.66	0.73
1:4:77:LYS:N	2:4:348:HOH:O	2.03	0.73
1:4:216:VAL:CG1	1:4:217:ILE:HG22	2.10	0.73
1:4:276:ASP:CG	1:4:277:VAL:N	2.44	0.73
1:2:31:ASP:OD1	1:2:32:PRO:O	2.06	0.73
1:3:17:ARG:CG	1:3:43:PHE:HE2	1.97	0.73
1:3:293:ALA:O	1:3:294:LYS:HB3	1.87	0.73
1:4:129:CYS:CA	1:4:132:ASN:HD22	2.01	0.73
1:2:132:ASN:HD21	1:2:133:LEU:CD2	2.00	0.73
1:2:138:LYS:HE3	1:2:330:VAL:CG1	2.18	0.73
1:2:277:VAL:CG2	1:4:41:TYR:CE1	2.55	0.73
1:3:152:CYS:SG	1:3:239:VAL:HG13	2.27	0.73
1:3:251:TYR:CE1	1:3:255:LYS:HD3	2.24	0.73
1:3:295:ALA:CA	1:3:297:ILE:HD12	2.19	0.73
1:4:11:ILE:CD1	1:4:11:ILE:N	2.51	0.73
1:3:272:TYR:HA	1:3:291:PHE:O	1.88	0.73
1:4:211:LYS:CE	1:4:211:LYS:CA	2.66	0.73
1:1:145:ASN:C	1:1:145:ASN:HD22	1.96	0.73
1:1:156:VAL:HG22	1:1:258:MET:HE2	1.71	0.73
1:1:193:ARG:HH11	1:1:204:PRO:HG2	1.53	0.73
1:1:327:MET:O	1:1:331:ASP:HB2	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:159:VAL:CG2	1:2:266:LEU:HD21	2.18	0.73
1:3:276:ASP:OD1	1:3:277:VAL:HG22	1.88	0.73
1:1:294:LYS:C	1:1:297:ILE:CD1	2.62	0.73
1:2:81:ILE:HD13	1:2:82:PRO:O	1.89	0.73
1:2:248:GLU:HA	1:2:302:THR:HG21	1.69	0.73
1:3:53:LYS:HE2	1:3:53:LYS:N	2.02	0.73
1:3:328:GLN:O	1:3:329:LYS:C	2.31	0.73
1:1:180:THR:OG1	1:1:181:GLN:N	2.22	0.73
1:1:272:TYR:HA	1:1:291:PHE:O	1.88	0.73
1:2:135:LYS:HD2	1:2:135:LYS:O	1.89	0.73
1:2:311:ASP:O	1:2:313:GLU:N	2.21	0.73
1:3:7:GLY:O	1:3:8:PHE:HB3	1.88	0.73
1:3:105:SER:O	1:3:106:ALA:C	2.31	0.73
1:3:129:CYS:CA	1:3:132:ASN:ND2	2.51	0.73
1:3:262:SER:O	1:3:267:GLN:HA	1.89	0.73
1:4:248:GLU:HG2	1:4:302:THR:HG22	1.69	0.73
1:1:127:PHE:CA	1:1:132:ASN:HB2	2.18	0.72
1:1:161:HIS:CG	1:1:162:GLU:N	2.52	0.72
1:1:276:ASP:CG	1:1:277:VAL:HG22	2.14	0.72
1:1:292:ASP:OD2	1:1:295:ALA:CB	2.35	0.72
1:2:266:LEU:CD2	1:2:270:LEU:HD12	2.19	0.72
1:4:75:GLU:HB2	2:4:347:HOH:O	1.89	0.72
1:4:138:LYS:H	1:4:138:LYS:CD	2.00	0.72
1:4:190:LYS:HD2	2:4:367:HOH:O	1.87	0.72
1:4:227:MET:HE1	1:4:229:PHE:CZ	2.24	0.72
1:4:288:SER:HB2	1:4:319:ARG:NH1	2.03	0.72
1:2:284:GLY:HA2	1:2:314:PHE:CE1	2.24	0.72
1:3:81:ILE:HD12	1:3:83:TRP:CE2	2.24	0.72
1:3:294:LYS:O	1:3:297:ILE:CD1	2.37	0.72
1:1:145:ASN:HB2	1:1:323:LEU:HD21	1.70	0.72
1:3:126:MET:HE3	1:3:212:ALA:HB2	1.68	0.72
1:4:44:LYS:HG3	1:4:56:VAL:CG2	2.12	0.72
1:2:196:ARG:HG2	1:2:196:ARG:HH11	1.52	0.72
1:2:266:LEU:HD23	1:2:270:LEU:CD1	2.20	0.72
1:3:81:ILE:HD13	1:3:82:PRO:CD	2.18	0.72
1:3:220:LEU:HB3	1:3:223:LYS:HG2	1.71	0.72
1:4:113:LYS:CB	1:4:114:LYS:CE	2.67	0.72
1:4:294:LYS:H	1:4:297:ILE:HG21	1.54	0.72
1:4:297:ILE:C	1:4:297:ILE:CD1	2.62	0.72
1:1:276:ASP:O	1:1:278:VAL:CG1	2.28	0.72
1:3:150:THR:HG22	1:3:151:ASN:N	2.04	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:200:GLN:OE1	1:4:48:THR:CG2	2.38	0.72
1:4:173:THR:CG2	1:4:228:ALA:HB2	2.19	0.72
1:2:283:ILE:O	1:2:284:GLY:C	2.33	0.72
1:3:101:ILE:HG21	2:3:380:HOH:O	1.89	0.72
1:4:188:SER:C	1:4:190:LYS:N	2.44	0.72
1:1:51:VAL:O	1:1:52:PHE:HB2	1.89	0.72
1:1:65:VAL:CG1	1:1:70:ILE:HD13	2.19	0.72
1:1:277:VAL:HG21	1:3:41:TYR:CZ	2.25	0.72
1:2:19:ALA:HA	1:2:24:ALA:HB3	1.72	0.72
1:2:76:MET:O	1:2:77:LYS:CD	2.37	0.72
1:1:193:ARG:CD	1:4:277:VAL:HA	2.20	0.72
1:1:295:ALA:N	1:1:297:ILE:HD12	2.04	0.72
1:2:95:THR:HG22	1:2:97:VAL:HG23	1.71	0.72
1:2:251:TYR:CE1	1:2:255:LYS:HD3	2.23	0.72
1:2:296:GLY:H	1:2:297:ILE:HD13	1.55	0.72
1:4:127:PHE:HB3	1:4:132:ASN:HB2	1.71	0.72
1:4:200:GLN:O	2:4:448:HOH:O	2.07	0.72
1:1:11:ILE:H	1:1:11:ILE:CD1	2.03	0.72
1:3:239:VAL:HG12	1:3:310:TYR:HE1	1.55	0.72
1:1:36:LEU:HD11	1:1:62:ALA:C	2.14	0.71
1:1:71:THR:C	1:1:72:VAL:CG1	2.62	0.71
1:2:11:ILE:HG22	1:2:15:VAL:HG21	1.71	0.71
1:2:126:MET:HB3	1:2:215:LYS:HD2	1.72	0.71
1:2:132:ASN:HD21	1:2:133:LEU:HD21	1.55	0.71
1:2:244:ARG:CD	1:3:244:ARG:NH1	2.53	0.71
1:2:250:SER:O	1:2:251:TYR:C	2.33	0.71
1:4:118:SER:O	1:4:118:SER:OG	2.08	0.71
1:1:273:THR:CG2	1:1:290:ILE:HD11	2.20	0.71
1:3:78:PRO:CG	1:3:98:PHE:CE2	2.70	0.71
1:4:78:PRO:C	1:4:80:ASN:N	2.47	0.71
1:4:101:ILE:HG23	1:4:142:VAL:HG11	1.71	0.71
1:2:225:THR:CG2	1:3:298:GLN:CD	2.62	0.71
1:2:177:VAL:HG13	1:2:232:PRO:O	1.91	0.71
1:3:161:HIS:O	1:3:163:ASN:N	2.24	0.71
1:4:164:PHE:O	1:4:165:GLU:CB	2.38	0.71
1:1:319:ARG:O	1:1:322:ASP:N	2.23	0.71
1:2:145:ASN:O	1:2:146:ALA:O	2.08	0.71
1:2:189:ALA:O	1:2:190:LYS:NZ	2.22	0.71
1:2:244:ARG:NH1	1:3:244:ARG:HG3	2.04	0.71
1:4:138:LYS:CE	1:4:330:VAL:CG1	2.69	0.71
1:1:280:SER:O	1:1:281:ASP:O	2.08	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:235:ASP:O	1:2:235:ASP:OD1	2.09	0.71
1:1:167:VAL:CG2	1:1:244:ARG:HG2	2.20	0.71
1:1:277:VAL:CA	1:4:193:ARG:HG3	2.15	0.71
1:1:309:TRP:CD1	1:1:309:TRP:H	2.08	0.71
1:3:167:VAL:CG1	1:3:245:LEU:O	2.38	0.71
1:4:142:VAL:HG22	1:4:142:VAL:O	1.91	0.71
1:4:282:PHE:CE1	1:4:290:ILE:HD13	2.26	0.71
1:1:265:PRO:HG2	2:1:442:HOH:O	1.90	0.71
1:3:117:ILE:C	1:3:119:ALA:H	1.97	0.71
1:3:220:LEU:O	1:3:221:ASP:C	2.33	0.71
1:4:8:PHE:CZ	1:4:39:MET:HB2	2.25	0.71
1:4:105:SER:O	1:4:108:PHE:CD1	2.43	0.71
1:4:211:LYS:HA	1:4:211:LYS:HZ3	1.54	0.71
1:4:273:THR:N	1:4:291:PHE:O	2.20	0.71
1:1:26:VAL:O	1:1:27:VAL:HB	1.90	0.71
1:1:320:VAL:O	1:1:324:LEU:HB2	1.91	0.71
1:2:131:VAL:HG12	1:2:158:LYS:HZ1	1.51	0.71
1:2:269:PHE:O	1:2:288:SER:CB	2.39	0.71
1:2:270:LEU:HD23	1:2:271:GLY:H	1.54	0.71
1:4:78:PRO:HG3	1:4:98:PHE:HE2	1.54	0.71
1:4:78:PRO:CD	1:4:98:PHE:CE2	2.74	0.71
1:1:2:LYS:CE	1:1:87:GLY:O	2.38	0.70
1:1:138:LYS:CD	1:1:138:LYS:H	2.04	0.70
1:2:232:PRO:CG	1:3:232:PRO:HB2	2.20	0.70
1:2:244:ARG:HG3	1:3:244:ARG:NH2	2.06	0.70
1:4:53:LYS:HD2	1:4:53:LYS:C	2.16	0.70
1:4:146:ALA:CB	1:4:150:THR:HG21	2.21	0.70
1:3:14:LEU:O	1:3:18:ALA:N	2.24	0.70
1:3:196:ARG:HD2	1:4:47:SER:OG	1.89	0.70
1:1:2:LYS:HB2	1:1:89:GLU:HB2	1.73	0.70
1:2:30:ASN:OD1	1:2:81:ILE:CG1	2.35	0.70
1:2:108:PHE:O	1:2:109:LYS:C	2.33	0.70
1:3:239:VAL:HG12	1:3:310:TYR:CE1	2.26	0.70
1:4:131:VAL:HG21	1:4:216:VAL:HG22	1.74	0.70
1:1:44:LYS:HD2	1:1:56:VAL:CG1	2.21	0.70
1:2:125:PRO:HD2	1:2:143:VAL:HA	1.73	0.70
1:2:161:HIS:HB2	1:2:166:ILE:HD12	1.71	0.70
1:3:71:THR:CG2	1:3:73:PHE:CE1	2.75	0.70
1:4:26:VAL:O	1:4:27:VAL:CG1	2.38	0.70
1:4:127:PHE:CE1	1:4:140:MET:HE1	2.26	0.70
1:4:137:SER:HB3	1:4:138:LYS:NZ	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:95:THR:HA	2:1:436:HOH:O	1.90	0.70
1:1:108:PHE:O	1:1:111:GLY:N	2.25	0.70
1:1:261:ALA:O	1:1:263:GLU:N	2.24	0.70
1:2:220:LEU:HA	1:2:223:LYS:HZ2	1.55	0.70
1:4:232:PRO:O	1:4:233:THR:C	2.32	0.70
1:1:253:ASP:C	1:1:255:LYS:N	2.45	0.70
1:2:156:VAL:HG22	1:2:258:MET:CE	2.22	0.70
1:2:211:LYS:HA	1:2:211:LYS:NZ	2.07	0.70
1:2:301:LYS:O	1:2:302:THR:HG23	1.90	0.70
1:3:51:VAL:O	1:3:52:PHE:HB2	1.90	0.70
1:3:94:SER:O	1:3:96:GLY:N	2.24	0.70
1:4:137:SER:HA	1:4:138:LYS:HE3	1.72	0.70
1:4:277:VAL:O	1:4:278:VAL:C	2.35	0.70
1:1:3:ILE:O	1:1:27:VAL:HG23	1.91	0.70
1:2:4:GLY:N	1:2:27:VAL:CG2	2.55	0.70
1:2:81:ILE:HD12	1:2:83:TRP:CZ2	2.26	0.70
1:2:159:VAL:O	1:2:163:ASN:HB2	1.90	0.70
1:3:37:GLU:HA	1:3:40:VAL:CG1	2.21	0.70
1:1:1:SER:CB	1:1:25:GLN:HB2	2.22	0.70
1:1:75:GLU:O	2:1:438:HOH:O	2.09	0.70
1:2:94:SER:O	1:2:95:THR:C	2.34	0.70
1:2:298:GLN:NE2	1:3:225:THR:CG2	2.54	0.70
1:3:286:ASN:OD1	1:3:318:GLN:NE2	2.25	0.70
1:3:322:ASP:O	1:3:323:LEU:C	2.34	0.70
1:4:1:SER:HB3	1:4:25:GLN:NE2	2.00	0.70
1:4:76:MET:O	1:4:77:LYS:CD	2.40	0.70
1:1:71:THR:HG21	1:1:73:PHE:CD1	2.26	0.70
1:1:296:GLY:CA	1:4:227:MET:HE3	2.22	0.70
1:2:54:GLY:CA	1:2:66:ASP:OD1	2.39	0.70
1:3:105:SER:O	1:3:108:PHE:HD1	1.74	0.70
1:3:232:PRO:O	1:3:233:THR:O	2.08	0.70
1:1:47:SER:OG	1:2:185:ASP:OD2	2.10	0.70
1:2:156:VAL:HG22	1:2:258:MET:HE2	1.74	0.70
1:2:168:GLU:OE2	1:2:244:ARG:CZ	2.40	0.70
1:2:173:THR:O	1:2:228:ALA:HA	1.92	0.70
1:4:270:LEU:HD23	1:4:271:GLY:H	1.53	0.70
1:4:318:GLN:OE1	1:4:318:GLN:HA	1.90	0.70
1:1:127:PHE:HB3	1:1:132:ASN:CG	2.17	0.69
1:1:171:MET:SD	1:1:209:ALA:CB	2.78	0.69
1:2:128:VAL:H	1:2:132:ASN:CB	2.05	0.69
1:4:150:THR:HG21	1:4:212:ALA:HB3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:145:ASN:OD1	1:1:323:LEU:HD23	1.92	0.69
1:1:203:ILE:O	1:1:204:PRO:O	2.10	0.69
1:2:235:ASP:OD2	1:2:311:ASP:OD1	2.10	0.69
1:2:329:LYS:HZ2	1:2:329:LYS:HB3	1.56	0.69
1:3:8:PHE:CD1	1:3:29:VAL:CG1	2.74	0.69
1:1:276:ASP:O	1:1:277:VAL:C	2.35	0.69
1:1:297:ILE:HD13	1:1:297:ILE:O	1.91	0.69
1:2:244:ARG:CG	1:3:244:ARG:NH2	2.55	0.69
1:1:298:GLN:OE1	1:4:225:THR:HG23	1.92	0.69
1:2:127:PHE:HD1	1:2:143:VAL:HG23	1.57	0.69
1:2:294:LYS:C	1:2:297:ILE:HD12	2.16	0.69
1:1:44:LYS:O	1:1:51:VAL:HA	1.92	0.69
1:1:272:TYR:CE2	1:1:293:ALA:HB2	2.27	0.69
1:1:325:LYS:O	1:1:327:MET:N	2.25	0.69
1:2:113:LYS:HB3	1:2:114:LYS:HG2	1.73	0.69
1:2:296:GLY:N	1:2:297:ILE:CD1	2.55	0.69
1:3:78:PRO:C	1:3:80:ASN:H	2.01	0.69
1:4:204:PRO:HG3	1:4:229:PHE:HE2	1.57	0.69
1:1:119:ALA:HB1	1:1:120:PRO:HD3	1.72	0.69
1:2:95:THR:HG22	1:2:97:VAL:N	2.08	0.69
1:3:8:PHE:CD2	1:3:8:PHE:C	2.70	0.69
1:1:97:VAL:O	1:1:98:PHE:CG	2.45	0.69
1:2:74:ASN:HA	2:2:407:HOH:O	1.92	0.69
1:2:126:MET:CB	1:2:215:LYS:HZ2	2.06	0.69
1:2:216:VAL:HG12	1:2:217:ILE:HG22	1.75	0.69
1:3:19:ALA:HB1	1:3:24:ALA:HB3	1.73	0.69
1:3:276:ASP:CG	1:3:277:VAL:N	2.47	0.69
1:1:17:ARG:HB3	1:1:43:PHE:CE2	2.28	0.69
1:1:54:GLY:CA	1:1:66:ASP:OD2	2.40	0.69
1:1:319:ARG:HA	1:1:322:ASP:OD2	1.93	0.69
1:2:244:ARG:CZ	1:3:244:ARG:HG3	2.22	0.69
1:2:277:VAL:CG2	1:4:41:TYR:HE1	1.97	0.69
1:4:44:LYS:HG2	1:4:56:VAL:HG11	1.75	0.69
1:4:301:LYS:HZ3	1:4:301:LYS:HB2	1.58	0.69
1:2:84:SER:O	1:2:86:ALA:HB3	1.93	0.69
1:3:212:ALA:O	1:3:216:VAL:N	2.26	0.69
1:3:255:LYS:HB3	1:3:255:LYS:NZ	2.08	0.69
1:3:275:ASP:C	1:3:276:ASP:OD2	2.35	0.69
1:3:296:GLY:N	1:3:297:ILE:CD1	2.56	0.69
1:3:296:GLY:N	1:3:297:ILE:HD12	2.07	0.69
1:4:211:LYS:HE2	1:4:211:LYS:CA	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:113:LYS:HB3	1:2:114:LYS:CG	2.23	0.68
1:2:255:LYS:CE	1:2:293:ALA:HB1	2.19	0.68
1:3:9:GLY:O	1:3:13:ARG:HB2	1.93	0.68
1:4:325:LYS:O	1:4:327:MET:N	2.25	0.68
1:1:225:THR:CB	1:4:298:GLN:OE1	2.40	0.68
1:2:284:GLY:HA2	1:2:314:PHE:HE1	1.58	0.68
1:3:8:PHE:CE1	1:3:29:VAL:HG11	2.29	0.68
1:4:118:SER:C	1:4:316:TYR:HH	1.99	0.68
1:1:9:GLY:HA2	1:1:13:ARG:HH21	1.56	0.68
1:1:13:ARG:O	1:1:16:LEU:N	2.25	0.68
1:1:193:ARG:NH1	1:4:295:ALA:CB	2.53	0.68
1:1:266:LEU:O	1:1:267:GLN:C	2.37	0.68
1:1:292:ASP:OD1	1:1:292:ASP:O	2.10	0.68
1:1:295:ALA:HB1	1:4:193:ARG:HH12	1.56	0.68
1:3:27:VAL:O	1:3:28:ALA:HB2	1.92	0.68
1:1:71:THR:C	1:1:72:VAL:HG12	2.18	0.68
1:2:34:ILE:HD11	1:2:39:MET:HG3	1.75	0.68
1:4:131:VAL:O	1:4:132:ASN:C	2.36	0.68
1:4:136:TYR:C	1:4:137:SER:OG	2.35	0.68
1:1:105:SER:O	1:1:106:ALA:C	2.34	0.68
1:2:6:ASN:HD22	1:2:93:GLU:CD	2.01	0.68
1:2:105:SER:O	1:2:106:ALA:C	2.36	0.68
1:2:277:VAL:O	1:2:278:VAL:C	2.33	0.68
1:3:115:VAL:HB	1:3:142:VAL:HG23	1.75	0.68
1:3:134:GLU:C	1:3:136:TYR:N	2.52	0.68
1:1:129:CYS:O	1:1:133:LEU:CG	2.42	0.68
1:4:73:PHE:HB2	1:4:81:ILE:HD11	1.75	0.68
1:1:26:VAL:HG11	1:1:70:ILE:HG21	1.76	0.68
1:1:71:THR:HG22	1:1:72:VAL:H	1.55	0.68
1:1:213:VAL:HA	1:1:216:VAL:HG12	1.75	0.68
1:2:11:ILE:HG22	1:2:15:VAL:HG23	1.76	0.68
1:2:124:ALA:C	1:2:125:PRO:O	2.26	0.68
1:2:149:THR:O	1:2:152:CYS:HB3	1.93	0.68
1:2:216:VAL:HG13	1:2:217:ILE:HG22	1.74	0.68
1:2:296:GLY:N	1:2:297:ILE:HD12	2.09	0.68
1:4:53:LYS:HE2	1:4:53:LYS:N	2.07	0.68
1:4:236:VAL:O	1:4:237:SER:OG	2.11	0.68
1:1:225:THR:HG21	1:4:298:GLN:NE2	2.09	0.68
1:2:6:ASN:CB	1:2:30:ASN:HD21	2.07	0.68
1:2:193:ARG:HH12	1:3:295:ALA:HB1	1.59	0.68
1:3:8:PHE:HD2	1:3:8:PHE:C	2.01	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:2:LYS:NZ	1:4:2:LYS:HB3	1.99	0.68
1:4:236:VAL:HG12	1:4:237:SER:H	1.59	0.68
1:2:31:ASP:O	1:2:34:ILE:HG23	1.93	0.68
1:4:34:ILE:HG23	1:4:34:ILE:O	1.94	0.68
1:4:131:VAL:HG12	1:4:158:LYS:HZ3	1.58	0.68
1:4:209:ALA:O	1:4:213:VAL:HB	1.94	0.68
1:1:11:ILE:HD12	1:1:11:ILE:N	2.09	0.68
1:2:277:VAL:HB	1:4:41:TYR:OH	1.94	0.68
1:3:156:VAL:CG2	1:3:258:MET:HE2	2.24	0.68
1:3:318:GLN:OE1	1:3:318:GLN:HA	1.93	0.68
1:1:41:TYR:CZ	1:3:277:VAL:HG21	2.28	0.67
1:1:131:VAL:O	1:1:132:ASN:C	2.36	0.67
1:3:113:LYS:HB3	1:3:114:LYS:CE	2.24	0.67
1:4:51:VAL:CA	2:4:340:HOH:O	2.38	0.67
1:4:127:PHE:HD1	1:4:143:VAL:CG2	2.07	0.67
1:2:3:ILE:HD13	1:2:324:LEU:HD12	1.75	0.67
1:2:168:GLU:OE2	1:2:244:ARG:NE	2.27	0.67
1:3:51:VAL:C	2:3:370:HOH:O	2.21	0.67
1:3:81:ILE:HG23	1:3:83:TRP:NE1	2.08	0.67
1:3:173:THR:HG22	1:3:227:MET:O	1.93	0.67
1:3:183:THR:HG22	2:3:383:HOH:O	1.93	0.67
1:2:104:ALA:O	1:2:105:SER:C	2.37	0.67
1:2:112:ALA:O	1:2:113:LYS:CB	2.41	0.67
1:2:244:ARG:HD3	1:3:244:ARG:NH1	2.09	0.67
1:3:243:VAL:CG2	1:3:304:VAL:HG12	2.19	0.67
1:4:273:THR:CG2	1:4:290:ILE:HD11	2.24	0.67
1:1:129:CYS:HG	1:1:269:PHE:HE1	1.36	0.67
1:1:251:TYR:O	1:1:254:ILE:HB	1.95	0.67
1:2:83:TRP:C	1:2:86:ALA:HB3	2.19	0.67
1:2:158:LYS:O	1:2:162:GLU:HG2	1.94	0.67
1:3:127:PHE:CE2	1:3:136:TYR:HB2	2.29	0.67
1:4:17:ARG:NE	2:4:339:HOH:O	2.23	0.67
1:4:52:PHE:C	1:4:53:LYS:NZ	2.52	0.67
1:1:44:LYS:HD2	1:1:56:VAL:HG13	1.77	0.67
1:1:227:MET:HE3	1:4:296:GLY:CA	2.25	0.67
1:1:297:ILE:H	1:1:297:ILE:HD12	1.55	0.67
1:1:314:PHE:HB2	1:1:317:SER:HB2	1.74	0.67
1:2:132:ASN:CG	1:2:133:LEU:H	2.03	0.67
1:3:32:PRO:HA	1:3:74:ASN:CG	2.19	0.67
1:3:81:ILE:CG2	1:3:83:TRP:NE1	2.57	0.67
1:3:211:LYS:HA	1:3:211:LYS:NZ	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:105:SER:O	1:4:107:HIS:N	2.27	0.67
1:4:250:SER:O	1:4:251:TYR:C	2.38	0.67
1:4:329:LYS:NZ	1:4:330:VAL:N	2.42	0.67
1:1:138:LYS:H	1:1:138:LYS:HD3	1.58	0.67
1:1:177:VAL:HA	1:1:181:GLN:OE1	1.94	0.67
1:2:161:HIS:O	1:2:162:GLU:C	2.38	0.67
1:2:236:VAL:O	1:2:312:ASN:OD1	2.13	0.67
1:3:273:THR:O	1:3:293:ALA:HB3	1.95	0.67
1:4:135:LYS:HD2	1:4:135:LYS:O	1.94	0.67
1:1:78:PRO:HD3	1:1:98:PHE:CZ	2.29	0.67
1:1:178:THR:OG1	1:1:180:THR:N	2.28	0.67
1:2:220:LEU:O	1:2:223:LYS:HG2	1.95	0.67
1:3:189:ALA:C	1:3:190:LYS:HE2	2.20	0.67
1:4:292:ASP:CG	1:4:295:ALA:HB3	2.19	0.67
1:1:59:GLU:HB3	1:1:64:VAL:CG1	2.24	0.67
1:1:71:THR:HG21	1:1:73:PHE:CZ	2.29	0.67
1:2:74:ASN:HB2	2:2:395:HOH:O	1.95	0.67
1:2:185:ASP:OD2	1:2:196:ARG:HD2	1.95	0.67
1:4:54:GLY:O	1:4:56:VAL:HG12	1.93	0.67
1:4:200:GLN:C	1:4:201:ASN:HD22	2.03	0.67
1:2:93:GLU:OE2	1:2:98:PHE:HB2	1.95	0.67
1:2:126:MET:HB2	1:2:215:LYS:NZ	2.10	0.67
1:2:181:GLN:HE22	1:2:230:ARG:HB2	1.60	0.67
1:3:251:TYR:O	1:3:254:ILE:CB	2.43	0.67
1:4:237:SER:OG	1:4:312:ASN:OD1	2.12	0.67
1:1:128:VAL:C	1:1:132:ASN:HB3	2.17	0.67
1:1:129:CYS:O	1:1:133:LEU:HG	1.94	0.67
1:2:64:VAL:O	1:2:64:VAL:CG2	2.42	0.67
1:2:252:ASP:O	1:2:255:LYS:N	2.25	0.67
1:3:32:PRO:HG3	1:3:75:GLU:O	1.94	0.67
1:4:113:LYS:CD	1:4:114:LYS:HZ2	1.91	0.67
1:1:101:ILE:O	1:1:105:SER:CB	2.43	0.66
1:1:188:SER:C	1:1:190:LYS:N	2.51	0.66
1:2:178:THR:OG1	1:2:180:THR:HG23	1.94	0.66
1:2:180:THR:OG1	1:2:181:GLN:N	2.27	0.66
1:4:266:LEU:O	1:4:267:GLN:C	2.38	0.66
1:4:276:ASP:O	1:4:278:VAL:N	2.28	0.66
1:1:2:LYS:HE2	1:1:87:GLY:O	1.95	0.66
1:1:41:TYR:OH	1:2:196:ARG:NH1	2.26	0.66
1:2:252:ASP:C	1:2:252:ASP:OD1	2.38	0.66
1:4:3:ILE:C	1:4:27:VAL:HG23	2.20	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:131:VAL:CG1	1:1:158:LYS:HE2	2.24	0.66
1:1:287:ARG:O	1:1:319:ARG:NH1	2.27	0.66
1:2:41:TYR:OH	1:4:277:VAL:CG1	2.42	0.66
1:3:252:ASP:O	1:3:253:ASP:C	2.39	0.66
1:3:297:ILE:HA	1:3:305:LYS:O	1.94	0.66
1:4:150:THR:HG21	1:4:212:ALA:CB	2.25	0.66
1:4:274:GLU:C	1:4:276:ASP:H	2.01	0.66
1:2:33:PHE:CZ	1:2:76:MET:SD	2.88	0.66
1:2:232:PRO:HB2	1:3:232:PRO:HG2	1.77	0.66
1:2:250:SER:O	1:2:253:ASP:N	2.29	0.66
1:2:328:GLN:CA	1:2:328:GLN:NE2	2.58	0.66
1:3:164:PHE:CE2	1:3:249:CYS:CB	2.78	0.66
1:4:156:VAL:HG21	1:4:308:SER:OG	1.95	0.66
1:4:239:VAL:HG13	1:4:310:TYR:HE1	1.60	0.66
1:1:1:SER:C	1:1:25:GLN:HG2	2.19	0.66
1:1:14:LEU:O	1:1:18:ALA:HB2	1.95	0.66
1:1:250:SER:C	1:1:252:ASP:N	2.47	0.66
1:3:2:LYS:NZ	1:3:2:LYS:HB3	2.10	0.66
1:3:276:ASP:CG	1:3:277:VAL:H	1.88	0.66
1:4:39:MET:CE	1:4:72:VAL:HB	2.26	0.66
1:4:113:LYS:CB	1:4:114:LYS:HD2	2.18	0.66
1:1:53:LYS:HE2	1:1:53:LYS:N	2.10	0.66
1:2:59:GLU:O	1:2:61:GLY:N	2.28	0.66
1:2:113:LYS:HB3	1:2:114:LYS:HD2	1.76	0.66
1:2:281:ASP:O	1:2:283:ILE:HB	1.94	0.66
1:3:173:THR:CG2	1:3:228:ALA:HB2	2.25	0.66
1:3:252:ASP:HA	1:3:255:LYS:CG	2.25	0.66
1:4:292:ASP:OD1	1:4:307:VAL:HG11	1.95	0.66
1:1:149:THR:HG23	1:1:310:TYR:OH	1.94	0.66
1:3:3:ILE:CD1	1:3:24:ALA:HB1	2.26	0.66
1:3:287:ARG:O	1:3:288:SER:HB2	1.96	0.66
1:4:66:ASP:C	1:4:68:LYS:HD3	2.20	0.66
1:4:109:LYS:O	1:4:110:GLY:C	2.39	0.66
1:1:52:PHE:N	2:1:430:HOH:O	2.28	0.66
1:2:3:ILE:O	1:2:27:VAL:HG23	1.96	0.66
1:2:295:ALA:HB2	1:3:193:ARG:NH2	2.10	0.66
1:2:332:SER:O	1:2:333:ALA:HB2	1.96	0.66
1:3:1:SER:HB3	1:3:25:GLN:NE2	2.11	0.66
1:4:30:ASN:OD1	1:4:81:ILE:CG1	2.44	0.66
1:4:133:LEU:O	1:4:136:TYR:HB3	1.95	0.66
1:1:128:VAL:HG23	1:1:216:VAL:HG21	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:66:ASP:HB2	1:2:68:LYS:HE2	1.77	0.66
1:3:101:ILE:HG23	2:3:381:HOH:O	1.96	0.66
1:3:153:LEU:O	1:3:154:ALA:C	2.39	0.66
1:4:8:PHE:HZ	1:4:39:MET:CB	2.08	0.66
1:4:127:PHE:HD1	1:4:143:VAL:HG23	1.60	0.66
1:2:16:LEU:C	1:2:18:ALA:H	2.02	0.66
1:2:55:GLU:OE2	1:2:55:GLU:HA	1.94	0.66
1:2:127:PHE:CD1	1:2:143:VAL:HG23	2.30	0.66
1:3:216:VAL:HG13	1:3:217:ILE:N	2.11	0.66
1:4:325:LYS:O	1:4:326:HIS:C	2.39	0.66
1:1:59:GLU:O	1:1:61:GLY:N	2.29	0.65
1:1:188:SER:O	1:1:189:ALA:C	2.39	0.65
1:3:128:VAL:N	1:3:132:ASN:HB3	2.10	0.65
1:3:173:THR:HG23	1:3:228:ALA:CB	2.25	0.65
1:4:34:ILE:HD11	1:4:42:MET:SD	2.36	0.65
1:3:32:PRO:HG3	1:3:75:GLU:C	2.22	0.65
1:3:277:VAL:HG23	1:3:278:VAL:N	2.10	0.65
1:4:66:ASP:O	1:4:68:LYS:CD	2.45	0.65
1:4:295:ALA:N	1:4:297:ILE:HG23	2.10	0.65
1:4:311:ASP:O	1:4:312:ASN:C	2.40	0.65
1:1:277:VAL:HG11	1:3:41:TYR:CZ	2.31	0.65
1:1:285:ASP:OD2	1:1:285:ASP:C	2.38	0.65
1:2:181:GLN:HG2	1:2:198:ALA:HB2	1.77	0.65
1:3:328:GLN:O	1:3:329:LYS:O	2.14	0.65
1:4:53:LYS:C	1:4:53:LYS:CD	2.69	0.65
1:4:170:LEU:CD2	1:4:225:THR:CG2	2.74	0.65
1:1:132:ASN:HD21	1:1:133:LEU:CD2	2.05	0.65
1:2:185:ASP:HA	1:2:196:ARG:HA	1.78	0.65
1:4:8:PHE:HD2	1:4:8:PHE:C	2.04	0.65
1:4:145:ASN:C	1:4:145:ASN:HD22	2.04	0.65
1:1:277:VAL:HG23	1:1:278:VAL:N	2.07	0.65
1:1:303:PHE:HE2	1:4:303:PHE:CE2	2.14	0.65
1:1:319:ARG:HG2	1:1:319:ARG:HH11	1.61	0.65
1:2:213:VAL:O	1:2:216:VAL:HG12	1.96	0.65
1:2:4:GLY:HA2	1:2:27:VAL:CG2	2.26	0.65
1:2:65:VAL:C	1:2:66:ASP:OD2	2.39	0.65
1:2:155:PRO:O	1:2:159:VAL:HG23	1.96	0.65
1:3:69:LYS:O	1:3:69:LYS:HG2	1.94	0.65
1:3:84:SER:OG	1:3:111:GLY:CA	2.43	0.65
1:4:44:LYS:CE	1:4:45:TYR:CE2	2.79	0.65
1:4:83:TRP:HA	1:4:86:ALA:CB	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:108:PHE:O	1:4:111:GLY:N	2.29	0.65
1:4:224:LEU:HD21	1:4:241:LEU:HD11	1.79	0.65
1:1:76:MET:O	1:1:77:LYS:HB2	1.96	0.65
1:1:142:VAL:O	1:1:142:VAL:HG13	1.95	0.65
1:1:309:TRP:CD1	1:1:309:TRP:N	2.63	0.65
1:2:16:LEU:C	1:2:18:ALA:N	2.53	0.65
1:2:292:ASP:OD1	1:2:295:ALA:HB3	1.97	0.65
1:3:243:VAL:HG22	1:3:304:VAL:CG1	2.24	0.65
1:4:33:PHE:HZ	1:4:76:MET:SD	2.19	0.65
1:4:130:GLY:HA3	1:4:158:LYS:NZ	2.12	0.65
1:1:106:ALA:O	1:1:107:HIS:C	2.39	0.65
1:1:164:PHE:O	1:1:165:GLU:CB	2.46	0.65
1:1:189:ALA:O	1:1:190:LYS:HD3	1.97	0.65
1:3:188:SER:O	1:3:190:LYS:N	2.30	0.65
1:3:188:SER:HB2	1:3:195:GLY:HA3	1.79	0.65
1:1:17:ARG:CG	1:1:43:PHE:CE2	2.67	0.64
1:1:101:ILE:CG1	1:1:142:VAL:HG11	2.27	0.64
1:1:129:CYS:O	1:1:132:ASN:ND2	2.28	0.64
1:3:175:HIS:CB	1:3:230:ARG:HH21	2.10	0.64
1:3:252:ASP:O	1:3:255:LYS:CG	2.45	0.64
1:4:82:PRO:HB2	1:4:85:LYS:O	1.96	0.64
1:4:276:ASP:CG	1:4:277:VAL:H	2.01	0.64
1:2:193:ARG:CB	1:3:277:VAL:HG12	2.25	0.64
1:3:46:ASP:HB3	1:3:50:GLY:N	2.05	0.64
1:3:66:ASP:HB2	1:3:68:LYS:HD3	1.77	0.64
1:4:128:VAL:O	1:4:132:ASN:HB3	1.97	0.64
1:2:53:LYS:NZ	1:2:53:LYS:HB3	2.12	0.64
1:2:204:PRO:HA	1:2:228:ALA:O	1.97	0.64
1:3:50:GLY:C	1:3:51:VAL:CG2	2.70	0.64
1:4:307:VAL:O	1:4:307:VAL:CG1	2.44	0.64
1:1:244:ARG:CZ	1:4:244:ARG:CZ	2.76	0.64
1:3:127:PHE:CG	1:3:132:ASN:HB2	2.33	0.64
1:3:131:VAL:N	1:3:158:LYS:NZ	2.45	0.64
1:4:328:GLN:O	1:4:332:SER:N	2.29	0.64
1:3:146:ALA:CB	1:3:150:THR:HG21	2.27	0.64
1:4:8:PHE:CD2	1:4:8:PHE:C	2.75	0.64
1:4:185:ASP:OD1	1:4:185:ASP:N	2.30	0.64
1:1:90:TYR:CZ	1:1:328:GLN:CD	2.76	0.64
1:1:325:LYS:O	1:1:328:GLN:N	2.30	0.64
1:3:270:LEU:C	1:3:270:LEU:CD2	2.70	0.64
1:3:276:ASP:O	1:3:278:VAL:CG1	2.45	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:27:VAL:CG2	1:1:28:ALA:N	2.38	0.64
1:1:153:LEU:O	1:1:154:ALA:C	2.41	0.64
1:3:46:ASP:CB	1:3:50:GLY:HA2	2.28	0.64
1:3:127:PHE:HB2	1:3:323:LEU:HD21	1.78	0.64
1:4:4:GLY:CA	1:4:27:VAL:HG23	2.28	0.64
1:4:71:THR:HG21	1:4:73:PHE:CE1	2.31	0.64
1:4:217:ILE:HG12	1:4:220:LEU:HD22	1.80	0.64
1:1:294:LYS:C	1:1:297:ILE:HD12	2.23	0.64
1:3:196:ARG:CG	1:3:196:ARG:HH11	2.08	0.64
1:4:250:SER:O	1:4:252:ASP:N	2.31	0.64
1:2:117:ILE:HD12	1:2:144:SER:HB3	1.79	0.64
1:2:244:ARG:HH12	1:3:244:ARG:HG3	1.60	0.64
1:4:108:PHE:HA	1:4:112:ALA:HB3	1.79	0.64
1:4:146:ALA:HB1	1:4:150:THR:HG21	1.79	0.64
1:2:173:THR:HG23	1:2:228:ALA:CB	2.28	0.64
1:3:14:LEU:O	1:3:18:ALA:CB	2.46	0.64
1:3:83:TRP:CA	1:3:86:ALA:HB3	2.28	0.64
1:3:127:PHE:CB	1:3:132:ASN:CB	2.57	0.64
1:3:168:GLU:HG2	1:3:244:ARG:HD2	1.79	0.64
1:3:175:HIS:CG	1:3:230:ARG:NH2	2.61	0.64
1:3:235:ASP:OD2	1:3:313:GLU:HB2	1.98	0.64
1:1:196:ARG:NH2	1:4:281:ASP:OD2	2.31	0.63
1:1:277:VAL:O	1:1:278:VAL:CG2	2.45	0.63
1:4:217:ILE:CD1	1:4:220:LEU:CD2	2.75	0.63
1:2:132:ASN:CG	1:2:133:LEU:N	2.55	0.63
1:2:236:VAL:O	1:2:237:SER:CB	2.28	0.63
1:3:2:LYS:HB3	1:3:2:LYS:HZ3	1.63	0.63
1:3:81:ILE:HD12	1:3:83:TRP:CD2	2.33	0.63
1:3:134:GLU:O	1:3:135:LYS:C	2.40	0.63
1:3:265:PRO:C	1:3:267:GLN:N	2.56	0.63
1:4:95:THR:CG2	1:4:97:VAL:HG23	2.28	0.63
1:4:283:ILE:O	1:4:284:GLY:O	2.17	0.63
1:1:121:SER:OG	1:1:124:ALA:HB3	1.97	0.63
1:1:129:CYS:HA	1:1:132:ASN:ND2	2.12	0.63
1:1:193:ARG:NE	1:4:277:VAL:CA	2.60	0.63
1:1:252:ASP:O	1:1:255:LYS:CB	2.46	0.63
1:2:14:LEU:HA	1:2:17:ARG:HB2	1.79	0.63
1:2:193:ARG:CD	1:3:277:VAL:HA	2.28	0.63
1:4:13:ARG:O	1:4:16:LEU:N	2.30	0.63
1:4:17:ARG:HG2	1:4:43:PHE:HE2	1.62	0.63
1:4:126:MET:HG3	1:4:146:ALA:HB2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:129:CYS:HB3	1:1:269:PHE:CE1	2.34	0.63
1:1:298:GLN:CD	1:4:225:THR:HG23	2.23	0.63
1:2:33:PHE:CZ	1:2:76:MET:CE	2.70	0.63
1:2:66:ASP:CB	1:2:68:LYS:HE2	2.28	0.63
1:3:127:PHE:CD2	1:3:132:ASN:HB2	2.33	0.63
1:4:7:GLY:O	1:4:8:PHE:HB3	1.98	0.63
1:4:52:PHE:O	1:4:53:LYS:NZ	2.27	0.63
1:1:65:VAL:HG11	1:1:70:ILE:HD13	1.79	0.63
1:1:85:LYS:HG3	1:1:85:LYS:O	1.99	0.63
1:1:150:THR:OG1	1:1:212:ALA:HB3	1.98	0.63
1:2:10:ARG:O	1:2:14:LEU:CD2	2.47	0.63
1:2:41:TYR:OH	1:4:277:VAL:HG21	1.98	0.63
1:3:6:ASN:CA	1:3:30:ASN:HD21	2.08	0.63
1:3:184:VAL:O	1:3:184:VAL:CG1	2.45	0.63
1:4:78:PRO:HD3	1:4:98:PHE:CE2	2.33	0.63
1:4:248:GLU:HG2	1:4:302:THR:CG2	2.28	0.63
1:1:126:MET:CB	1:1:215:LYS:HZ2	2.02	0.63
1:1:145:ASN:CB	1:1:323:LEU:HD23	2.28	0.63
1:2:131:VAL:HG12	1:2:158:LYS:HZ3	1.63	0.63
1:2:244:ARG:CG	1:3:244:ARG:NH1	2.58	0.63
1:3:98:PHE:HA	1:3:103:LYS:HB3	1.81	0.63
1:3:127:PHE:HD2	1:3:132:ASN:CA	2.12	0.63
1:3:134:GLU:C	1:3:136:TYR:H	2.06	0.63
1:4:127:PHE:CD1	1:4:143:VAL:HG23	2.32	0.63
1:3:276:ASP:OD1	1:3:277:VAL:CG2	2.47	0.63
1:4:239:VAL:CG1	1:4:310:TYR:CE1	2.79	0.63
1:1:9:GLY:HA2	1:1:13:ARG:NH2	2.14	0.63
1:1:126:MET:HE2	1:1:215:LYS:CD	2.29	0.63
1:2:117:ILE:HD11	1:2:142:VAL:HG22	1.81	0.63
1:2:131:VAL:HG12	1:2:158:LYS:CE	2.28	0.63
1:2:175:HIS:HA	1:2:237:SER:OG	1.99	0.63
1:2:272:TYR:HA	1:2:291:PHE:O	1.98	0.63
1:3:65:VAL:O	1:3:68:LYS:HG2	1.99	0.63
1:3:91:ILE:HD11	1:3:112:ALA:HB1	1.81	0.63
1:3:188:SER:O	1:3:189:ALA:C	2.41	0.63
1:4:55:GLU:O	1:4:66:ASP:N	2.30	0.63
1:1:54:GLY:HA2	1:1:66:ASP:OD1	1.99	0.63
1:1:294:LYS:O	1:1:297:ILE:HD11	1.99	0.63
1:2:26:VAL:HG23	1:2:27:VAL:N	2.12	0.63
1:3:180:THR:O	1:3:182:LYS:N	2.32	0.63
1:4:208:GLY:HA3	1:4:211:LYS:HG3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:239:VAL:HG12	1:4:310:TYR:HE1	1.60	0.63
1:1:250:SER:O	1:1:251:TYR:C	2.41	0.62
1:1:305:LYS:HB2	1:1:305:LYS:NZ	2.12	0.62
1:2:100:THR:O	1:2:103:LYS:N	2.32	0.62
1:3:81:ILE:HD12	1:3:83:TRP:CZ2	2.34	0.62
1:3:125:PRO:HG2	1:3:140:MET:HE2	1.80	0.62
1:4:57:LYS:HD2	1:4:58:MET:HE1	1.80	0.62
1:1:89:GLU:HB3	1:1:90:TYR:CD1	2.34	0.62
1:1:126:MET:CE	1:1:215:LYS:HZ2	2.12	0.62
1:1:161:HIS:CD2	1:1:162:GLU:H	2.15	0.62
1:1:277:VAL:O	1:1:278:VAL:C	2.42	0.62
1:1:329:LYS:HZ1	1:1:330:VAL:N	1.95	0.62
1:2:33:PHE:C	1:2:34:ILE:HG22	2.18	0.62
1:2:211:LYS:HA	1:2:211:LYS:HZ2	1.63	0.62
1:2:251:TYR:O	1:2:254:ILE:HB	1.98	0.62
1:2:277:VAL:HA	1:3:193:ARG:CG	2.29	0.62
1:3:188:SER:HB3	1:3:191:ASP:O	1.97	0.62
1:3:287:ARG:O	1:3:319:ARG:NH1	2.32	0.62
1:4:251:TYR:HB2	1:4:299:LEU:HB2	1.80	0.62
1:2:36:LEU:HD21	1:2:62:ALA:C	2.25	0.62
1:2:78:PRO:C	1:2:80:ASN:H	2.05	0.62
1:2:84:SER:O	1:2:86:ALA:N	2.32	0.62
1:1:90:TYR:CD1	1:1:90:TYR:N	2.68	0.62
1:1:153:LEU:HD21	1:1:241:LEU:CD2	2.30	0.62
1:1:322:ASP:O	1:1:323:LEU:C	2.41	0.62
1:4:6:ASN:OD1	1:4:30:ASN:ND2	2.32	0.62
1:2:4:GLY:CA	1:2:27:VAL:HG21	2.29	0.62
1:2:161:HIS:O	1:2:165:GLU:N	2.31	0.62
1:2:244:ARG:CZ	1:3:244:ARG:CZ	2.77	0.62
1:3:196:ARG:NH1	1:3:196:ARG:CG	2.42	0.62
1:3:279:SER:C	1:3:281:ASP:N	2.57	0.62
1:4:170:LEU:HD21	1:4:225:THR:CG2	2.30	0.62
1:4:204:PRO:HG3	1:4:229:PHE:CE2	2.32	0.62
1:1:71:THR:CG2	1:1:72:VAL:H	2.09	0.62
1:1:145:ASN:HB2	1:1:323:LEU:HD23	1.80	0.62
1:1:285:ASP:OD2	1:1:285:ASP:O	2.18	0.62
1:3:2:LYS:HG3	1:3:89:GLU:CG	2.27	0.62
1:3:25:GLN:C	1:3:26:VAL:O	2.38	0.62
1:3:84:SER:O	1:3:85:LYS:C	2.41	0.62
1:3:89:GLU:HB2	1:3:90:TYR:HD1	1.64	0.62
1:3:253:ASP:HB2	2:3:385:HOH:O	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:39:MET:HE3	1:4:72:VAL:HB	1.81	0.62
1:4:207:THR:OG1	1:4:208:GLY:N	2.20	0.62
1:4:261:ALA:O	1:4:262:SER:C	2.43	0.62
1:4:273:THR:O	1:4:293:ALA:N	2.29	0.62
1:2:32:PRO:C	1:2:33:PHE:CG	2.74	0.62
1:2:232:PRO:HB2	1:3:232:PRO:CG	2.30	0.62
1:3:71:THR:CG2	1:3:73:PHE:CZ	2.80	0.62
1:3:108:PHE:O	1:3:111:GLY:N	2.33	0.62
1:4:44:LYS:HB3	1:4:44:LYS:NZ	2.10	0.62
1:4:251:TYR:HB2	1:4:299:LEU:HB3	1.82	0.62
1:1:277:VAL:CA	1:4:193:ARG:CD	2.73	0.62
1:1:295:ALA:CB	1:4:193:ARG:NH1	2.63	0.62
1:2:273:THR:HB	1:2:290:ILE:HD11	1.82	0.62
1:3:52:PHE:C	1:3:53:LYS:HE2	2.25	0.62
1:4:11:ILE:H	1:4:11:ILE:HD12	1.59	0.62
1:4:52:PHE:CD1	1:4:53:LYS:CE	2.83	0.62
1:4:83:TRP:C	1:4:86:ALA:HB3	2.24	0.62
1:4:134:GLU:OE2	1:4:134:GLU:O	2.17	0.62
1:1:4:GLY:N	1:1:27:VAL:HG21	2.15	0.62
1:1:57:LYS:O	1:1:64:VAL:HG13	1.99	0.62
1:1:108:PHE:HA	1:1:112:ALA:HB3	1.81	0.62
1:1:127:PHE:HZ	1:1:140:MET:SD	2.22	0.62
1:1:144:SER:OG	1:1:145:ASN:N	2.25	0.62
1:1:181:GLN:O	1:2:183:THR:HG23	2.00	0.62
1:1:270:LEU:CD2	1:1:270:LEU:C	2.73	0.62
1:2:126:MET:HB2	1:2:215:LYS:HZ2	1.64	0.62
1:2:193:ARG:NH1	1:2:204:PRO:HG2	2.14	0.62
1:3:74:ASN:OD1	1:3:75:GLU:N	2.33	0.62
1:4:3:ILE:CG2	1:4:4:GLY:H	2.10	0.62
1:4:159:VAL:O	1:4:160:LEU:C	2.41	0.62
1:1:52:PHE:O	1:1:53:LYS:HB3	2.00	0.62
1:2:28:ALA:HA	1:2:71:THR:O	1.99	0.62
1:3:49:HIS:CD2	1:3:313:GLU:OE1	2.53	0.62
1:3:196:ARG:CD	1:4:47:SER:OG	2.47	0.62
1:4:170:LEU:CD2	1:4:225:THR:HG22	2.29	0.62
1:4:220:LEU:CA	1:4:223:LYS:HZ3	2.00	0.62
1:4:250:SER:O	1:4:253:ASP:N	2.33	0.62
1:1:193:ARG:HH11	1:1:204:PRO:CG	2.11	0.61
1:1:248:GLU:HG2	1:1:302:THR:CG2	2.30	0.61
1:1:270:LEU:HD23	1:1:270:LEU:C	2.20	0.61
1:1:279:SER:C	1:1:281:ASP:H	2.06	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:135:LYS:HZ1	1:2:140:MET:HE1	1.64	0.61
