



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:49 AM UTC

PDB ID : 4WIM / pdb_00004wim
Title : Crystal Structure of the GMP Synthetase from Plasmodium falciparum
Authors : Ballut, L.; Violot, S.; Haser, R.; Aghajari, N.
Deposited on : 2014-09-26
Resolution : 3.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

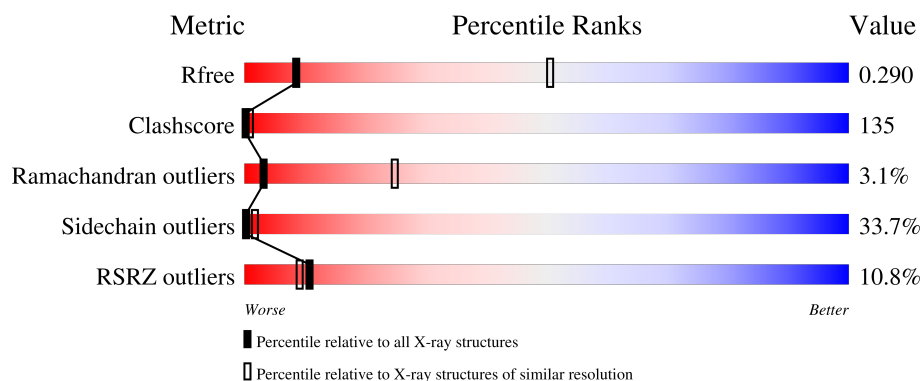
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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

Mol	Chain	Length	Quality of chain
1	A	568	11% 15% 29% 32% 15% 8%
1	B	568	8% 20% 30% 26% 9% 15%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7304 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 GMP synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	520	Total	C	N	O	S	0	0	0
			3941	2532	649	743	17			
1	B	480	Total	C	N	O	S	0	0	0
			3340	2115	570	645	10			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	MET	-	initiating methionine	UNP Q8IJR9
A	-11	ARG	-	expression tag	UNP Q8IJR9
A	-10	GLY	-	expression tag	UNP Q8IJR9
A	-9	SER	-	expression tag	UNP Q8IJR9
A	-8	HIS	-	expression tag	UNP Q8IJR9
A	-7	HIS	-	expression tag	UNP Q8IJR9
A	-6	HIS	-	expression tag	UNP Q8IJR9
A	-5	HIS	-	expression tag	UNP Q8IJR9
A	-4	HIS	-	expression tag	UNP Q8IJR9
A	-3	HIS	-	expression tag	UNP Q8IJR9
A	-2	GLY	-	expression tag	UNP Q8IJR9
A	-1	SER	-	expression tag	UNP Q8IJR9
A	0	MET	-	expression tag	UNP Q8IJR9
A	1	ALA	-	expression tag	UNP Q8IJR9
B	-12	MET	-	initiating methionine	UNP Q8IJR9
B	-11	ARG	-	expression tag	UNP Q8IJR9
B	-10	GLY	-	expression tag	UNP Q8IJR9
B	-9	SER	-	expression tag	UNP Q8IJR9
B	-8	HIS	-	expression tag	UNP Q8IJR9
B	-7	HIS	-	expression tag	UNP Q8IJR9
B	-6	HIS	-	expression tag	UNP Q8IJR9
B	-5	HIS	-	expression tag	UNP Q8IJR9
B	-4	HIS	-	expression tag	UNP Q8IJR9
B	-3	HIS	-	expression tag	UNP Q8IJR9
B	-2	GLY	-	expression tag	UNP Q8IJR9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	SER	-	expression tag	UNP Q8IJR9
B	0	MET	-	expression tag	UNP Q8IJR9
B	1	ALA	-	expression tag	UNP Q8IJR9

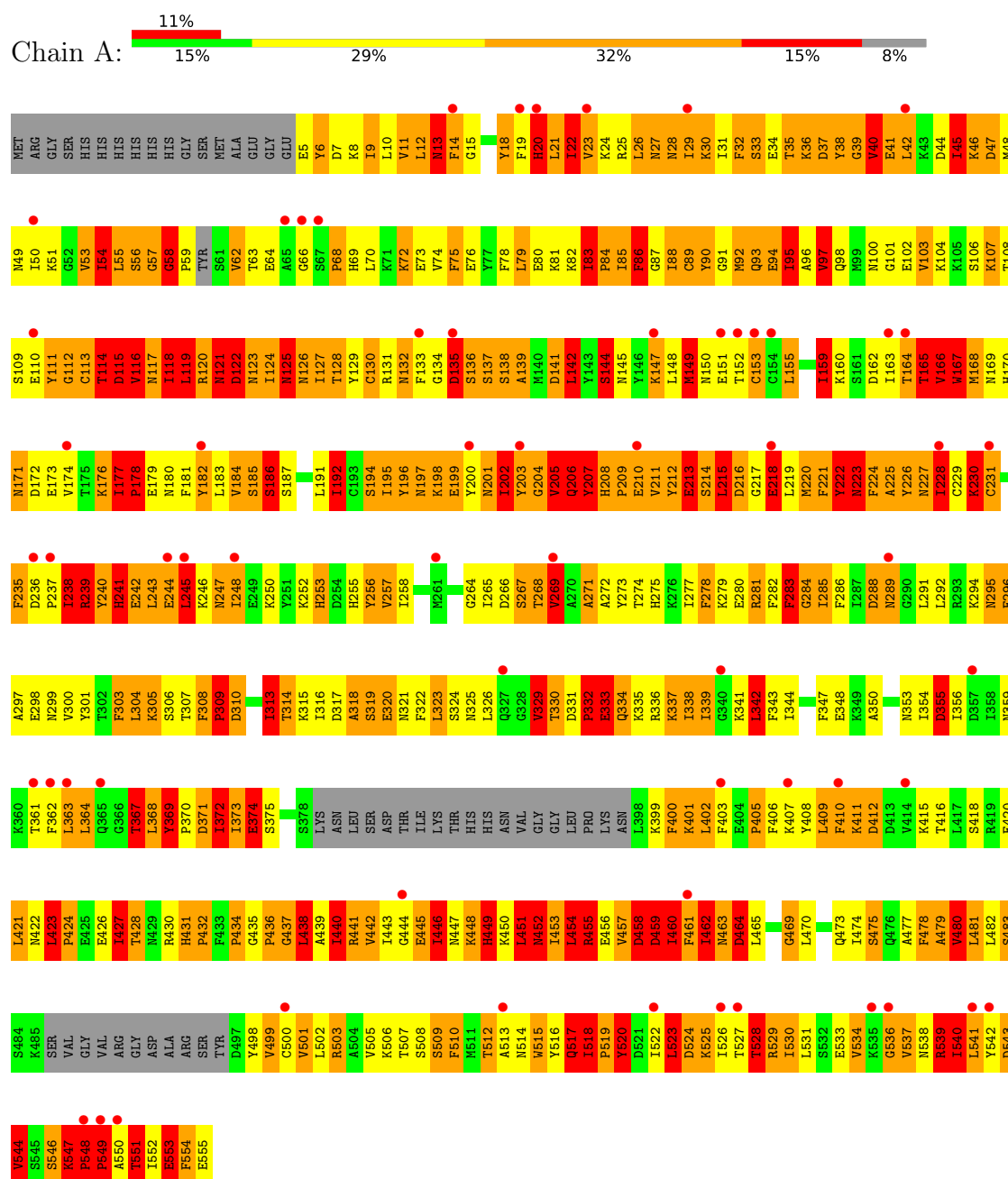
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	14	Total 14	O 14	0	0
2	B	9	Total 9	O 9	0	0

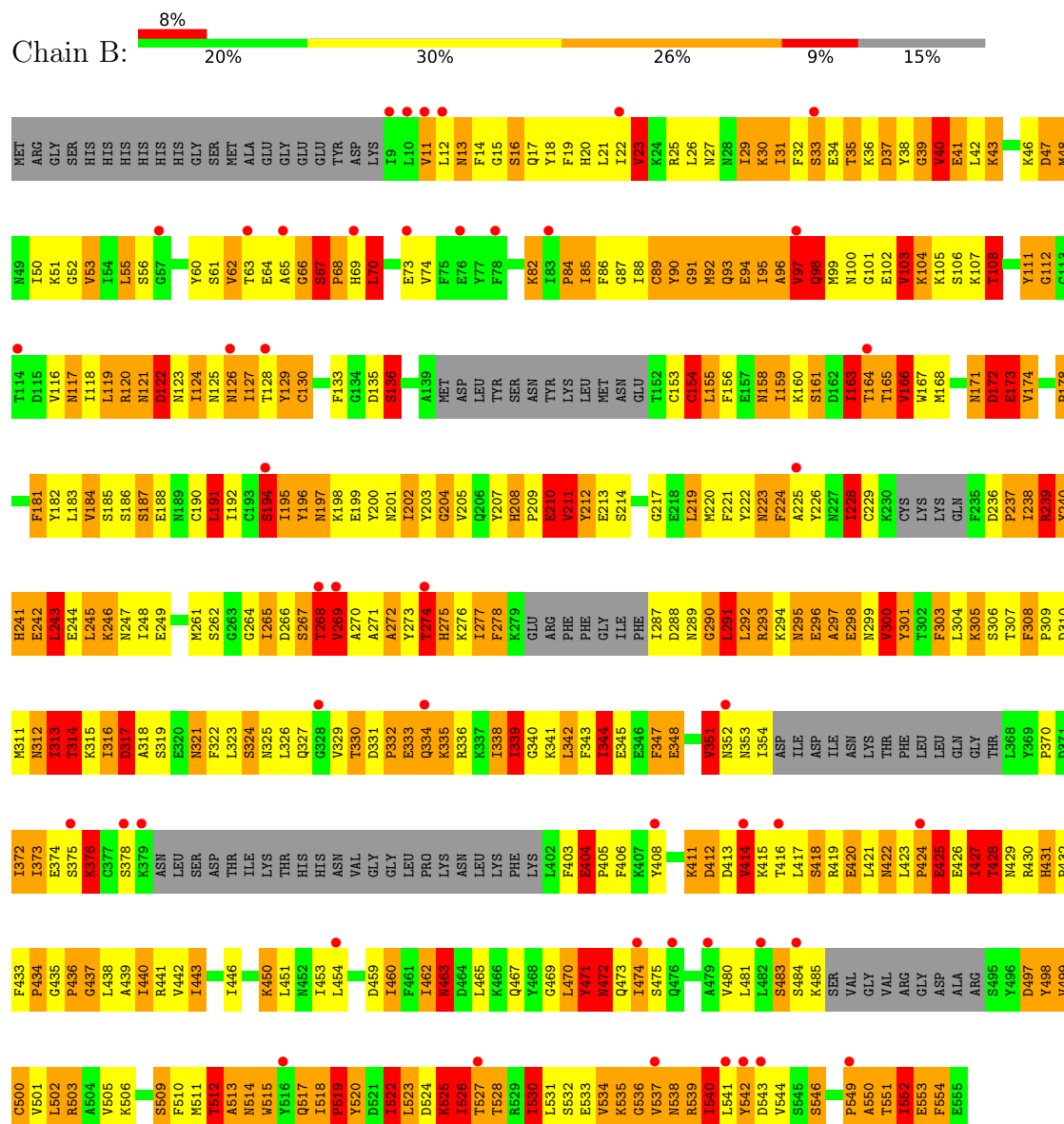
3 Residue-property plots

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: GMP synthetase



- Molecule 1: GMP synthetase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	43.45Å 68.55Å 102.08Å 101.11° 99.17° 93.71°	Depositor
Resolution (Å)	49.30 – 3.60 49.30 – 3.60	Depositor EDS
% Data completeness (in resolution range)	89.4 (49.30-3.60) 89.7 (49.30-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 3.57Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.281 , 0.293 0.282 , 0.290	Depositor DCC
R_{free} test set	595 reflections (4.53%)	wwPDB-VP
Wilson B-factor (Å ²)	125.1	Xtriage
Anisotropy	0.434	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 300.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	7304	wwPDB-VP
Average B, all atoms (Å ²)	115.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.66% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	2.42	190/4017 (4.7%)	2.45	310/5449 (5.7%)
1	B	2.02	72/3394 (2.1%)	2.24	198/4633 (4.3%)
All	All	2.25	262/7411 (3.5%)	2.36	508/10082 (5.0%)