1:2:220:LEU:HA	1:2:223:LYS:NZ	2.14	0.61
1:3:330:VAL:O	1:3:331:ASP:C	2.43	0.61
1:4:73:PHE:CD2	1:4:81:ILE:CD1	2.82	0.61
1:1:165:GLU:OE1	1:1:167:VAL:HG12	1.99	0.61
1:1:303:PHE:CE2	1:4:303:PHE:CE2	2.89	0.61
1:2:243:VAL:HG23	1:2:245:LEU:CD2	2.28	0.61
1:3:128:VAL:O	1:3:132:ASN:HB3	1.99	0.61
1:3:241:LEU:O	1:3:305:LYS:HA	2.00	0.61
1:3:309:TRP:CD1	1:3:309:TRP:H	2.17	0.61
1:1:10:ARG:HH12	1:1:46:ASP:CG	2.07	0.61
1:1:193:ARG:HE	1:4:277:VAL:HA	1.66	0.61
1:1:209:ALA:O	1:1:213:VAL:HB	2.01	0.61
1:1:213:VAL:C	1:1:216:VAL:HG12	2.25	0.61
1:1:303:PHE:CE2	1:4:303:PHE:HE2	2.17	0.61
1:4:108:PHE:O	1:4:110:GLY:N	2.33	0.61
1:4:138:LYS:HD3	1:4:330:VAL:HG12	1.83	0.61
1:4:183:THR:O	1:4:183:THR:HG22	1.99	0.61
1:1:81:ILE:CG2	1:1:83:TRP:NE1	2.63	0.61
1:1:131:VAL:HG12	1:1:158:LYS:NZ	2.16	0.61
1:1:324:LEU:HD12	1:1:324:LEU:O	2.00	0.61
1:3:6:ASN:OD1	1:3:30:ASN:ND2	2.33	0.61
1:3:20:LEU:C	1:3:22:CYS:H	2.07	0.61
1:3:152:CYS:HA	1:3:289:SER:HB2	1.80	0.61
1:3:282:PHE:O	1:3:283:ILE:C	2.42	0.61
1:2:276:ASP:OD1	1:2:277:VAL:CG1	2.48	0.61
1:3:11:ILE:HG22	1:3:15:VAL:CG2	2.30	0.61
1:3:53:LYS:NZ	1:3:53:LYS:CB	2.59	0.61
1:1:165:GLU:O	1:1:166:ILE:O	2.17	0.61
1:1:282:PHE:CZ	1:1:290:ILE:CD1	2.84	0.61
1:2:127:PHE:CZ	1:2:136:TYR:HB2	2.35	0.61
1:2:132:ASN:ND2	1:2:133:LEU:HG	2.15	0.61
1:3:83:TRP:CA	1:3:86:ALA:CB	2.79	0.61
1:4:83:TRP:CA	1:4:86:ALA:CB	2.78	0.61
1:4:321:ILE:CG2	1:4:325:LYS:HE3	2.31	0.61
1:1:127:PHE:CE1	1:1:143:VAL:HG21	2.34	0.61
1:2:243:VAL:CG2	1:2:245:LEU:HD23	2.28	0.61
1:3:172:THR:O	1:3:240:ASP:N	2.30	0.61
1:3:270:LEU:CD2	1:3:271:GLY:N	2.51	0.61
1:1:128:VAL:CG2	1:1:216:VAL:HG21	2.31	0.61
1:1:193:ARG:HA	1:4:277:VAL:HG12	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:83:TRP:C	1:3:86:ALA:HB3	2.25	0.61
1:4:185:ASP:HA	1:4:196:ARG:HA	1.81	0.61
1:1:272:TYR:CE2	1:1:293:ALA:CB	2.83	0.61
1:2:127:PHE:CB	1:2:132:ASN:HB2	2.31	0.61
1:3:26:VAL:C	1:3:27:VAL:CG1	2.57	0.61
1:4:125:PRO:CG	1:4:140:MET:HE3	2.25	0.61
1:4:127:PHE:HB2	1:4:323:LEU:HD21	1.83	0.61
1:4:161:HIS:O	1:4:165:GLU:HA	2.01	0.61
1:4:281:ASP:O	1:4:283:ILE:N	2.33	0.61
1:1:188:SER:C	1:1:190:LYS:H	2.08	0.61
1:1:243:VAL:CG2	1:1:304:VAL:HG11	2.30	0.61
1:2:319:ARG:NH1	1:2:319:ARG:HG2	2.15	0.61
1:3:33:PHE:CZ	1:3:76:MET:SD	2.94	0.61
1:3:278:VAL:O	1:3:279:SER:OG	2.17	0.61
1:4:161:HIS:O	1:4:165:GLU:CA	2.49	0.61
1:4:281:ASP:HA	2:4:357:HOH:O	2.00	0.61
1:4:318:GLN:OE1	1:4:318:GLN:CA	2.47	0.61
1:1:17:ARG:HB3	1:1:43:PHE:HZ	1.62	0.60
1:3:66:ASP:C	1:3:68:LYS:HD3	2.25	0.60
1:3:239:VAL:CG1	1:3:310:TYR:CE1	2.83	0.60
1:3:296:GLY:H	1:3:297:ILE:CD1	2.14	0.60
1:4:46:ASP:O	1:4:50:GLY:HA2	2.00	0.60
1:4:65:VAL:O	1:4:68:LYS:HD3	2.01	0.60
1:4:85:LYS:O	1:4:86:ALA:CB	2.47	0.60
1:1:253:ASP:O	1:1:254:ILE:C	2.42	0.60
1:1:273:THR:HG22	1:1:290:ILE:HD12	1.81	0.60
1:2:154:ALA:HB3	1:2:155:PRO:HD3	1.83	0.60
1:3:33:PHE:HZ	1:3:76:MET:SD	2.23	0.60
1:3:125:PRO:O	1:3:144:SER:HB3	2.01	0.60
1:3:136:TYR:CD2	1:3:140:MET:SD	2.94	0.60
1:3:283:ILE:HD11	2:3:388:HOH:O	2.01	0.60
1:4:106:ALA:O	1:4:107:HIS:C	2.43	0.60
1:4:113:LYS:C	1:4:114:LYS:HE3	2.26	0.60
1:4:292:ASP:O	1:4:294:LYS:N	2.34	0.60
1:1:293:ALA:O	1:1:294:LYS:CB	2.47	0.60
1:1:295:ALA:HB1	1:4:193:ARG:NH1	2.15	0.60
1:1:321:ILE:O	1:1:325:LYS:HG3	2.00	0.60
1:2:91:ILE:HD12	1:2:91:ILE:N	2.14	0.60
1:2:173:THR:CG2	1:2:228:ALA:CB	2.79	0.60
1:3:11:ILE:O	1:3:15:VAL:HG23	2.00	0.60
1:3:75:GLU:C	2:3:378:HOH:O	2.43	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:113:LYS:HG2	1:3:114:LYS:HZ2	1.65	0.60
1:3:119:ALA:HB1	1:3:120:PRO:CD	2.31	0.60
1:3:146:ALA:O	1:3:316:TYR:HE1	1.84	0.60
1:3:216:VAL:O	1:3:218:PRO:CD	2.50	0.60
1:3:272:TYR:HE1	1:3:274:GLU:OE2	1.84	0.60
1:1:59:GLU:HB3	1:1:64:VAL:HG11	1.84	0.60
1:1:90:TYR:HA	1:1:114:LYS:O	2.00	0.60
1:2:66:ASP:OD2	1:2:66:ASP:N	2.33	0.60
1:2:208:GLY:HA3	1:2:211:LYS:HG2	1.83	0.60
1:3:250:SER:HA	1:3:299:LEU:CD1	2.30	0.60
1:3:275:ASP:O	1:3:275:ASP:OD2	2.18	0.60
1:3:294:LYS:CA	1:3:297:ILE:HG13	2.30	0.60
1:4:227:MET:CE	1:4:229:PHE:CZ	2.84	0.60
1:4:220:LEU:O	1:4:221:ASP:C	2.45	0.60
1:1:19:ALA:CA	1:1:24:ALA:HB3	2.31	0.60
1:1:126:MET:HE2	1:1:215:LYS:NZ	2.17	0.60
1:1:196:ARG:HG3	1:1:197:GLY:H	1.66	0.60
1:2:4:GLY:CA	1:2:27:VAL:CG2	2.80	0.60
1:2:25:GLN:O	1:2:26:VAL:O	2.20	0.60
1:2:113:LYS:CE	1:2:114:LYS:HZ1	2.12	0.60
1:3:127:PHE:CB	1:3:323:LEU:HD21	2.30	0.60
1:3:178:THR:OG1	1:3:181:GLN:HB2	2.01	0.60
1:1:319:ARG:NH1	1:1:319:ARG:HG2	2.15	0.60
1:3:132:ASN:OD1	1:3:133:LEU:HD23	2.02	0.60
1:4:127:PHE:HE1	1:4:140:MET:CE	2.15	0.60
1:1:251:TYR:O	1:1:252:ASP:C	2.45	0.60
1:2:44:LYS:NZ	1:2:45:TYR:CE2	2.69	0.60
1:2:89:GLU:O	1:2:114:LYS:HG3	2.02	0.60
1:3:4:GLY:CA	1:3:27:VAL:HG23	2.29	0.60
1:3:11:ILE:N	1:3:11:ILE:HD12	2.16	0.60
1:3:128:VAL:C	1:3:132:ASN:HD22	2.08	0.60
1:4:2:LYS:HZ1	1:4:88:ALA:HA	1.66	0.60
1:4:59:GLU:O	1:4:60:ASP:C	2.44	0.60
1:4:243:VAL:HG23	1:4:304:VAL:CG1	2.28	0.60
1:1:8:PHE:CE1	1:1:39:MET:SD	2.95	0.60
1:1:119:ALA:HB1	1:1:120:PRO:HD2	1.84	0.60
1:1:163:ASN:OD1	1:1:163:ASN:O	2.20	0.60
1:3:131:VAL:O	1:3:131:VAL:HG23	2.02	0.60
1:4:113:LYS:CG	1:4:114:LYS:HE3	2.32	0.60
1:4:116:VAL:HG11	1:4:324:LEU:HD22	1.82	0.60
1:4:150:THR:HG23	1:4:212:ALA:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:83:TRP:HA	1:1:86:ALA:CB	2.30	0.60
1:1:276:ASP:C	1:1:277:VAL:CG2	2.74	0.60
1:2:104:ALA:CB	1:2:142:VAL:HG21	2.32	0.60
1:2:127:PHE:HB3	1:2:132:ASN:HB2	1.84	0.60
1:2:272:TYR:OH	1:2:274:GLU:CD	2.45	0.60
1:4:8:PHE:CZ	1:4:39:MET:CB	2.84	0.60
1:4:127:PHE:CZ	1:4:135:LYS:NZ	2.70	0.60
1:4:132:ASN:CG	1:4:133:LEU:HD23	2.26	0.60
1:1:1:SER:OG	1:1:25:GLN:CB	2.36	0.59
1:1:200:GLN:OE1	1:2:48:THR:HG23	2.02	0.59
1:3:26:VAL:HB	1:3:70:ILE:CG2	2.32	0.59
1:3:101:ILE:HD13	2:3:380:HOH:O	2.02	0.59
1:1:112:ALA:O	1:1:113:LYS:HG3	2.01	0.59
1:1:193:ARG:NH1	1:1:204:PRO:CG	2.65	0.59
1:2:54:GLY:O	1:2:56:VAL:N	2.34	0.59
1:2:125:PRO:HB2	1:2:143:VAL:HG23	1.84	0.59
1:2:216:VAL:CG1	1:2:217:ILE:N	2.65	0.59
1:2:277:VAL:CG2	1:2:278:VAL:H	2.08	0.59
1:3:22:CYS:SG	1:3:321:ILE:HG21	2.41	0.59
1:3:52:PHE:CA	2:3:370:HOH:O	2.29	0.59
1:4:66:ASP:O	1:4:68:LYS:HD3	2.01	0.59
1:1:31:ASP:HB3	1:1:34:ILE:CG2	2.32	0.59
1:1:74:ASN:OD1	1:1:75:GLU:N	2.35	0.59
1:1:295:ALA:CA	1:1:297:ILE:HD12	2.33	0.59
1:2:6:ASN:CG	1:2:30:ASN:HD21	2.10	0.59
1:2:126:MET:HE3	1:2:212:ALA:HA	1.84	0.59
1:4:1:SER:CB	1:4:25:GLN:HE21	2.04	0.59
1:4:77:LYS:O	2:4:348:HOH:O	2.11	0.59
1:4:188:SER:HB3	1:4:191:ASP:C	2.27	0.59
1:2:16:LEU:O	1:2:18:ALA:N	2.35	0.59
1:2:319:ARG:O	1:2:320:VAL:C	2.46	0.59
1:3:74:ASN:HB2	2:3:365:HOH:O	2.01	0.59
1:3:173:THR:O	1:3:228:ALA:HA	2.02	0.59
1:4:53:LYS:NZ	1:4:53:LYS:CB	2.52	0.59
1:1:281:ASP:O	1:1:283:ILE:HB	2.01	0.59
1:2:154:ALA:HB3	1:2:155:PRO:CD	2.33	0.59
1:2:165:GLU:O	1:2:166:ILE:HB	2.02	0.59
1:3:78:PRO:O	1:3:81:ILE:HG22	2.02	0.59
1:4:64:VAL:O	1:4:64:VAL:HG22	2.01	0.59
1:1:30:ASN:ND2	1:1:30:ASN:O	2.35	0.59
1:1:113:LYS:CB	1:1:114:LYS:HD2	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:298:GLN:HE22	1:3:225:THR:CG2	2.14	0.59
1:3:126:MET:CE	1:3:212:ALA:HA	2.32	0.59
1:4:44:LYS:CG	1:4:56:VAL:HG11	2.32	0.59
1:4:101:ILE:HG23	1:4:142:VAL:CG1	2.32	0.59
1:4:153:LEU:HD21	1:4:241:LEU:HD13	1.84	0.59
1:4:160:LEU:HD22	1:4:245:LEU:HD21	1.85	0.59
1:1:244:ARG:HH22	1:4:244:ARG:CG	2.16	0.59
1:1:251:TYR:CD2	1:1:254:ILE:HG21	2.37	0.59
1:2:242:THR:HA	1:2:304:VAL:O	2.02	0.59
1:3:78:PRO:HG3	1:3:98:PHE:CD2	2.38	0.59
1:3:287:ARG:HH11	1:3:290:ILE:HG21	1.66	0.59
1:3:325:LYS:O	1:3:328:GLN:N	2.36	0.59
1:4:320:VAL:O	1:4:324:LEU:HB2	2.02	0.59
1:4:329:LYS:C	1:4:329:LYS:HZ2	2.07	0.59
1:1:41:TYR:CE1	1:3:277:VAL:CG2	2.74	0.59
1:1:311:ASP:O	1:1:313:GLU:N	2.35	0.59
1:2:40:VAL:HG22	1:2:41:TYR:N	2.18	0.59
1:2:127:PHE:CE2	1:2:136:TYR:CB	2.82	0.59
1:2:127:PHE:CA	1:2:132:ASN:HB2	2.33	0.59
1:4:3:ILE:HG22	1:4:4:GLY:N	2.17	0.59
1:4:251:TYR:OH	1:4:291:PHE:HZ	1.78	0.59
1:4:270:LEU:CD2	1:4:271:GLY:N	2.44	0.59
1:1:108:PHE:O	1:1:109:LYS:C	2.46	0.59
1:2:4:GLY:HA2	1:2:27:VAL:HG22	1.85	0.59
1:4:52:PHE:O	1:4:53:LYS:CB	2.45	0.59
1:4:56:VAL:O	1:4:56:VAL:HG22	2.02	0.59
1:4:185:ASP:C	1:4:195:GLY:O	2.46	0.59
1:1:277:VAL:HG12	1:4:193:ARG:HG3	1.85	0.59
1:2:297:ILE:H	1:2:297:ILE:HD12	1.64	0.59
1:3:126:MET:HE3	1:3:212:ALA:CB	2.33	0.59
1:3:329:LYS:HZ2	1:3:329:LYS:HB3	1.68	0.59
1:4:128:VAL:HG13	1:4:151:ASN:ND2	2.18	0.59
1:1:210:ALA:HB2	1:1:224:LEU:O	2.03	0.58
1:2:44:LYS:CD	1:2:56:VAL:HG21	2.32	0.58
1:2:208:GLY:HA3	1:2:211:LYS:CG	2.33	0.58
1:2:293:ALA:O	1:2:294:LYS:CG	2.50	0.58
1:2:298:GLN:OE1	1:3:225:THR:HG23	2.03	0.58
1:3:46:ASP:CB	1:3:50:GLY:H	2.09	0.58
1:3:49:HIS:HD2	1:3:313:GLU:OE1	1.83	0.58
1:4:53:LYS:CD	1:4:54:GLY:N	2.63	0.58
1:4:132:ASN:HD21	1:4:133:LEU:CD2	2.12	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:112:ALA:O	1:1:113:LYS:CB	2.52	0.58
1:2:250:SER:C	1:2:252:ASP:N	2.55	0.58
1:3:132:ASN:ND2	1:3:133:LEU:HG	2.18	0.58
1:3:265:PRO:O	1:3:267:GLN:N	2.36	0.58
1:2:185:ASP:HA	1:2:195:GLY:O	2.04	0.58
1:4:42:MET:CG	1:4:42:MET:O	2.49	0.58
1:4:325:LYS:O	1:4:328:GLN:N	2.37	0.58
1:1:44:LYS:HG2	1:1:56:VAL:HG21	1.85	0.58
1:1:93:GLU:OE2	1:1:98:PHE:CD2	2.56	0.58
1:1:212:ALA:O	1:1:216:VAL:CB	2.48	0.58
1:1:276:ASP:OD1	1:1:277:VAL:CG2	2.52	0.58
1:1:296:GLY:N	1:1:297:ILE:HD12	2.18	0.58
1:2:44:LYS:O	1:2:51:VAL:HA	2.04	0.58
1:3:78:PRO:HD3	1:3:98:PHE:CZ	2.38	0.58
1:3:132:ASN:CG	1:3:133:LEU:H	2.11	0.58
1:3:164:PHE:HZ	1:3:253:ASP:HB3	1.68	0.58
1:4:34:ILE:HD12	1:4:42:MET:SD	2.43	0.58
1:4:126:MET:HB2	1:4:215:LYS:HD3	1.85	0.58
1:4:132:ASN:HD21	1:4:133:LEU:HD21	1.67	0.58
1:1:181:GLN:O	1:2:183:THR:CG2	2.51	0.58
1:2:3:ILE:HD13	1:2:324:LEU:HD11	1.83	0.58
1:3:90:TYR:N	1:3:90:TYR:CD1	2.71	0.58
1:3:118:SER:O	1:3:118:SER:OG	2.20	0.58
1:3:119:ALA:HB1	1:3:120:PRO:HD3	1.85	0.58
1:2:95:THR:CG2	1:2:97:VAL:HG23	2.34	0.58
1:2:126:MET:CB	1:2:215:LYS:NZ	2.66	0.58
1:3:241:LEU:HG	1:3:243:VAL:HG13	1.85	0.58
1:1:167:VAL:HG22	1:1:244:ARG:HG2	1.84	0.58
1:1:252:ASP:C	1:1:252:ASP:OD1	2.46	0.58
1:3:146:ALA:HB1	1:3:150:THR:HG21	1.85	0.58
1:3:155:PRO:O	1:3:159:VAL:HG23	2.03	0.58
1:3:299:LEU:CD2	1:3:300:SER:H	2.14	0.58
1:4:127:PHE:CE2	1:4:135:LYS:HG3	2.38	0.58
1:4:250:SER:C	1:4:252:ASP:N	2.61	0.58
1:1:31:ASP:HB3	1:1:34:ILE:HG23	1.84	0.58
1:2:10:ARG:NH1	1:2:46:ASP:OD2	2.36	0.58
1:2:44:LYS:HB3	1:2:56:VAL:HG21	1.86	0.58
1:2:244:ARG:CD	1:3:244:ARG:HH12	2.15	0.58
1:3:78:PRO:C	1:3:80:ASN:N	2.59	0.58
1:4:127:PHE:CD1	1:4:143:VAL:CG2	2.85	0.58
1:4:236:VAL:CG1	1:4:237:SER:H	2.16	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:259:LYS:C	1:4:261:ALA:N	2.62	0.58
1:1:161:HIS:O	1:1:163:ASN:N	2.35	0.58
1:1:232:PRO:O	1:1:233:THR:C	2.45	0.58
1:2:265:PRO:C	1:2:267:GLN:H	2.12	0.58
1:3:145:ASN:HD22	1:3:145:ASN:C	2.10	0.58
1:3:292:ASP:OD1	1:3:292:ASP:C	2.47	0.58
1:3:326:HIS:O	1:3:327:MET:C	2.46	0.58
1:4:53:LYS:HD2	1:4:54:GLY:CA	2.33	0.58
1:1:261:ALA:C	1:1:263:GLU:N	2.59	0.58
1:2:91:ILE:HD13	1:2:115:VAL:CG2	2.22	0.58
1:3:77:LYS:O	1:3:80:ASN:HB2	2.03	0.58
1:3:279:SER:O	1:3:281:ASP:N	2.29	0.58
1:3:287:ARG:HH11	1:3:290:ILE:CG2	2.17	0.58
1:3:295:ALA:C	1:3:297:ILE:HD12	2.29	0.58
1:2:150:THR:HG21	1:2:212:ALA:CB	2.34	0.57
1:2:231:VAL:HB	1:3:231:VAL:HG12	1.86	0.57
1:2:266:LEU:HD13	2:2:412:HOH:O	2.04	0.57
1:3:145:ASN:O	1:3:316:TYR:OH	2.19	0.57
1:1:305:LYS:HD3	1:4:227:MET:SD	2.44	0.57
1:2:128:VAL:H	1:2:132:ASN:HB2	1.69	0.57
1:2:285:ASP:C	1:2:285:ASP:OD2	2.45	0.57
1:3:168:GLU:OE2	1:3:244:ARG:NE	2.37	0.57
1:3:249:CYS:SG	1:3:254:ILE:HD11	2.44	0.57
1:4:128:VAL:C	1:4:132:ASN:HB3	2.30	0.57
1:1:28:ALA:HB1	1:1:73:PHE:CE2	2.39	0.57
1:1:30:ASN:C	1:1:30:ASN:HD22	2.08	0.57
1:1:113:LYS:C	1:1:114:LYS:CE	2.66	0.57
1:2:84:SER:O	1:2:85:LYS:C	2.45	0.57
1:2:128:VAL:H	1:2:132:ASN:HB3	1.69	0.57
1:2:131:VAL:O	1:2:132:ASN:C	2.47	0.57
1:3:220:LEU:HA	1:3:223:LYS:HZ2	1.68	0.57
1:3:274:GLU:C	1:3:276:ASP:H	2.11	0.57
1:4:176:ALA:O	1:4:177:VAL:O	2.23	0.57
1:1:7:GLY:O	1:1:8:PHE:CB	2.40	0.57
1:1:126:MET:HE2	1:1:215:LYS:CE	2.34	0.57
1:1:232:PRO:HB2	1:4:232:PRO:HB2	1.86	0.57
1:1:252:ASP:O	1:1:255:LYS:CG	2.53	0.57
1:4:269:PHE:O	1:4:288:SER:HB3	2.02	0.57
1:4:319:ARG:O	1:4:322:ASP:N	2.36	0.57
1:2:325:LYS:O	1:2:326:HIS:C	2.47	0.57
1:3:41:TYR:OH	1:4:196:ARG:NH1	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:126:MET:HA	1:4:144:SER:O	2.04	0.57
1:1:172:THR:O	1:1:240:ASP:N	2.34	0.57
1:1:205:SER:CB	1:1:228:ALA:HB3	2.33	0.57
1:2:298:GLN:CD	1:3:225:THR:HG23	2.30	0.57
1:3:32:PRO:O	1:3:33:PHE:CD1	2.58	0.57
1:3:216:VAL:O	1:3:218:PRO:HD2	2.05	0.57
1:3:291:PHE:CE2	1:3:306:VAL:HB	2.39	0.57
1:3:296:GLY:N	1:3:297:ILE:HG23	2.20	0.57
1:3:319:ARG:NH1	1:3:319:ARG:HG2	2.19	0.57
1:4:38:TYR:O	1:4:42:MET:HB2	2.04	0.57
1:4:251:TYR:OH	1:4:291:PHE:CZ	2.55	0.57
1:1:41:TYR:HE1	1:3:277:VAL:CG2	2.13	0.57
1:1:188:SER:HB2	1:1:192:TRP:HA	1.86	0.57
1:2:161:HIS:CA	1:2:166:ILE:HG13	2.35	0.57
1:3:95:THR:CG2	1:3:97:VAL:HG22	2.34	0.57
1:4:6:ASN:HD22	1:4:93:GLU:CD	2.13	0.57
1:4:11:ILE:H	1:4:11:ILE:HD13	1.66	0.57
1:4:276:ASP:OD1	1:4:277:VAL:N	2.38	0.57
1:1:152:CYS:SG	1:1:239:VAL:HG11	2.43	0.57
1:2:193:ARG:HH12	1:3:295:ALA:CB	2.17	0.57
1:3:258:MET:CG	1:3:270:LEU:HD11	2.32	0.57
1:4:305:LYS:NZ	1:4:305:LYS:HB2	2.18	0.57
1:1:52:PHE:O	1:1:53:LYS:HE2	2.05	0.57
1:1:213:VAL:HA	1:1:216:VAL:CG1	2.35	0.57
1:3:36:LEU:O	1:3:40:VAL:HG12	2.04	0.57
1:4:4:GLY:N	1:4:27:VAL:CG2	2.68	0.57
1:4:44:LYS:HE3	1:4:45:TYR:CD2	2.39	0.57
1:1:109:LYS:O	1:1:110:GLY:C	2.48	0.57
1:1:298:GLN:CD	1:4:225:THR:CG2	2.78	0.57
1:2:244:ARG:HG3	1:3:244:ARG:CZ	2.34	0.57
1:3:55:GLU:HB2	1:3:66:ASP:HA	1.87	0.57
1:4:104:ALA:O	1:4:106:ALA:N	2.37	0.57
1:1:127:PHE:CD2	1:1:136:TYR:HB2	2.36	0.56
1:1:128:VAL:H	1:1:132:ASN:HB3	1.70	0.56
1:1:251:TYR:N	1:1:299:LEU:CD1	2.67	0.56
1:1:277:VAL:CG1	1:3:41:TYR:OH	2.49	0.56
1:2:52:PHE:C	1:2:53:LYS:HE2	2.30	0.56
1:2:65:VAL:O	1:2:68:LYS:HD3	2.04	0.56
1:2:244:ARG:HH22	1:3:244:ARG:CG	2.17	0.56
1:3:90:TYR:CD2	1:3:328:GLN:NE2	2.69	0.56
1:3:138:LYS:HZ2	1:3:330:VAL:HG11	1.63	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:22:CYS:SG	1:4:318:GLN:NE2	2.78	0.56
1:4:76:MET:O	1:4:76:MET:HG3	2.05	0.56
1:4:193:ARG:O	1:4:203:ILE:CG2	2.53	0.56
1:1:168:GLU:OE2	1:1:244:ARG:CZ	2.53	0.56
1:1:277:VAL:CA	1:4:193:ARG:HD3	2.34	0.56
1:2:188:SER:HB3	1:2:192:TRP:HA	1.86	0.56
1:2:251:TYR:CZ	1:2:297:ILE:HB	2.40	0.56
1:2:318:GLN:OE1	1:2:318:GLN:CA	2.45	0.56
1:3:161:HIS:CG	1:3:162:GLU:N	2.72	0.56
1:1:17:ARG:CB	1:1:43:PHE:CE2	2.88	0.56
1:1:26:VAL:HB	1:1:70:ILE:HG22	1.86	0.56
1:1:34:ILE:CG1	1:1:39:MET:HE2	2.35	0.56
1:1:225:THR:CG2	1:4:298:GLN:CD	2.79	0.56
1:2:153:LEU:HD12	1:2:171:MET:SD	2.45	0.56
1:2:193:ARG:NH1	1:3:295:ALA:HB1	2.20	0.56
1:2:210:ALA:O	1:2:211:LYS:C	2.48	0.56
1:2:216:VAL:O	1:2:218:PRO:HD2	2.04	0.56
1:2:276:ASP:C	1:2:277:VAL:HG22	2.31	0.56
1:3:282:PHE:CE2	1:3:309:TRP:CG	2.92	0.56
1:4:54:GLY:HA3	1:4:66:ASP:OD2	2.05	0.56
1:4:79:GLU:N	1:4:79:GLU:OE1	2.39	0.56
1:4:126:MET:HE2	1:4:212:ALA:HA	1.87	0.56
1:4:128:VAL:H	1:4:132:ASN:HB3	1.70	0.56
1:4:231:VAL:O	1:4:232:PRO:C	2.49	0.56
1:4:236:VAL:O	1:4:237:SER:CB	2.51	0.56
1:1:126:MET:CG	1:1:146:ALA:HB2	2.35	0.56
1:2:30:ASN:CG	1:2:81:ILE:HG13	2.29	0.56
1:2:44:LYS:HD3	1:2:56:VAL:HG21	1.88	0.56
1:1:14:LEU:O	1:1:18:ALA:N	2.39	0.56
1:1:193:ARG:CG	1:4:277:VAL:HA	2.36	0.56
1:1:248:GLU:HG2	1:1:302:THR:HG22	1.87	0.56
1:2:19:ALA:CA	1:2:24:ALA:HB3	2.35	0.56
1:2:30:ASN:HA	1:2:73:PHE:O	2.06	0.56
1:2:137:SER:CB	1:2:138:LYS:NZ	2.67	0.56
1:2:161:HIS:CG	1:2:165:GLU:O	2.57	0.56
1:2:243:VAL:HG22	1:2:304:VAL:HG12	1.87	0.56
1:3:164:PHE:CD2	1:3:249:CYS:HB3	2.40	0.56
1:4:117:ILE:HD12	1:4:121:SER:OG	2.04	0.56
1:4:127:PHE:CB	1:4:132:ASN:HB2	2.34	0.56
1:4:187:PRO:O	1:4:187:PRO:CG	2.53	0.56
1:4:328:GLN:O	1:4:332:SER:HB2	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:8:PHE:HZ	1:1:39:MET:HB3	1.71	0.56
1:2:41:TYR:HH	1:4:277:VAL:HG11	1.69	0.56
1:2:145:ASN:O	1:2:146:ALA:C	2.49	0.56
1:2:277:VAL:HA	1:3:193:ARG:HG3	1.87	0.56
1:3:154:ALA:HB1	1:3:155:PRO:HD3	1.84	0.56
1:3:271:GLY:O	1:3:272:TYR:HB3	2.05	0.56
1:4:137:SER:HB3	1:4:138:LYS:HZ1	1.69	0.56
1:4:216:VAL:HG13	1:4:217:ILE:N	2.18	0.56
1:4:314:PHE:HA	1:4:317:SER:OG	2.06	0.56
1:1:22:CYS:SG	1:1:321:ILE:CG2	2.92	0.56
1:1:216:VAL:CG1	1:1:217:ILE:N	2.69	0.56
1:3:145:ASN:O	1:3:146:ALA:C	2.49	0.56
1:4:2:LYS:HZ3	1:4:88:ALA:HA	1.65	0.56
1:4:212:ALA:O	1:4:216:VAL:N	2.39	0.56
1:4:255:LYS:CD	1:4:293:ALA:HB1	2.34	0.56
1:1:8:PHE:HD1	1:1:29:VAL:HG11	1.70	0.56
1:1:175:HIS:CD2	1:1:230:ARG:NH2	2.74	0.56
1:2:116:VAL:HA	1:2:143:VAL:O	2.05	0.56
1:3:89:GLU:HB2	1:3:90:TYR:CD1	2.40	0.56
1:3:126:MET:HE3	1:3:212:ALA:CA	2.35	0.56
1:3:252:ASP:C	1:3:254:ILE:N	2.62	0.56
1:3:287:ARG:NH1	1:3:290:ILE:CD1	2.68	0.56
1:3:299:LEU:CD2	1:3:304:VAL:HG23	2.35	0.56
1:4:239:VAL:HG13	1:4:310:TYR:CE1	2.41	0.56
1:4:272:TYR:HA	1:4:291:PHE:O	2.05	0.56
1:2:11:ILE:O	1:2:15:VAL:HG23	2.05	0.56
1:2:296:GLY:O	1:2:307:VAL:CG2	2.51	0.56
1:3:167:VAL:HG22	1:3:168:GLU:H	1.70	0.56
1:3:227:MET:HE1	1:3:229:PHE:CZ	2.41	0.56
1:4:134:GLU:C	1:4:136:TYR:N	2.63	0.56
1:1:53:LYS:NZ	1:1:53:LYS:CB	2.60	0.56
1:1:159:VAL:HB	1:1:258:MET:HE3	1.88	0.56
1:1:164:PHE:O	1:1:165:GLU:HB2	2.06	0.56
1:1:213:VAL:CA	1:1:216:VAL:HG12	2.36	0.56
1:1:217:ILE:HG12	1:1:220:LEU:HD22	1.86	0.56
1:2:113:LYS:HB3	1:2:114:LYS:HE3	1.86	0.56
1:2:277:VAL:CA	1:3:193:ARG:NE	2.68	0.56
1:3:4:GLY:N	1:3:27:VAL:HG21	2.20	0.56
1:3:184:VAL:O	1:3:184:VAL:HG13	2.06	0.56
1:4:19:ALA:HB1	1:4:24:ALA:HB3	1.87	0.56
1:4:52:PHE:CD1	1:4:53:LYS:HE3	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:133:LEU:HD23	1:4:133:LEU:H	1.71	0.56
1:4:292:ASP:O	1:4:297:ILE:HG21	2.06	0.56
1:1:46:ASP:O	1:1:50:GLY:HA3	2.06	0.55
1:1:95:THR:HG23	1:1:97:VAL:HG23	1.87	0.55
1:1:167:VAL:HG13	1:1:245:LEU:O	2.06	0.55
1:2:14:LEU:H	1:2:14:LEU:HD13	1.70	0.55
1:2:91:ILE:CD1	1:2:114:LYS:O	2.50	0.55
1:2:93:GLU:OE2	1:2:98:PHE:CD2	2.59	0.55
1:2:185:ASP:OD1	1:2:185:ASP:N	2.39	0.55
1:2:299:LEU:CG	1:2:304:VAL:HG23	2.35	0.55
1:3:114:LYS:HE3	1:3:114:LYS:N	2.18	0.55
1:3:302:THR:O	1:3:302:THR:OG1	2.24	0.55
1:4:232:PRO:O	1:4:233:THR:O	2.24	0.55
1:4:235:ASP:CG	1:4:311:ASP:OD1	2.49	0.55
1:1:52:PHE:C	1:1:53:LYS:CE	2.64	0.55
1:1:71:THR:HG22	1:1:72:VAL:O	2.05	0.55
1:1:220:LEU:CB	1:1:223:LYS:HZ2	2.19	0.55
1:1:282:PHE:HZ	1:1:290:ILE:HD13	1.64	0.55
1:1:314:PHE:HB2	1:1:317:SER:CB	2.37	0.55
1:3:3:ILE:CG2	1:3:4:GLY:H	2.14	0.55
1:4:28:ALA:HB1	1:4:73:PHE:CE2	2.40	0.55
1:4:105:SER:O	1:4:106:ALA:C	2.49	0.55
1:1:133:LEU:O	1:1:136:TYR:HB3	2.06	0.55
1:3:44:LYS:O	1:3:51:VAL:CA	2.52	0.55
1:3:127:PHE:CE1	1:3:140:MET:HE1	2.40	0.55
1:3:128:VAL:O	1:3:132:ASN:CB	2.53	0.55
1:3:131:VAL:HG12	1:3:158:LYS:CE	2.36	0.55
1:3:188:SER:O	1:3:191:ASP:N	2.40	0.55
1:3:259:LYS:HG3	1:3:272:TYR:CD1	2.41	0.55
1:4:17:ARG:NH1	2:4:452:HOH:O	2.39	0.55
1:4:134:GLU:O	1:4:135:LYS:C	2.48	0.55
1:1:93:GLU:OE2	1:1:98:PHE:HD2	1.88	0.55
1:1:116:VAL:HA	1:1:143:VAL:O	2.06	0.55
1:1:282:PHE:HD1	1:1:285:ASP:OD1	1.90	0.55
1:2:104:ALA:HB3	1:2:142:VAL:HG21	1.88	0.55
1:2:293:ALA:O	1:2:294:LYS:HG2	2.06	0.55
1:1:128:VAL:HG11	1:1:154:ALA:HB2	1.88	0.55
1:1:283:ILE:O	1:1:283:ILE:HG22	2.07	0.55
1:2:9:GLY:O	1:2:10:ARG:C	2.49	0.55
1:2:83:TRP:HD1	1:2:112:ALA:HB2	1.72	0.55
1:2:109:LYS:O	1:2:110:GLY:C	2.50	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:178:THR:O	1:3:179:ALA:C	2.49	0.55
1:4:26:VAL:CA	1:4:27:VAL:HG12	2.36	0.55
1:1:105:SER:O	1:1:107:HIS:N	2.39	0.55
1:2:295:ALA:HB2	1:3:193:ARG:HH12	1.66	0.55
1:4:2:LYS:HZ1	1:4:87:GLY:C	2.13	0.55
1:4:3:ILE:C	1:4:27:VAL:CG2	2.80	0.55
1:4:182:LYS:HE3	1:4:187:PRO:HG3	1.89	0.55
1:4:287:ARG:O	1:4:288:SER:CB	2.53	0.55
1:1:8:PHE:CZ	1:1:39:MET:HB3	2.41	0.55
1:1:83:TRP:CZ2	1:1:91:ILE:HG21	2.41	0.55
1:1:112:ALA:O	1:1:113:LYS:HB2	2.07	0.55
1:1:319:ARG:O	1:1:320:VAL:C	2.50	0.55
1:2:65:VAL:O	1:2:66:ASP:HB2	2.06	0.55
1:4:143:VAL:HG22	1:4:144:SER:N	2.20	0.55
1:4:181:GLN:HE21	1:4:203:ILE:CD1	1.99	0.55
1:4:251:TYR:H	1:4:299:LEU:HG	1.72	0.55
1:4:292:ASP:HB3	1:4:307:VAL:HG13	1.87	0.55
1:4:313:GLU:O	1:4:317:SER:OG	2.24	0.55
1:4:78:PRO:HG3	1:4:98:PHE:CD2	2.39	0.55
1:4:95:THR:HG22	1:4:97:VAL:HG23	1.88	0.55
1:1:2:LYS:HA	1:1:25:GLN:HG2	1.89	0.55
1:1:54:GLY:HA2	1:1:66:ASP:CG	2.31	0.55
1:2:276:ASP:O	1:2:277:VAL:C	2.49	0.55
1:2:294:LYS:HA	1:2:297:ILE:HG13	1.88	0.55
1:3:1:SER:O	1:3:25:GLN:NE2	2.40	0.55
1:3:59:GLU:O	1:3:61:GLY:N	2.40	0.55
1:3:84:SER:OG	1:3:111:GLY:C	2.49	0.55
1:4:4:GLY:CA	1:4:27:VAL:HG21	2.37	0.55
1:4:287:ARG:O	1:4:319:ARG:NH1	2.40	0.55
1:1:227:MET:HE2	1:1:228:ALA:H	1.71	0.55
1:2:39:MET:O	1:2:42:MET:N	2.40	0.55
1:2:94:SER:O	1:2:96:GLY:N	2.40	0.55
1:2:132:ASN:ND2	1:2:133:LEU:CG	2.69	0.55
1:2:192:TRP:CD1	1:2:192:TRP:H	2.25	0.55
1:3:101:ILE:HG22	1:3:102:GLU:N	2.21	0.55
1:3:161:HIS:C	1:3:163:ASN:N	2.64	0.55
1:3:270:LEU:HD23	1:3:271:GLY:CA	2.36	0.55
1:4:252:ASP:O	1:4:255:LYS:N	2.40	0.55
1:1:79:GLU:HB2	1:1:109:LYS:HD3	1.89	0.54
1:2:3:ILE:HG22	1:2:4:GLY:O	2.06	0.54
1:2:113:LYS:HB3	1:2:114:LYS:CE	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:138:LYS:HZ2	1:2:138:LYS:H	1.54	0.54
1:2:188:SER:HB3	1:2:192:TRP:CA	2.37	0.54
1:3:236:VAL:O	1:3:237:SER:CB	2.42	0.54
1:3:297:ILE:CD1	1:3:297:ILE:N	2.69	0.54
1:4:201:ASN:HB3	1:4:203:ILE:CG1	2.37	0.54
1:4:316:TYR:CE2	1:4:320:VAL:HG23	2.42	0.54
1:1:3:ILE:CG2	1:1:4:GLY:H	2.10	0.54
1:2:221:ASP:OD2	1:2:221:ASP:O	2.25	0.54
1:3:39:MET:O	1:3:42:MET:N	2.40	0.54
1:3:44:LYS:HG2	1:3:56:VAL:HG21	1.88	0.54
1:3:120:PRO:HD2	1:3:120:PRO:O	2.07	0.54
1:3:190:LYS:HE2	1:3:190:LYS:N	2.23	0.54
1:3:266:LEU:O	1:3:267:GLN:O	2.25	0.54
1:4:265:PRO:C	2:4:453:HOH:O	2.51	0.54
1:1:19:ALA:O	1:1:24:ALA:HB3	2.06	0.54
1:1:19:ALA:C	1:1:24:ALA:HB3	2.31	0.54
1:1:56:VAL:O	1:1:57:LYS:HE2	2.07	0.54
1:1:81:ILE:HG23	1:1:83:TRP:NE1	2.22	0.54
1:1:276:ASP:OD1	1:1:277:VAL:CG1	2.54	0.54
1:2:322:ASP:O	1:2:323:LEU:C	2.51	0.54
1:3:105:SER:C	1:3:107:HIS:N	2.63	0.54
1:3:161:HIS:CA	1:3:166:ILE:HG13	2.38	0.54
1:3:175:HIS:HB3	1:3:230:ARG:HH21	1.72	0.54
1:3:272:TYR:CE1	1:3:274:GLU:OE2	2.61	0.54
1:4:66:ASP:HB3	1:4:68:LYS:HE2	1.89	0.54
1:1:1:SER:HB3	1:1:25:GLN:HE21	1.73	0.54
1:1:89:GLU:HB3	1:1:90:TYR:HD1	1.69	0.54
1:1:101:ILE:CB	1:1:142:VAL:HG11	2.37	0.54
1:1:142:VAL:CG1	1:1:142:VAL:O	2.55	0.54
1:2:36:LEU:HD12	1:2:36:LEU:O	2.07	0.54
1:2:91:ILE:HG21	1:2:107:HIS:NE2	2.23	0.54
1:3:259:LYS:HG3	1:3:272:TYR:CE1	2.43	0.54
1:4:8:PHE:HD1	1:4:29:VAL:HG11	1.72	0.54
1:4:217:ILE:CD1	1:4:220:LEU:HD22	2.38	0.54
1:1:3:ILE:HG13	1:1:25:GLN:O	2.08	0.54
1:1:26:VAL:CG1	1:1:70:ILE:CG2	2.80	0.54
1:1:93:GLU:OE2	1:1:98:PHE:HB2	2.08	0.54
1:1:145:ASN:CB	1:1:323:LEU:CD2	2.78	0.54
1:1:225:THR:HG21	1:4:298:GLN:CD	2.32	0.54
1:3:164:PHE:CE2	1:3:249:CYS:HB2	2.43	0.54
1:4:271:GLY:O	1:4:272:TYR:HB3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:30:ASN:HD22	1:1:30:ASN:N	2.04	0.54
1:1:50:GLY:C	1:1:51:VAL:HG23	2.33	0.54
1:1:216:VAL:HG13	1:1:217:ILE:N	2.21	0.54
1:1:272:TYR:OH	1:1:274:GLU:CG	2.56	0.54
1:1:296:GLY:HA2	1:4:227:MET:HG2	1.88	0.54
1:2:3:ILE:CD1	1:2:324:LEU:HD12	2.36	0.54
1:3:106:ALA:O	1:3:107:HIS:C	2.50	0.54
1:3:183:THR:O	1:3:184:VAL:HB	2.07	0.54
1:3:255:LYS:HB3	1:3:255:LYS:HZ2	1.72	0.54
1:3:325:LYS:O	1:3:326:HIS:C	2.50	0.54
1:4:44:LYS:CE	1:4:45:TYR:HE2	2.20	0.54
1:4:78:PRO:CD	1:4:98:PHE:CZ	2.90	0.54
1:4:251:TYR:HB2	1:4:299:LEU:CG	2.38	0.54
1:1:263:GLU:O	1:1:264:GLY:O	2.26	0.54
1:1:324:LEU:O	1:1:324:LEU:CD1	2.56	0.54
1:3:187:PRO:HG2	1:3:187:PRO:O	2.07	0.54
1:3:282:PHE:CE2	1:3:309:TRP:CD1	2.96	0.54
1:1:101:ILE:HG13	1:1:123:ASP:OD1	2.08	0.54
1:1:295:ALA:O	1:1:307:VAL:HG11	2.07	0.54
1:2:294:LYS:CA	1:2:297:ILE:HG13	2.38	0.54
1:3:8:PHE:CZ	1:3:39:MET:CG	2.89	0.54
1:3:113:LYS:CG	1:3:114:LYS:HZ2	2.21	0.54
1:3:249:CYS:SG	1:3:250:SER:N	2.79	0.54
1:4:105:SER:C	1:4:107:HIS:N	2.66	0.54
1:4:171:MET:O	1:4:227:MET:N	2.32	0.54
1:4:182:LYS:HE2	1:4:187:PRO:HG2	1.90	0.54
1:1:128:VAL:N	1:1:132:ASN:HB3	2.22	0.54
1:1:141:THR:OG1	1:1:142:VAL:HB	2.08	0.54
1:1:154:ALA:CB	1:1:155:PRO:CD	2.65	0.54
1:2:97:VAL:C	1:2:98:PHE:CD1	2.78	0.54
1:2:296:GLY:HA2	1:3:227:MET:SD	2.47	0.54
1:3:8:PHE:HD1	1:3:29:VAL:CG1	2.17	0.54
1:3:220:LEU:HD12	1:3:223:LYS:HG3	1.89	0.54
1:3:329:LYS:HZ3	1:3:330:VAL:N	2.05	0.54
1:4:6:ASN:O	1:4:94:SER:HB3	2.08	0.54
1:4:126:MET:CG	1:4:146:ALA:HB2	2.37	0.54
1:4:175:HIS:CG	1:4:230:ARG:HH21	2.26	0.54
1:4:279:SER:C	1:4:281:ASP:N	2.65	0.54
1:4:314:PHE:HB2	1:4:317:SER:HB2	1.89	0.54
1:1:14:LEU:HA	1:1:17:ARG:CG	2.35	0.54
1:1:70:ILE:O	1:1:70:ILE:HG12	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:217:ILE:HG23	1:2:220:LEU:HD23	1.90	0.54
1:3:167:VAL:CG2	1:3:168:GLU:N	2.71	0.54
1:4:57:LYS:CD	1:4:58:MET:HE1	2.38	0.54
1:4:113:LYS:HG2	1:4:114:LYS:HE3	1.90	0.54
1:4:127:PHE:HD2	1:4:132:ASN:HA	1.72	0.54
1:4:152:CYS:SG	1:4:239:VAL:HG13	2.48	0.54
1:1:253:ASP:C	1:1:255:LYS:H	2.13	0.53
1:1:328:GLN:HE21	1:1:328:GLN:HA	1.73	0.53
1:2:58:MET:HA	1:2:62:ALA:O	2.08	0.53
1:2:78:PRO:C	1:2:80:ASN:N	2.64	0.53
1:2:152:CYS:SG	1:2:152:CYS:O	2.66	0.53
1:3:81:ILE:CG2	1:3:83:TRP:CE2	2.92	0.53
1:3:117:ILE:C	1:3:119:ALA:N	2.66	0.53
1:3:305:LYS:O	1:3:305:LYS:HG2	2.05	0.53
1:4:220:LEU:CA	1:4:223:LYS:NZ	2.67	0.53
1:4:292:ASP:OD1	1:4:295:ALA:HB3	2.08	0.53
1:1:189:ALA:C	1:1:190:LYS:HD3	2.34	0.53
1:1:211:LYS:HA	1:1:211:LYS:HZ2	1.68	0.53
1:3:56:VAL:O	1:3:56:VAL:CG1	2.55	0.53
1:3:74:ASN:HA	2:3:377:HOH:O	2.08	0.53
1:3:280:SER:O	2:3:387:HOH:O	2.19	0.53
1:4:8:PHE:HD1	1:4:29:VAL:CG1	2.21	0.53
1:4:17:ARG:HG2	1:4:43:PHE:CE2	2.43	0.53
1:4:301:LYS:HB2	1:4:301:LYS:NZ	2.21	0.53
1:1:5:ILE:HG23	1:1:92:VAL:CG1	2.38	0.53
1:1:101:ILE:HG22	1:1:105:SER:HG	1.70	0.53
1:1:129:CYS:CB	1:1:269:PHE:CE1	2.90	0.53
1:1:153:LEU:O	1:1:154:ALA:O	2.25	0.53
1:2:152:CYS:SG	1:2:239:VAL:HG12	2.48	0.53
1:2:297:ILE:HD13	1:2:297:ILE:O	2.07	0.53
1:2:301:LYS:O	1:2:302:THR:CG2	2.56	0.53
1:4:1:SER:CB	1:4:25:GLN:HB2	2.36	0.53
1:4:39:MET:O	1:4:43:PHE:N	2.40	0.53
1:1:104:ALA:O	1:1:105:SER:C	2.50	0.53
1:2:282:PHE:O	1:2:283:ILE:C	2.51	0.53
1:3:18:ALA:O	1:3:19:ALA:C	2.51	0.53
1:3:83:TRP:HA	1:3:86:ALA:HB1	1.90	0.53
1:3:254:ILE:O	1:3:255:LYS:O	2.27	0.53
1:4:42:MET:O	1:4:42:MET:HG2	2.07	0.53
1:4:161:HIS:O	1:4:162:GLU:C	2.50	0.53
1:1:296:GLY:N	1:1:297:ILE:CD1	2.71	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:113:LYS:CG	1:2:114:LYS:CE	2.81	0.53
1:2:213:VAL:O	1:2:214:GLY:C	2.52	0.53
1:2:271:GLY:O	1:2:272:TYR:HB3	2.09	0.53
1:2:298:GLN:OE1	1:3:226:GLY:N	2.41	0.53
1:3:155:PRO:HB3	1:3:266:LEU:HD23	1.90	0.53
1:3:196:ARG:NE	1:4:47:SER:OG	2.42	0.53
1:1:8:PHE:CD1	1:1:29:VAL:HG11	2.43	0.53
1:1:44:LYS:CG	1:1:56:VAL:HG11	2.38	0.53
1:2:243:VAL:CG2	1:2:245:LEU:CD2	2.87	0.53
1:4:238:VAL:HG22	1:4:307:VAL:HG22	1.91	0.53
1:1:101:ILE:HG23	1:1:142:VAL:HG21	1.90	0.53
1:1:161:HIS:CG	1:1:162:GLU:H	2.24	0.53
1:1:252:ASP:O	1:1:255:LYS:CA	2.56	0.53
1:2:117:ILE:C	1:2:119:ALA:H	2.17	0.53
1:3:52:PHE:C	1:3:53:LYS:HZ3	2.17	0.53
1:3:205:SER:CB	1:3:228:ALA:HB3	2.33	0.53
1:4:276:ASP:OD1	1:4:277:VAL:CG2	2.52	0.53
1:2:296:GLY:CA	1:2:307:VAL:HG21	2.37	0.53
1:3:132:ASN:CG	1:3:133:LEU:N	2.67	0.53
1:3:156:VAL:HG22	1:3:258:MET:CE	2.32	0.53
1:4:259:LYS:C	1:4:261:ALA:H	2.15	0.53
1:4:259:LYS:O	1:4:261:ALA:N	2.41	0.53
1:1:263:GLU:O	1:1:264:GLY:C	2.52	0.53
1:4:117:ILE:HG13	1:4:144:SER:HB2	1.91	0.53
1:1:56:VAL:O	1:1:57:LYS:CE	2.57	0.53
1:2:56:VAL:O	1:2:56:VAL:HG22	2.08	0.53
1:2:283:ILE:O	1:2:283:ILE:HG22	2.07	0.53
1:3:6:ASN:HD22	1:3:93:GLU:CD	2.17	0.53
1:3:278:VAL:HA	1:3:281:ASP:OD2	2.08	0.53
1:4:171:MET:HA	1:4:240:ASP:O	2.09	0.53
1:2:177:VAL:HA	1:2:181:GLN:OE1	2.09	0.52
1:3:129:CYS:O	1:3:133:LEU:CG	2.57	0.52
1:3:235:ASP:CG	1:3:235:ASP:O	2.51	0.52
1:4:71:THR:CG2	1:4:73:PHE:CE1	2.92	0.52
1:4:131:VAL:O	1:4:132:ASN:O	2.27	0.52
1:4:153:LEU:HD13	1:4:213:VAL:HG21	1.90	0.52
1:4:177:VAL:HG13	1:4:231:VAL:O	2.08	0.52
1:1:44:LYS:HD2	1:1:56:VAL:HG11	1.90	0.52
1:1:220:LEU:HA	1:1:223:LYS:CE	2.35	0.52
1:1:265:PRO:CG	2:1:442:HOH:O	2.54	0.52
1:2:216:VAL:HG12	1:2:217:ILE:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:41:TYR:CZ	1:4:277:VAL:HG11	2.45	0.52
1:3:129:CYS:O	1:3:130:GLY:C	2.52	0.52
1:3:200:GLN:C	1:3:201:ASN:ND2	2.58	0.52
1:4:4:GLY:N	1:4:27:VAL:HG21	2.24	0.52
1:4:247:LYS:O	1:4:248:GLU:C	2.49	0.52
1:1:11:ILE:CD1	1:1:11:ILE:N	2.72	0.52
1:1:164:PHE:HZ	1:1:253:ASP:HB3	1.74	0.52
1:2:186:GLY:N	1:2:195:GLY:O	2.43	0.52
1:2:327:MET:HB3	1:2:331:ASP:OD2	2.09	0.52
1:3:152:CYS:SG	1:3:239:VAL:CG1	2.97	0.52
1:3:181:GLN:HE21	1:3:203:ILE:HD13	1.74	0.52
1:1:193:ARG:NH2	1:4:295:ALA:CB	2.59	0.52
1:1:294:LYS:C	1:1:297:ILE:HD11	2.34	0.52
1:2:119:ALA:HB1	1:2:120:PRO:CD	2.39	0.52
1:2:231:VAL:HB	1:3:231:VAL:CG1	2.38	0.52
1:2:251:TYR:CA	1:2:299:LEU:HD12	2.33	0.52
1:3:82:PRO:O	1:3:83:TRP:CG	2.62	0.52
1:3:126:MET:HE3	1:3:212:ALA:HA	1.91	0.52
1:4:104:ALA:CB	1:4:142:VAL:HG21	2.39	0.52
1:4:104:ALA:HB3	1:4:142:VAL:HG21	1.92	0.52
1:4:40:VAL:CG2	1:4:41:TYR:N	2.72	0.52
1:4:182:LYS:HE2	1:4:187:PRO:O	2.09	0.52
1:4:322:ASP:O	1:4:323:LEU:C	2.52	0.52
1:1:90:TYR:HD1	1:1:90:TYR:H	1.57	0.52
1:1:127:PHE:CD1	1:1:143:VAL:CG2	2.92	0.52
1:2:3:ILE:O	1:2:27:VAL:CG2	2.54	0.52
1:2:227:MET:CE	1:3:296:GLY:HA3	2.40	0.52
1:2:269:PHE:O	1:2:288:SER:HB2	2.08	0.52
1:4:98:PHE:HA	1:4:103:LYS:HB3	1.91	0.52
1:1:178:THR:O	1:1:179:ALA:C	2.52	0.52
1:2:14:LEU:HD13	1:2:14:LEU:N	2.24	0.52
1:2:28:ALA:HB1	1:2:73:PHE:CE2	2.44	0.52
1:2:113:LYS:CB	1:2:114:LYS:HG2	2.39	0.52
1:3:14:LEU:O	1:3:18:ALA:HB2	2.09	0.52
1:3:68:LYS:O	1:3:70:ILE:HG23	2.09	0.52
1:4:34:ILE:O	1:4:34:ILE:CG2	2.57	0.52
1:4:183:THR:HB	1:4:184:VAL:CG1	2.37	0.52
1:4:327:MET:O	1:4:328:GLN:C	2.52	0.52
1:1:27:VAL:H	1:1:70:ILE:HB	1.75	0.52
1:1:63:LEU:HD22	1:1:65:VAL:HG12	1.92	0.52
1:1:193:ARG:CB	1:4:277:VAL:HG12	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:36:LEU:HD12	1:2:36:LEU:C	2.35	0.52
1:2:78:PRO:CD	1:2:98:PHE:CE2	2.92	0.52
1:2:81:ILE:HD13	1:2:82:PRO:HD2	1.92	0.52
1:2:176:ALA:O	1:2:177:VAL:O	2.28	0.52
1:3:294:LYS:C	1:3:297:ILE:HD11	2.29	0.52
1:4:132:ASN:CG	1:4:133:LEU:H	2.18	0.52
1:1:3:ILE:C	1:1:27:VAL:CG2	2.83	0.52
1:2:113:LYS:C	1:2:114:LYS:CG	2.73	0.52
1:2:270:LEU:HD23	1:2:271:GLY:N	2.25	0.52
1:2:277:VAL:HG11	1:4:41:TYR:CZ	2.45	0.52
1:3:296:GLY:N	1:3:297:ILE:HD13	2.25	0.52
1:4:32:PRO:CB	1:4:74:ASN:HD21	2.20	0.52
1:4:78:PRO:HD3	1:4:98:PHE:HE2	1.75	0.52
1:1:39:MET:O	1:1:43:PHE:N	2.44	0.51
1:1:160:LEU:O	1:1:164:PHE:N	2.42	0.51
1:1:205:SER:O	1:1:206:SER:C	2.53	0.51
1:1:244:ARG:CZ	1:4:244:ARG:NE	2.73	0.51
1:2:6:ASN:CA	1:2:30:ASN:ND2	2.68	0.51
1:2:51:VAL:CG2	2:2:401:HOH:O	2.57	0.51
1:2:173:THR:HG22	1:2:228:ALA:HB2	1.91	0.51
1:2:298:GLN:CD	1:3:225:THR:CG2	2.83	0.51
1:3:83:TRP:N	1:3:86:ALA:CB	2.73	0.51
1:4:114:LYS:CD	1:4:114:LYS:N	2.70	0.51
1:1:117:ILE:HB	1:1:144:SER:HB2	1.90	0.51
1:1:128:VAL:HG13	1:1:151:ASN:HD22	1.74	0.51
1:1:188:SER:OG	1:1:195:GLY:CA	2.58	0.51
1:1:208:GLY:HA3	1:1:211:LYS:HG3	1.85	0.51
1:1:211:LYS:NZ	1:1:211:LYS:CA	2.62	0.51
1:1:276:ASP:C	1:1:277:VAL:HG22	2.32	0.51
1:2:97:VAL:O	1:2:98:PHE:CE1	2.54	0.51
1:2:113:LYS:HG2	1:2:114:LYS:CE	2.26	0.51
1:2:113:LYS:CE	1:2:114:LYS:NZ	2.69	0.51
1:2:236:VAL:HG22	1:2:311:ASP:HA	1.92	0.51
1:2:277:VAL:CB	1:4:41:TYR:OH	2.56	0.51
1:3:2:LYS:HZ1	1:3:87:GLY:C	2.10	0.51
1:3:79:GLU:HB2	1:3:109:LYS:HB3	1.91	0.51
1:3:171:MET:CG	1:3:172:THR:N	2.66	0.51
1:4:57:LYS:O	1:4:64:VAL:HG13	2.10	0.51
1:1:32:PRO:HA	1:1:74:ASN:CG	2.32	0.51
1:2:46:ASP:O	1:2:50:GLY:CA	2.59	0.51
1:4:89:GLU:HG3	1:4:90:TYR:CE1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:89:GLU:CG	1:4:90:TYR:HD1	2.15	0.51
1:1:54:GLY:CA	1:1:66:ASP:CG	2.83	0.51
1:1:74:ASN:HB2	2:1:425:HOH:O	2.11	0.51
1:1:272:TYR:OH	1:1:274:GLU:HG2	2.10	0.51
1:1:309:TRP:H	1:1:309:TRP:HD1	1.55	0.51
1:2:200:GLN:C	1:2:201:ASN:HD22	2.18	0.51
1:3:20:LEU:C	1:3:22:CYS:N	2.69	0.51
1:3:26:VAL:HG11	1:3:68:LYS:HG3	1.92	0.51
1:3:188:SER:HB2	1:3:195:GLY:CA	2.39	0.51
1:3:276:ASP:O	1:3:278:VAL:CG2	2.55	0.51
1:4:89:GLU:OE1	1:4:90:TYR:CE1	2.55	0.51
1:1:113:LYS:HB3	1:1:114:LYS:NZ	2.26	0.51
1:1:205:SER:HB3	1:1:228:ALA:CB	2.38	0.51
1:1:255:LYS:HD2	1:1:293:ALA:HB1	1.93	0.51
1:1:270:LEU:HA	1:1:289:SER:O	2.10	0.51
1:1:328:GLN:HE21	1:1:328:GLN:CA	2.23	0.51
1:2:225:THR:CB	1:3:298:GLN:HE22	2.23	0.51
1:2:272:TYR:HH	1:2:274:GLU:CD	2.18	0.51
1:2:327:MET:O	1:2:328:GLN:C	2.53	0.51
1:3:3:ILE:HD11	1:3:24:ALA:HB1	1.91	0.51
1:3:78:PRO:HD3	1:3:98:PHE:CE2	2.46	0.51
1:3:172:THR:N	1:3:240:ASP:O	2.36	0.51
1:1:117:ILE:HD11	1:1:142:VAL:O	2.10	0.51
1:1:160:LEU:CD2	1:1:254:ILE:HD12	2.37	0.51
1:2:54:GLY:O	1:2:56:VAL:HG12	2.10	0.51
1:2:137:SER:O	1:2:140:MET:CG	2.58	0.51
1:2:153:LEU:O	1:2:153:LEU:CD2	2.54	0.51
1:2:153:LEU:CD2	1:2:157:ALA:HB2	2.40	0.51
1:2:188:SER:CB	1:2:192:TRP:HA	2.41	0.51
1:2:196:ARG:NH2	1:3:281:ASP:OD2	2.43	0.51
1:2:329:LYS:NZ	1:2:330:VAL:N	2.58	0.51
1:3:82:PRO:HB2	1:3:85:LYS:O	2.11	0.51
1:4:251:TYR:CE1	1:4:297:ILE:HG12	2.44	0.51
1:1:113:LYS:CB	1:1:114:LYS:CE	2.86	0.51
1:1:236:VAL:HG12	1:1:237:SER:N	2.26	0.51
1:1:288:SER:HB2	1:1:319:ARG:NH1	2.25	0.51
1:2:295:ALA:CA	1:2:297:ILE:HD12	2.40	0.51
1:3:207:THR:HG1	1:3:208:GLY:H	1.54	0.51
1:4:27:VAL:CG2	1:4:28:ALA:N	2.45	0.51
1:1:175:HIS:O	1:1:231:VAL:CG2	2.58	0.51
1:2:153:LEU:O	1:2:154:ALA:C	2.54	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:225:THR:HG21	1:3:298:GLN:HE22	1.66	0.51
1:3:83:TRP:HA	1:3:86:ALA:CB	2.40	0.51
1:3:250:SER:O	1:3:251:TYR:C	2.54	0.51
1:4:129:CYS:O	1:4:130:GLY:C	2.53	0.51
1:1:159:VAL:O	1:1:160:LEU:C	2.52	0.51
1:1:196:ARG:NH2	1:4:281:ASP:CG	2.69	0.51
1:2:27:VAL:HG13	1:2:28:ALA:O	2.10	0.51
1:2:188:SER:O	1:2:190:LYS:C	2.54	0.51
1:2:188:SER:HB2	1:2:195:GLY:HA3	1.93	0.51
1:2:242:THR:C	1:2:243:VAL:CG1	2.83	0.51
1:3:153:LEU:HD23	1:3:156:VAL:HG12	1.93	0.51
1:3:168:GLU:OE2	1:3:244:ARG:CZ	2.59	0.51
1:4:265:PRO:CA	2:4:453:HOH:O	2.57	0.51
1:1:32:PRO:O	1:1:34:ILE:HG22	2.11	0.51
1:1:90:TYR:N	1:1:90:TYR:HD1	2.09	0.51
1:2:7:GLY:O	1:2:8:PHE:HB3	2.10	0.51
1:2:53:LYS:HE2	1:2:53:LYS:N	2.26	0.51
1:2:127:PHE:HA	1:2:132:ASN:HB2	1.92	0.51
1:2:276:ASP:OD1	1:2:277:VAL:HG22	2.10	0.51
1:3:103:LYS:O	1:3:106:ALA:HB3	2.11	0.51
1:3:127:PHE:HD2	1:3:132:ASN:HA	1.74	0.51
1:3:184:VAL:O	1:3:185:ASP:O	2.29	0.51
1:3:301:LYS:NZ	1:3:301:LYS:HB2	2.25	0.51
1:4:89:GLU:CG	1:4:90:TYR:CD1	2.86	0.51
1:1:16:LEU:C	1:1:18:ALA:N	2.69	0.50
1:1:44:LYS:O	1:1:51:VAL:CA	2.58	0.50
1:2:32:PRO:O	1:2:34:ILE:HG22	2.10	0.50
1:2:235:ASP:CG	1:2:313:GLU:HG3	2.35	0.50
1:2:281:ASP:O	1:2:283:ILE:CB	2.58	0.50
1:2:303:PHE:HE2	1:3:303:PHE:CE2	2.29	0.50
1:4:169:GLY:C	1:4:224:LEU:HD23	2.36	0.50
1:4:175:HIS:N	1:4:229:PHE:O	2.44	0.50
1:2:181:GLN:HE22	1:2:230:ARG:CB	2.25	0.50
1:2:272:TYR:CE2	1:2:293:ALA:HB2	2.46	0.50
1:3:81:ILE:HD12	1:3:83:TRP:CH2	2.47	0.50
1:3:283:ILE:O	1:3:284:GLY:C	2.53	0.50
1:4:217:ILE:CG1	1:4:220:LEU:HD22	2.40	0.50
1:1:3:ILE:C	1:1:27:VAL:HG23	2.35	0.50
1:1:11:ILE:O	1:1:15:VAL:HG23	2.10	0.50
1:1:145:ASN:O	1:1:146:ALA:C	2.55	0.50
1:1:235:ASP:CG	1:1:235:ASP:O	2.52	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:149:THR:O	1:2:152:CYS:N	2.44	0.50
1:3:9:GLY:HA2	1:3:13:ARG:NH2	2.25	0.50
1:3:14:LEU:HA	1:3:17:ARG:HG3	1.92	0.50
1:3:38:TYR:O	1:3:42:MET:N	2.41	0.50
1:3:168:GLU:CG	1:3:244:ARG:HD2	2.41	0.50
1:3:213:VAL:HA	1:3:216:VAL:HG12	1.93	0.50
1:3:329:LYS:HB3	1:3:329:LYS:NZ	2.27	0.50
1:4:125:PRO:CG	1:4:140:MET:CE	2.74	0.50
1:1:19:ALA:HA	1:1:24:ALA:HB3	1.91	0.50
1:1:66:ASP:O	1:1:68:LYS:CD	2.53	0.50
1:3:117:ILE:HG22	1:3:119:ALA:O	2.11	0.50
1:3:129:CYS:O	1:3:133:LEU:CD1	2.59	0.50
1:3:250:SER:HA	1:3:299:LEU:HD12	1.92	0.50
1:3:266:LEU:O	1:3:267:GLN:C	2.54	0.50
1:4:134:GLU:O	1:4:136:TYR:N	2.45	0.50
1:4:180:THR:CG2	1:4:181:GLN:H	2.21	0.50
1:4:243:VAL:CG2	1:4:304:VAL:CG1	2.89	0.50
1:1:92:VAL:O	1:1:92:VAL:HG12	2.10	0.50
1:1:329:LYS:HZ2	1:1:330:VAL:N	2.05	0.50
1:2:6:ASN:HA	1:2:30:ASN:HD22	1.71	0.50
1:3:2:LYS:HZ3	1:3:88:ALA:HA	1.75	0.50
1:3:116:VAL:HA	1:3:143:VAL:O	2.11	0.50
1:4:98:PHE:HA	1:4:103:LYS:CD	2.41	0.50
1:4:218:PRO:C	1:4:220:LEU:H	2.18	0.50
1:1:16:LEU:C	1:1:18:ALA:H	2.20	0.50
1:1:112:ALA:O	1:1:113:LYS:CG	2.59	0.50
1:1:119:ALA:CB	1:1:120:PRO:CD	2.75	0.50
1:1:148:CYS:SG	1:1:149:THR:N	2.84	0.50
1:2:319:ARG:HG2	1:2:319:ARG:HH11	1.74	0.50
1:3:156:VAL:HA	1:3:258:MET:HE3	1.94	0.50
1:3:161:HIS:HB2	1:3:166:ILE:CD1	2.36	0.50
1:3:174:VAL:HG12	1:3:231:VAL:HG21	1.92	0.50
1:3:239:VAL:CG1	1:3:310:TYR:HE1	2.20	0.50
1:4:221:ASP:C	1:4:221:ASP:OD2	2.55	0.50
1:1:71:THR:HG22	1:1:72:VAL:C	2.37	0.50
1:1:129:CYS:HB3	1:1:269:PHE:CD1	2.45	0.50
1:1:175:HIS:CG	1:1:230:ARG:HH21	2.30	0.50
1:2:161:HIS:HB2	1:2:166:ILE:CD1	2.41	0.50
1:3:68:LYS:O	1:3:70:ILE:CG2	2.59	0.50
1:4:78:PRO:CG	1:4:98:PHE:HE2	2.16	0.50
1:4:95:THR:HG22	1:4:97:VAL:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:243:VAL:CG2	1:4:304:VAL:HG12	2.34	0.50
1:1:173:THR:O	1:1:228:ALA:HA	2.11	0.50
1:2:46:ASP:HB3	1:2:50:GLY:N	2.23	0.50
1:2:102:GLU:C	1:2:102:GLU:OE1	2.54	0.50
1:2:117:ILE:HD12	1:2:144:SER:CB	2.41	0.50
1:3:43:PHE:HE1	1:3:65:VAL:HG21	1.77	0.50
1:4:10:ARG:O	1:4:14:LEU:HD23	2.12	0.50
1:4:259:LYS:O	1:4:260:THR:C	2.54	0.50
1:4:276:ASP:O	1:4:277:VAL:C	2.55	0.50
1:1:134:GLU:OE2	1:1:134:GLU:O	2.30	0.50
1:1:266:LEU:HD23	1:1:270:LEU:HB2	1.92	0.50
1:1:277:VAL:CG1	1:4:193:ARG:HG3	2.41	0.50
1:1:295:ALA:HB2	1:4:193:ARG:CZ	2.40	0.50
1:2:73:PHE:CE1	1:2:82:PRO:HG2	2.46	0.50
1:2:329:LYS:NZ	1:2:329:LYS:HB3	2.23	0.50
1:4:17:ARG:CG	1:4:43:PHE:HE2	2.24	0.50
1:4:108:PHE:CG	1:4:109:LYS:N	2.80	0.50
1:1:157:ALA:O	1:1:158:LYS:C	2.55	0.49
1:2:28:ALA:HB1	1:2:73:PHE:HE2	1.77	0.49
1:2:75:GLU:HB3	2:2:408:HOH:O	2.11	0.49
1:2:192:TRP:H	1:2:192:TRP:HD1	1.59	0.49
1:3:129:CYS:CA	1:3:132:ASN:HD22	2.21	0.49
1:4:297:ILE:HD13	1:4:298:GLN:N	2.27	0.49
1:1:30:ASN:ND2	1:1:30:ASN:C	2.69	0.49
1:1:101:ILE:HG12	1:1:142:VAL:CG1	2.43	0.49
1:1:176:ALA:O	1:1:177:VAL:C	2.55	0.49
1:1:304:VAL:HG12	1:1:304:VAL:O	2.11	0.49
1:2:4:GLY:HA2	1:2:27:VAL:HG21	1.92	0.49
1:2:13:ARG:C	1:2:15:VAL:N	2.69	0.49
1:3:135:LYS:HG3	1:3:135:LYS:O	2.11	0.49
1:4:238:VAL:CG2	1:4:307:VAL:HG22	2.42	0.49
1:4:251:TYR:HB2	1:4:299:LEU:HG	1.93	0.49
1:1:150:THR:HG21	1:1:212:ALA:HB1	1.95	0.49
1:3:117:ILE:O	1:3:119:ALA:N	2.40	0.49
1:3:276:ASP:O	1:3:278:VAL:N	2.45	0.49
1:4:76:MET:O	1:4:76:MET:CG	2.60	0.49
1:4:170:LEU:CD2	1:4:225:THR:HG23	2.42	0.49
1:1:124:ALA:O	1:1:125:PRO:C	2.53	0.49
1:2:149:THR:O	1:2:152:CYS:CB	2.60	0.49
1:2:272:TYR:CD1	1:2:272:TYR:C	2.89	0.49
1:3:71:THR:C	1:3:72:VAL:HG12	2.36	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:115:VAL:HG12	1:3:116:VAL:N	2.27	0.49
1:3:181:GLN:NE2	1:3:203:ILE:HD13	2.28	0.49
1:4:127:PHE:HD2	1:4:132:ASN:CA	2.25	0.49
1:4:272:TYR:H	1:4:291:PHE:H	1.58	0.49
1:1:170:LEU:O	1:1:241:LEU:HA	2.12	0.49
1:2:1:SER:C	1:2:2:LYS:CG	2.77	0.49
1:2:188:SER:O	1:2:189:ALA:C	2.56	0.49
1:2:328:GLN:O	1:2:332:SER:HB2	2.13	0.49
1:3:27:VAL:O	1:3:28:ALA:CB	2.60	0.49
1:3:38:TYR:O	1:3:42:MET:HB2	2.12	0.49
1:3:292:ASP:OD2	1:3:295:ALA:CB	2.54	0.49
1:1:181:GLN:O	1:1:182:LYS:C	2.56	0.49
1:2:46:ASP:O	1:2:50:GLY:HA3	2.13	0.49
1:2:279:SER:O	1:2:281:ASP:N	2.42	0.49
1:3:81:ILE:HG21	1:3:83:TRP:CE2	2.48	0.49
1:3:282:PHE:O	1:3:285:ASP:HB3	2.12	0.49
1:4:83:TRP:HA	1:4:86:ALA:HB3	1.84	0.49
1:4:272:TYR:CD2	1:4:291:PHE:HD1	2.30	0.49
1:1:81:ILE:HD12	1:1:82:PRO:O	2.12	0.49
1:2:30:ASN:ND2	1:2:30:ASN:O	2.46	0.49
1:2:66:ASP:C	1:2:68:LYS:HD3	2.35	0.49
1:3:37:GLU:HA	1:3:40:VAL:HG13	1.95	0.49
1:3:84:SER:O	1:3:86:ALA:N	2.45	0.49
1:3:199:ALA:HB2	2:3:383:HOH:O	2.12	0.49
1:3:319:ARG:CG	1:3:319:ARG:HH11	2.23	0.49
1:4:165:GLU:O	1:4:166:ILE:HB	2.12	0.49
1:1:193:ARG:CA	1:4:277:VAL:HG12	2.42	0.49
1:2:129:CYS:CB	1:2:269:PHE:CE1	2.96	0.49
1:2:205:SER:OG	1:2:206:SER:O	2.29	0.49
1:3:95:THR:HA	2:3:376:HOH:O	2.13	0.49
1:3:155:PRO:HB3	1:3:266:LEU:CD2	2.43	0.49
1:4:73:PHE:CD2	1:4:81:ILE:HD11	2.47	0.49
1:1:132:ASN:ND2	1:1:133:LEU:CG	2.75	0.49
1:1:219:GLU:O	1:1:223:LYS:CE	2.61	0.49
1:1:236:VAL:HG12	1:1:237:SER:H	1.78	0.49
1:1:322:ASP:O	1:1:323:LEU:O	2.30	0.49
1:1:329:LYS:HZ2	1:1:329:LYS:C	2.21	0.49
1:2:55:GLU:HB3	1:2:67:GLY:H	1.77	0.49
1:2:126:MET:CG	1:2:146:ALA:HB2	2.43	0.49
1:2:279:SER:C	1:2:281:ASP:H	2.20	0.49
1:3:100:THR:O	1:3:101:ILE:C	2.54	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:116:VAL:HG11	1:3:324:LEU:HD22	1.93	0.49
1:3:159:VAL:O	1:3:163:ASN:CB	2.61	0.49
1:3:241:LEU:HG	1:3:243:VAL:CG1	2.41	0.49
1:3:295:ALA:O	1:3:307:VAL:HG11	2.12	0.49
1:3:314:PHE:CG	1:3:314:PHE:O	2.63	0.49
1:3:319:ARG:NH1	1:3:319:ARG:CG	2.75	0.49
1:4:77:LYS:HA	1:4:77:LYS:HD2	1.52	0.49
1:4:81:ILE:CG2	1:4:83:TRP:NE1	2.76	0.49
1:4:218:PRO:O	1:4:220:LEU:N	2.46	0.49
1:4:314:PHE:O	1:4:314:PHE:CG	2.63	0.49
1:2:11:ILE:O	1:2:15:VAL:CG2	2.61	0.49
1:2:126:MET:HG3	1:2:146:ALA:HB2	1.95	0.49
1:2:129:CYS:SG	1:2:269:PHE:CE1	3.05	0.49
1:2:298:GLN:OE1	1:3:225:THR:CG2	2.60	0.49
1:3:273:THR:OG1	1:3:274:GLU:N	2.46	0.49
1:3:290:ILE:O	1:3:308:SER:OG	2.31	0.49
1:3:291:PHE:HE2	1:3:306:VAL:HB	1.78	0.49
1:4:100:THR:O	1:4:103:LYS:N	2.46	0.49
1:4:131:VAL:HG22	1:4:132:ASN:N	2.28	0.49
1:4:159:VAL:HB	1:4:258:MET:HE3	1.95	0.49
1:4:282:PHE:HE1	1:4:290:ILE:HD13	1.76	0.49
1:1:295:ALA:C	1:1:297:ILE:HD12	2.38	0.48
1:2:51:VAL:HB	2:2:400:HOH:O	2.13	0.48
1:2:66:ASP:HB2	1:2:68:LYS:CE	2.42	0.48
1:2:150:THR:HG21	1:2:212:ALA:HB1	1.94	0.48
1:2:174:VAL:CG2	1:2:238:VAL:HG13	2.43	0.48
1:2:261:ALA:O	1:2:262:SER:C	2.56	0.48
1:3:37:GLU:HA	1:3:40:VAL:HG11	1.92	0.48
1:3:74:ASN:O	1:3:75:GLU:HG2	2.13	0.48
1:3:221:ASP:O	1:3:221:ASP:OD2	2.31	0.48
1:3:250:SER:O	1:3:253:ASP:N	2.45	0.48
1:4:30:ASN:HD22	1:4:30:ASN:C	2.10	0.48
1:4:170:LEU:HD23	1:4:225:THR:HG22	1.95	0.48
1:1:188:SER:O	1:1:190:LYS:CA	2.56	0.48
1:1:238:VAL:HG23	1:1:309:TRP:CD2	2.48	0.48
1:1:277:VAL:CB	1:3:41:TYR:OH	2.60	0.48
1:2:10:ARG:HD3	1:2:10:ARG:HA	1.53	0.48
1:2:150:THR:O	1:2:151:ASN:C	2.54	0.48
1:2:177:VAL:HG13	1:2:233:THR:O	2.13	0.48
1:2:272:TYR:OH	1:2:274:GLU:OE2	2.24	0.48
1:3:55:GLU:O	1:3:66:ASP:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:104:ALA:C	1:3:106:ALA:N	2.64	0.48
1:3:217:ILE:HG23	1:3:220:LEU:HD23	1.95	0.48
1:4:83:TRP:HA	1:4:86:ALA:HB1	1.95	0.48
1:4:330:VAL:O	1:4:331:ASP:C	2.56	0.48
1:1:91:ILE:O	1:1:115:VAL:HA	2.12	0.48
1:1:101:ILE:O	1:1:105:SER:HB2	2.13	0.48
1:1:193:ARG:HG3	1:4:277:VAL:HG12	1.95	0.48
1:1:248:GLU:HG2	1:1:302:THR:HG21	1.96	0.48
1:1:277:VAL:HG11	1:3:41:TYR:HH	1.78	0.48
1:2:40:VAL:CG2	1:2:41:TYR:N	2.76	0.48
1:2:129:CYS:HA	1:2:132:ASN:HD22	1.77	0.48
1:3:167:VAL:CG2	1:3:168:GLU:H	2.25	0.48
1:3:301:LYS:NZ	1:3:301:LYS:CB	2.76	0.48
1:4:39:MET:O	1:4:40:VAL:C	2.56	0.48
1:4:129:CYS:SG	1:4:269:PHE:CE1	3.07	0.48
1:1:131:VAL:O	1:1:133:LEU:N	2.46	0.48
1:1:186:GLY:C	1:2:42:MET:HE1	2.38	0.48
1:1:296:GLY:H	1:1:297:ILE:CD1	2.26	0.48
1:2:41:TYR:OH	1:4:277:VAL:CB	2.61	0.48
1:2:93:GLU:OE2	1:2:98:PHE:CB	2.62	0.48
1:2:319:ARG:HH11	1:2:319:ARG:CG	2.27	0.48
1:3:292:ASP:OD1	1:3:292:ASP:O	2.31	0.48
1:4:8:PHE:CD1	1:4:29:VAL:HG11	2.48	0.48
1:4:155:PRO:O	1:4:159:VAL:HG23	2.13	0.48
1:1:34:ILE:HD11	1:1:39:MET:CG	2.40	0.48
1:1:282:PHE:CE1	1:1:290:ILE:HD13	2.49	0.48
1:3:117:ILE:HB	1:3:144:SER:CA	2.38	0.48
1:3:330:VAL:C	1:3:332:SER:N	2.69	0.48
1:4:1:SER:C	1:4:25:GLN:HB2	2.38	0.48
1:4:4:GLY:N	1:4:27:VAL:HG23	2.29	0.48
1:4:32:PRO:HB3	1:4:74:ASN:OD1	2.12	0.48
1:4:124:ALA:O	1:4:215:LYS:NZ	2.40	0.48
1:4:153:LEU:O	1:4:154:ALA:C	2.56	0.48
1:4:217:ILE:HD11	1:4:220:LEU:CD2	2.43	0.48
1:4:310:TYR:HB2	1:4:312:ASN:H	1.78	0.48
1:1:41:TYR:CG	1:1:41:TYR:O	2.66	0.48
1:1:170:LEU:HD22	1:1:170:LEU:HA	1.51	0.48
1:1:215:LYS:CD	1:1:215:LYS:O	2.62	0.48
1:1:292:ASP:OD1	1:1:295:ALA:CA	2.60	0.48
1:3:8:PHE:HZ	1:3:39:MET:HG2	1.71	0.48
1:3:113:LYS:CE	1:3:114:LYS:HZ2	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:130:GLY:HA3	1:3:158:LYS:HZ1	1.79	0.48
1:3:259:LYS:HD2	1:3:272:TYR:CE1	2.48	0.48
1:4:236:VAL:HG11	1:4:280:SER:HA	1.96	0.48
1:4:310:TYR:HB2	1:4:311:ASP:H	1.47	0.48
1:4:329:LYS:NZ	1:4:330:VAL:CA	2.77	0.48
1:1:292:ASP:HB3	1:1:307:VAL:HG13	1.96	0.48
1:2:83:TRP:CD1	1:2:112:ALA:HB2	2.49	0.48
1:2:104:ALA:O	1:2:107:HIS:N	2.46	0.48
1:2:173:THR:HG22	1:2:227:MET:O	2.14	0.48
1:2:190:LYS:HD3	2:2:427:HOH:O	2.13	0.48
1:2:196:ARG:HH11	1:2:196:ARG:CG	2.16	0.48
1:2:277:VAL:CG2	1:2:278:VAL:N	2.71	0.48
1:3:19:ALA:CB	1:3:24:ALA:HB3	2.42	0.48
1:3:169:GLY:C	1:3:224:LEU:HD23	2.39	0.48
1:3:276:ASP:OD2	1:3:276:ASP:N	2.47	0.48
1:1:244:ARG:HH22	1:4:244:ARG:HG3	1.78	0.48
1:2:27:VAL:CG2	1:2:28:ALA:H	2.23	0.48
1:3:53:LYS:HD2	1:3:54:GLY:N	2.29	0.48
1:3:164:PHE:CE2	1:3:249:CYS:HB3	2.49	0.48
1:3:287:ARG:NH1	1:3:290:ILE:HD12	2.28	0.48
1:4:17:ARG:CG	1:4:43:PHE:CE2	2.97	0.48
1:4:215:LYS:HG2	1:4:215:LYS:O	2.13	0.48
1:4:216:VAL:CG1	1:4:217:ILE:N	2.76	0.48
1:1:5:ILE:HG23	1:1:92:VAL:HG11	1.95	0.48
1:1:44:LYS:CD	1:1:56:VAL:HG11	2.43	0.48
1:1:79:GLU:HB2	1:1:109:LYS:HB3	1.95	0.48
1:1:225:THR:HG21	1:4:298:GLN:HE22	1.76	0.48
1:2:6:ASN:ND2	1:2:93:GLU:CD	2.68	0.48
1:2:27:VAL:HG22	1:2:28:ALA:N	2.29	0.48
1:2:70:ILE:HG12	1:2:70:ILE:O	2.13	0.48
1:2:153:LEU:CD2	1:2:153:LEU:C	2.87	0.48
1:2:201:ASN:HD22	1:2:201:ASN:N	2.10	0.48
1:3:19:ALA:HB1	1:3:24:ALA:CB	2.42	0.48
1:3:81:ILE:HG23	1:3:83:TRP:CE2	2.49	0.48
1:3:121:SER:HG	1:3:124:ALA:HB3	1.76	0.48
1:1:213:VAL:HG11	1:1:224:LEU:HD13	1.95	0.48
1:1:318:GLN:OE1	1:1:318:GLN:CA	2.53	0.48
1:2:161:HIS:O	1:2:163:ASN:N	2.47	0.48
1:2:184:VAL:O	1:2:185:ASP:HB2	2.13	0.48
1:2:185:ASP:CA	1:2:195:GLY:O	2.62	0.48
1:3:285:ASP:C	1:3:285:ASP:OD2	2.57	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:295:ALA:C	1:3:297:ILE:CG2	2.76	0.48
1:4:59:GLU:O	1:4:61:GLY:N	2.47	0.48
1:4:66:ASP:O	1:4:68:LYS:CE	2.62	0.48
1:4:183:THR:C	1:4:184:VAL:HG12	2.38	0.48
1:4:305:LYS:HB2	1:4:305:LYS:HZ3	1.77	0.48
1:1:32:PRO:HB2	1:1:33:PHE:CE1	2.49	0.47
1:1:305:LYS:CD	1:4:227:MET:SD	3.01	0.47
1:2:18:ALA:O	1:2:19:ALA:C	2.57	0.47
1:3:287:ARG:NH1	1:3:290:ILE:HD13	2.29	0.47
1:4:6:ASN:ND2	1:4:93:GLU:OE1	2.47	0.47
1:4:127:PHE:CE2	1:4:136:TYR:HB2	2.48	0.47
1:4:180:THR:HG23	1:4:181:GLN:N	2.21	0.47
1:1:53:LYS:CD	1:1:54:GLY:N	2.70	0.47
1:1:175:HIS:O	1:1:231:VAL:HG23	2.14	0.47
1:2:1:SER:HB3	1:2:25:GLN:HE21	1.78	0.47
1:2:255:LYS:HB3	1:2:255:LYS:HZ3	1.80	0.47
1:3:130:GLY:O	1:3:133:LEU:HD12	2.15	0.47
1:3:171:MET:HA	1:3:240:ASP:O	2.14	0.47
1:4:14:LEU:O	1:4:18:ALA:N	2.46	0.47
1:4:217:ILE:HG12	1:4:217:ILE:O	2.13	0.47
1:4:282:PHE:O	1:4:283:ILE:C	2.56	0.47
1:1:8:PHE:HB2	1:1:12:GLY:C	2.39	0.47
1:1:127:PHE:CZ	1:1:140:MET:SD	3.04	0.47
1:1:196:ARG:NH1	1:2:41:TYR:OH	2.47	0.47
1:2:295:ALA:HB2	1:3:193:ARG:NH1	2.24	0.47
1:3:104:ALA:O	1:3:106:ALA:N	2.45	0.47
1:3:105:SER:O	1:3:108:PHE:CD1	2.62	0.47
1:4:8:PHE:N	1:4:31:ASP:OD2	2.47	0.47
1:4:31:ASP:HB3	1:4:34:ILE:CG2	2.43	0.47
1:4:65:VAL:O	1:4:66:ASP:HB2	2.12	0.47
1:1:8:PHE:CD2	1:1:13:ARG:HG2	2.50	0.47
1:1:26:VAL:HB	1:1:70:ILE:CG2	2.43	0.47
1:1:113:LYS:HG2	1:1:114:LYS:HZ1	1.80	0.47
1:1:233:THR:HG21	1:4:202:ILE:HD11	1.96	0.47
1:1:250:SER:O	1:1:253:ASP:N	2.48	0.47
1:1:273:THR:O	1:1:293:ALA:HB3	2.15	0.47
1:1:296:GLY:HA2	1:4:227:MET:CG	2.44	0.47
1:2:81:ILE:CG2	1:2:83:TRP:NE1	2.77	0.47
1:2:303:PHE:HE2	1:3:303:PHE:CZ	2.32	0.47
1:3:27:VAL:CG2	1:3:28:ALA:O	2.59	0.47
1:3:100:THR:HG23	1:3:103:LYS:HD3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:211:LYS:HA	1:3:211:LYS:HZ3	1.79	0.47
1:1:138:LYS:CD	1:1:330:VAL:HG12	2.45	0.47
1:2:201:ASN:HB3	1:2:203:ILE:HG13	1.96	0.47
1:2:211:LYS:HA	1:2:211:LYS:HZ3	1.80	0.47
1:3:97:VAL:O	1:3:97:VAL:HG23	2.13	0.47
1:3:299:LEU:HD23	1:3:304:VAL:HG23	1.96	0.47
1:4:138:LYS:HE3	1:4:330:VAL:CG1	2.45	0.47
1:1:26:VAL:HG21	1:1:68:LYS:HG3	1.96	0.47
1:1:301:LYS:O	1:1:302:THR:HG22	2.15	0.47
1:1:328:GLN:N	1:1:328:GLN:HE21	2.13	0.47
1:2:66:ASP:HB3	2:2:402:HOH:O	2.13	0.47
1:2:126:MET:HB3	1:2:215:LYS:CD	2.44	0.47
1:2:193:ARG:NH2	1:3:295:ALA:CB	2.58	0.47
1:3:28:ALA:HB1	1:3:73:PHE:CE2	2.49	0.47
1:3:32:PRO:HB3	1:3:74:ASN:OD1	2.15	0.47
1:3:283:ILE:CD1	2:3:388:HOH:O	2.59	0.47
1:1:6:ASN:CB	1:1:30:ASN:HD21	2.28	0.47
1:1:101:ILE:O	1:1:102:GLU:C	2.57	0.47
1:1:101:ILE:C	1:1:105:SER:HG	2.14	0.47
1:1:134:GLU:O	1:1:135:LYS:C	2.57	0.47
1:1:174:VAL:CG1	1:1:231:VAL:CG2	2.89	0.47
1:1:188:SER:O	1:1:190:LYS:C	2.57	0.47
1:1:262:SER:O	1:1:267:GLN:HA	2.15	0.47
1:1:320:VAL:O	1:1:324:LEU:CB	2.62	0.47
1:2:25:GLN:HB2	1:2:25:GLN:HE21	1.31	0.47
1:2:150:THR:C	1:2:152:CYS:N	2.69	0.47
1:2:167:VAL:HG22	1:2:244:ARG:HG2	1.96	0.47
1:2:244:ARG:NH2	1:3:244:ARG:CG	2.70	0.47
1:2:249:CYS:SG	1:2:250:SER:N	2.88	0.47
1:2:326:HIS:O	1:2:327:MET:C	2.57	0.47
1:3:2:LYS:NZ	1:3:88:ALA:HA	2.30	0.47
1:3:34:ILE:HD11	1:3:39:MET:HG2	1.95	0.47
1:3:120:PRO:CD	1:3:120:PRO:O	2.62	0.47
1:3:146:ALA:O	1:3:316:TYR:CE1	2.67	0.47
1:3:149:THR:O	1:3:152:CYS:HB3	2.15	0.47
1:3:231:VAL:HA	1:3:232:PRO:HD2	1.77	0.47
1:3:314:PHE:HB2	1:3:317:SER:HB2	1.97	0.47
1:4:108:PHE:O	1:4:109:LYS:O	2.30	0.47
1:4:218:PRO:C	1:4:220:LEU:N	2.72	0.47
1:4:327:MET:O	1:4:331:ASP:N	2.47	0.47
1:1:73:PHE:CD2	1:1:81:ILE:HD11	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:8:PHE:CZ	1:2:39:MET:CG	2.91	0.47
1:3:11:ILE:O	1:3:12:GLY:C	2.58	0.47
1:3:101:ILE:HG12	1:3:142:VAL:HG13	1.96	0.47
1:4:170:LEU:HD21	1:4:225:THR:HG22	1.95	0.47
1:4:175:HIS:O	1:4:231:VAL:HG22	2.15	0.47
1:4:178:THR:O	1:4:179:ALA:C	2.58	0.47
1:1:14:LEU:CA	1:1:17:ARG:HG3	2.37	0.47
1:1:59:GLU:HB3	1:1:64:VAL:HG12	1.95	0.47
1:1:298:GLN:OE1	1:4:225:THR:CG2	2.61	0.47
1:2:17:ARG:CG	1:2:43:PHE:HE2	2.11	0.47
1:2:33:PHE:CD2	1:2:33:PHE:N	2.77	0.47
1:2:50:GLY:C	1:2:51:VAL:O	2.56	0.47
1:2:78:PRO:CG	1:2:98:PHE:HE2	2.17	0.47
1:2:137:SER:CB	1:2:138:LYS:HZ1	2.28	0.47
1:2:294:LYS:N	1:2:297:ILE:HG13	2.29	0.47
1:2:311:ASP:O	1:2:314:PHE:N	2.48	0.47
1:1:52:PHE:CA	1:1:53:LYS:HE2	2.42	0.47
1:1:101:ILE:N	1:1:123:ASP:OD1	2.36	0.47
1:1:129:CYS:HB2	1:1:319:ARG:HD3	1.96	0.47
1:1:282:PHE:O	1:1:283:ILE:C	2.57	0.47
1:2:25:GLN:C	1:2:26:VAL:O	2.58	0.47
1:2:73:PHE:CD1	1:2:82:PRO:HG2	2.50	0.47
1:2:130:GLY:C	1:2:158:LYS:NZ	2.73	0.47
1:2:201:ASN:N	1:2:201:ASN:ND2	2.62	0.47
1:2:247:LYS:C	1:2:248:GLU:O	2.57	0.47
1:3:26:VAL:CA	1:3:27:VAL:HG12	2.44	0.47
1:3:36:LEU:HD21	1:3:58:MET:HB3	1.97	0.47
1:3:270:LEU:HD23	1:3:271:GLY:H	1.67	0.47
1:4:66:ASP:O	1:4:68:LYS:HE2	2.15	0.47
1:1:105:SER:C	1:1:107:HIS:N	2.74	0.46
1:1:328:GLN:O	1:1:329:LYS:C	2.56	0.46
1:2:27:VAL:HG13	1:2:28:ALA:C	2.39	0.46
1:2:74:ASN:CA	2:2:407:HOH:O	2.53	0.46
1:2:133:LEU:O	1:2:136:TYR:HB3	2.15	0.46
1:2:184:VAL:O	1:2:184:VAL:HG13	2.15	0.46
1:2:197:GLY:O	1:2:201:ASN:HB2	2.15	0.46
1:2:252:ASP:O	1:2:255:LYS:HB2	2.15	0.46
1:3:74:ASN:OD1	1:3:74:ASN:C	2.59	0.46
1:3:188:SER:HB3	1:3:192:TRP:N	2.29	0.46
1:4:7:GLY:O	1:4:8:PHE:CB	2.63	0.46
1:4:38:TYR:O	1:4:42:MET:CB	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:188:SER:HB3	1:1:191:ASP:O	2.15	0.46
1:1:193:ARG:HG3	1:4:277:VAL:HA	1.97	0.46
1:2:44:LYS:HG3	1:2:56:VAL:HG11	1.97	0.46
1:2:71:THR:HG22	1:2:72:VAL:N	2.30	0.46
1:2:83:TRP:CA	1:2:86:ALA:CB	2.93	0.46
1:2:251:TYR:HB2	1:2:299:LEU:CB	2.38	0.46
1:3:321:ILE:O	1:3:324:LEU:CB	2.63	0.46
1:4:131:VAL:HG12	1:4:158:LYS:CE	2.44	0.46
1:1:108:PHE:O	1:1:110:GLY:N	2.48	0.46
1:1:161:HIS:O	1:1:165:GLU:N	2.42	0.46
1:1:279:SER:C	1:1:281:ASP:N	2.72	0.46
1:2:78:PRO:O	1:2:81:ILE:HG22	2.15	0.46
1:2:325:LYS:O	1:2:327:MET:N	2.48	0.46
1:2:332:SER:O	1:2:333:ALA:CB	2.63	0.46
1:3:16:LEU:HD21	1:3:70:ILE:HD12	1.97	0.46
1:3:26:VAL:O	1:3:27:VAL:HB	2.14	0.46
1:3:81:ILE:HG21	1:3:83:TRP:CZ2	2.50	0.46
1:3:151:ASN:O	1:3:155:PRO:HD2	2.15	0.46
1:3:156:VAL:HA	1:3:258:MET:CE	2.44	0.46
1:4:189:ALA:O	1:4:190:LYS:HD3	2.15	0.46
1:1:11:ILE:HG21	1:1:118:SER:OG	2.15	0.46
1:1:36:LEU:O	1:1:40:VAL:HG13	2.15	0.46
1:1:132:ASN:ND2	1:1:133:LEU:HG	2.30	0.46
1:1:160:LEU:HA	1:1:160:LEU:HD23	1.53	0.46
1:1:281:ASP:C	1:1:283:ILE:N	2.73	0.46
1:2:127:PHE:HD2	1:2:132:ASN:CB	2.29	0.46
1:2:165:GLU:O	1:2:166:ILE:CB	2.63	0.46
1:2:251:TYR:HE1	1:2:255:LYS:HD3	1.79	0.46
1:2:295:ALA:C	1:2:297:ILE:HD12	2.39	0.46
1:3:78:PRO:HD2	1:3:79:GLU:H	1.80	0.46
1:3:138:LYS:HZ1	1:3:330:VAL:CG1	2.09	0.46
1:4:127:PHE:HZ	1:4:135:LYS:HZ3	1.62	0.46
1:4:131:VAL:HG12	1:4:158:LYS:HZ1	1.73	0.46
1:4:145:ASN:ND2	1:4:145:ASN:O	2.47	0.46
1:1:8:PHE:CA	1:1:12:GLY:HA3	2.39	0.46
1:1:295:ALA:HB2	1:4:193:ARG:HH12	1.79	0.46
1:2:90:TYR:CZ	1:2:328:GLN:NE2	2.83	0.46
1:2:230:ARG:C	1:2:231:VAL:HG13	2.39	0.46
1:3:16:LEU:HD21	1:3:70:ILE:HD11	1.93	0.46
1:4:33:PHE:CZ	1:4:76:MET:SD	3.06	0.46
1:4:52:PHE:CG	1:4:53:LYS:HE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:120:PRO:O	1:4:120:PRO:HG2	2.15	0.46
1:4:131:VAL:CG2	1:4:216:VAL:HG22	2.45	0.46
1:4:235:ASP:OD2	1:4:311:ASP:OD1	2.33	0.46
1:4:251:TYR:O	1:4:254:ILE:HB	2.16	0.46
1:1:28:ALA:HB1	1:1:73:PHE:HE2	1.77	0.46
1:1:168:GLU:HG3	1:1:244:ARG:HD2	1.94	0.46
1:1:266:LEU:HD23	1:1:270:LEU:CB	2.45	0.46
1:1:304:VAL:HG13	1:1:305:LYS:N	2.20	0.46
1:3:71:THR:C	1:3:72:VAL:CG1	2.80	0.46
1:3:81:ILE:HD12	1:3:83:TRP:CE3	2.50	0.46
1:3:108:PHE:CG	1:3:109:LYS:N	2.84	0.46
1:3:322:ASP:O	1:3:323:LEU:O	2.34	0.46
1:4:236:VAL:CG1	1:4:237:SER:N	2.77	0.46
1:1:153:LEU:HD21	1:1:241:LEU:HD22	1.98	0.46
1:2:36:LEU:HD21	1:2:62:ALA:CA	2.46	0.46
1:2:128:VAL:N	1:2:132:ASN:HB2	2.30	0.46
1:2:164:PHE:HZ	1:2:253:ASP:HB3	1.80	0.46
1:2:242:THR:C	1:2:243:VAL:HG13	2.41	0.46
1:3:6:ASN:CB	1:3:30:ASN:HD21	2.29	0.46
1:3:27:VAL:H	1:3:70:ILE:HB	1.81	0.46
1:3:29:VAL:O	1:3:30:ASN:HB3	2.16	0.46
1:3:66:ASP:O	1:3:67:GLY:C	2.59	0.46
1:4:212:ALA:O	1:4:216:VAL:HG12	2.15	0.46
1:4:227:MET:HE1	1:4:229:PHE:CE1	2.49	0.46
1:4:251:TYR:CB	1:4:299:LEU:HG	2.46	0.46
1:1:282:PHE:HZ	1:1:290:ILE:CD1	2.27	0.46
1:1:294:LYS:HA	1:1:297:ILE:HG13	1.98	0.46
1:1:312:ASN:O	1:1:313:GLU:C	2.58	0.46
1:1:318:GLN:O	1:1:321:ILE:HB	2.16	0.46
1:1:324:LEU:HD12	1:1:324:LEU:C	2.41	0.46
1:2:169:GLY:O	1:2:170:LEU:HD23	2.16	0.46
1:3:81:ILE:CD1	1:3:82:PRO:O	2.59	0.46
1:3:148:CYS:SG	1:3:175:HIS:HE1	2.39	0.46
1:3:161:HIS:O	1:3:165:GLU:N	2.46	0.46
1:3:255:LYS:NZ	1:3:255:LYS:CB	2.77	0.46
1:3:287:ARG:HH12	1:3:290:ILE:CD1	2.28	0.46
1:3:321:ILE:O	1:3:324:LEU:HB3	2.15	0.46
1:4:53:LYS:N	1:4:53:LYS:CE	2.77	0.46
1:4:152:CYS:SG	1:4:239:VAL:CG1	3.04	0.46
1:1:82:PRO:HB2	1:1:85:LYS:O	2.16	0.46
1:1:244:ARG:NH2	1:4:244:ARG:CG	2.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:276:ASP:OD1	1:1:277:VAL:CB	2.64	0.46
1:1:292:ASP:OD1	1:1:307:VAL:HG11	2.14	0.46