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

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

All (262) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	332	PRO	N-CD	-20.34	1.19	1.47
1	A	118	ILE	CA-CB	-14.99	1.39	1.54
1	A	54	ILE	CA-CB	-14.64	1.33	1.55
1	A	462	ILE	CA-CB	-13.85	1.36	1.54
1	A	522	ILE	CA-CB	-12.88	1.38	1.54
1	A	501	VAL	CA-CB	-12.37	1.39	1.54
1	B	517	GLN	CA-C	-11.13	1.38	1.52
1	A	331	ASP	CA-C	-11.02	1.41	1.53
1	B	265	ILE	CA-CB	-10.14	1.41	1.54
1	A	519	PRO	CA-C	-9.96	1.41	1.52
1	A	478	PHE	C-O	-9.33	1.12	1.23
1	B	552	ILE	CA-CB	-9.29	1.42	1.54
1	A	480	VAL	CA-CB	-9.28	1.39	1.55
1	A	116	VAL	CA-CB	-9.22	1.42	1.55
1	A	202	ILE	CA-CB	-9.21	1.43	1.54
1	A	339	ILE	CA-CB	-9.20	1.43	1.54
1	A	530	ILE	CA-CB	-9.13	1.43	1.54
1	A	285	ILE	C-O	-9.09	1.14	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	9	ILE	CA-CB	-8.97	1.43	1.54
1	A	166	VAL	CA-CB	-8.74	1.46	1.55
1	A	284	GLY	C-O	-8.70	1.14	1.23
1	B	502	LEU	C-O	-8.41	1.14	1.24
1	B	519	PRO	N-CD	-8.39	1.35	1.47
1	A	427	ILE	CA-CB	-8.35	1.44	1.54
1	B	427	ILE	CA-CB	-8.34	1.45	1.54
1	A	32	PHE	CA-C	-8.28	1.42	1.52
1	B	550	ALA	CA-C	-8.27	1.42	1.52
1	B	268	THR	N-CA	-8.24	1.36	1.46
1	B	514	ASN	C-O	8.17	1.33	1.23
1	A	458	ASP	C-O	-8.14	1.14	1.24
1	B	515	TRP	CA-C	-8.05	1.42	1.52
1	A	286	PHE	C-O	-8.03	1.14	1.24
1	B	344	ILE	CA-CB	-8.00	1.43	1.54
1	A	83	ILE	C-O	-7.98	1.15	1.24
1	A	75	PHE	CA-C	-7.95	1.42	1.52
1	B	238	ILE	CA-CB	-7.92	1.44	1.54
1	A	369	TYR	CA-C	-7.90	1.42	1.52
1	A	30	LYS	CA-C	-7.77	1.43	1.53
1	A	529	ARG	CA-C	-7.76	1.43	1.52
1	B	174	VAL	CA-C	-7.74	1.43	1.52
1	A	116	VAL	CA-C	-7.69	1.44	1.52
1	A	442	VAL	CA-CB	-7.67	1.44	1.54
1	B	542	TYR	C-O	-7.67	1.13	1.23
1	A	38	TYR	CA-C	-7.62	1.43	1.52
1	A	124	ILE	CA-C	-7.59	1.43	1.52
1	A	225	ALA	CA-C	-7.56	1.43	1.52
1	A	128	THR	CA-CB	-7.53	1.42	1.53
1	A	13	ASN	CA-C	-7.52	1.43	1.52
1	B	333	GLU	CA-C	-7.52	1.43	1.52
1	A	517	GLN	CA-C	-7.50	1.43	1.52
1	A	83	ILE	CA-CB	-7.47	1.45	1.54
1	A	205	VAL	C-O	7.38	1.32	1.24
1	B	530	ILE	CA-CB	-7.37	1.44	1.54
1	A	479	ALA	CA-CB	-7.34	1.41	1.53
1	A	83	ILE	CA-C	-7.34	1.46	1.53
1	A	288	ASP	CA-C	-7.25	1.43	1.52
1	A	196	TYR	C-O	-7.16	1.14	1.23
1	A	218	GLU	CA-C	-7.16	1.43	1.52
1	B	522	ILE	CA-CB	-7.15	1.45	1.54
1	A	53	VAL	CA-CB	-7.14	1.42	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	314	THR	CA-CB	-7.10	1.41	1.53
1	A	457	VAL	CA-CB	-7.05	1.45	1.54
1	A	519	PRO	C-O	-7.03	1.15	1.23
1	A	410	PHE	CA-C	-6.98	1.44	1.52
1	A	20	HIS	C-O	-6.97	1.16	1.24
1	A	103	VAL	CA-CB	-6.93	1.43	1.55
1	A	458	ASP	CA-C	-6.93	1.43	1.52
1	A	318	ALA	CA-CB	-6.92	1.41	1.53
1	B	164	THR	CA-CB	-6.91	1.42	1.53
1	A	525	LYS	C-O	-6.90	1.16	1.24
1	A	118	ILE	CA-C	-6.87	1.43	1.53
1	B	296	GLU	C-O	-6.84	1.16	1.24
1	B	550	ALA	C-O	-6.82	1.15	1.23
1	B	29	ILE	CA-C	-6.71	1.44	1.52
1	B	300	VAL	CA-CB	-6.71	1.46	1.54
1	A	22	ILE	CA-CB	-6.69	1.46	1.54
1	A	518	ILE	CA-CB	-6.67	1.49	1.54
1	A	205	VAL	CA-CB	-6.65	1.46	1.54
1	A	201	ASN	CA-C	-6.65	1.44	1.53
1	B	197	ASN	CA-C	-6.64	1.44	1.52
1	A	29	ILE	CA-CB	-6.64	1.47	1.54
1	A	411	LYS	CA-C	-6.63	1.43	1.52
1	A	34	GLU	C-O	-6.62	1.15	1.23
1	A	522	ILE	N-CA	-6.59	1.38	1.46
1	A	530	ILE	CA-C	-6.58	1.44	1.52
1	A	117	ASN	C-O	-6.58	1.16	1.24
1	B	238	ILE	CA-C	-6.58	1.44	1.52
1	A	32	PHE	C-O	-6.57	1.15	1.23
1	A	95	ILE	N-CA	-6.55	1.39	1.46
1	A	350	ALA	C-O	6.55	1.31	1.24
1	A	458	ASP	N-CA	-6.55	1.38	1.46
1	A	197	ASN	C-O	6.50	1.32	1.24
1	A	20	HIS	CA-C	-6.46	1.44	1.52
1	A	537	VAL	CA-CB	-6.45	1.46	1.54
1	B	211	VAL	CA-CB	-6.45	1.45	1.54
1	A	453	ILE	CA-CB	-6.44	1.46	1.54
1	B	513	ALA	CA-C	6.44	1.60	1.52
1	B	552	ILE	C-O	-6.43	1.16	1.24
1	B	518	ILE	CA-CB	-6.39	1.46	1.54
1	A	428	THR	C-O	-6.38	1.16	1.24
1	B	29	ILE	CA-CB	-6.36	1.45	1.54
1	B	518	ILE	CA-C	-6.35	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	90	TYR	CA-C	-6.32	1.43	1.52
1	A	520	TYR	CA-C	-6.32	1.44	1.52
1	A	547	LYS	C-N	6.29	1.40	1.33
1	A	520	TYR	C-O	-6.26	1.16	1.24
1	A	84	PRO	C-O	-6.26	1.15	1.23
1	B	526	ILE	CA-CB	-6.24	1.46	1.54
1	A	452	ASN	CA-C	-6.20	1.44	1.52
1	A	454	LEU	C-O	-6.20	1.15	1.24
1	A	524	ASP	CA-C	-6.19	1.45	1.52
1	B	436	PRO	CA-C	-6.18	1.45	1.52
1	A	222	TYR	CA-C	-6.18	1.45	1.52
1	A	411	LYS	C-O	-6.18	1.16	1.24
1	A	409	LEU	CA-C	-6.17	1.45	1.52
1	A	40	VAL	CA-CB	-6.17	1.47	1.54
1	A	90	TYR	C-O	-6.16	1.16	1.24
1	A	409	LEU	C-O	-6.11	1.16	1.23
1	A	540	ILE	CA-C	6.10	1.59	1.52
1	A	364	LEU	CA-C	-6.09	1.45	1.52
1	A	526	ILE	CA-C	-6.07	1.45	1.52
1	A	303	PHE	CA-C	-6.07	1.44	1.52
1	A	527	THR	N-CA	-6.04	1.39	1.46
1	B	512	THR	CA-CB	-6.04	1.43	1.53
1	B	433	PHE	CA-C	-6.04	1.45	1.52
1	A	239	ARG	CA-C	-6.03	1.44	1.52
1	A	421	LEU	CA-C	-6.00	1.44	1.52
1	A	239	ARG	N-CA	-5.99	1.38	1.46
1	A	424	PRO	CA-C	-5.97	1.45	1.52
1	A	363	LEU	C-O	-5.97	1.16	1.23
1	A	223	ASN	CA-C	-5.97	1.45	1.52
1	A	460	ILE	CA-CB	-5.97	1.47	1.54
1	B	515	TRP	CA-CB	-5.96	1.44	1.53
1	A	185	SER	CA-C	5.96	1.60	1.52
1	A	226	TYR	N-CA	-5.95	1.39	1.46
1	A	41	GLU	CA-C	-5.93	1.45	1.53
1	A	329	VAL	CA-CB	-5.93	1.47	1.54
1	B	347	PHE	CA-C	-5.91	1.45	1.52
1	B	308	PHE	CA-C	-5.91	1.45	1.52
1	B	299	ASN	C-O	-5.90	1.17	1.24
1	B	105	LYS	CA-C	-5.85	1.45	1.53
1	A	101	GLY	CA-C	-5.83	1.46	1.52
1	A	500	CYS	CA-C	-5.83	1.45	1.52
1	B	454	LEU	CA-C	-5.81	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	128	THR	N-CA	-5.80	1.39	1.46
1	A	187	SER	CA-C	5.80	1.59	1.52
1	A	529	ARG	C-O	-5.79	1.17	1.24
1	B	40	VAL	C-O	-5.78	1.18	1.24
1	A	462	ILE	C-O	-5.76	1.17	1.24
1	A	534	VAL	CA-CB	-5.76	1.47	1.54
1	A	339	ILE	CA-C	-5.74	1.45	1.52
1	B	161	SER	CA-C	-5.74	1.45	1.52
1	B	450	LYS	C-O	-5.72	1.17	1.24
1	A	295	ASN	CA-C	-5.72	1.43	1.52
1	A	464	ASP	C-N	-5.71	1.26	1.33
1	B	277	ILE	CA-CB	-5.71	1.47	1.54
1	A	84	PRO	CA-C	-5.71	1.45	1.52
1	A	36	LYS	CA-C	-5.71	1.45	1.52
1	A	446	ILE	CA-CB	-5.70	1.47	1.54
1	A	138	SER	CA-C	-5.70	1.45	1.52
1	B	194	SER	CA-C	-5.70	1.45	1.52
1	A	338	ILE	CA-C	-5.68	1.46	1.52
1	B	502	LEU	CA-C	-5.68	1.46	1.52
1	B	450	LYS	N-CA	-5.67	1.39	1.46
1	B	463	ASN	CA-C	-5.67	1.45	1.52
1	A	534	VAL	C-O	-5.67	1.18	1.24
1	A	285	ILE	CA-CB	-5.66	1.47	1.54
1	A	412	ASP	C-O	-5.66	1.17	1.24
1	A	522	ILE	CA-C	-5.66	1.45	1.52
1	A	94	GLU	C-O	-5.66	1.17	1.24
1	A	462	ILE	CA-C	-5.66	1.45	1.52
1	A	480	VAL	CA-C	-5.64	1.46	1.52
1	A	92	MET	CA-C	-5.63	1.45	1.52
1	A	155	LEU	C-O	-5.62	1.16	1.24
1	A	441	ARG	CA-C	-5.58	1.45	1.52
1	A	272	ALA	CA-C	-5.56	1.45	1.52
1	A	131	ARG	N-CA	-5.53	1.39	1.46
1	B	351	VAL	CA-C	-5.53	1.45	1.52
1	A	316	ILE	C-O	-5.52	1.18	1.24
1	A	446	ILE	C-O	-5.52	1.18	1.24
1	A	411	LYS	N-CA	-5.52	1.39	1.46
1	A	520	TYR	N-CA	-5.51	1.39	1.46
1	A	93	GLN	CA-C	-5.50	1.45	1.52
1	B	313	ILE	CA-C	-5.50	1.45	1.52
1	B	519	PRO	C-O	-5.49	1.17	1.23
1	A	451	LEU	N-CA	-5.49	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	92	MET	C-O	-5.48	1.17	1.24
1	B	53	VAL	CA-CB	-5.46	1.47	1.54
1	A	544	VAL	CA-C	5.45	1.60	1.52
1	A	315	LYS	C-O	-5.45	1.17	1.23
1	A	522	ILE	C-O	-5.42	1.17	1.24
1	A	272	ALA	CA-CB	-5.42	1.44	1.53
1	B	103	VAL	CA-C	-5.42	1.45	1.52
1	A	256	TYR	CA-C	5.41	1.60	1.53
1	A	549	PRO	N-CD	5.40	1.55	1.47
1	A	455	ARG	CA-C	-5.39	1.45	1.52
1	A	342	LEU	C-O	-5.39	1.17	1.24
1	A	482	LEU	C-O	-5.39	1.17	1.23
1	A	528	THR	CA-CB	-5.38	1.45	1.53
1	A	72	LYS	C-O	-5.37	1.17	1.24
1	A	461	PHE	C-O	-5.36	1.18	1.24
1	B	210	GLU	C-O	-5.36	1.17	1.23
1	A	75	PHE	C-O	-5.36	1.17	1.24
1	A	155	LEU	CA-C	-5.36	1.44	1.52
1	A	94	GLU	C-N	-5.36	1.27	1.33
1	A	503	ARG	C-O	-5.35	1.17	1.23
1	A	13	ASN	N-CA	-5.35	1.39	1.46
1	A	337	LYS	N-CA	-5.35	1.40	1.46
1	A	176	LYS	C-O	-5.35	1.17	1.23
1	A	13	ASN	CA-CB	-5.34	1.46	1.53
1	A	220	MET	C-O	-5.33	1.17	1.24
1	B	187	SER	C-O	-5.33	1.17	1.23
1	A	272	ALA	C-O	-5.32	1.17	1.24
1	A	208	HIS	CA-C	-5.31	1.45	1.52
1	B	550	ALA	CA-CB	-5.30	1.43	1.53
1	A	186	SER	N-CA	5.29	1.52	1.46
1	A	215	LEU	N-CA	-5.28	1.40	1.46
1	B	451	LEU	N-CA	-5.27	1.40	1.46
1	B	499	VAL	CA-CB	-5.27	1.47	1.55
1	A	353	ASN	C-O	-5.26	1.17	1.24
1	A	554	PHE	C-O	-5.26	1.18	1.24
1	B	454	LEU	N-CA	-5.26	1.39	1.46
1	A	529	ARG	N-CA	-5.26	1.40	1.46
1	B	437	GLY	C-O	-5.25	1.17	1.23
1	A	356	ILE	CA-CB	-5.24	1.49	1.55
1	A	269	VAL	CA-CB	-5.23	1.48	1.54
1	A	518	ILE	C-O	-5.22	1.18	1.23
1	A	337	LYS	CA-C	-5.22	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	268	THR	C-O	-5.22	1.18	1.24
1	A	479	ALA	N-CA	-5.21	1.39	1.46
1	B	327	GLN	CA-C	5.20	1.60	1.52
1	A	530	ILE	C-O	-5.18	1.18	1.24
1	B	313	ILE	C-O	-5.16	1.18	1.24
1	B	414	VAL	C-O	-5.15	1.17	1.24
1	A	40	VAL	CA-C	-5.15	1.46	1.52
1	B	239	ARG	N-CA	-5.14	1.40	1.46
1	A	223	ASN	N-CA	-5.13	1.40	1.46
1	A	33	SER	CA-C	-5.12	1.46	1.52
1	A	208	HIS	C-O	-5.12	1.18	1.24
1	A	548	PRO	N-CD	5.12	1.54	1.47
1	A	272	ALA	N-CA	-5.12	1.40	1.46
1	A	56	SER	CA-CB	-5.11	1.44	1.53
1	A	322	PHE	CA-C	-5.10	1.46	1.52
1	B	450	LYS	CA-C	-5.10	1.46	1.52
1	A	422	ASN	CA-C	-5.09	1.45	1.53
1	A	527	THR	CA-CB	-5.09	1.45	1.53
1	A	178	PRO	CA-C	-5.08	1.46	1.52
1	B	471	TYR	C-O	-5.08	1.18	1.24
1	A	228	ILE	CA-CB	-5.07	1.48	1.54
1	B	462	ILE	CA-CB	-5.07	1.48	1.54
1	A	159	ILE	CA-CB	-5.07	1.47	1.54
1	A	13	ASN	C-O	-5.05	1.18	1.24
1	B	303	PHE	CA-C	-5.05	1.46	1.52
1	A	424	PRO	C-O	-5.05	1.17	1.23
1	B	542	TYR	CA-C	-5.04	1.46	1.53
1	A	437	GLY	C-O	-5.04	1.16	1.24
1	B	267	SER	CA-C	-5.04	1.46	1.52
1	A	13	ASN	CB-CG	-5.03	1.39	1.52
1	A	202	ILE	C-O	-5.03	1.18	1.24
1	A	499	VAL	CA-C	-5.03	1.46	1.52
1	A	14	PHE	C-O	-5.01	1.17	1.24
1	A	271	ALA	CA-C	-5.00	1.46	1.52