1:1:318:GLN:O	1:1:322:ASP:OD2	2.34	0.46
1:2:76:MET:O	1:2:77:LYS:CG	2.64	0.46
1:2:131:VAL:HG12	1:2:158:LYS:HE2	1.97	0.46
1:2:136:TYR:CZ	1:2:327:MET:HG2	2.51	0.46
1:2:185:ASP:HA	1:2:196:ARG:CA	2.46	0.46
1:2:188:SER:C	1:2:190:LYS:N	2.69	0.46
1:2:220:LEU:HA	1:2:223:LYS:HG3	1.98	0.46
1:3:142:VAL:HG11	2:3:381:HOH:O	2.16	0.46
1:3:185:ASP:C	1:3:195:GLY:O	2.59	0.46
1:4:127:PHE:HB2	1:4:323:LEU:CD2	2.46	0.46
1:4:180:THR:OG1	1:4:181:GLN:N	2.46	0.46
1:4:196:ARG:HG3	1:4:197:GLY:N	2.16	0.46
1:4:314:PHE:HB2	1:4:317:SER:CB	2.45	0.46
1:1:15:VAL:HA	1:1:18:ALA:HB2	1.98	0.46
1:2:78:PRO:HG3	1:2:98:PHE:CD2	2.47	0.46
1:2:106:ALA:O	1:2:107:HIS:O	2.34	0.46
1:2:256:ALA:O	1:2:257:ALA:C	2.57	0.46
1:2:295:ALA:O	1:2:307:VAL:HG11	2.16	0.46
1:3:65:VAL:C	1:3:66:ASP:OD2	2.59	0.46
1:3:152:CYS:HB3	1:3:239:VAL:HG11	1.96	0.46
1:3:172:THR:HB	1:3:240:ASP:HB3	1.97	0.46
1:4:7:GLY:H	1:4:30:ASN:ND2	2.14	0.46
1:4:265:PRO:C	1:4:267:GLN:H	2.24	0.46
1:1:84:SER:O	1:1:86:ALA:N	2.49	0.45
1:1:202:ILE:HD12	1:4:233:THR:HG21	1.85	0.45
1:2:6:ASN:HA	1:2:30:ASN:HD21	1.75	0.45
1:2:292:ASP:OD1	1:2:292:ASP:O	2.33	0.45
1:3:138:LYS:HZ2	1:3:138:LYS:HG2	1.41	0.45
1:3:190:LYS:CE	1:3:190:LYS:HA	2.45	0.45
1:4:19:ALA:CA	1:4:24:ALA:HB3	2.46	0.45
1:4:74:ASN:HB2	2:4:457:HOH:O	2.16	0.45
1:4:79:GLU:H	1:4:79:GLU:CD	2.24	0.45
1:4:175:HIS:O	1:4:231:VAL:CG2	2.64	0.45
1:4:294:LYS:HZ2	1:4:294:LYS:HG3	1.61	0.45
1:1:233:THR:HG21	1:4:202:ILE:CD1	2.46	0.45
1:1:277:VAL:O	1:4:193:ARG:HD3	2.16	0.45
1:2:8:PHE:CE2	1:2:34:ILE:CD1	2.99	0.45
1:2:89:GLU:O	1:2:114:LYS:CG	2.65	0.45
1:3:124:ALA:C	1:3:125:PRO:O	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:216:VAL:O	1:3:218:PRO:HD3	2.15	0.45
1:3:299:LEU:O	1:3:300:SER:CB	2.64	0.45
1:4:65:VAL:CG2	1:4:66:ASP:OD2	2.64	0.45
1:4:130:GLY:HA3	1:4:158:LYS:HZ2	1.79	0.45
1:1:4:GLY:CA	1:1:27:VAL:CG2	2.79	0.45
1:1:128:VAL:O	1:1:132:ASN:N	2.49	0.45
1:1:220:LEU:O	1:1:223:LYS:HD3	2.17	0.45
1:1:324:LEU:CD1	1:1:324:LEU:C	2.88	0.45
1:2:104:ALA:C	1:2:106:ALA:N	2.74	0.45
1:3:242:THR:C	1:3:243:VAL:HG13	2.41	0.45
1:3:283:ILE:CG1	2:3:388:HOH:O	2.64	0.45
1:4:77:LYS:O	1:4:80:ASN:HB2	2.17	0.45
1:4:107:HIS:O	1:4:108:PHE:C	2.59	0.45
1:4:292:ASP:HB3	1:4:307:VAL:CG1	2.47	0.45
1:1:3:ILE:HG13	1:1:25:GLN:HB3	1.99	0.45
1:1:51:VAL:O	1:1:52:PHE:CB	2.59	0.45
1:1:161:HIS:C	1:1:163:ASN:N	2.72	0.45
1:1:285:ASP:O	1:1:286:ASN:C	2.60	0.45
1:1:328:GLN:O	1:1:329:LYS:O	2.34	0.45
1:2:213:VAL:HA	1:2:216:VAL:HG12	1.98	0.45
1:2:281:ASP:OD1	1:3:196:ARG:NH2	2.49	0.45
1:3:55:GLU:HB3	1:3:67:GLY:H	1.80	0.45
1:3:129:CYS:C	1:3:132:ASN:ND2	2.75	0.45
1:3:285:ASP:OD2	1:3:287:ARG:HB2	2.17	0.45
1:4:2:LYS:C	1:4:3:ILE:HG13	2.42	0.45
1:4:26:VAL:HG21	1:4:68:LYS:HG3	1.99	0.45
1:4:164:PHE:CE2	1:4:249:CYS:HB3	2.51	0.45
1:4:217:ILE:O	1:4:220:LEU:HB2	2.16	0.45
1:2:137:SER:O	1:2:140:MET:HG2	2.17	0.45
1:2:266:LEU:O	1:2:267:GLN:C	2.60	0.45
1:3:11:ILE:HG22	1:3:15:VAL:HG21	1.97	0.45
1:3:32:PRO:C	1:3:33:PHE:CG	2.95	0.45
1:3:143:VAL:HG11	1:3:327:MET:SD	2.57	0.45
1:3:220:LEU:O	1:3:223:LYS:HD3	2.15	0.45
1:3:282:PHE:HE2	1:3:309:TRP:CD2	2.35	0.45
1:4:329:LYS:NZ	1:4:329:LYS:O	2.37	0.45
1:1:85:LYS:O	1:1:86:ALA:HB2	2.17	0.45
1:1:152:CYS:SG	1:1:239:VAL:HG13	2.54	0.45
1:1:153:LEU:O	1:1:153:LEU:HD23	2.17	0.45
1:1:252:ASP:O	1:1:255:LYS:HB2	2.17	0.45
1:1:295:ALA:HB2	1:4:193:ARG:NH1	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:7:GLY:HA2	1:2:31:ASP:HB2	1.98	0.45
1:2:59:GLU:HB2	1:2:64:VAL:CG1	2.47	0.45
1:2:97:VAL:O	1:2:98:PHE:HD1	1.78	0.45
1:2:134:GLU:C	1:2:136:TYR:N	2.71	0.45
1:2:149:THR:HA	1:2:310:TYR:CZ	2.52	0.45
1:2:215:LYS:O	1:2:215:LYS:HD3	2.16	0.45
1:3:55:GLU:O	1:3:65:VAL:CA	2.58	0.45
1:3:78:PRO:CD	1:3:98:PHE:CE2	2.99	0.45
1:3:79:GLU:HG3	1:3:109:LYS:CD	2.47	0.45
1:3:95:THR:HG21	1:3:97:VAL:CG2	2.47	0.45
1:3:114:LYS:H	1:3:114:LYS:HG2	1.45	0.45
1:3:145:ASN:C	1:3:146:ALA:O	2.56	0.45
1:4:36:LEU:CD1	1:4:63:LEU:HB2	2.46	0.45
1:4:160:LEU:HA	1:4:160:LEU:HD23	1.72	0.45
1:1:76:MET:O	1:1:77:LYS:HD3	2.17	0.45
1:2:164:PHE:O	1:2:165:GLU:CB	2.61	0.45
1:2:280:SER:O	1:2:281:ASP:O	2.35	0.45
1:3:77:LYS:C	2:3:378:HOH:O	2.60	0.45
1:3:170:LEU:O	1:3:241:LEU:HD12	2.16	0.45
1:3:212:ALA:O	1:3:215:LYS:C	2.60	0.45
1:3:314:PHE:HA	1:3:317:SER:OG	2.16	0.45
1:4:54:GLY:HA3	1:4:66:ASP:CG	2.42	0.45
1:4:188:SER:O	1:4:189:ALA:C	2.60	0.45
1:4:201:ASN:HB3	1:4:203:ILE:HG12	1.97	0.45
1:4:329:LYS:C	1:4:329:LYS:HD2	2.38	0.45
1:1:253:ASP:O	1:1:255:LYS:N	2.48	0.45
1:1:290:ILE:O	1:1:308:SER:HA	2.16	0.45
1:2:51:VAL:HG23	2:2:401:HOH:O	2.15	0.45
1:2:101:ILE:O	1:2:105:SER:CB	2.65	0.45
1:2:263:GLU:O	1:2:264:GLY:C	2.60	0.45
1:2:274:GLU:C	1:2:276:ASP:H	2.23	0.45
1:3:33:PHE:HZ	1:3:76:MET:CE	2.30	0.45
1:4:272:TYR:CZ	1:4:293:ALA:HB2	2.51	0.45
1:1:19:ALA:HA	1:1:24:ALA:CB	2.46	0.45
1:1:115:VAL:CG1	1:1:116:VAL:N	2.75	0.45
1:1:154:ALA:N	1:1:155:PRO:HD2	2.32	0.45
1:1:174:VAL:HG12	1:1:231:VAL:HG21	1.95	0.45
1:1:237:SER:O	1:1:310:TYR:CD1	2.70	0.45
1:1:299:LEU:O	1:1:300:SER:HB3	2.16	0.45
1:1:323:LEU:O	1:1:324:LEU:C	2.60	0.45
1:2:3:ILE:HG13	1:2:25:GLN:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:299:LEU:HG	1:2:304:VAL:HG23	1.99	0.45
1:3:39:MET:O	1:3:43:PHE:N	2.48	0.45
1:3:46:ASP:HB2	1:3:50:GLY:HA2	1.98	0.45
1:3:188:SER:C	1:3:190:LYS:N	2.74	0.45
1:3:190:LYS:HD3	2:3:337:HOH:O	2.17	0.45
1:3:318:GLN:O	1:3:319:ARG:C	2.60	0.45
1:4:17:ARG:HH22	1:4:46:ASP:HB2	1.81	0.45
1:4:18:ALA:O	1:4:19:ALA:C	2.60	0.45
1:4:52:PHE:C	1:4:53:LYS:HE2	2.41	0.45
1:4:142:VAL:O	1:4:142:VAL:CG2	2.63	0.45
1:4:193:ARG:O	1:4:203:ILE:HG23	2.16	0.45
1:4:201:ASN:HD22	1:4:201:ASN:N	2.15	0.45
1:2:117:ILE:H	1:2:117:ILE:HG13	1.44	0.45
1:3:132:ASN:O	1:3:133:LEU:C	2.59	0.45
1:3:185:ASP:OD2	1:3:196:ARG:HD3	2.17	0.45
1:3:188:SER:HA	1:3:191:ASP:OD2	2.16	0.45
1:3:269:PHE:O	1:3:288:SER:HB3	2.17	0.45
1:4:52:PHE:C	1:4:53:LYS:CE	2.90	0.45
1:4:238:VAL:HG22	1:4:307:VAL:CG2	2.46	0.45
1:1:39:MET:C	1:1:42:MET:H	2.25	0.44
1:1:129:CYS:HA	1:1:132:ASN:HD22	1.81	0.44
1:1:157:ALA:O	1:1:159:VAL:N	2.50	0.44
1:1:175:HIS:CD2	1:1:230:ARG:HH21	2.35	0.44
1:2:38:TYR:O	1:2:42:MET:HB2	2.16	0.44
1:3:126:MET:HE2	1:3:212:ALA:HA	1.99	0.44
1:3:128:VAL:HG11	1:3:154:ALA:HB1	1.99	0.44
1:4:116:VAL:HG11	1:4:324:LEU:CD2	2.47	0.44
1:1:105:SER:O	1:1:108:PHE:HD1	1.99	0.44
1:1:225:THR:HG23	1:4:298:GLN:OE1	2.14	0.44
1:2:22:CYS:SG	1:2:321:ILE:HG21	2.57	0.44
1:2:100:THR:OG1	1:2:103:LYS:HD2	2.17	0.44
1:2:117:ILE:CD1	1:2:142:VAL:HG22	2.46	0.44
1:3:36:LEU:HD11	1:3:63:LEU:HB2	1.98	0.44
1:3:128:VAL:C	1:3:132:ASN:ND2	2.73	0.44
1:4:14:LEU:H	1:4:14:LEU:HD22	1.82	0.44
1:4:83:TRP:CE2	1:4:91:ILE:HG12	2.51	0.44
1:4:239:VAL:HG22	1:4:308:SER:HB2	1.99	0.44
1:4:319:ARG:NH1	1:4:319:ARG:HG2	2.32	0.44
1:1:180:THR:O	1:1:181:GLN:C	2.60	0.44
1:1:285:ASP:O	1:1:285:ASP:CG	2.59	0.44
1:2:58:MET:HE2	1:2:58:MET:HB2	1.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:276:ASP:CG	1:2:277:VAL:HG22	2.43	0.44
1:3:98:PHE:HA	1:3:103:LYS:HG2	1.97	0.44
1:3:129:CYS:C	1:3:132:ASN:HD22	2.26	0.44
1:3:171:MET:CA	1:3:240:ASP:O	2.65	0.44
1:4:3:ILE:HD12	1:4:24:ALA:HB1	1.99	0.44
1:4:39:MET:O	1:4:42:MET:N	2.50	0.44
1:4:52:PHE:CE1	1:4:53:LYS:CE	2.94	0.44
1:4:97:VAL:O	1:4:98:PHE:CB	2.65	0.44
1:1:202:ILE:HD11	1:4:233:THR:CB	2.46	0.44
1:1:242:THR:HA	1:1:304:VAL:O	2.17	0.44
1:2:77:LYS:O	1:2:80:ASN:HB2	2.17	0.44
1:2:109:LYS:HG2	1:2:110:GLY:N	2.32	0.44
1:3:26:VAL:HG11	1:3:68:LYS:CG	2.48	0.44
1:3:39:MET:O	1:3:40:VAL:C	2.60	0.44
1:1:168:GLU:CG	1:1:244:ARG:CD	2.88	0.44
1:2:117:ILE:HB	1:2:144:SER:HB2	1.99	0.44
1:3:57:LYS:HA	1:3:57:LYS:HD3	1.87	0.44
1:3:329:LYS:NZ	1:3:330:VAL:N	2.66	0.44
1:4:28:ALA:CB	1:4:83:TRP:CZ3	2.91	0.44
1:4:172:THR:O	1:4:240:ASP:N	2.41	0.44
1:4:233:THR:HA	1:4:234:PRO:HD2	1.87	0.44
1:1:11:ILE:CG2	1:1:15:VAL:CG2	2.90	0.44
1:1:295:ALA:O	1:1:307:VAL:HG21	2.18	0.44
1:2:52:PHE:C	2:2:400:HOH:O	2.55	0.44
1:2:181:GLN:CD	1:2:198:ALA:HB1	2.42	0.44
1:2:193:ARG:O	1:2:203:ILE:HG23	2.18	0.44
1:3:4:GLY:N	1:3:27:VAL:CG2	2.78	0.44
1:3:186:GLY:O	1:3:195:GLY:CA	2.66	0.44
1:3:319:ARG:O	1:3:320:VAL:O	2.35	0.44
1:4:325:LYS:C	1:4:327:MET:N	2.74	0.44
1:1:168:GLU:OE2	1:1:244:ARG:NE	2.50	0.44
1:1:181:GLN:HB3	1:1:198:ALA:CB	2.48	0.44
1:1:301:LYS:C	1:1:302:THR:HG22	2.42	0.44
1:2:9:GLY:O	1:2:10:ARG:O	2.35	0.44
1:2:145:ASN:ND2	1:2:145:ASN:C	2.60	0.44
1:3:46:ASP:HB3	1:3:50:GLY:HA2	1.98	0.44
1:3:211:LYS:HE2	1:3:211:LYS:N	2.31	0.44
1:3:227:MET:HE1	1:3:229:PHE:CE2	2.53	0.44
1:3:251:TYR:N	1:3:299:LEU:CD1	2.69	0.44
1:4:7:GLY:H	1:4:30:ASN:HD22	1.65	0.44
1:4:52:PHE:CE2	1:4:66:ASP:OD2	2.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:78:PRO:HD3	1:4:98:PHE:CZ	2.51	0.44
1:4:193:ARG:O	1:4:203:ILE:HG21	2.17	0.44
1:4:267:GLN:HB3	1:4:268:GLY:H	1.43	0.44
1:4:292:ASP:OD1	1:4:295:ALA:O	2.35	0.44
1:1:138:LYS:HD3	1:1:138:LYS:N	2.29	0.44
1:2:66:ASP:O	1:2:68:LYS:HD2	2.16	0.44
1:3:44:LYS:CG	1:3:56:VAL:HG21	2.46	0.44
1:3:216:VAL:HG12	1:3:217:ILE:HG22	2.00	0.44
1:3:273:THR:O	1:3:293:ALA:CB	2.64	0.44
1:4:73:PHE:HD2	1:4:81:ILE:CD1	2.29	0.44
1:4:75:GLU:CB	2:4:347:HOH:O	2.38	0.44
1:4:203:ILE:O	1:4:204:PRO:C	2.61	0.44
1:1:41:TYR:C	1:1:41:TYR:CD2	2.92	0.44
1:1:141:THR:OG1	1:1:142:VAL:N	2.51	0.44
1:1:252:ASP:O	1:1:253:ASP:C	2.60	0.44
1:1:325:LYS:C	1:1:327:MET:N	2.74	0.44
1:2:127:PHE:CD2	1:2:132:ASN:OD1	2.71	0.44
1:2:159:VAL:HG21	1:2:266:LEU:HD21	1.95	0.44
1:2:270:LEU:CD2	1:2:271:GLY:N	2.80	0.44
1:3:81:ILE:CG1	1:3:82:PRO:HD2	2.48	0.44
1:3:172:THR:O	1:3:240:ASP:HB2	2.17	0.44
1:4:188:SER:O	1:4:190:LYS:C	2.61	0.44
1:4:281:ASP:CA	2:4:357:HOH:O	2.63	0.44
1:4:298:GLN:HE21	1:4:299:LEU:N	2.16	0.44
1:1:101:ILE:HG23	1:1:142:VAL:CB	2.48	0.43
1:1:183:THR:CG2	1:2:181:GLN:O	2.66	0.43
1:2:44:LYS:O	1:2:51:VAL:CA	2.66	0.43
1:2:138:LYS:HE3	1:2:330:VAL:HG12	1.95	0.43
1:3:1:SER:HB3	1:3:25:GLN:HE22	1.81	0.43
1:3:46:ASP:HB3	1:3:50:GLY:CA	2.48	0.43
1:3:146:ALA:HB3	1:3:150:THR:HG21	1.98	0.43
1:3:160:LEU:O	1:3:164:PHE:N	2.51	0.43
1:4:6:ASN:CA	1:4:30:ASN:HD21	2.19	0.43
1:4:19:ALA:CB	1:4:24:ALA:HB3	2.48	0.43
1:4:39:MET:CE	1:4:72:VAL:CG2	2.96	0.43
1:4:83:TRP:N	1:4:86:ALA:CB	2.81	0.43
1:4:126:MET:HE3	1:4:212:ALA:HB2	1.99	0.43
1:1:16:LEU:O	1:1:18:ALA:N	2.51	0.43
1:1:128:VAL:HG11	1:1:154:ALA:CB	2.48	0.43
1:2:13:ARG:O	1:2:17:ARG:N	2.47	0.43
1:2:54:GLY:C	1:2:56:VAL:N	2.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:161:HIS:O	1:2:165:GLU:CA	2.66	0.43
1:2:267:GLN:CG	1:2:268:GLY:N	2.73	0.43
1:2:275:ASP:C	1:2:276:ASP:OD2	2.61	0.43
1:3:26:VAL:O	1:3:27:VAL:CB	2.66	0.43
1:3:245:LEU:HD23	1:3:245:LEU:HA	1.84	0.43
1:4:239:VAL:HG12	1:4:310:TYR:CE1	2.47	0.43
1:1:251:TYR:O	1:1:252:ASP:O	2.35	0.43
1:2:244:ARG:HA	1:3:244:ARG:HH22	1.84	0.43
1:2:262:SER:O	1:2:267:GLN:HA	2.18	0.43
1:3:126:MET:HG2	1:3:212:ALA:HB2	2.01	0.43
1:3:283:ILE:HG13	2:3:388:HOH:O	2.18	0.43
1:3:311:ASP:O	1:3:314:PHE:N	2.51	0.43
1:3:319:ARG:HG2	1:3:319:ARG:HH11	1.84	0.43
1:4:52:PHE:CD1	1:4:53:LYS:HE2	2.52	0.43
1:4:129:CYS:O	1:4:133:LEU:HG	2.18	0.43
1:4:130:GLY:HA3	1:4:158:LYS:HZ1	1.82	0.43
1:4:146:ALA:HB3	1:4:150:THR:HG21	2.00	0.43
1:1:10:ARG:HD3	1:1:10:ARG:HA	1.62	0.43
1:1:34:ILE:CD1	1:1:39:MET:HG2	2.44	0.43
1:1:38:TYR:O	1:1:42:MET:N	2.51	0.43
1:1:50:GLY:O	1:1:51:VAL:HG23	2.18	0.43
1:1:269:PHE:CD2	1:1:269:PHE:N	2.86	0.43
1:1:272:TYR:OH	1:1:274:GLU:OE1	2.35	0.43
1:1:292:ASP:HB2	1:1:309:TRP:HE1	1.82	0.43
1:2:52:PHE:C	1:2:53:LYS:CE	2.91	0.43
1:2:184:VAL:C	1:2:185:ASP:OD1	2.61	0.43
1:3:79:GLU:HG3	1:3:109:LYS:HD2	2.00	0.43
1:3:95:THR:HG21	1:3:97:VAL:HG22	2.00	0.43
1:4:312:ASN:O	1:4:313:GLU:C	2.59	0.43
1:1:30:ASN:ND2	1:1:30:ASN:N	2.66	0.43
1:1:170:LEU:O	1:1:241:LEU:HD12	2.18	0.43
1:1:175:HIS:CB	1:1:230:ARG:HH21	2.31	0.43
1:1:184:VAL:O	1:1:185:ASP:O	2.37	0.43
1:1:202:ILE:HD11	1:4:233:THR:HB	1.99	0.43
1:2:36:LEU:CD2	1:2:62:ALA:HA	2.48	0.43
1:2:153:LEU:HD23	1:2:153:LEU:C	2.35	0.43
1:2:227:MET:HG2	1:3:305:LYS:HE3	2.01	0.43
1:2:236:VAL:N	2:2:418:HOH:O	2.52	0.43
1:4:104:ALA:C	1:4:106:ALA:N	2.75	0.43
1:1:107:HIS:O	1:1:108:PHE:C	2.62	0.43
1:1:163:ASN:OD1	1:1:163:ASN:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:193:ARG:HD3	1:4:277:VAL:O	2.17	0.43
1:1:220:LEU:CD1	1:1:223:LYS:NZ	2.81	0.43
1:1:251:TYR:CE2	1:1:254:ILE:HG21	2.53	0.43
1:1:277:VAL:C	1:1:278:VAL:HG22	2.41	0.43
1:1:286:ASN:N	1:1:286:ASN:HD22	2.14	0.43
1:2:247:LYS:O	1:2:248:GLU:C	2.60	0.43
1:3:29:VAL:HG12	1:3:30:ASN:N	2.34	0.43
1:3:145:ASN:ND2	1:3:145:ASN:C	2.73	0.43
1:3:178:THR:HG1	1:3:181:GLN:HB2	1.84	0.43
1:3:211:LYS:NZ	2:3:384:HOH:O	2.51	0.43
1:4:145:ASN:C	1:4:145:ASN:ND2	2.73	0.43
1:4:146:ALA:CB	1:4:212:ALA:HB2	2.49	0.43
1:1:76:MET:O	1:1:77:LYS:CB	2.64	0.43
1:1:129:CYS:C	1:1:132:ASN:HD22	2.21	0.43
1:1:188:SER:CB	1:1:191:ASP:C	2.84	0.43
1:1:298:GLN:CD	1:4:225:THR:OG1	2.61	0.43
1:2:202:ILE:HD11	1:3:233:THR:HG21	2.00	0.43
1:2:292:ASP:OD1	1:2:292:ASP:C	2.62	0.43
1:3:44:LYS:HD2	1:3:56:VAL:HG11	1.99	0.43
1:4:152:CYS:HA	1:4:289:SER:CB	2.49	0.43
1:4:190:LYS:HD3	1:4:190:LYS:HA	1.64	0.43
1:1:36:LEU:HD11	1:1:62:ALA:CA	2.49	0.43
1:1:220:LEU:HD13	1:1:223:LYS:NZ	2.33	0.43
1:1:278:VAL:HG23	1:1:309:TRP:CZ2	2.54	0.43
1:1:310:TYR:HB2	1:1:311:ASP:H	1.22	0.43
1:2:34:ILE:HG12	1:2:39:MET:CE	2.49	0.43
1:2:41:TYR:OH	1:4:277:VAL:CG2	2.65	0.43
1:2:71:THR:HG21	1:2:73:PHE:CE1	2.53	0.43
1:2:133:LEU:H	1:2:133:LEU:HG	1.23	0.43
1:2:244:ARG:NE	1:3:244:ARG:CZ	2.82	0.43
1:3:224:LEU:CD2	1:3:241:LEU:HD11	2.49	0.43
1:3:276:ASP:HB3	1:3:294:LYS:HD3	2.00	0.43
1:4:3:ILE:HA	1:4:90:TYR:O	2.19	0.43
1:4:14:LEU:O	1:4:15:VAL:C	2.62	0.43
1:4:30:ASN:OD1	1:4:81:ILE:HG21	2.18	0.43
1:4:238:VAL:HB	1:4:309:TRP:CE3	2.53	0.43
1:4:293:ALA:O	1:4:294:LYS:CB	2.56	0.43
1:1:208:GLY:HA2	1:1:211:LYS:HG2	1.91	0.43
1:2:319:ARG:O	1:2:322:ASP:N	2.52	0.43
1:3:44:LYS:HE3	1:3:44:LYS:HB3	1.68	0.43
1:3:269:PHE:CD2	1:3:269:PHE:N	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:318:GLN:O	1:3:321:ILE:CB	2.57	0.43
1:4:211:LYS:HE2	1:4:211:LYS:HA	1.84	0.43
1:1:319:ARG:O	1:1:323:LEU:N	2.49	0.43
1:2:84:SER:O	1:2:86:ALA:CB	2.63	0.43
1:2:101:ILE:HD11	1:2:124:ALA:HA	2.01	0.43
1:2:271:GLY:O	1:2:272:TYR:CB	2.66	0.43
1:2:276:ASP:C	1:2:277:VAL:CG2	2.91	0.43
1:2:327:MET:O	1:2:331:ASP:N	2.52	0.43
1:3:52:PHE:C	1:3:53:LYS:CE	2.92	0.43
1:1:57:LYS:HD3	1:1:57:LYS:HA	1.78	0.42
1:1:101:ILE:CG1	1:1:142:VAL:CG1	2.95	0.42
1:1:133:LEU:HG	1:1:133:LEU:H	1.30	0.42
1:1:227:MET:HE2	1:1:227:MET:HB2	1.85	0.42
1:2:252:ASP:O	1:2:255:LYS:CB	2.67	0.42
1:4:119:ALA:CB	1:4:120:PRO:CD	2.50	0.42
1:4:137:SER:CA	1:4:138:LYS:HE3	2.45	0.42
1:4:156:VAL:HA	1:4:258:MET:CE	2.50	0.42
1:1:97:VAL:C	1:1:98:PHE:CD1	2.93	0.42
1:1:156:VAL:CG2	1:1:258:MET:HE2	2.46	0.42
1:1:282:PHE:O	1:1:285:ASP:HB3	2.19	0.42
1:2:93:GLU:OE2	1:2:98:PHE:HD2	2.00	0.42
1:2:329:LYS:C	1:2:329:LYS:HZ2	2.26	0.42
1:3:37:GLU:C	1:3:40:VAL:HG13	2.44	0.42
1:4:70:ILE:O	1:4:71:THR:C	2.62	0.42
1:4:184:VAL:O	1:4:185:ASP:O	2.37	0.42
1:1:125:PRO:HB2	1:1:127:PHE:CE1	2.54	0.42
1:1:175:HIS:HB3	1:1:230:ARG:HH21	1.83	0.42
1:2:66:ASP:CB	2:2:402:HOH:O	2.68	0.42
1:2:196:ARG:HH21	1:3:281:ASP:CG	2.26	0.42
1:4:32:PRO:O	1:4:33:PHE:CB	2.68	0.42
1:4:95:THR:HG21	1:4:97:VAL:HG23	2.01	0.42
1:1:129:CYS:CA	1:1:132:ASN:HD22	2.33	0.42
1:2:76:MET:C	2:2:408:HOH:O	2.35	0.42
1:2:127:PHE:HD2	1:2:132:ASN:CA	2.32	0.42
1:2:131:VAL:N	1:2:158:LYS:NZ	2.67	0.42
1:2:235:ASP:O	1:2:236:VAL:HG23	2.20	0.42
1:2:300:SER:O	1:2:301:LYS:CB	2.66	0.42
1:3:53:LYS:N	1:3:53:LYS:CE	2.76	0.42
1:3:186:GLY:O	1:3:195:GLY:HA3	2.19	0.42
1:3:307:VAL:H	1:3:307:VAL:HG12	1.63	0.42
1:3:320:VAL:O	1:3:321:ILE:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:10:ARG:HD3	1:4:10:ARG:HA	1.57	0.42
1:4:74:ASN:OD1	1:4:74:ASN:C	2.56	0.42
1:4:180:THR:O	1:4:181:GLN:C	2.62	0.42
1:4:271:GLY:O	1:4:272:TYR:CB	2.67	0.42
1:1:16:LEU:O	1:1:19:ALA:HB3	2.18	0.42
1:1:231:VAL:O	1:1:232:PRO:C	2.62	0.42
1:1:251:TYR:CD2	1:1:254:ILE:CG2	3.03	0.42
1:1:322:ASP:CG	2:1:449:HOH:O	2.62	0.42
1:2:34:ILE:O	1:2:39:MET:HE3	2.19	0.42
1:2:101:ILE:HB	1:2:123:ASP:OD1	2.19	0.42
1:2:104:ALA:O	1:2:106:ALA:N	2.51	0.42
1:2:135:LYS:O	1:2:135:LYS:CD	2.63	0.42
1:3:108:PHE:O	1:3:110:GLY:N	2.52	0.42
1:3:318:GLN:O	1:3:321:ILE:N	2.52	0.42
1:1:135:LYS:NZ	1:1:140:MET:HE1	2.34	0.42
1:1:160:LEU:CD2	1:1:254:ILE:CD1	2.97	0.42
1:1:296:GLY:HA2	1:4:227:MET:HE3	1.99	0.42
1:1:329:LYS:NZ	1:1:330:VAL:CA	2.82	0.42
1:2:81:ILE:HG23	1:2:83:TRP:NE1	2.34	0.42
1:3:132:ASN:OD1	1:3:133:LEU:CD2	2.66	0.42
1:3:255:LYS:HZ2	1:3:255:LYS:CB	2.32	0.42
1:3:314:PHE:HB2	1:3:317:SER:CB	2.50	0.42
1:4:14:LEU:O	1:4:18:ALA:HB2	2.20	0.42
1:4:152:CYS:HA	1:4:289:SER:HB3	2.01	0.42
1:4:208:GLY:HA2	1:4:211:LYS:HG2	1.98	0.42
1:4:329:LYS:HD2	1:4:329:LYS:HA	1.54	0.42
1:1:101:ILE:HG12	1:1:142:VAL:HG11	1.97	0.42
1:1:168:GLU:HG3	1:1:244:ARG:CD	2.50	0.42
1:1:282:PHE:O	1:1:285:ASP:CB	2.67	0.42
1:1:298:GLN:CD	1:4:225:THR:HG1	2.26	0.42
1:2:11:ILE:CD1	1:2:11:ILE:N	2.42	0.42
1:2:31:ASP:HA	1:2:32:PRO:HD2	1.73	0.42
1:2:51:VAL:HG21	2:2:401:HOH:O	2.18	0.42
1:2:77:LYS:HA	1:2:77:LYS:HD2	1.64	0.42
1:2:232:PRO:HG2	1:3:232:PRO:CB	2.41	0.42
1:2:303:PHE:CE2	1:3:303:PHE:CE2	3.08	0.42
1:3:43:PHE:CE1	1:3:65:VAL:HG21	2.54	0.42
1:3:101:ILE:CB	1:3:123:ASP:OD1	2.42	0.42
1:3:281:ASP:C	1:3:283:ILE:N	2.75	0.42
1:4:8:PHE:CZ	1:4:39:MET:HB3	2.54	0.42
1:4:115:VAL:HG12	1:4:116:VAL:N	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:165:GLU:OE1	1:4:167:VAL:HG12	2.19	0.42
1:4:319:ARG:HA	1:4:322:ASP:OD2	2.20	0.42
1:1:233:THR:HG22	1:1:236:VAL:H	1.85	0.42
1:1:251:TYR:CZ	1:1:255:LYS:HD3	2.55	0.42
1:2:150:THR:CG2	1:2:212:ALA:HB3	2.50	0.42
1:2:252:ASP:O	1:2:253:ASP:C	2.62	0.42
1:3:161:HIS:O	1:3:164:PHE:N	2.47	0.42
1:3:272:TYR:CE2	1:3:293:ALA:CB	2.98	0.42
1:1:68:LYS:O	1:1:70:ILE:HG23	2.20	0.42
1:1:101:ILE:HD13	1:1:142:VAL:CG1	2.49	0.42
1:1:167:VAL:HG23	1:1:244:ARG:HG2	2.01	0.42
1:2:131:VAL:HG22	1:2:132:ASN:H	1.85	0.42
1:3:66:ASP:O	1:3:68:LYS:HD2	2.17	0.42
1:3:156:VAL:HG12	1:3:157:ALA:N	2.34	0.42
1:3:175:HIS:HA	1:3:237:SER:OG	2.19	0.42
1:4:9:GLY:HA2	1:4:13:ARG:NH2	2.35	0.42
1:4:11:ILE:O	1:4:12:GLY:C	2.62	0.42
1:4:99:THR:O	1:4:121:SER:OG	2.36	0.42
1:4:119:ALA:O	1:4:144:SER:OG	2.33	0.42
1:4:170:LEU:HD23	1:4:170:LEU:HA	1.80	0.42
1:4:276:ASP:OD2	1:4:277:VAL:HG22	2.19	0.42
1:1:1:SER:CB	1:1:25:GLN:HE21	2.33	0.42
1:1:243:VAL:HG23	1:1:304:VAL:HG12	1.94	0.42
1:2:214:GLY:O	1:2:216:VAL:N	2.53	0.42
1:2:235:ASP:O	1:2:236:VAL:CG2	2.67	0.42
1:3:90:TYR:CE2	1:3:328:GLN:CD	2.98	0.42
1:3:250:SER:O	1:3:252:ASP:N	2.53	0.42
1:4:20:LEU:HD21	1:4:26:VAL:HG13	2.01	0.42
1:4:97:VAL:C	1:4:98:PHE:CD1	2.98	0.42
1:4:138:LYS:CE	1:4:138:LYS:H	2.33	0.42
1:4:282:PHE:CE2	1:4:309:TRP:CD1	3.08	0.42
1:1:115:VAL:HG12	1:1:116:VAL:N	2.29	0.41
1:1:165:GLU:OE1	1:1:167:VAL:CG1	2.65	0.41
1:2:20:LEU:HA	1:2:20:LEU:HD23	1.83	0.41
1:2:27:VAL:HG22	1:2:28:ALA:H	1.83	0.41
1:2:76:MET:O	1:2:77:LYS:CB	2.68	0.41
1:2:177:VAL:CG1	1:2:232:PRO:O	2.66	0.41
1:2:193:ARG:HG3	1:3:277:VAL:HA	2.01	0.41
1:2:213:VAL:HG13	1:2:217:ILE:CG2	2.49	0.41
1:2:266:LEU:O	1:2:269:PHE:N	2.51	0.41
1:2:316:TYR:O	1:2:319:ARG:HB2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:205:SER:HB3	1:3:228:ALA:CB	2.41	0.41
1:3:255:LYS:HB3	1:3:255:LYS:HZ3	1.79	0.41
1:4:66:ASP:CB	1:4:68:LYS:HE2	2.48	0.41
1:4:138:LYS:CD	1:4:330:VAL:CG1	2.98	0.41
1:4:188:SER:HB3	1:4:191:ASP:CA	2.50	0.41
1:4:319:ARG:NH1	1:4:319:ARG:CG	2.80	0.41
1:1:214:GLY:C	1:1:216:VAL:H	2.27	0.41
1:2:131:VAL:CG2	1:2:132:ASN:N	2.83	0.41
1:2:213:VAL:HA	1:2:216:VAL:CG1	2.50	0.41
1:2:244:ARG:CA	1:3:244:ARG:HH22	2.31	0.41
1:3:127:PHE:CA	1:3:132:ASN:HB3	2.50	0.41
1:4:17:ARG:HG3	1:4:43:PHE:CD2	2.55	0.41
1:1:32:PRO:CA	1:1:74:ASN:ND2	2.62	0.41
1:1:43:PHE:CE1	1:1:52:PHE:CE2	3.08	0.41
1:1:78:PRO:C	1:1:80:ASN:H	2.26	0.41
1:1:316:TYR:O	1:1:317:SER:C	2.62	0.41
1:2:129:CYS:O	1:2:130:GLY:C	2.64	0.41
1:2:136:TYR:OH	1:2:331:ASP:OD2	2.32	0.41
1:2:170:LEU:HD22	1:2:170:LEU:HA	1.87	0.41
1:3:184:VAL:C	1:3:185:ASP:O	2.62	0.41
1:3:241:LEU:HD21	1:3:243:VAL:HG11	2.02	0.41
1:3:313:GLU:O	1:3:317:SER:OG	2.38	0.41
1:4:39:MET:HE1	1:4:72:VAL:HB	2.02	0.41
1:4:55:GLU:H	1:4:66:ASP:HA	1.85	0.41
1:4:117:ILE:HG21	1:4:117:ILE:HD13	1.76	0.41
1:1:82:PRO:O	1:1:83:TRP:CG	2.74	0.41
1:1:319:ARG:HH11	1:1:319:ARG:CG	2.27	0.41
1:2:74:ASN:CB	2:2:395:HOH:O	2.62	0.41
1:2:227:MET:HE3	1:2:227:MET:HB2	1.94	0.41
1:2:294:LYS:H	1:2:297:ILE:HG13	1.85	0.41
1:2:295:ALA:HB2	1:3:193:ARG:CZ	2.50	0.41
1:3:19:ALA:CA	1:3:24:ALA:HB3	2.50	0.41
1:3:25:GLN:HG3	1:3:26:VAL:N	2.35	0.41
1:3:97:VAL:O	1:3:98:PHE:CD1	2.73	0.41
1:3:158:LYS:HE2	1:3:158:LYS:HB2	1.78	0.41
1:3:251:TYR:CD1	1:3:255:LYS:HD3	2.55	0.41
1:3:304:VAL:HG13	1:3:305:LYS:N	2.35	0.41
1:1:27:VAL:HG22	1:1:28:ALA:CA	2.46	0.41
1:1:78:PRO:HG3	1:1:98:PHE:CE2	2.56	0.41
1:1:187:PRO:HA	1:2:38:TYR:OH	2.20	0.41
1:1:279:SER:O	1:1:281:ASP:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:282:PHE:CD1	1:1:285:ASP:OD1	2.72	0.41
1:2:2:LYS:NZ	1:2:87:GLY:O	2.53	0.41
1:3:128:VAL:H	1:3:132:ASN:HB3	1.84	0.41
1:4:124:ALA:C	1:4:125:PRO:O	2.64	0.41
1:4:138:LYS:CD	1:4:138:LYS:N	2.78	0.41
1:4:174:VAL:HG12	1:4:231:VAL:HG21	2.03	0.41
1:4:174:VAL:O	1:4:237:SER:HA	2.20	0.41
1:1:2:LYS:CA	1:1:25:GLN:HG2	2.50	0.41
1:1:18:ALA:O	1:1:19:ALA:C	2.63	0.41
1:1:66:ASP:CA	2:1:432:HOH:O	2.62	0.41
1:1:143:VAL:CG2	1:1:144:SER:N	2.79	0.41
1:2:39:MET:O	1:2:40:VAL:C	2.61	0.41
1:2:242:THR:O	1:2:243:VAL:HG12	2.21	0.41
1:3:3:ILE:CG2	1:3:4:GLY:N	2.82	0.41
1:3:57:LYS:O	1:3:64:VAL:HG13	2.21	0.41
1:3:104:ALA:HB3	1:3:142:VAL:HG21	2.02	0.41
1:3:224:LEU:HD21	1:3:241:LEU:HD11	2.01	0.41
1:4:46:ASP:O	1:4:50:GLY:CA	2.69	0.41
1:4:113:LYS:C	1:4:114:LYS:CD	2.94	0.41
1:4:113:LYS:CG	1:4:114:LYS:CE	2.97	0.41
1:4:149:THR:O	1:4:152:CYS:N	2.54	0.41
1:1:127:PHE:CZ	1:1:136:TYR:HB2	2.43	0.41
1:1:127:PHE:HD1	1:1:143:VAL:CG2	2.34	0.41
1:1:171:MET:CE	1:1:209:ALA:HB2	2.49	0.41
1:1:281:ASP:C	1:1:283:ILE:H	2.27	0.41
1:2:113:LYS:CA	1:2:114:LYS:HG2	2.48	0.41
1:2:128:VAL:N	1:2:132:ASN:CB	2.80	0.41
1:2:225:THR:CB	1:3:298:GLN:NE2	2.84	0.41
1:2:276:ASP:OD1	1:2:277:VAL:CG2	2.69	0.41
1:3:77:LYS:N	2:3:378:HOH:O	1.76	0.41
1:3:113:LYS:HE2	1:3:114:LYS:NZ	2.36	0.41
1:3:159:VAL:O	1:3:160:LEU:C	2.63	0.41
1:3:188:SER:CB	1:3:192:TRP:HA	2.51	0.41
1:3:213:VAL:HA	1:3:216:VAL:CG1	2.51	0.41
1:4:299:LEU:HD13	1:4:299:LEU:C	2.45	0.41
1:1:33:PHE:CZ	1:1:76:MET:SD	3.13	0.41
1:1:294:LYS:CA	1:1:297:ILE:HG13	2.50	0.41
1:2:8:PHE:HZ	1:2:39:MET:CB	2.34	0.41
1:2:126:MET:HB3	1:2:215:LYS:NZ	2.36	0.41
1:2:143:VAL:HG22	1:2:144:SER:N	2.36	0.41
1:3:77:LYS:HA	1:3:78:PRO:HD3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:81:ILE:HD12	1:3:83:TRP:CZ3	2.56	0.41
1:4:93:GLU:OE2	1:4:98:PHE:HB2	2.20	0.41
1:4:175:HIS:HB3	1:4:230:ARG:HE	1.85	0.41
1:1:14:LEU:HG	1:1:314:PHE:HB3	2.02	0.41
1:1:46:ASP:HB3	1:1:50:GLY:N	2.28	0.41
1:1:131:VAL:H	1:1:131:VAL:HG13	1.62	0.41
1:1:145:ASN:ND2	1:1:145:ASN:C	2.66	0.41
1:1:182:LYS:HA	1:1:182:LYS:HD2	1.74	0.41
1:1:213:VAL:O	1:1:217:ILE:CG2	2.69	0.41
1:1:244:ARG:NH2	1:4:244:ARG:HG3	2.35	0.41
1:1:301:LYS:C	1:1:302:THR:CG2	2.94	0.41
1:1:304:VAL:CG1	1:1:304:VAL:O	2.58	0.41
1:2:74:ASN:OD1	1:2:75:GLU:N	2.53	0.41
1:2:149:THR:O	1:2:152:CYS:CA	2.68	0.41
1:2:213:VAL:HG13	1:2:217:ILE:HG23	2.03	0.41
1:2:231:VAL:HA	1:2:232:PRO:HD2	1.88	0.41
1:2:269:PHE:CE1	1:2:319:ARG:NH2	2.89	0.41
1:2:299:LEU:CD2	1:2:300:SER:H	2.27	0.41
1:3:8:PHE:CE1	1:3:39:MET:SD	3.14	0.41
1:3:13:ARG:HD3	1:3:42:MET:O	2.21	0.41
1:3:81:ILE:HG21	1:3:83:TRP:NE1	2.36	0.41
1:3:255:LYS:HG2	1:3:255:LYS:H	1.49	0.41
1:3:264:GLY:HA3	1:3:265:PRO:HD3	1.84	0.41
1:3:276:ASP:OD1	1:3:277:VAL:CB	2.68	0.41
1:3:286:ASN:N	1:3:286:ASN:HD22	2.17	0.41
1:3:316:TYR:O	1:3:319:ARG:HB2	2.21	0.41
1:4:2:LYS:O	1:4:3:ILE:HG13	2.21	0.41
1:4:39:MET:HE2	1:4:72:VAL:HG21	2.03	0.41
1:4:101:ILE:HD13	1:4:101:ILE:HG21	1.82	0.41
1:4:132:ASN:O	1:4:133:LEU:C	2.63	0.41
1:4:183:THR:C	1:4:184:VAL:CG1	2.93	0.41
1:4:216:VAL:CG1	1:4:217:ILE:H	2.34	0.41
1:4:275:ASP:CG	1:4:275:ASP:O	2.63	0.41
1:1:65:VAL:HG12	1:1:70:ILE:HD13	1.98	0.41
1:1:81:ILE:HG21	1:1:83:TRP:NE1	2.34	0.41
1:1:127:PHE:CE2	1:1:136:TYR:CA	3.03	0.41
1:1:272:TYR:H	1:1:291:PHE:H	1.69	0.41
1:2:132:ASN:HD21	1:2:133:LEU:HD23	1.82	0.41
1:2:181:GLN:CG	1:2:198:ALA:CB	2.94	0.41
1:2:181:GLN:NE2	1:2:230:ARG:HB2	2.32	0.41
1:2:299:LEU:HD23	1:2:299:LEU:HA	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:254:ILE:O	1:3:255:LYS:C	2.63	0.41
1:4:81:ILE:HG22	1:4:83:TRP:NE1	2.35	0.41
1:4:156:VAL:O	1:4:160:LEU:HB2	2.21	0.41
1:4:159:VAL:HG11	1:4:258:MET:HG3	2.02	0.41
1:4:173:THR:HG22	1:4:227:MET:O	2.20	0.41
1:4:280:SER:HB3	2:4:358:HOH:O	2.20	0.41
1:1:28:ALA:HB3	1:1:83:TRP:HZ3	1.86	0.40
1:2:208:GLY:CA	1:2:211:LYS:HG2	2.51	0.40
1:2:305:LYS:HD3	1:3:227:MET:SD	2.61	0.40
1:3:114:LYS:HE3	1:3:114:LYS:CA	2.50	0.40
1:3:131:VAL:N	1:3:158:LYS:HZ1	2.18	0.40
1:4:37:GLU:H	1:4:37:GLU:HG3	1.42	0.40
1:4:138:LYS:HD3	1:4:330:VAL:CG1	2.49	0.40
1:4:251:TYR:HE1	1:4:255:LYS:HE3	1.85	0.40
1:4:265:PRO:HG2	2:4:352:HOH:O	2.21	0.40
1:1:128:VAL:HG13	1:1:151:ASN:ND2	2.35	0.40
1:2:1:SER:O	1:2:2:LYS:CG	2.45	0.40
1:2:44:LYS:HZ2	1:2:44:LYS:HG2	1.46	0.40
1:2:217:ILE:HA	1:2:218:PRO:HD2	1.82	0.40
1:2:276:ASP:HB2	1:2:277:VAL:H	1.14	0.40
1:3:113:LYS:C	1:3:114:LYS:CD	2.94	0.40
1:3:299:LEU:CD2	1:3:303:PHE:O	2.69	0.40
1:4:1:SER:O	1:4:2:LYS:HG2	2.22	0.40
1:4:49:HIS:NE2	1:4:313:GLU:OE1	2.53	0.40
1:4:126:MET:CB	1:4:215:LYS:HD3	2.49	0.40
1:4:133:LEU:CD2	1:4:133:LEU:H	2.25	0.40
1:4:136:TYR:CZ	1:4:327:MET:HG2	2.56	0.40
1:4:252:ASP:O	1:4:253:ASP:C	2.65	0.40
1:4:285:ASP:OD2	1:4:285:ASP:C	2.64	0.40
1:1:185:ASP:OD2	1:1:196:ARG:HD2	2.20	0.40
1:2:26:VAL:CG2	1:2:27:VAL:N	2.83	0.40
1:2:52:PHE:O	1:2:53:LYS:HB3	2.21	0.40
1:2:215:LYS:CD	1:2:215:LYS:O	2.69	0.40
1:3:17:ARG:NH2	2:3:369:HOH:O	2.52	0.40
1:3:112:ALA:O	1:3:113:LYS:CB	2.69	0.40
1:3:127:PHE:HB3	1:3:323:LEU:HD21	2.02	0.40
1:3:188:SER:HB3	1:3:192:TRP:HA	2.02	0.40
1:3:203:ILE:HG22	1:3:203:ILE:O	2.21	0.40
1:4:17:ARG:NH2	1:4:46:ASP:HB2	2.36	0.40
1:4:177:VAL:HG22	1:4:233:THR:O	2.21	0.40
1:4:323:LEU:HD13	1:4:327:MET:SD	2.62	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:184:VAL:O	1:1:184:VAL:CG1	2.69	0.40
1:2:66:ASP:O	1:2:68:LYS:CE	2.67	0.40
1:2:160:LEU:HD21	1:2:254:ILE:HD12	2.02	0.40
1:2:223:LYS:HG2	1:2:223:LYS:H	1.56	0.40
1:2:227:MET:SD	1:3:296:GLY:CA	3.09	0.40
1:2:310:TYR:HB2	1:2:311:ASP:H	1.47	0.40
1:3:250:SER:HA	1:3:299:LEU:HD11	2.02	0.40
1:4:16:LEU:C	1:4:18:ALA:N	2.79	0.40
1:4:94:SER:O	1:4:96:GLY:N	2.54	0.40
1:4:175:HIS:CG	1:4:230:ARG:NH2	2.88	0.40
1:4:285:ASP:OD2	1:4:287:ARG:HB2	2.21	0.40
1:1:59:GLU:C	1:1:61:GLY:N	2.77	0.40
1:1:145:ASN:O	1:1:145:ASN:CG	2.57	0.40
1:1:161:HIS:O	1:1:164:PHE:N	2.54	0.40
1:2:131:VAL:H	1:2:131:VAL:HG13	1.47	0.40
1:2:166:ILE:N	1:2:245:LEU:O	2.45	0.40
1:2:173:THR:HG23	1:2:228:ALA:HB2	1.85	0.40
1:2:227:MET:SD	1:3:305:LYS:HD3	2.61	0.40
1:3:32:PRO:CB	1:3:74:ASN:OD1	2.69	0.40
1:3:33:PHE:C	1:3:34:ILE:HG22	2.46	0.40
1:3:48:THR:HG22	1:4:200:GLN:OE1	2.21	0.40
1:3:84:SER:HG	1:3:111:GLY:C	2.26	0.40
1:3:252:ASP:C	1:3:252:ASP:OD1	2.64	0.40
1:4:5:ILE:HD12	1:4:16:LEU:HG	2.04	0.40
1:4:314:PHE:CA	1:4:317:SER:OG	2.69	0.40