All (508) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	159	ILE	N-CA-C	-26.40	85.07	110.42
1	A	279	LYS	N-CA-C	20.09	133.25	111.36
1	B	67	SER	N-CA-C	-18.37	88.47	109.60
1	A	167	TRP	N-CA-C	-16.91	81.33	108.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	319	SER	N-CA-C	16.57	128.80	111.07
1	A	124	ILE	N-CA-C	-16.51	94.57	110.42
1	A	191	LEU	N-CA-C	16.25	128.69	111.14
1	A	353	ASN	N-CA-C	-15.62	94.23	113.28
1	A	244	GLU	N-CA-C	-15.45	92.57	111.11
1	A	267	SER	N-CA-C	15.11	127.24	111.07
1	B	437	GLY	N-CA-C	-14.86	94.90	112.73
1	B	30	LYS	N-CA-C	-14.61	90.48	110.35
1	B	427	ILE	N-CA-C	-14.03	97.01	113.42
1	A	458	ASP	N-CA-C	-13.98	96.12	111.36
1	A	113	CYS	N-CA-C	-13.50	89.75	109.59
1	A	118	ILE	CB-CA-C	-13.50	93.99	111.13
1	A	455	ARG	N-CA-C	-13.48	96.59	111.28
1	A	245	LEU	N-CA-C	13.28	125.28	111.07
1	A	218	GLU	N-CA-C	-13.03	97.16	111.36
1	B	520	TYR	N-CA-C	12.80	124.76	111.07
1	B	21	LEU	N-CA-C	-12.79	96.98	111.82
1	A	332	PRO	N-CA-CB	-12.77	89.84	103.25
1	B	265	ILE	CB-CA-C	-12.56	95.18	112.14
1	B	161	SER	N-CA-C	-12.46	92.23	110.42
1	B	500	CYS	N-CA-C	12.26	128.04	109.41
1	A	171	ASN	N-CA-C	-12.21	95.30	113.61
1	A	86	PHE	N-CA-C	-12.11	90.92	108.96
1	B	552	ILE	N-CA-C	12.05	122.89	110.72
1	A	427	ILE	N-CA-C	11.93	122.79	110.62
1	A	508	SER	N-CA-C	-11.93	96.85	111.40
1	A	29	ILE	N-CA-C	-11.86	92.31	110.09
1	B	171	ASN	N-CA-C	-11.82	98.99	113.41
1	B	91	GLY	N-CA-C	-11.77	98.47	112.83
1	A	87	GLY	N-CA-C	-11.56	88.77	110.97
1	B	112	GLY	N-CA-C	11.56	140.58	113.18
1	B	126	ASN	N-CA-C	11.44	126.73	113.01
1	B	174	VAL	N-CA-C	-11.43	92.17	108.17
1	A	526	ILE	CB-CA-C	-11.41	97.37	111.97
1	A	338	ILE	CB-CA-C	-11.37	97.42	111.97
1	A	196	TYR	N-CA-C	11.36	127.78	108.23
1	A	45	ILE	N-CA-C	-11.36	94.70	109.80
1	A	166	VAL	N-CA-C	-11.35	92.22	107.88
1	B	224	PHE	N-CA-C	-11.26	99.01	111.28
1	B	332	PRO	N-CA-C	11.18	129.46	113.47
1	A	22	ILE	CB-CA-C	-11.14	97.72	111.97
1	A	456	GLU	N-CA-C	11.07	123.34	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	332	PRO	CA-N-CD	10.90	127.26	112.00
1	A	54	ILE	N-CA-C	-10.81	92.96	108.42
1	A	481	LEU	N-CA-C	10.80	127.16	110.42
1	B	47	ASP	N-CA-C	-10.76	96.91	111.54
1	A	119	LEU	N-CA-C	10.71	126.32	107.80
1	A	153	CYS	N-CA-C	10.55	126.49	112.88
1	A	224	PHE	CA-C-N	-10.50	106.79	120.44
1	A	224	PHE	C-N-CA	-10.50	106.79	120.44
1	B	219	LEU	CA-C-N	-10.50	106.79	120.44
1	B	219	LEU	C-N-CA	-10.50	106.79	120.44
1	B	15	GLY	N-CA-C	10.49	129.80	115.32
1	B	278	PHE	N-CA-C	10.49	126.47	109.59
1	B	296	GLU	N-CA-C	-10.44	99.90	111.28
1	A	115	ASP	N-CA-C	-10.41	96.79	110.53
1	A	28	ASN	N-CA-C	-10.34	98.70	111.11
1	A	533	GLU	N-CA-C	10.33	124.39	111.69
1	A	202	ILE	CB-CA-C	-10.24	95.57	110.83
1	A	283	PHE	N-CA-C	10.23	126.37	108.56
1	B	66	GLY	N-CA-C	-10.17	100.41	114.64
1	B	334	GLN	CA-C-N	-10.10	107.31	120.44
1	B	334	GLN	C-N-CA	-10.10	107.31	120.44
1	A	329	VAL	CB-CA-C	-10.00	96.36	110.96
1	A	449	HIS	N-CA-C	9.94	121.88	111.14
1	A	212	TYR	N-CA-C	-9.93	98.71	113.61
1	B	534	VAL	N-CA-C	9.92	120.64	108.53
1	B	272	ALA	CA-C-N	-9.91	107.55	120.44
1	B	272	ALA	C-N-CA	-9.91	107.55	120.44
1	B	333	GLU	N-CA-C	-9.90	100.49	111.28
1	B	274	THR	N-CA-C	9.89	121.65	111.07
1	A	57	GLY	N-CA-C	-9.75	93.59	111.14
1	A	530	ILE	CB-CA-C	-9.74	99.50	111.97
1	B	339	ILE	N-CA-C	-9.61	100.82	110.62
1	B	436	PRO	N-CA-C	-9.60	96.24	111.03
1	B	228	ILE	N-CA-C	-9.56	103.83	113.10
1	A	168	MET	N-CA-C	9.52	123.35	108.79
1	A	540	ILE	CB-CA-C	9.52	124.81	110.62
1	A	216	ASP	N-CA-C	-9.42	100.88	112.38
1	A	58	GLY	N-CA-C	-9.42	93.12	112.34
1	A	26	LEU	N-CA-C	-9.37	101.04	111.07
1	A	522	ILE	CB-CA-C	-9.37	99.49	112.14
1	B	330	THR	CB-CA-C	-9.32	98.15	111.85
1	A	549	PRO	CA-N-CD	-9.28	98.51	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	532	SER	N-CA-C	9.24	123.81	112.54
1	A	208	HIS	CB-CA-C	-9.18	100.97	110.33
1	A	313	ILE	N-CA-C	9.13	120.89	108.84
1	A	356	ILE	N-CA-C	9.02	120.55	107.75
1	B	103	VAL	CB-CA-C	-8.98	96.56	111.29
1	A	436	PRO	N-CA-C	-8.97	102.16	114.27
1	A	442	VAL	N-CA-C	-8.92	94.73	107.75
1	B	552	ILE	CB-CA-C	-8.85	100.00	112.22
1	A	541	LEU	N-CA-C	-8.83	95.83	109.52
1	A	200	TYR	N-CA-C	-8.82	101.48	113.30
1	A	544	VAL	N-CA-C	8.79	124.03	113.22
1	A	530	ILE	N-CA-C	8.74	118.81	110.42
1	B	554	PHE	N-CA-C	8.70	121.86	111.33
1	A	230	LYS	N-CA-C	8.66	120.33	111.07
1	B	204	GLY	N-CA-C	-8.64	92.70	113.18
1	A	241	HIS	N-CA-C	-8.61	101.90	111.28
1	A	83	ILE	CA-C-N	8.59	128.45	120.21
1	A	83	ILE	C-N-CA	8.59	128.45	120.21
1	B	122	ASP	N-CA-C	-8.58	101.87	111.14
1	A	401	LYS	N-CA-C	-8.58	97.63	110.24
1	A	309	PRO	N-CA-C	8.55	125.69	113.47
1	B	472	ASN	N-CA-C	-8.54	102.87	113.20
1	B	404	GLU	N-CA-C	-8.52	97.22	109.48
1	A	138	SER	N-CA-C	-8.48	97.78	110.24
1	A	88	ILE	CB-CA-C	-8.42	99.52	111.40
1	B	277	ILE	CB-CA-C	-8.40	101.01	112.02
1	A	509	SER	N-CA-C	8.39	119.32	108.24
1	A	338	ILE	N-CA-C	8.37	118.46	110.42
1	A	309	PRO	CB-CA-C	-8.37	99.75	113.06
1	B	342	LEU	N-CA-C	-8.36	102.11	111.14
1	A	354	ILE	N-CA-C	-8.34	95.01	106.85
1	A	239	ARG	N-CA-C	-8.30	102.16	111.71
1	B	420	GLU	N-CA-C	-8.22	103.04	113.72
1	A	122	ASP	N-CA-C	-8.22	102.29	111.82
1	A	209	PRO	N-CA-C	-8.18	104.13	114.35
1	B	497	ASP	N-CA-C	8.13	121.60	108.76
1	B	535	LYS	N-CA-C	-8.12	96.94	109.52
1	B	62	VAL	N-CA-C	8.08	118.86	110.62
1	B	11	VAL	N-CA-C	-8.02	95.80	108.86
1	A	242	GLU	N-CA-C	8.01	120.02	111.28
1	B	474	ILE	N-CA-C	7.97	119.41	108.89
1	A	192	ILE	N-CA-C	7.95	118.73	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	40	VAL	N-CA-C	-7.93	98.66	109.37
1	A	231	CYS	N-CA-C	-7.92	100.31	111.24
1	B	481	LEU	N-CA-C	7.91	122.56	108.24
1	A	151	GLU	N-CA-C	7.91	119.68	111.14
1	A	227	ASN	N-CA-C	7.86	123.13	112.68
1	A	369	TYR	CB-CA-C	-7.84	94.72	110.17
1	A	116	VAL	CB-CA-C	-7.83	96.83	110.38
1	A	285	ILE	CB-CA-C	-7.83	98.90	110.33
1	A	228	ILE	N-CA-C	-7.82	102.91	110.42
1	A	203	TYR	CB-CA-C	-7.82	100.35	111.85
1	A	530	ILE	CA-C-N	-7.80	109.82	120.28
1	A	530	ILE	C-N-CA	-7.80	109.82	120.28
1	A	141	ASP	N-CA-C	7.78	119.39	111.07
1	B	514	ASN	N-CA-C	-7.78	95.84	109.06
1	B	98	GLN	N-CA-C	-7.74	102.81	111.71
1	A	46	LYS	N-CA-C	7.71	122.83	112.88
1	B	154	CYS	N-CA-C	-7.70	102.02	111.33
1	A	203	TYR	N-CA-C	7.67	121.14	108.49
1	A	198	LYS	N-CA-C	7.61	122.41	113.20
1	B	108	THR	N-CA-C	-7.59	101.21	111.54
1	A	31	ILE	N-CA-C	7.59	119.27	108.42
1	B	351	VAL	CB-CA-C	-7.58	101.91	112.14
1	A	11	VAL	CB-CA-C	-7.57	98.87	111.29
1	B	338	ILE	CB-CA-C	-7.55	102.13	112.02
1	A	53	VAL	N-CA-C	-7.55	96.58	108.81
1	A	364	LEU	N-CA-C	-7.53	97.85	109.52
1	B	318	ALA	N-CA-C	7.50	122.04	108.17
1	A	288	ASP	N-CA-C	-7.48	99.20	110.28
1	B	341	LYS	N-CA-C	-7.45	104.17	113.18
1	B	29	ILE	CB-CA-C	-7.44	99.10	111.29
1	B	100	ASN	N-CA-C	7.43	119.38	111.28
1	B	553	GLU	N-CA-C	-7.42	96.64	108.73
1	A	252	LYS	N-CA-C	7.42	119.15	111.14
1	A	55	LEU	N-CA-C	-7.35	97.88	109.50
1	A	8	LYS	N-CA-C	7.34	126.43	110.80
1	A	42	LEU	N-CA-C	-7.31	103.92	112.92
1	B	43	LYS	N-CA-C	-7.31	104.24	113.01
1	A	117	ASN	N-CA-C	7.30	121.10	108.76
1	B	317	ASP	N-CA-C	7.30	121.63	112.87
1	B	344	ILE	N-CA-C	-7.28	101.94	111.05
1	A	132	ASN	N-CA-C	7.26	120.35	110.55
1	B	63	THR	N-CA-C	-7.25	104.52	113.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	242	GLU	N-CA-C	-7.24	103.32	111.07
1	A	9	ILE	N-CA-C	7.23	118.89	108.48
1	A	524	ASP	CA-C-N	-7.23	110.59	120.28
1	A	524	ASP	C-N-CA	-7.23	110.59	120.28
1	A	329	VAL	N-CA-C	7.14	118.16	107.80
1	B	549	PRO	N-CA-C	7.12	130.61	112.10
1	A	204	GLY	N-CA-C	7.12	130.05	113.18
1	A	518	ILE	CB-CA-C	7.10	117.33	110.16
1	A	355	ASP	N-CA-C	7.09	120.67	109.39
1	A	166	VAL	N-CA-CB	-7.07	100.66	111.05
1	B	183	LEU	N-CA-C	7.07	120.45	109.07
1	A	412	ASP	CA-C-N	7.06	129.74	120.28
1	A	412	ASP	C-N-CA	7.06	129.74	120.28
1	B	33	SER	N-CA-C	7.05	119.58	108.79
1	A	240	TYR	CA-C-N	-7.04	110.84	120.28
1	A	240	TYR	C-N-CA	-7.04	110.84	120.28
1	B	84	PRO	CA-C-O	-7.00	113.44	121.56
1	A	120	ARG	N-CA-C	-6.99	99.12	109.81
1	B	173	GLU	N-CA-C	-6.93	100.02	110.28
1	A	548	PRO	C-N-CD	6.91	135.80	120.60
1	B	551	THR	N-CA-C	6.91	119.65	110.53
1	B	436	PRO	CA-C-N	-6.90	112.32	119.98
1	B	436	PRO	C-N-CA	-6.90	112.32	119.98
1	A	515	TRP	CA-C-N	6.89	131.15	120.75
1	A	515	TRP	C-N-CA	6.89	131.15	120.75
1	B	198	LYS	N-CA-C	-6.85	104.60	114.12
1	A	462	ILE	CB-CA-C	-6.83	102.79	112.22
1	A	515	TRP	N-CA-C	6.81	119.83	108.73
1	A	197	ASN	N-CA-C	6.80	119.78	108.96
1	A	126	ASN	N-CA-C	-6.78	103.13	111.33
1	A	445	GLU	N-CA-C	-6.77	100.25	110.28
1	A	253	HIS	N-CA-C	6.74	118.71	111.36
1	B	533	GLU	N-CA-C	6.74	118.71	111.36
1	B	518	ILE	CA-C-N	6.73	126.49	119.76
1	B	518	ILE	C-N-CA	6.73	126.49	119.76
1	B	330	THR	N-CA-C	6.73	119.59	108.49
1	A	313	ILE	CB-CA-C	-6.73	102.32	111.33
1	B	237	PRO	CB-CA-C	-6.71	102.39	113.06
1	A	333	GLU	N-CA-C	-6.71	104.20	112.38
1	A	460	ILE	CB-CA-C	-6.70	103.39	111.97
1	A	213	GLU	N-CA-C	-6.69	104.86	113.16
1	B	223	ASN	N-CA-C	6.68	118.64	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	50	ILE	N-CA-C	-6.68	99.55	107.70
1	B	536	GLY	N-CA-C	-6.66	105.31	114.64
1	A	238	ILE	CB-CA-C	-6.66	103.16	112.14
1	A	551	THR	N-CA-C	-6.62	98.87	109.39
1	A	124	ILE	CA-C-N	-6.61	110.04	121.66
1	A	124	ILE	C-N-CA	-6.61	110.04	121.66
1	A	479	ALA	N-CA-C	-6.60	100.66	110.23
1	A	285	ILE	CA-C-O	-6.59	113.38	120.36
1	B	538	ASN	N-CA-C	6.56	118.51	111.36
1	A	41	GLU	N-CA-C	-6.55	102.08	110.53
1	B	172	ASP	N-CA-C	6.55	120.29	107.98
1	B	411	LYS	N-CA-C	6.55	119.42	111.82
1	B	238	ILE	CB-CA-C	-6.54	103.20	112.22
1	A	364	LEU	CA-CB-CG	-6.54	93.42	116.30
1	A	135	ASP	N-CA-C	6.52	119.16	108.52
1	A	296	GLU	CA-C-N	-6.52	111.96	120.44
1	A	296	GLU	C-N-CA	-6.52	111.96	120.44
1	B	35	THR	N-CA-C	6.51	119.79	109.50
1	B	269	VAL	CB-CA-C	-6.51	103.63	111.97
1	B	269	VAL	N-CA-C	6.50	116.67	110.42
1	A	9	ILE	CB-CA-C	-6.50	100.94	110.62
1	A	411	LYS	CA-C-N	-6.49	111.07	120.29
1	A	411	LYS	C-N-CA	-6.49	111.07	120.29
1	A	12	LEU	N-CA-C	6.48	119.68	109.96
1	A	462	ILE	CA-C-N	-6.46	112.05	120.44
1	A	462	ILE	C-N-CA	-6.46	112.05	120.44
1	B	525	LYS	CA-C-N	-6.44	111.64	120.46
1	B	525	LYS	C-N-CA	-6.44	111.64	120.46
1	A	128	THR	N-CA-C	-6.43	103.87	112.94
1	B	105	LYS	N-CA-C	6.42	118.84	110.43
1	A	18	TYR	N-CA-C	-6.41	104.77	112.59
1	B	513	ALA	N-CA-C	-6.41	98.63	108.76
1	A	206	GLN	N-CA-C	-6.40	105.42	112.72
1	B	519	PRO	N-CA-CB	-6.40	97.39	103.34
1	A	101	GLY	N-CA-C	-6.39	101.45	112.06
1	A	178	PRO	CB-CA-C	-6.35	103.58	111.64
1	B	96	ALA	N-CA-C	-6.35	104.36	111.28
1	A	372	ILE	N-CA-C	-6.35	103.11	111.05
1	B	433	PHE	N-CA-C	-6.35	95.79	109.81
1	A	47	ASP	N-CA-C	-6.33	100.41	113.31
1	B	518	ILE	N-CA-C	-6.33	95.22	108.88
1	A	124	ILE	CB-CA-C	-6.32	103.88	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	432	PRO	CA-C-O	-6.28	114.40	121.43
1	A	350	ALA	CA-C-O	6.26	127.40	120.82
1	A	459	ASP	CA-C-N	-6.24	112.69	120.56
1	A	459	ASP	C-N-CA	-6.24	112.69	120.56
1	B	124	ILE	CB-CA-C	-6.23	103.86	112.02
1	A	118	ILE	N-CA-C	-6.23	100.75	110.09
1	B	300	VAL	CB-CA-C	-6.22	104.01	111.97
1	A	547	LYS	CA-C-N	-6.22	113.98	120.38
1	A	547	LYS	C-N-CA	-6.22	113.98	120.38
1	A	144	SER	N-CA-C	-6.20	104.52	111.28
1	B	23	VAL	N-CA-C	6.20	116.94	110.62
1	A	426	GLU	N-CA-C	6.19	118.03	111.28
1	A	440	ILE	CB-CA-C	6.17	120.74	112.22
1	A	441	ARG	N-CA-C	-6.16	105.62	113.01
1	A	280	GLU	N-CA-C	6.15	120.79	113.16
1	A	79	LEU	CA-C-N	-6.15	109.80	121.54
1	A	79	LEU	C-N-CA	-6.15	109.80	121.54
1	A	150	ASN	N-CA-C	6.14	118.64	110.53
1	B	298	GLU	N-CA-C	-6.13	104.67	111.36
1	A	221	PHE	CB-CA-C	-6.12	100.62	110.79
1	A	448	LYS	N-CA-C	6.12	117.94	111.28
1	B	155	LEU	CA-C-N	-6.11	114.84	123.03
1	B	155	LEU	C-N-CA	-6.11	114.84	123.03
1	A	243	LEU	CA-CB-CG	-6.11	94.92	116.30
1	A	267	SER	N-CA-CB	-6.10	101.16	110.01
1	A	405	PRO	N-CA-C	6.08	122.16	113.47
1	A	517	GLN	CA-C-N	6.07	128.13	122.85
1	A	517	GLN	C-N-CA	6.07	128.13	122.85
1	A	75	PHE	CA-C-N	-6.06	111.68	120.29
1	A	75	PHE	C-N-CA	-6.06	111.68	120.29
1	A	353	ASN	N-CA-CB	6.06	119.97	110.46
1	A	199	GLU	N-CA-C	-6.06	106.50	114.31
1	A	520	TYR	CA-C-N	-6.06	112.56	120.44
1	A	520	TYR	C-N-CA	-6.06	112.56	120.44
1	A	281	ARG	CA-C-N	-6.05	114.24	122.77
1	A	281	ARG	C-N-CA	-6.05	114.24	122.77
1	A	373	ILE	N-CA-C	6.05	116.83	110.72
1	B	414	VAL	N-CA-C	-6.05	103.53	111.09
1	A	208	HIS	O-C-N	6.05	127.24	120.83
1	A	100	ASN	CA-C-N	-6.04	116.02	122.67
1	A	100	ASN	C-N-CA	-6.04	116.02	122.67
1	B	239	ARG	CB-CA-C	-6.04	101.14	110.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	542	TYR	CA-C-O	-6.04	113.62	120.32
1	B	301	TYR	N-CA-C	-6.02	105.42	112.89
1	A	423	LEU	N-CA-C	-6.01	100.21	109.41
1	B	418	SER	CA-C-N	-6.01	112.22	122.56
1	B	418	SER	C-N-CA	-6.01	112.22	122.56
1	A	480	VAL	CB-CA-C	-6.01	101.08	110.69
1	B	65	ALA	N-CA-C	5.99	118.91	110.23
1	A	427	ILE	CB-CA-C	-5.98	104.07	112.14
1	A	554	PHE	N-CA-C	5.98	117.47	111.07
1	B	297	ALA	N-CA-C	5.98	117.79	111.28
1	B	469	GLY	N-CA-C	5.98	123.57	115.32
1	B	300	VAL	N-CA-C	5.97	116.16	110.42
1	B	336	ARG	N-CA-C	5.97	117.87	111.36
1	B	515	TRP	CB-CA-C	-5.97	100.01	109.80
1	A	126	ASN	CA-C-N	-5.96	111.25	121.97
1	A	126	ASN	C-N-CA	-5.96	111.25	121.97
1	A	165	THR	N-CA-C	-5.95	100.92	110.14
1	B	534	VAL	CB-CA-C	-5.95	102.22	110.91
1	B	376	LYS	N-CA-C	5.94	118.27	111.02
1	B	272	ALA	N-CA-C	5.94	117.42	111.07
1	A	524	ASP	N-CA-C	-5.91	104.74	111.07
1	B	268	THR	CA-C-N	-5.90	113.13	120.56
1	B	268	THR	C-N-CA	-5.90	113.13	120.56
1	B	467	GLN	N-CA-C	5.90	117.79	111.36
1	A	222	TYR	CB-CA-C	-5.89	101.63	110.88
1	A	66	GLY	N-CA-C	5.89	123.73	115.43
1	B	470	LEU	N-CA-C	-5.88	106.26	113.50
1	B	243	LEU	N-CA-C	5.87	117.35	111.07
1	B	348	GLU	N-CA-C	5.86	117.67	111.28
1	B	509	SER	N-CA-C	5.86	116.29	108.38
1	A	534	VAL	CB-CA-C	-5.86	102.96	110.98
1	A	85	ILE	N-CA-C	-5.85	99.19	108.90
1	A	84	PRO	CA-C-O	-5.85	114.06	122.31
1	A	63	THR	CB-CA-C	-5.83	100.35	110.09
1	A	37	ASP	N-CA-C	-5.83	100.68	109.95
1	B	119	LEU	N-CA-C	5.83	117.64	108.96
1	A	438	LEU	CA-C-N	-5.81	112.88	120.44
1	A	438	LEU	C-N-CA	-5.81	112.88	120.44
1	B	103	VAL	N-CA-C	5.81	121.43	109.34
1	B	340	GLY	N-CA-C	5.81	119.24	112.50
1	A	544	VAL	N-CA-CB	-5.81	103.24	112.07