All (31) 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)
1:2:108:PHE:CE2	1:4:138:LYS:O[1_565]	0.55	1.65
1:2:102:GLU:CB	2:4:351:HOH:O[1_565]	0.85	1.35
1:2:123:ASP:CB	1:4:108:PHE:CE2[1_565]	0.92	1.28
1:2:80:ASN:OD1	1:3:139:ASP:OD2[1_665]	0.98	1.22
1:2:108:PHE:CZ	1:4:138:LYS:O[1_565]	1.03	1.17
1:2:123:ASP:CB	1:4:108:PHE:CZ[1_565]	1.11	1.09
1:2:108:PHE:CE2	1:4:138:LYS:C[1_565]	1.29	0.91
1:3:102:GLU:N	2:2:403:HOH:O[1_445]	1.37	0.83
1:3:102:GLU:CA	2:2:403:HOH:O[1_445]	1.48	0.72
1:2:80:ASN:OD1	1:3:139:ASP:CG[1_665]	1.60	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:123:ASP:CA	1:4:108:PHE:CE2[1_565]	1.70	0.50
1:2:85:LYS:CE	2:3:380:HOH:O[1_665]	1.72	0.48
1:2:80:ASN:CG	1:3:139:ASP:OD2[1_665]	1.73	0.47
1:2:108:PHE:CZ	1:4:138:LYS:C[1_565]	1.74	0.46
1:3:101:ILE:C	2:2:403:HOH:O[1_445]	1.78	0.42
1:2:102:GLU:CG	2:4:351:HOH:O[1_565]	1.79	0.41
1:2:80:ASN:CG	1:3:139:ASP:OD1[1_665]	1.81	0.39
1:2:108:PHE:CE1	1:4:139:ASP:CA[1_565]	1.91	0.29
1:2:108:PHE:CD2	1:4:138:LYS:O[1_565]	1.91	0.29
1:3:267:GLN:OE1	1:4:247:LYS:CE[1_455]	1.96	0.24
1:2:80:ASN:CG	1:3:139:ASP:CG[1_665]	2.03	0.17
1:3:101:ILE:O	2:2:403:HOH:O[1_445]	2.03	0.17
1:2:80:ASN:ND2	1:3:139:ASP:OD1[1_665]	2.05	0.15
1:2:108:PHE:CZ	1:4:139:ASP:N[1_565]	2.05	0.15
1:2:106:ALA:O	1:4:139:ASP:OD1[1_565]	2.06	0.14
1:2:108:PHE:CZ	1:4:139:ASP:CA[1_565]	2.06	0.14
1:2:80:ASN:OD1	1:3:139:ASP:OD1[1_665]	2.07	0.13
1:1:90:TYR:OH	2:4:343:HOH:O[1_566]	2.09	0.11
1:2:80:ASN:ND2	1:3:139:ASP:OD2[1_665]	2.15	0.05
1:2:85:LYS:NZ	2:3:380:HOH:O[1_665]	2.16	0.04
1:1:134:GLU:OE1	1:2:135:LYS:CB[1_556]	2.18	0.02