1	A	164	THR	CB-CA-C	-5.78	98.33	109.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	423	LEU	CA-C-N	5.77	126.09	119.92
1	A	423	LEU	C-N-CA	5.77	126.09	119.92
1	B	460	ILE	N-CA-C	-5.77	104.74	110.62
1	A	424	PRO	O-C-N	5.76	129.88	122.91
1	B	335	LYS	N-CA-C	-5.76	104.91	111.07
1	B	526	ILE	CB-CA-C	-5.76	104.37	112.14
1	A	510	PHE	N-CA-C	5.73	117.53	111.28
1	A	164	THR	N-CA-C	-5.73	100.06	109.40
1	A	194	SER	N-CA-C	5.72	119.15	109.76
1	A	424	PRO	CA-C-O	-5.72	114.79	121.95
1	A	215	LEU	N-CA-CB	-5.71	101.73	110.12
1	B	332	PRO	CA-C-N	-5.71	112.63	120.28
1	B	332	PRO	C-N-CA	-5.71	112.63	120.28
1	B	305	LYS	CA-C-N	-5.70	113.03	120.44
1	B	305	LYS	C-N-CA	-5.70	113.03	120.44
1	A	421	LEU	CB-CA-C	-5.69	100.58	110.09
1	A	529	ARG	CB-CA-C	-5.68	101.97	110.88
1	A	517	GLN	N-CA-C	-5.67	101.35	110.14
1	A	121	ASN	N-CA-C	5.67	117.46	111.28
1	A	374	GLU	N-CA-C	-5.65	106.47	113.19
1	A	177	ILE	CB-CA-C	-5.64	101.09	111.36
1	A	214	SER	CB-CA-C	-5.64	103.56	111.85
1	B	37	ASP	CA-C-N	-5.62	112.95	120.54
1	B	37	ASP	C-N-CA	-5.62	112.95	120.54
1	A	501	VAL	CA-C-N	5.62	130.47	122.72
1	A	501	VAL	C-N-CA	5.62	130.47	122.72
1	B	531	LEU	CA-CB-CG	5.62	135.96	116.30
1	A	284	GLY	O-C-N	-5.62	117.37	122.93
1	A	553	GLU	N-CA-C	-5.62	100.63	109.50
1	B	240	TYR	N-CA-C	5.61	117.40	111.28
1	A	308	PHE	CA-C-N	5.60	124.80	118.97
1	A	308	PHE	C-N-CA	5.60	124.80	118.97
1	B	53	VAL	CB-CA-C	-5.60	101.87	110.50
1	A	103	VAL	N-CA-C	5.60	117.88	108.81
1	A	536	GLY	N-CA-C	5.60	123.16	115.27
1	A	207	TYR	N-CA-C	-5.59	101.90	109.95
1	B	471	TYR	CA-C-N	-5.59	110.76	121.94
1	B	471	TYR	C-N-CA	-5.59	110.76	121.94
1	B	238	ILE	N-CA-C	-5.58	105.08	110.72
1	A	114	THR	CB-CA-C	-5.57	100.91	110.16
1	A	330	THR	CB-CA-C	-5.57	98.35	109.99
1	B	540	ILE	N-CA-C	-5.57	100.28	108.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	539	ARG	N-CA-C	-5.56	100.62	109.23
1	A	68	PRO	N-CA-C	5.55	119.91	111.19
1	A	247	ASN	CB-CA-C	5.55	120.01	110.79
1	A	525	LYS	N-CA-C	5.53	117.31	111.28
1	B	422	ASN	N-CA-C	5.52	119.01	111.39
1	A	523	LEU	N-CA-C	5.51	117.36	111.36
1	A	334	GLN	N-CA-C	-5.50	105.37	111.36
1	B	515	TRP	O-C-N	5.49	129.48	123.22
1	A	255	HIS	N-CA-C	5.48	117.83	108.90
1	B	34	GLU	N-CA-C	-5.48	100.75	109.07
1	B	509	SER	CA-C-N	5.46	127.59	120.28
1	B	509	SER	C-N-CA	5.46	127.59	120.28
1	A	21	LEU	CB-CA-C	5.44	119.83	110.79
1	A	499	VAL	CB-CA-C	-5.43	102.40	110.33
1	B	267	SER	CB-CA-C	-5.43	102.36	110.88
1	B	428	THR	CB-CA-C	-5.43	101.17	110.24
1	A	230	LYS	CA-C-N	-5.43	114.70	122.68
1	A	230	LYS	C-N-CA	-5.43	114.70	122.68
1	B	335	LYS	CA-C-N	-5.42	112.59	120.29
1	B	335	LYS	C-N-CA	-5.42	112.59	120.29
1	B	187	SER	N-CA-C	5.42	117.04	108.96
1	B	130	CYS	N-CA-C	-5.41	105.90	112.88
1	A	421	LEU	CB-CG-CD2	-5.41	94.48	110.70
1	A	305	LYS	CB-CA-C	-5.40	101.83	110.79
1	B	483	SER	N-CA-C	5.40	119.43	112.41
1	B	431	HIS	N-CA-CB	-5.39	100.77	110.37
1	B	237	PRO	N-CA-C	5.39	121.17	113.47
1	A	125	ASN	N-CA-C	5.39	119.91	113.23
1	B	499	VAL	N-CA-C	5.39	115.93	108.23
1	A	26	LEU	N-CA-CB	5.38	117.82	110.01
1	A	205	VAL	CA-C-O	5.38	126.19	120.48
1	A	412	ASP	CB-CA-C	5.38	120.00	110.85
1	A	45	ILE	CB-CA-C	-5.38	103.86	111.28
1	B	39	GLY	CA-C-N	-5.37	113.48	120.63
1	B	39	GLY	C-N-CA	-5.37	113.48	120.63
1	A	420	GLU	N-CA-C	-5.37	105.99	112.54
1	A	111	TYR	CB-CA-C	-5.37	110.41	116.63
1	A	424	PRO	CA-C-N	5.37	127.91	120.29
1	A	424	PRO	C-N-CA	5.37	127.91	120.29
1	A	503	ARG	CB-CG-CD	5.36	123.63	111.30
1	A	208	HIS	CA-C-N	5.36	126.39	120.45
1	A	208	HIS	C-N-CA	5.36	126.39	120.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	70	LEU	N-CA-CB	-5.35	102.11	109.97
1	B	434	PRO	N-CA-C	-5.33	103.75	111.22
1	B	412	ASP	N-CA-CB	-5.33	102.28	110.01
1	B	530	ILE	CB-CA-C	-5.33	104.86	112.22
1	B	276	LYS	CA-C-N	-5.33	113.74	120.56
1	B	276	LYS	C-N-CA	-5.33	113.74	120.56
1	A	268	THR	CA-C-N	-5.31	113.19	120.46
1	A	268	THR	C-N-CA	-5.31	113.19	120.46
1	A	310	ASP	N-CA-C	5.29	117.65	107.44
1	B	197	ASN	CA-C-N	-5.29	113.92	122.23
1	B	197	ASN	C-N-CA	-5.29	113.92	122.23
1	A	278	PHE	CA-C-N	5.29	127.80	120.29
1	A	278	PHE	C-N-CA	5.29	127.80	120.29
1	A	130	CYS	N-CA-C	-5.28	105.70	113.61
1	A	269	VAL	N-CA-C	5.27	116.00	110.62
1	B	158	ASN	CA-C-N	-5.27	113.92	120.56
1	B	158	ASN	C-N-CA	-5.27	113.92	120.56
1	A	441	ARG	CA-C-N	-5.26	116.10	123.10
1	A	441	ARG	C-N-CA	-5.26	116.10	123.10
1	B	278	PHE	N-CA-CB	-5.25	102.24	110.69
1	B	424	PRO	N-CA-C	-5.25	103.21	111.34
1	A	325	ASN	CA-C-N	-5.24	115.17	123.24
1	A	325	ASN	C-N-CA	-5.24	115.17	123.24
1	B	531	LEU	N-CA-C	-5.23	105.47	111.07
1	B	194	SER	N-CA-C	-5.23	100.57	108.52
1	B	97	VAL	N-CA-C	5.23	115.95	110.62
1	A	112	GLY	CA-C-N	-5.22	113.72	121.24
1	A	112	GLY	C-N-CA	-5.22	113.72	121.24
1	A	539	ARG	NE-CZ-NH2	5.21	123.89	119.20
1	B	503	ARG	N-CA-C	5.21	117.74	109.24
1	A	95	ILE	N-CA-CB	-5.21	104.46	110.55
1	A	342	LEU	CA-CB-CG	-5.21	98.08	116.30
1	A	367	THR	N-CA-C	5.21	116.88	108.34
1	A	185	SER	N-CA-C	5.19	117.63	108.75
1	B	436	PRO	CB-CA-C	-5.19	105.10	111.64
1	A	342	LEU	N-CA-C	5.19	117.02	111.36
1	A	30	LYS	CA-C-N	-5.19	114.76	122.23
1	A	30	LYS	C-N-CA	-5.19	114.76	122.23
1	B	373	ILE	CA-C-N	-5.19	113.33	120.28
1	B	373	ILE	C-N-CA	-5.19	113.33	120.28
1	A	478	PHE	CA-C-N	-5.17	113.37	120.71
1	A	478	PHE	C-N-CA	-5.17	113.37	120.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	125	ASN	N-CA-CB	5.17	118.50	110.44
1	A	320	GLU	N-CA-C	5.16	117.65	111.71
1	A	139	ALA	N-CA-C	-5.16	105.74	111.36
1	B	462	ILE	N-CA-C	-5.15	106.01	113.07
1	A	24	LYS	N-CA-C	5.15	116.58	111.07
1	B	425	GLU	N-CA-C	-5.15	103.89	110.53
1	A	185	SER	CA-CB-OG	-5.14	100.82	111.10
1	B	181	PHE	N-CA-C	5.13	117.30	107.75
1	B	314	THR	N-CA-C	-5.13	103.76	110.53
1	A	56	SER	CA-C-O	-5.13	115.25	120.99
1	A	469	GLY	N-CA-C	5.12	122.42	115.30
1	A	226	TYR	N-CA-C	5.12	117.52	111.33
1	A	119	LEU	CB-CA-C	-5.12	103.15	110.62
1	A	182	TYR	N-CA-C	5.12	118.35	110.42
1	A	97	VAL	CA-C-N	-5.11	113.78	122.56
1	A	97	VAL	C-N-CA	-5.11	113.78	122.56
1	A	316	ILE	CB-CA-C	-5.10	103.54	110.42
1	A	431	HIS	N-CA-C	-5.10	98.55	109.81
1	B	167	TRP	N-CA-C	-5.10	101.00	109.46
1	A	343	PHE	N-CA-C	-5.09	105.81	111.36
1	B	375	SER	N-CA-C	5.08	116.51	111.07
1	A	409	LEU	N-CA-C	-5.08	100.59	108.42
1	B	378	SER	N-CA-C	5.08	116.81	111.28
1	B	125	ASN	N-CA-C	-5.08	105.87	111.71
1	B	121	ASN	CB-CA-C	5.07	117.93	109.56
1	A	39	GLY	N-CA-C	-5.06	101.19	113.18
1	B	551	THR	CA-C-N	5.06	127.61	120.42
1	B	551	THR	C-N-CA	5.06	127.61	120.42
1	A	196	TYR	N-CA-CB	-5.05	102.92	110.24
1	A	142	LEU	CA-CB-CG	-5.04	98.67	116.30
1	A	63	THR	N-CA-C	-5.04	106.83	113.17
1	A	402	LEU	N-CA-C	5.04	117.03	110.53
1	A	434	PRO	N-CA-C	5.03	120.53	113.53
1	A	454	LEU	CA-C-N	-5.01	113.56	120.28
1	A	454	LEU	C-N-CA	-5.01	113.56	120.28
1	A	315	LYS	N-CA-C	-5.01	99.51	108.13
1	A	123	ASN	N-CA-C	-5.01	107.12	113.18
1	A	128	THR	N-CA-CB	-5.01	102.72	110.98
1	A	139	ALA	O-C-N	5.01	127.86	122.15
1	B	13	ASN	N-CA-C	5.01	116.89	108.73
1	A	64	GLU	N-CA-C	-5.00	100.74	108.90
1	B	347	PHE	CB-CA-C	-5.00	103.03	110.88