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	1	331/333 (99%)	177 (54%)	70 (21%)	84 (25%)	0	0
1	2	331/333 (99%)	180 (54%)	75 (23%)	76 (23%)	0	0
1	3	331/333 (99%)	175 (53%)	70 (21%)	86 (26%)	0	0
1	4	331/333 (99%)	180 (54%)	73 (22%)	78 (24%)	0	0
All	All	1324/1332 (99%)	712 (54%)	288 (22%)	324 (24%)	0	0

All (324) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	8	PHE
1	1	10	ARG
1	1	27	VAL
1	1	50	GLY
1	1	51	VAL
1	1	52	PHE
1	1	53	LYS
1	1	77	LYS
1	1	83	TRP
1	1	84	SER
1	1	86	ALA
1	1	89	GLU
1	1	95	THR
1	1	98	PHE
1	1	113	LYS
1	1	125	PRO
1	1	133	LEU
1	1	138	LYS
1	1	146	ALA
1	1	147	SER
1	1	158	LYS
1	1	161	HIS
1	1	177	VAL
1	1	184	VAL
1	1	189	ALA
1	1	198	ALA
1	1	204	PRO
1	1	211	LYS
1	1	221	ASP
1	1	237	SER
1	1	252	ASP
1	1	264	GLY
1	1	267	GLN
1	1	276	ASP
1	1	277	VAL
1	1	278	VAL
1	1	280	SER
1	1	281	ASP
1	1	282	PHE
1	1	294	LYS
1	1	311	ASP
1	1	312	ASN