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	134	GLY	Peptide
1	A	135	ASP	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3941	0	3629	1029	1
1	B	3340	0	2831	846	1
2	A	14	0	0	4	0
2	B	9	0	0	4	0
All	All	7304	0	6460	1854	1

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 135.

All (1854) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:VAL:CG1	1:A:207:TYR:HD2	1.05	1.67
1:A:461:PHE:CE2	1:A:502:LEU:HD23	1.12	1.59
1:A:166:VAL:CG1	1:A:207:TYR:CD2	1.86	1.56
1:B:70:LEU:CD1	1:B:94:GLU:CD	1.77	1.55
1:B:92:MET:HA	1:B:95:ILE:CD1	1.35	1.55
1:A:502:LEU:CD1	1:A:540:ILE:HD11	1.35	1.54
1:A:166:VAL:HG11	1:A:207:TYR:CD2	1.38	1.51
1:A:461:PHE:CE2	1:A:502:LEU:CD2	1.93	1.50
1:A:92:MET:HA	1:A:95:ILE:CG2	1.43	1.47
1:B:46:LYS:N	1:B:48:MET:HG3	1.27	1.45
1:B:68:PRO:CD	1:B:90:TYR:OH	1.65	1.44
1:B:440:ILE:HD12	1:B:441:ARG:N	1.14	1.44
1:A:543:ASP:HB2	1:B:541:LEU:CD2	1.46	1.43
1:A:205:VAL:CG2	1:A:207:TYR:CD1	2.02	1.43
1:B:291:LEU:HD12	1:B:437:GLY:C	0.99	1.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:MET:C	1:A:95:ILE:HG23	1.46	1.40
1:B:291:LEU:HD13	1:B:437:GLY:N	1.35	1.38
1:A:181:PHE:CE1	1:A:195:ILE:O	1.78	1.36
1:B:503:ARG:NH1	1:B:543:ASP:OD2	1.58	1.36
1:A:205:VAL:CG2	1:A:207:TYR:HD1	1.36	1.36
1:A:10:LEU:O	1:A:54:ILE:HG22	1.25	1.35
1:A:454:LEU:C	1:A:454:LEU:HD12	1.50	1.35
1:B:518:ILE:HD13	1:B:523:LEU:CD2	1.54	1.35
1:A:92:MET:CA	1:A:95:ILE:CG2	2.02	1.34
1:B:291:LEU:CG	1:B:437:GLY:HA3	1.56	1.34
1:B:499:VAL:CG1	1:B:539:ARG:O	1.74	1.34
1:A:461:PHE:HE2	1:A:502:LEU:CD2	1.30	1.33
1:A:512:THR:CG2	1:A:547:LYS:NZ	1.92	1.33
1:A:91:GLY:O	1:A:95:ILE:HG22	1.15	1.31
1:A:116:VAL:CG1	1:A:164:THR:O	1.78	1.30
1:A:211:VAL:HG12	1:A:213:GLU:N	1.46	1.30
1:A:320:GLU:HA	1:A:323:LEU:CD2	1.59	1.30
1:A:116:VAL:HG12	1:A:164:THR:O	1.27	1.30
1:A:512:THR:CG2	1:A:547:LYS:HZ2	1.44	1.30
1:B:499:VAL:HG13	1:B:539:ARG:O	1.16	1.30
1:A:411:LYS:NZ	1:A:432:PRO:HG2	1.45	1.30
1:B:46:LYS:H	1:B:48:MET:CG	1.42	1.30
1:A:363:LEU:C	1:A:364:LEU:HD12	1.56	1.29
1:B:429:ASN:CB	1:B:472:ASN:OD1	1.79	1.29
1:A:205:VAL:HG23	1:A:207:TYR:CD1	1.66	1.28
1:B:224:PHE:O	1:B:228:ILE:HG13	1.34	1.27
1:A:207:TYR:OH	1:A:220:MET:SD	1.93	1.27
1:B:221:PHE:O	1:B:225:ALA:HB2	1.32	1.27
1:B:46:LYS:O	1:B:48:MET:HG2	1.35	1.26
1:B:243:LEU:C	1:B:243:LEU:HD23	1.58	1.26
1:B:297:ALA:C	1:B:300:VAL:HG13	1.56	1.26
1:A:181:PHE:CE1	1:A:195:ILE:HB	1.71	1.26
1:B:294:LYS:CG	1:B:295:ASN:OD1	1.82	1.26
1:A:461:PHE:CD2	1:A:502:LEU:HD23	1.70	1.25
1:B:297:ALA:HA	1:B:300:VAL:CG1	1.65	1.25
1:B:440:ILE:HD12	1:B:440:ILE:C	1.55	1.25
1:A:451:LEU:O	1:A:451:LEU:HD23	1.34	1.24
1:A:470:LEU:O	1:A:474:ILE:HG13	1.25	1.24
1:B:62:VAL:HA	1:B:67:SER:OG	1.32	1.24
1:B:440:ILE:CD1	1:B:441:ARG:N	1.99	1.24
1:A:25:ARG:O	1:A:29:ILE:HG13	1.32	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:ASP:OD1	1:A:237:PRO:HD2	1.36	1.23
1:A:25:ARG:CZ	1:A:211:VAL:O	1.86	1.23
1:A:211:VAL:CG1	1:A:213:GLU:H	1.49	1.23
1:A:181:PHE:CD2	1:A:197:ASN:HB2	1.74	1.23
1:A:264:GLY:O	1:A:267:SER:OG	1.56	1.22
1:A:25:ARG:NH2	1:A:211:VAL:H	1.37	1.22
1:A:524:ASP:O	1:A:528:THR:HG22	1.38	1.22
1:B:245:LEU:HD12	1:B:245:LEU:O	1.37	1.22
1:B:243:LEU:HD23	1:B:244:GLU:N	1.53	1.22
1:B:221:PHE:O	1:B:225:ALA:CB	1.86	1.21
1:A:11:VAL:HA	1:A:54:ILE:CG2	1.72	1.20
1:A:85:ILE:C	1:A:86:PHE:HD1	1.48	1.20
1:A:192:ILE:HD12	1:A:192:ILE:O	1.38	1.20
1:B:437:GLY:O	1:B:438:LEU:HD12	1.36	1.20
1:B:70:LEU:HD12	1:B:94:GLU:CD	1.65	1.20
1:B:36:LYS:CB	1:B:40:VAL:HG13	1.71	1.20
1:A:363:LEU:O	1:A:364:LEU:HD12	1.42	1.19
1:A:323:LEU:HG	1:A:324:SER:N	1.55	1.19
1:A:451:LEU:HD23	1:A:451:LEU:C	1.58	1.19
1:A:242:GLU:C	1:A:243:LEU:HD23	1.66	1.19
1:B:29:ILE:O	1:B:31:ILE:HG23	1.36	1.19
1:B:97:VAL:CG1	1:B:102:GLU:OE1	1.91	1.19
1:A:423:LEU:HB3	1:A:424:PRO:HD2	1.18	1.18
1:A:92:MET:C	1:A:95:ILE:CG2	2.17	1.17
1:A:183:LEU:HD13	1:A:192:ILE:CD1	1.74	1.17
1:A:543:ASP:CB	1:B:541:LEU:CD2	2.22	1.17
1:A:92:MET:O	1:A:95:ILE:HG23	1.02	1.17
1:A:423:LEU:HB3	1:A:424:PRO:CD	1.72	1.17
1:B:91:GLY:O	1:B:95:ILE:HG23	1.39	1.17
1:A:461:PHE:CD2	1:A:502:LEU:CD2	2.26	1.17
1:B:70:LEU:CD1	1:B:94:GLU:OE2	1.90	1.17
1:A:25:ARG:NH1	1:A:211:VAL:O	1.78	1.17
1:B:420:GLU:O	1:B:421:LEU:HD23	1.43	1.17
1:A:446:ILE:N	1:A:446:ILE:HD12	1.61	1.16
1:A:195:ILE:HD12	1:A:195:ILE:N	1.60	1.16
1:A:434:PRO:CG	1:A:553:GLU:OE1	1.94	1.16
1:A:19:PHE:CZ	1:A:35:THR:HG22	1.81	1.15
1:A:369:TYR:HB3	1:A:370:PRO:CD	1.76	1.15
1:B:194:SER:O	1:B:195:ILE:HD12	1.47	1.15
1:B:26:LEU:O	1:B:31:ILE:HG21	1.47	1.15
1:B:92:MET:O	1:B:95:ILE:HG12	1.45	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:LEU:HD12	1:A:470:LEU:N	1.52	1.14
1:A:546:SER:OG	2:A:601:HOH:O	1.61	1.14
1:A:225:ALA:O	1:A:229:CYS:O	1.64	1.14
1:A:301:TYR:CE1	1:A:313:ILE:HG21	1.81	1.14
1:A:408:TYR:O	1:A:409:LEU:HD12	1.44	1.14
1:B:103:VAL:CG1	1:B:173:GLU:O	1.96	1.14
1:B:419:ARG:NH1	1:B:422:ASN:OD1	1.81	1.14
1:B:530:ILE:N	1:B:530:ILE:HD12	1.60	1.14
1:A:502:LEU:HD12	1:A:540:ILE:HD11	1.23	1.13
1:B:103:VAL:CG1	1:B:104:LYS:H	1.53	1.13
1:A:205:VAL:HG21	1:A:207:TYR:CD1	1.73	1.13
1:A:210:GLU:O	1:A:211:VAL:HG23	1.47	1.13
1:A:301:TYR:HE1	1:A:313:ILE:HG21	1.05	1.13
1:B:29:ILE:HG22	1:B:30:LYS:O	1.46	1.13
1:B:261:MET:SD	1:B:271:ALA:CB	2.38	1.12
1:B:485:LYS:CB	1:B:499:VAL:CG2	2.26	1.12
1:B:294:LYS:HG2	1:B:295:ASN:OD1	1.38	1.12
1:B:420:GLU:C	1:B:421:LEU:HD23	1.75	1.12
1:A:147:LYS:O	1:A:148:LEU:HD12	1.47	1.11
1:B:68:PRO:HD2	1:B:90:TYR:OH	1.30	1.11
1:B:92:MET:HA	1:B:95:ILE:HD13	1.19	1.11
1:A:320:GLU:CA	1:A:323:LEU:HD23	1.81	1.11
1:A:183:LEU:HD13	1:A:192:ILE:HD11	1.16	1.11
1:B:165:THR:O	1:B:166:VAL:HG13	1.48	1.11
1:B:440:ILE:HD12	1:B:441:ARG:CA	1.79	1.11
1:B:70:LEU:HD11	1:B:94:GLU:CD	1.69	1.11
1:B:70:LEU:HD12	1:B:94:GLU:OE2	1.45	1.10
1:B:243:LEU:CD2	1:B:247:ASN:HD21	1.64	1.10
1:A:292:LEU:O	1:A:455:ARG:HG2	1.50	1.10
1:A:301:TYR:HE1	1:A:313:ILE:CG2	1.64	1.10
1:B:166:VAL:HG12	1:B:214:SER:CA	1.79	1.10
1:A:92:MET:O	1:A:95:ILE:CG2	1.98	1.10
1:A:215:LEU:HD12	1:A:215:LEU:N	1.65	1.10
1:A:502:LEU:CD1	1:A:540:ILE:CD1	2.28	1.10
1:A:320:GLU:HA	1:A:323:LEU:HD23	1.20	1.10
1:A:369:TYR:HB3	1:A:370:PRO:HD3	1.10	1.10
1:A:439:ALA:O	1:A:442:VAL:HG12	1.49	1.10
1:B:245:LEU:HD12	1:B:245:LEU:C	1.75	1.10
1:A:19:PHE:HZ	1:A:35:THR:HG22	0.99	1.09
1:A:166:VAL:HG13	1:A:207:TYR:CD2	1.69	1.09
1:B:437:GLY:C	1:B:438:LEU:HD12	1.75	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:ALA:CA	1:B:300:VAL:CG1	2.29	1.09
1:A:320:GLU:CA	1:A:323:LEU:CD2	2.30	1.09
1:A:326:LEU:CG	1:A:338:ILE:CD1	2.30	1.09
1:B:92:MET:CA	1:B:95:ILE:CD1	2.29	1.09
1:A:291:LEU:C	1:A:292:LEU:HD12	1.76	1.09
1:A:305:LYS:HG2	1:A:306:SER:N	1.60	1.09
1:A:367:THR:O	1:A:406:PHE:O	1.69	1.09
1:B:211:VAL:HG13	1:B:213:GLU:H	1.13	1.09
1:A:223:ASN:OD1	1:A:227:ASN:ND2	1.86	1.09
1:A:454:LEU:HD12	1:A:454:LEU:O	1.49	1.09
1:A:452:ASN:HA	1:A:455:ARG:NH2	1.66	1.08
1:B:97:VAL:HG13	1:B:102:GLU:OE1	1.53	1.08
1:A:332:PRO:HG2	1:A:333:GLU:H	0.92	1.08
1:B:211:VAL:HG13	1:B:212:TYR:N	1.63	1.08
1:B:534:VAL:HG12	1:B:535:LYS:N	1.64	1.08
1:B:196:TYR:CD1	1:B:196:TYR:C	2.29	1.08