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Mol	Chain	Res	Type
1	1	326	HIS
1	2	26	VAL
1	2	27	VAL
1	2	50	GLY
1	2	51	VAL
1	2	53	LYS
1	2	60	ASP
1	2	77	LYS
1	2	86	ALA
1	2	95	THR
1	2	98	PHE
1	2	106	ALA
1	2	107	HIS
1	2	132	ASN
1	2	133	LEU
1	2	146	ALA
1	2	147	SER
1	2	177	VAL
1	2	181	GLN
1	2	184	VAL
1	2	189	ALA
1	2	192	TRP
1	2	204	PRO
1	2	211	LYS
1	2	221	ASP
1	2	233	THR
1	2	237	SER
1	2	251	TYR
1	2	267	GLN
1	2	276	ASP
1	2	277	VAL
1	2	278	VAL
1	2	281	ASP
1	2	282	PHE
1	2	311	ASP
1	2	312	ASN
1	2	326	HIS
1	3	26	VAL
1	3	27	VAL
1	3	50	GLY
1	3	52	PHE
1	3	53	LYS

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Mol	Chain	Res	Type
1	3	60	ASP
1	3	77	LYS
1	3	83	TRP
1	3	86	ALA
1	3	95	THR
1	3	98	PHE
1	3	106	ALA
1	3	109	LYS
1	3	133	LEU
1	3	135	LYS
1	3	146	ALA
1	3	154	ALA
1	3	161	HIS
1	3	165	GLU
1	3	181	GLN
1	3	184	VAL
1	3	211	LYS
1	3	221	ASP
1	3	233	THR
1	3	237	SER
1	3	251	TYR
1	3	252	ASP
1	3	255	LYS
1	3	267	GLN
1	3	276	ASP
1	3	277	VAL
1	3	278	VAL
1	3	279	SER
1	3	282	PHE
1	3	294	LYS
1	3	301	LYS
1	3	311	ASP
1	3	312	ASN
1	3	326	HIS
1	3	330	VAL
1	3	331	ASP
1	4	26	VAL
1	4	27	VAL
1	4	50	GLY
1	4	51	VAL
1	4	52	PHE
1	4	53	LYS