1:B:313:ILE:C	1:B:313:ILE:HD12	1.77	1.08
1:A:25:ARG:NH2	1:A:211:VAL:O	1.87	1.08
1:A:512:THR:HG22	1:A:547:LYS:HZ2	0.91	1.08
1:A:7:ASP:O	1:A:49:ASN:O	1.70	1.07
1:B:419:ARG:HH11	1:B:422:ASN:HA	1.13	1.07
1:B:94:GLU:OE1	1:B:95:ILE:HA	1.54	1.07
1:A:438:LEU:HD21	1:A:454:LEU:HD11	1.22	1.07
1:A:155:LEU:HD23	1:A:155:LEU:O	1.53	1.07
1:B:12:LEU:O	1:B:56:SER:CB	2.03	1.07
1:B:296:GLU:O	1:B:300:VAL:HG12	1.54	1.07
1:B:70:LEU:CD1	1:B:94:GLU:CG	2.33	1.06
1:A:411:LYS:NZ	1:A:432:PRO:CG	2.17	1.06
1:B:500:CYS:SG	1:B:501:VAL:N	2.29	1.06
1:B:518:ILE:CD1	1:B:523:LEU:CD2	2.33	1.06
1:B:154:CYS:HB2	1:B:203:TYR:OH	1.54	1.06
1:B:534:VAL:HG12	1:B:535:LYS:O	1.56	1.06
1:B:29:ILE:HG22	1:B:30:LYS:N	1.68	1.05
1:B:326:LEU:CB	1:B:446:ILE:HD13	1.85	1.05
1:A:211:VAL:HG12	1:A:212:TYR:N	1.65	1.05
1:A:475:SER:OG	1:A:507:THR:OG1	1.72	1.05
1:B:212:TYR:C	1:B:212:TYR:CD1	2.29	1.05
1:B:246:LYS:HD2	1:B:246:LYS:O	1.55	1.05
1:B:292:LEU:HD12	1:B:293:ARG:H	1.14	1.05
1:A:265:ILE:O	1:A:269:VAL:HG23	1.56	1.05
1:A:291:LEU:O	1:A:292:LEU:HD12	1.56	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:LEU:HD11	1:B:223:ASN:HB2	1.09	1.05
1:A:228:ILE:HD12	1:A:228:ILE:N	1.66	1.05
1:B:89:CYS:SG	1:B:90:TYR:N	2.29	1.05
1:B:480:VAL:HG22	1:B:501:VAL:CB	1.85	1.05
1:B:163:ILE:HG23	1:B:164:THR:N	1.70	1.04
1:B:308:PHE:HA	1:B:311:MET:HE2	1.36	1.04
1:A:85:ILE:C	1:A:86:PHE:CD1	2.34	1.04
1:B:103:VAL:HG12	1:B:104:LYS:N	1.64	1.04
1:A:309:PRO:HG2	1:A:310:ASP:H	1.14	1.04
1:B:470:LEU:O	1:B:473:GLN:HB3	1.56	1.04
1:A:166:VAL:HG11	1:A:207:TYR:CG	1.92	1.03
1:B:261:MET:SD	1:B:271:ALA:HB1	1.96	1.03
1:A:478:PHE:CD1	1:A:480:VAL:HG23	1.94	1.03
1:A:534:VAL:O	1:A:534:VAL:HG13	1.54	1.03
1:A:228:ILE:CD1	1:A:228:ILE:H	1.63	1.03
1:A:326:LEU:CG	1:A:338:ILE:HD13	1.88	1.03
1:B:166:VAL:HG12	1:B:214:SER:HA	1.35	1.03
1:B:219:LEU:HD11	1:B:223:ASN:CB	1.89	1.03
1:B:246:LYS:HD2	1:B:246:LYS:C	1.82	1.03
1:B:485:LYS:CB	1:B:499:VAL:HG23	1.87	1.03
1:B:297:ALA:O	1:B:300:VAL:HG22	1.59	1.03
1:A:48:MET:HG3	1:A:48:MET:O	1.55	1.02
1:A:181:PHE:CG	1:A:197:ASN:HB2	1.93	1.02
1:A:450:LYS:O	1:A:453:ILE:HG12	1.57	1.02
1:B:92:MET:HA	1:B:95:ILE:HD11	1.05	1.02
1:B:219:LEU:HD12	1:B:219:LEU:O	1.58	1.02
1:B:465:LEU:CB	1:B:471:TYR:HB2	1.90	1.02
1:A:116:VAL:HG22	1:A:117:ASN:N	1.69	1.02
1:B:92:MET:CA	1:B:95:ILE:HD11	1.88	1.02
1:B:297:ALA:O	1:B:300:VAL:HG13	1.59	1.02
1:B:518:ILE:HG23	1:B:523:LEU:HG	1.41	1.02
1:A:451:LEU:C	1:A:451:LEU:CD2	2.29	1.02
1:A:502:LEU:HD11	1:A:540:ILE:CD1	1.88	1.02
1:B:166:VAL:CG1	1:B:214:SER:HA	1.88	1.02
1:A:243:LEU:HD23	1:A:243:LEU:N	1.61	1.01
1:B:291:LEU:HD11	1:B:437:GLY:HA2	1.06	1.01
1:A:205:VAL:HG23	1:A:207:TYR:H	1.21	1.01
1:B:166:VAL:CG1	1:B:214:SER:HB3	1.90	1.01
1:A:114:THR:HG22	1:A:114:THR:O	1.60	1.01
1:A:543:ASP:HA	1:B:541:LEU:CD2	1.90	1.01
1:B:166:VAL:CG1	1:B:214:SER:CB	2.38	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:THR:HG23	1:B:330:THR:O	1.58	1.01
1:A:92:MET:CA	1:A:95:ILE:HG21	1.75	1.01
1:A:194:SER:C	1:A:195:ILE:HD12	1.86	1.01
1:A:441:ARG:HD3	1:A:479:ALA:O	1.61	1.01
1:B:35:THR:OG1	1:B:376:LYS:HG3	1.59	1.01
1:B:94:GLU:CD	1:B:94:GLU:C	2.27	1.01
1:B:211:VAL:CG1	1:B:213:GLU:H	1.74	1.01
1:A:320:GLU:C	1:A:323:LEU:HD23	1.84	1.01
1:A:30:LYS:HG2	1:A:30:LYS:O	1.56	1.00
1:B:70:LEU:HD13	1:B:94:GLU:CD	1.79	1.00
1:B:243:LEU:HD23	1:B:244:GLU:CA	1.90	1.00
1:A:38:TYR:CD1	1:A:39:GLY:N	2.30	1.00
1:A:363:LEU:C	1:A:364:LEU:CD1	2.33	1.00
1:B:297:ALA:HA	1:B:300:VAL:HG11	1.01	1.00
1:A:198:LYS:HG3	1:A:198:LYS:O	1.60	1.00
1:A:502:LEU:HD11	1:A:540:ILE:HD11	1.00	1.00
1:A:205:VAL:CG2	1:A:207:TYR:H	1.73	1.00
1:A:228:ILE:HD12	1:A:228:ILE:H	1.19	1.00
1:A:222:TYR:C	1:A:222:TYR:HD1	1.70	0.99
1:A:512:THR:HG21	1:A:547:LYS:NZ	1.76	0.99
1:A:543:ASP:CB	1:B:541:LEU:HD21	1.85	0.99
1:B:518:ILE:CG2	1:B:523:LEU:HG	1.92	0.99
1:A:120:ARG:NH2	1:A:162:ASP:OD1	1.95	0.99
1:B:534:VAL:CG1	1:B:535:LYS:H	1.76	0.99
1:A:181:PHE:HE1	1:A:195:ILE:HB	1.03	0.99
1:B:312:ASN:H	1:B:312:ASN:ND2	1.54	0.99
1:A:211:VAL:CG1	1:A:212:TYR:H	1.73	0.99
1:A:224:PHE:HA	1:A:228:ILE:HD13	1.45	0.99
1:B:243:LEU:C	1:B:243:LEU:CD2	2.31	0.99
1:A:11:VAL:O	1:A:11:VAL:HG12	1.63	0.99
1:A:434:PRO:HG2	1:A:553:GLU:OE1	1.60	0.99
1:A:320:GLU:O	1:A:323:LEU:HD23	1.62	0.99
1:B:245:LEU:HG	1:B:246:LYS:N	1.76	0.99
1:B:291:LEU:CD1	1:B:437:GLY:HA2	1.56	0.99
1:B:518:ILE:HD13	1:B:523:LEU:HD21	1.03	0.99
1:B:332:PRO:HA	1:B:335:LYS:HG2	1.42	0.98
1:A:291:LEU:C	1:A:292:LEU:CD1	2.36	0.98
1:A:222:TYR:C	1:A:222:TYR:CD1	2.37	0.98
1:B:295:ASN:HA	1:B:298:GLU:CG	1.92	0.98
1:A:313:ILE:N	1:A:313:ILE:HD12	1.74	0.98
1:A:91:GLY:O	1:A:95:ILE:CG2	2.11	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:LEU:HD11	1:B:94:GLU:CG	1.92	0.98
1:B:554:PHE:O	1:B:554:PHE:HD1	1.44	0.98
1:A:258:ILE:HG13	1:A:361:THR:HG21	1.45	0.98
1:A:470:LEU:O	1:A:474:ILE:CG1	2.12	0.98
1:B:313:ILE:HD12	1:B:313:ILE:O	1.64	0.98
1:B:518:ILE:CD1	1:B:523:LEU:HD21	1.93	0.98
1:B:212:TYR:C	1:B:212:TYR:HD1	1.69	0.97
1:B:294:LYS:HG3	1:B:295:ASN:OD1	1.63	0.97
1:A:543:ASP:HB2	1:B:541:LEU:HD21	0.98	0.97
1:A:332:PRO:HG2	1:A:333:GLU:N	1.71	0.97
1:A:90:TYR:CE1	1:A:90:TYR:CE2	2.41	0.97
1:B:35:THR:OG1	1:B:376:LYS:HB3	1.63	0.97
1:B:403:PHE:O	1:B:405:PRO:HD3	1.63	0.97
1:B:480:VAL:O	1:B:500:CYS:SG	2.21	0.97
1:A:35:THR:O	1:A:36:LYS:HG2	1.64	0.97
1:B:313:ILE:HD11	1:B:315:LYS:CG	1.95	0.97
1:B:436:PRO:HB2	1:B:439:ALA:H	1.29	0.97
1:B:518:ILE:HG21	1:B:523:LEU:HD21	1.45	0.97
1:B:133:PHE:CE2	1:B:191:LEU:CD1	2.47	0.97
1:A:178:PRO:O	1:A:178:PRO:HG2	1.65	0.97
1:A:222:TYR:HD1	1:A:222:TYR:O	1.47	0.97
1:B:211:VAL:HG13	1:B:213:GLU:N	1.80	0.97
1:A:118:ILE:HG23	1:A:118:ILE:O	1.63	0.96
1:B:166:VAL:HG12	1:B:214:SER:CB	1.92	0.96
1:A:19:PHE:CZ	1:A:35:THR:CG2	2.46	0.96
1:A:502:LEU:HD12	1:A:540:ILE:CD1	1.93	0.96
1:B:440:ILE:C	1:B:440:ILE:CD1	2.30	0.96
1:B:312:ASN:H	1:B:312:ASN:HD22	1.13	0.96
1:B:297:ALA:C	1:B:300:VAL:CG1	2.38	0.96
1:B:196:TYR:C	1:B:196:TYR:HD1	1.70	0.96
1:B:331:ASP:O	1:B:335:LYS:N	1.99	0.96
1:A:179:GLU:HG2	1:A:180:ASN:H	1.29	0.96
1:A:235:PHE:O	1:A:235:PHE:HD1	1.46	0.96
1:B:19:PHE:HA	1:B:22:ILE:HD12	1.47	0.96
1:A:129:TYR:HE1	1:A:186:SER:HG	1.03	0.95
1:A:470:LEU:C	1:A:474:ILE:HG13	1.90	0.95
1:B:103:VAL:HG12	1:B:104:LYS:H	0.79	0.95
1:B:112:GLY:N	1:B:168:MET:O	1.97	0.95
1:B:243:LEU:CD2	1:B:247:ASN:ND2	2.30	0.95
1:A:118:ILE:CG1	1:A:119:LEU:N	2.30	0.95
1:A:465:LEU:HD21	1:A:474:ILE:HD12	1.47	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:GLN:HE21	1:B:172:ASP:HB2	1.31	0.95
1:B:211:VAL:CG1	1:B:213:GLU:N	2.30	0.95
1:A:501:VAL:HG22	1:A:541:LEU:HB2	1.49	0.95
1:A:452:ASN:CA	1:A:455:ARG:NH2	2.30	0.95
1:B:133:PHE:CD2	1:B:191:LEU:HD13	2.01	0.95
1:B:277:ILE:CG1	1:B:278:PHE:N	2.30	0.95
1:A:116:VAL:HG13	1:A:164:THR:O	1.64	0.95
1:B:36:LYS:CB	1:B:40:VAL:CG1	2.45	0.95
1:B:243:LEU:CD2	1:B:244:GLU:N	2.29	0.95
1:A:543:ASP:CA	1:B:541:LEU:CD2	2.44	0.94
1:B:238:ILE:CG2	1:B:239:ARG:N	2.30	0.94
1:B:289:ASN:CB	1:B:319:SER:HB2	1.97	0.94
1:B:324:SER:O	1:B:326:LEU:N	2.00	0.94
1:A:411:LYS:HZ2	1:A:432:PRO:HG2	1.19	0.94