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Mol	Chain	Res	Type
1	4	60	ASP
1	4	75	GLU
1	4	86	ALA
1	4	95	THR
1	4	98	PHE
1	4	106	ALA
1	4	107	HIS
1	4	112	ALA
1	4	132	ASN
1	4	133	LEU
1	4	147	SER
1	4	154	ALA
1	4	160	LEU
1	4	177	VAL
1	4	184	VAL
1	4	185	ASP
1	4	189	ALA
1	4	192	TRP
1	4	204	PRO
1	4	211	LYS
1	4	221	ASP
1	4	237	SER
1	4	265	PRO
1	4	267	GLN
1	4	276	ASP
1	4	277	VAL
1	4	278	VAL
1	4	280	SER
1	4	282	PHE
1	4	285	ASP
1	4	294	LYS
1	4	311	ASP
1	4	312	ASN
1	4	326	HIS
1	1	26	VAL
1	1	54	GLY
1	1	60	ASP
1	1	109	LYS
1	1	132	ASN
1	1	157	ALA
1	1	160	LEU
1	1	166	ILE

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Mol	Chain	Res	Type
1	1	181	GLN
1	1	185	ASP
1	1	197	GLY
1	1	219	GLU
1	1	262	SER
1	1	272	TYR
1	1	283	ILE
1	1	330	VAL
1	2	17	ARG
1	2	54	GLY
1	2	83	TRP
1	2	84	SER
1	2	108	PHE
1	2	112	ALA
1	2	113	LYS
1	2	125	PRO
1	2	129	CYS
1	2	130	GLY
1	2	161	HIS
1	2	215	LYS
1	2	219	GLU
1	2	264	GLY
1	2	265	PRO
1	2	280	SER
1	2	284	GLY
1	2	288	SER
1	2	294	LYS
1	2	300	SER
1	2	302	THR
1	3	8	PHE
1	3	13	ARG
1	3	51	VAL
1	3	112	ALA
1	3	113	LYS
1	3	118	SER
1	3	130	GLY
1	3	138	LYS
1	3	147	SER
1	3	189	ALA
1	3	198	ALA
1	3	204	PRO
1	3	219	GLU

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Mol	Chain	Res	Type
1	3	264	GLY
1	3	265	PRO
1	3	283	ILE
1	3	284	GLY
1	3	288	SER
1	3	300	SER
1	3	321	ILE
1	3	325	LYS
1	4	8	PHE
1	4	83	TRP
1	4	105	SER
1	4	108	PHE
1	4	113	LYS
1	4	118	SER
1	4	146	ALA
1	4	158	LYS
1	4	165	GLU
1	4	181	GLN
1	4	219	GLU
1	4	251	TYR
1	4	255	LYS
1	4	264	GLY
1	4	283	ILE
1	4	286	ASN
1	4	288	SER
1	1	108	PHE
1	1	162	GLU
1	1	165	GLU
1	1	233	THR
1	1	236	VAL
1	1	251	TYR
1	1	285	ASP
1	1	288	SER
1	1	301	LYS
1	1	310	TYR
1	2	138	LYS
1	2	279	SER
1	2	285	ASP
1	2	327	MET
1	3	162	GLU
1	3	232	PRO
1	3	249	CYS

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Mol	Chain	Res	Type
1	3	329	LYS
1	4	10	ARG
1	4	84	SER
1	4	109	LYS
1	4	110	GLY
1	4	130	GLY
1	4	180	THR
1	4	284	GLY
1	1	12	GLY
1	1	71	THR
1	1	106	ALA
1	1	268	GLY
1	1	287	ARG
1	1	329	LYS
1	2	52	PHE
1	2	166	ILE
1	2	236	VAL
1	2	328	GLN
1	3	12	GLY
1	3	28	ALA
1	3	166	ILE
1	3	185	ASP
1	3	253	ASP
1	3	272	TYR
1	3	280	SER
1	4	143	VAL
1	4	198	ALA
1	4	233	THR
1	4	236	VAL
1	4	279	SER
1	4	329	LYS
1	1	13	ARG
1	1	19	ALA
1	1	22	CYS
1	1	105	SER
1	1	154	ALA
1	1	279	SER
1	2	35	ALA
1	2	105	SER
1	2	109	LYS
1	2	154	ALA
1	2	180	THR

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Mol	Chain	Res	Type
1	3	39	MET
1	3	75	GLU
1	3	108	PHE
1	3	188	SER
1	3	281	ASP
1	3	287	ARG
1	4	138	LYS
1	4	161	HIS
1	4	166	ILE
1	4	205	SER
1	4	272	TYR
1	1	107	HIS
1	1	232	PRO
1	2	158	LYS
1	2	283	ILE
1	2	289	SER
1	2	330	VAL
1	3	236	VAL
1	3	289	SER
1	4	281	ASP
1	4	330	VAL
1	4	125	PRO
1	1	284	GLY
1	2	218	PRO
1	3	177	VAL
1	3	320	VAL
1	2	87	GLY
1	3	218	PRO
1	3	101	ILE
1	3	125	PRO

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	1	271/271 (100%)	160 (59%)	111 (41%)	0 0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2	271/271 (100%)	164 (60%)	107 (40%)	0	0
1	3	271/271 (100%)	166 (61%)	105 (39%)	0	0
1	4	271/271 (100%)	173 (64%)	98 (36%)	0	0
All	All	1084/1084 (100%)	663 (61%)	421 (39%)	0	0

All (421) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	3	ILE
1	1	8	PHE
1	1	11	ILE
1	1	14	LEU
1	1	16	LEU
1	1	26	VAL
1	1	30	ASN
1	1	33	PHE
1	1	34	ILE
1	1	37	GLU
1	1	39	MET
1	1	40	VAL
1	1	41	TYR
1	1	44	LYS
1	1	46	ASP
1	1	47	SER
1	1	51	VAL
1	1	53	LYS
1	1	57	LYS
1	1	58	MET
1	1	60	ASP
1	1	64	VAL
1	1	65	VAL
1	1	68	LYS
1	1	70	ILE
1	1	72	VAL
1	1	73	PHE
1	1	76	MET
1	1	77	LYS
1	1	78	PRO
1	1	81	ILE
1	1	84	SER
1	1	85	LYS

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Mol	Chain	Res	Type
1	1	90	TYR
1	1	91	ILE
1	1	92	VAL
1	1	97	VAL
1	1	99	THR
1	1	101	ILE
1	1	103	LYS
1	1	114	LYS
1	1	116	VAL
1	1	117	ILE
1	1	123	ASP
1	1	129	CYS
1	1	131	VAL
1	1	132	ASN
1	1	138	LYS
1	1	140	MET
1	1	141	THR
1	1	142	VAL
1	1	143	VAL
1	1	144	SER
1	1	145	ASN
1	1	153	LEU
1	1	156	VAL
1	1	165	GLU
1	1	170	LEU
1	1	171	MET
1	1	172	THR
1	1	178	THR
1	1	180	THR
1	1	183	THR
1	1	184	VAL
1	1	187	PRO
1	1	190	LYS
1	1	204	PRO
1	1	206	SER
1	1	211	LYS
1	1	215	LYS
1	1	220	LEU
1	1	223	LYS
1	1	224	LEU
1	1	227	MET
1	1	230	ARG

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Mol	Chain	Res	Type
1	1	231	VAL
1	1	232	PRO
1	1	238	VAL
1	1	239	VAL
1	1	244	ARG
1	1	253	ASP
1	1	255	LYS
1	1	258	MET
1	1	262	SER
1	1	263	GLU
1	1	266	LEU
1	1	270	LEU
1	1	273	THR
1	1	275	ASP
1	1	277	VAL
1	1	279	SER
1	1	290	ILE
1	1	292	ASP
1	1	297	ILE
1	1	298	GLN
1	1	299	LEU
1	1	301	LYS
1	1	302	THR
1	1	304	VAL
1	1	305	LYS
1	1	309	TRP
1	1	310	TYR
1	1	312	ASN
1	1	314	PHE
1	1	318	GLN
1	1	320	VAL
1	1	322	ASP
1	1	323	LEU
1	1	324	LEU
1	1	328	GLN
1	1	329	LYS
1	2	1	SER
1	2	2	LYS
1	2	3	ILE
1	2	8	PHE
1	2	10	ARG
1	2	11	ILE

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Mol	Chain	Res	Type
1	2	14	LEU
1	2	16	LEU
1	2	30	ASN
1	2	34	ILE
1	2	36	LEU
1	2	40	VAL
1	2	44	LYS
1	2	46	ASP
1	2	47	SER
1	2	51	VAL
1	2	53	LYS
1	2	58	MET
1	2	60	ASP
1	2	64	VAL
1	2	68	LYS
1	2	70	ILE
1	2	72	VAL
1	2	73	PHE
1	2	77	LYS
1	2	79	GLU
1	2	80	ASN
1	2	81	ILE
1	2	89	GLU
1	2	91	ILE
1	2	92	VAL
1	2	97	VAL
1	2	99	THR
1	2	101	ILE
1	2	102	GLU
1	2	108	PHE
1	2	109	LYS
1	2	114	LYS
1	2	116	VAL
1	2	117	ILE
1	2	123	ASP
1	2	128	VAL
1	2	131	VAL
1	2	132	ASN
1	2	138	LYS
1	2	139	ASP
1	2	140	MET
1	2	144	SER

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Mol	Chain	Res	Type
1	2	145	ASN
1	2	153	LEU
1	2	156	VAL
1	2	158	LYS
1	2	165	GLU
1	2	167	VAL
1	2	170	LEU
1	2	171	MET
1	2	172	THR
1	2	177	VAL
1	2	180	THR
1	2	183	THR
1	2	188	SER
1	2	190	LYS
1	2	205	SER
1	2	207	THR
1	2	211	LYS
1	2	215	LYS
1	2	216	VAL
1	2	220	LEU
1	2	223	LYS
1	2	225	THR
1	2	237	SER
1	2	238	VAL
1	2	239	VAL
1	2	243	VAL
1	2	245	LEU
1	2	247	LYS
1	2	253	ASP
1	2	255	LYS
1	2	258	MET
1	2	262	SER
1	2	263	GLU
1	2	266	LEU
1	2	270	LEU
1	2	274	GLU
1	2	275	ASP
1	2	279	SER
1	2	283	ILE
1	2	288	SER
1	2	289	SER
1	2	290	ILE

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Mol	Chain	Res	Type
1	2	292	ASP
1	2	297	ILE
1	2	298	GLN
1	2	299	LEU
1	2	300	SER
1	2	301	LYS
1	2	304	VAL
1	2	307	VAL
1	2	309	TRP
1	2	310	TYR
1	2	314	PHE
1	2	318	GLN
1	2	321	ILE
1	2	322	ASP
1	2	324	LEU
1	2	328	GLN
1	2	329	LYS
1	3	2	LYS
1	3	8	PHE
1	3	11	ILE
1	3	14	LEU
1	3	15	VAL
1	3	16	LEU
1	3	17	ARG
1	3	21	SER
1	3	27	VAL
1	3	30	ASN
1	3	34	ILE
1	3	37	GLU
1	3	40	VAL
1	3	44	LYS
1	3	46	ASP
1	3	51	VAL
1	3	53	LYS
1	3	55	GLU
1	3	58	MET
1	3	63	LEU
1	3	64	VAL
1	3	65	VAL
1	3	68	LYS
1	3	70	ILE
1	3	72	VAL

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Mol	Chain	Res	Type
1	3	80	ASN
1	3	81	ILE
1	3	85	LYS
1	3	90	TYR
1	3	91	ILE
1	3	95	THR
1	3	100	THR
1	3	101	ILE
1	3	105	SER
1	3	114	LYS
1	3	116	VAL
1	3	121	SER
1	3	125	PRO
1	3	126	MET
1	3	128	VAL
1	3	131	VAL
1	3	135	LYS
1	3	138	LYS
1	3	139	ASP
1	3	140	MET
1	3	143	VAL
1	3	145	ASN
1	3	150	THR
1	3	153	LEU
1	3	156	VAL
1	3	167	VAL
1	3	171	MET
1	3	172	THR
1	3	174	VAL
1	3	180	THR
1	3	184	VAL
1	3	187	PRO
1	3	188	SER
1	3	190	LYS
1	3	204	PRO
1	3	211	LYS
1	3	215	LYS
1	3	216	VAL
1	3	220	LEU
1	3	223	LYS
1	3	227	MET
1	3	230	ARG

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Mol	Chain	Res	Type
1	3	231	VAL
1	3	237	SER
1	3	238	VAL
1	3	239	VAL
1	3	253	ASP
1	3	254	ILE
1	3	255	LYS
1	3	258	MET
1	3	260	THR
1	3	263	GLU
1	3	266	LEU
1	3	270	LEU
1	3	274	GLU
1	3	275	ASP
1	3	283	ILE
1	3	288	SER
1	3	289	SER
1	3	290	ILE
1	3	292	ASP
1	3	294	LYS
1	3	297	ILE
1	3	298	GLN
1	3	299	LEU
1	3	301	LYS
1	3	302	THR
1	3	304	VAL
1	3	305	LYS
1	3	309	TRP
1	3	310	TYR
1	3	314	PHE
1	3	318	GLN
1	3	320	VAL
1	3	321	ILE
1	3	322	ASP
1	3	323	LEU
1	3	324	LEU
1	3	328	GLN
1	3	329	LYS
1	4	1	SER
1	4	2	LYS
1	4	8	PHE
1	4	11	ILE

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Mol	Chain	Res	Type
1	4	14	LEU
1	4	16	LEU
1	4	20	LEU
1	4	21	SER
1	4	25	GLN
1	4	26	VAL
1	4	27	VAL
1	4	29	VAL
1	4	30	ASN
1	4	37	GLU
1	4	40	VAL
1	4	43	PHE
1	4	53	LYS
1	4	56	VAL
1	4	58	MET
1	4	63	LEU
1	4	64	VAL
1	4	65	VAL
1	4	68	LYS
1	4	70	ILE
1	4	72	VAL
1	4	76	MET
1	4	77	LYS
1	4	79	GLU
1	4	81	ILE
1	4	97	VAL
1	4	99	THR
1	4	102	GLU
1	4	109	LYS
1	4	114	LYS
1	4	116	VAL
1	4	117	ILE
1	4	118	SER
1	4	120	PRO
1	4	126	MET
1	4	131	VAL
1	4	138	LYS
1	4	145	ASN
1	4	150	THR
1	4	151	ASN
1	4	153	LEU
1	4	156	VAL

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Mol	Chain	Res	Type
1	4	166	ILE
1	4	167	VAL
1	4	171	MET
1	4	172	THR
1	4	173	THR
1	4	180	THR
1	4	183	THR
1	4	191	ASP
1	4	196	ARG
1	4	204	PRO
1	4	205	SER
1	4	211	LYS
1	4	213	VAL
1	4	217	ILE
1	4	220	LEU
1	4	223	LYS
1	4	227	MET
1	4	230	ARG
1	4	231	VAL
1	4	232	PRO
1	4	236	VAL
1	4	239	VAL
1	4	253	ASP
1	4	258	MET
1	4	263	GLU
1	4	266	LEU
1	4	270	LEU
1	4	274	GLU
1	4	277	VAL
1	4	279	SER
1	4	283	ILE
1	4	286	ASN
1	4	289	SER
1	4	290	ILE
1	4	292	ASP
1	4	294	LYS
1	4	297	ILE
1	4	298	GLN
1	4	299	LEU
1	4	302	THR
1	4	305	LYS
1	4	310	TYR

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Mol	Chain	Res	Type
1	4	312	ASN
1	4	314	PHE
1	4	317	SER
1	4	318	GLN
1	4	323	LEU
1	4	324	LEU
1	4	328	GLN
1	4	329	LYS
1	4	331	ASP
1	4	332	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	25	GLN
1	1	30	ASN
1	1	107	HIS
1	1	132	ASN
1	1	175	HIS
1	1	201	ASN
1	1	312	ASN
1	1	326	HIS
1	1	328	GLN
1	2	6	ASN
1	2	25	GLN
1	2	30	ASN
1	2	49	HIS
1	2	132	ASN
1	2	175	HIS
1	2	181	GLN
1	2	201	ASN
1	2	328	GLN
1	3	6	ASN
1	3	25	GLN
1	3	30	ASN
1	3	49	HIS
1	3	175	HIS
1	3	201	ASN
1	3	326	HIS
1	3	328	GLN
1	4	25	GLN
1	4	80	ASN

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Mol	Chain	Res	Type
1	4	132	ASN
1	4	145	ASN
1	4	151	ASN
1	4	181	GLN
1	4	201	ASN
1	4	326	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	1	333/333 (100%)	-0.12	8 (2%) 59 49	2, 9, 28, 32	0
1	2	333/333 (100%)	-0.15	7 (2%) 63 54	2, 9, 28, 32	0
1	3	333/333 (100%)	-0.05	8 (2%) 59 49	2, 9, 28, 32	0
1	4	333/333 (100%)	-0.16	10 (3%) 52 42	2, 9, 28, 32	0
All	All	1332/1332 (100%)	-0.12	33 (2%) 58 48	2, 9, 28, 32	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1	110	GLY	6.2
1	4	86	ALA	5.6
1	3	112	ALA	5.2
1	3	86	ALA	4.3
1	2	212	ALA	4.3
1	4	110	GLY	4.3
1	4	333	ALA	4.0
1	3	54	GLY	3.9
1	3	191	ASP	3.9
1	3	84	SER	3.1
1	4	106	ALA	3.1
1	1	112	ALA	3.0
1	3	130	GLY	2.9
1	4	61	GLY	2.9
1	1	296	GLY	2.7
1	3	87	GLY	2.7
1	2	66	ASP	2.7
1	4	26	VAL	2.7
1	3	23	GLY	2.5
1	1	67	GLY	2.5
1	2	106	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	1	132	ASN	2.3
1	1	333	ALA	2.3
1	4	112	ALA	2.2
1	4	132	ASN	2.1
1	1	113	LYS	2.1
1	2	296	GLY	2.1
1	1	84	SER	2.1
1	2	21	SER	2.0
1	2	54	GLY	2.0
1	4	50	GLY	2.0
1	2	191	ASP	2.0
1	4	27	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.