1:A:258:ILE:HG13	1:A:361:THR:CG2	1.97	0.94
1:A:452:ASN:CB	1:A:455:ARG:NH2	2.30	0.94
1:A:454:LEU:C	1:A:454:LEU:CD1	2.31	0.94
1:A:123:ASN:HA	1:A:126:ASN:ND2	1.81	0.94
1:A:411:LYS:HZ1	1:A:432:PRO:CG	1.79	0.94
1:A:107:LYS:O	2:A:602:HOH:O	1.84	0.94
1:B:103:VAL:HG12	1:B:173:GLU:O	1.64	0.94
1:A:19:PHE:HZ	1:A:35:THR:CG2	1.81	0.94
1:A:285:ILE:HA	1:A:314:THR:OG1	1.68	0.94
1:B:211:VAL:CG1	1:B:212:TYR:N	2.30	0.94
1:B:509:SER:O	1:B:512:THR:O	1.86	0.94
1:B:243:LEU:HD21	1:B:247:ASN:HD21	1.33	0.94
1:B:300:VAL:CG2	1:B:301:TYR:N	2.29	0.94
1:B:35:THR:OG1	1:B:376:LYS:CB	2.16	0.93
1:A:347:PHE:CZ	1:A:363:LEU:CD1	2.52	0.93
1:A:114:THR:HG23	1:A:115:ASP:O	1.67	0.93
1:A:470:LEU:N	1:A:470:LEU:CD1	2.30	0.93
1:B:103:VAL:HG13	1:B:174:VAL:HA	1.48	0.93
1:B:530:ILE:H	1:B:530:ILE:CD1	1.81	0.93
1:A:116:VAL:CG2	1:A:117:ASN:N	2.30	0.93
1:A:434:PRO:HG3	1:A:553:GLU:OE1	1.68	0.93
1:B:62:VAL:CA	1:B:67:SER:OG	2.16	0.93
1:A:195:ILE:N	1:A:195:ILE:CD1	2.29	0.93
1:A:364:LEU:CD1	1:A:364:LEU:N	2.30	0.93
1:B:291:LEU:HG	1:B:292:LEU:H	1.34	0.93
1:A:211:VAL:HG12	1:A:212:TYR:H	1.28	0.93
1:A:543:ASP:HB2	1:B:541:LEU:HD22	1.45	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:HIS:CE1	1:A:477:ALA:H	1.86	0.93
1:A:165:THR:C	1:A:166:VAL:CG2	2.40	0.93
1:A:211:VAL:CG1	1:A:212:TYR:N	2.29	0.93
1:B:70:LEU:HD12	1:B:94:GLU:CG	1.98	0.93
1:B:194:SER:C	1:B:195:ILE:HD12	1.93	0.93
1:A:439:ALA:O	1:A:442:VAL:O	1.86	0.93
1:A:411:LYS:HZ1	1:A:432:PRO:HG2	1.24	0.93
1:A:438:LEU:CD2	1:A:454:LEU:HD11	1.99	0.93
1:B:29:ILE:CG2	1:B:30:LYS:N	2.30	0.93
1:A:264:GLY:HA2	1:A:430:ARG:CZ	2.00	0.92
1:A:547:LYS:HB3	1:A:548:PRO:CD	1.99	0.92
1:B:245:LEU:HA	1:B:248:ILE:CG1	1.99	0.92
1:A:332:PRO:CG	1:A:333:GLU:H	1.78	0.92
1:B:68:PRO:HD3	1:B:90:TYR:OH	1.69	0.92
1:A:439:ALA:C	1:A:442:VAL:HG12	1.95	0.92
1:B:181:PHE:HE1	1:B:199:GLU:HG3	1.34	0.92
1:A:313:ILE:N	1:A:313:ILE:CD1	2.30	0.92
1:B:465:LEU:C	1:B:471:TYR:HB2	1.95	0.92
1:B:291:LEU:CD1	1:B:437:GLY:CA	0.92	0.92
1:A:320:GLU:HA	1:A:323:LEU:HD22	1.48	0.92
1:A:205:VAL:HG23	1:A:207:TYR:HD1	0.74	0.91
1:A:283:PHE:CD1	1:A:283:PHE:N	2.37	0.91
1:A:450:LYS:HG2	1:A:451:LEU:N	1.82	0.91
1:B:35:THR:OG1	1:B:376:LYS:CG	2.18	0.91
1:B:90:TYR:CD1	1:B:90:TYR:C	2.45	0.91
1:B:92:MET:CA	1:B:95:ILE:HD13	1.97	0.91
1:B:133:PHE:CE2	1:B:191:LEU:HD13	2.05	0.91
1:A:445:GLU:C	1:A:446:ILE:HD12	1.96	0.91
1:B:525:LYS:HA	1:B:528:THR:CG2	2.01	0.91
1:A:51:LYS:NZ	1:A:82:LYS:O	2.03	0.91
1:A:408:TYR:C	1:A:409:LEU:HD12	1.95	0.91
1:B:166:VAL:CG1	1:B:214:SER:CA	2.47	0.90
1:A:106:SER:OG	1:A:173:GLU:HB2	1.71	0.90
1:A:465:LEU:HD11	1:A:474:ILE:CD1	2.00	0.90
1:B:471:TYR:CD1	1:B:471:TYR:C	2.44	0.90
1:B:133:PHE:HE2	1:B:191:LEU:HB2	1.35	0.90
1:A:309:PRO:HG2	1:A:310:ASP:N	1.84	0.90
1:A:441:ARG:HG3	1:A:480:VAL:HA	1.50	0.90
1:A:91:GLY:C	1:A:95:ILE:HG22	1.95	0.90
1:A:292:LEU:CD1	1:A:292:LEU:N	2.33	0.90
1:B:291:LEU:HD12	1:B:437:GLY:O	1.71	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:ASN:HB2	1:A:455:ARG:NH2	1.87	0.90
1:A:543:ASP:HA	1:B:541:LEU:HD23	1.50	0.90
1:B:98:GLN:C	1:B:98:GLN:NE2	2.30	0.90
1:B:219:LEU:HD12	1:B:223:ASN:H	1.34	0.90
1:B:419:ARG:NH1	1:B:422:ASN:HA	1.87	0.90
1:B:534:VAL:CG1	1:B:535:LYS:N	2.30	0.90
1:A:123:ASN:CG	1:A:126:ASN:ND2	2.30	0.90
1:A:512:THR:CG2	1:A:547:LYS:HZ1	1.76	0.90
1:A:301:TYR:HA	1:A:304:LEU:HD12	1.54	0.89
1:B:166:VAL:HG12	1:B:214:SER:HB3	1.51	0.89
1:A:181:PHE:CD1	1:A:195:ILE:O	2.24	0.89
1:B:309:PRO:HG2	1:B:310:ASP:H	1.35	0.89
1:A:461:PHE:HE2	1:A:502:LEU:HD22	1.38	0.89
1:B:194:SER:C	1:B:195:ILE:CD1	2.45	0.89
1:A:165:THR:C	1:A:166:VAL:HG23	1.96	0.89
1:B:524:ASP:O	1:B:528:THR:HG22	1.72	0.89
1:A:40:VAL:O	1:A:40:VAL:HG22	1.73	0.89
1:B:530:ILE:HD12	1:B:530:ILE:H	1.33	0.89
1:B:308:PHE:CB	1:B:311:MET:CE	2.49	0.89
1:A:461:PHE:CD2	1:A:502:LEU:HD21	2.06	0.89
1:B:70:LEU:HD11	1:B:94:GLU:HG2	1.55	0.88
1:A:470:LEU:HB3	1:A:474:ILE:CG1	2.04	0.88
1:B:68:PRO:CG	1:B:90:TYR:OH	2.21	0.88
1:A:37:ASP:O	1:A:40:VAL:HG12	1.73	0.88
1:B:277:ILE:CG1	1:B:278:PHE:H	1.85	0.88
1:A:181:PHE:CE1	1:A:195:ILE:CB	2.56	0.88
1:B:243:LEU:HD21	1:B:247:ASN:ND2	1.86	0.88
1:B:530:ILE:N	1:B:530:ILE:CD1	2.30	0.88
1:A:369:TYR:CB	1:A:370:PRO:CD	2.46	0.88
1:A:446:ILE:N	1:A:446:ILE:CD1	2.29	0.88
1:A:369:TYR:O	1:A:369:TYR:HD1	1.54	0.88
1:A:439:ALA:O	1:A:442:VAL:CG1	2.21	0.88
1:B:509:SER:O	2:B:601:HOH:O	1.90	0.88
1:A:97:VAL:HG13	1:A:97:VAL:O	1.74	0.88
1:A:25:ARG:NH2	1:A:211:VAL:N	2.22	0.88
1:B:52:GLY:HA3	1:B:228:ILE:HG21	1.56	0.88
1:B:52:GLY:N	1:B:228:ILE:CG2	2.36	0.88
1:B:518:ILE:CD1	1:B:523:LEU:HD23	2.02	0.88
1:A:452:ASN:HB2	1:A:455:ARG:HH22	1.39	0.88
1:B:313:ILE:C	1:B:313:ILE:CD1	2.44	0.88
1:A:10:LEU:O	1:A:54:ILE:CG2	2.20	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:TYR:C	1:B:90:TYR:HD1	1.81	0.87
1:A:111:TYR:CD2	1:A:112:GLY:N	2.42	0.87
1:A:215:LEU:HD12	1:A:215:LEU:H	1.30	0.87
1:B:297:ALA:CA	1:B:300:VAL:HG13	2.00	0.87
1:A:114:THR:HB	1:A:168:MET:HE2	1.57	0.87
1:A:194:SER:HB2	1:A:205:VAL:HA	1.57	0.87
1:A:11:VAL:HA	1:A:54:ILE:HG23	1.53	0.87
1:A:305:LYS:CG	1:A:306:SER:N	2.35	0.87
1:B:159:ILE:C	1:B:161:SER:H	1.82	0.87
1:A:86:PHE:HD1	1:A:86:PHE:N	1.73	0.87
1:B:294:LYS:HG2	1:B:295:ASN:N	1.87	0.87
1:B:324:SER:C	1:B:326:LEU:H	1.77	0.87
1:B:471:TYR:C	1:B:471:TYR:HD1	1.80	0.87
1:A:347:PHE:HZ	1:A:363:LEU:CD1	1.88	0.87
1:A:173:GLU:OE2	1:A:174:VAL:HG12	1.74	0.87
1:B:308:PHE:CA	1:B:311:MET:HE2	2.04	0.87
1:A:442:VAL:O	1:A:442:VAL:HG13	1.75	0.86
1:B:291:LEU:HD13	1:B:437:GLY:H	1.38	0.86
1:A:116:VAL:CG1	1:A:164:THR:C	2.48	0.86
1:A:181:PHE:HB3	1:A:197:ASN:CB	2.05	0.86
1:A:501:VAL:CG2	1:A:541:LEU:HD12	2.05	0.86
1:A:543:ASP:CA	1:B:541:LEU:HD22	2.06	0.86
1:A:235:PHE:O	1:A:235:PHE:CD1	2.29	0.86
1:B:300:VAL:HG22	1:B:301:TYR:N	1.90	0.86
1:A:480:VAL:O	1:A:501:VAL:O	1.94	0.86
1:B:243:LEU:HD23	1:B:244:GLU:HA	1.56	0.86
1:B:436:PRO:HG3	1:B:440:ILE:CG2	2.04	0.86
1:A:118:ILE:HG12	1:A:119:LEU:N	1.91	0.86
1:B:196:TYR:CD1	1:B:197:ASN:N	2.43	0.86
1:B:291:LEU:CD1	1:B:437:GLY:N	2.05	0.86
1:A:130:CYS:O	1:A:130:CYS:SG	2.34	0.85
1:A:470:LEU:HD12	1:A:470:LEU:H	1.36	0.85
1:A:499:VAL:HG23	1:A:499:VAL:O	1.74	0.85
1:A:110:GLU:O	1:A:111:TYR:CD1	2.29	0.85
1:A:407:LYS:O	1:A:408:TYR:CD1	2.29	0.85
1:A:441:ARG:CG	1:A:480:VAL:HA	2.07	0.85
1:B:26:LEU:O	1:B:31:ILE:CG2	2.23	0.85
1:B:90:TYR:CD1	1:B:90:TYR:O	2.29	0.85
1:B:430:ARG:O	1:B:432:PRO:HD3	1.76	0.85
1:B:51:LYS:C	1:B:228:ILE:HG23	2.00	0.85
1:A:25:ARG:HH22	1:A:211:VAL:H	1.22	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:LEU:CD1	1:B:94:GLU:HG2	2.06	0.85
1:B:111:TYR:O	1:B:111:TYR:CD1	2.29	0.85
1:B:201:ASN:O	1:B:203:TYR:CE1	2.30	0.85
1:A:196:TYR:O	1:A:196:TYR:CD2	2.29	0.85
1:A:278:PHE:O	1:A:278:PHE:CD1	2.29	0.85
1:A:478:PHE:CD1	1:A:478:PHE:O	2.29	0.85
1:B:196:TYR:CE1	1:B:197:ASN:O	2.30	0.85
1:A:181:PHE:HB3	1:A:197:ASN:CG	2.01	0.85
1:B:485:LYS:CB	1:B:499:VAL:HG21	2.06	0.85
1:B:554:PHE:O	1:B:554:PHE:CD1	2.29	0.85
1:B:554:PHE:HD1	1:B:554:PHE:C	1.82	0.85
1:A:423:LEU:CB	1:A:424:PRO:CD	2.48	0.85
1:B:241:HIS:C	1:B:241:HIS:ND1	2.34	0.85
1:A:132:ASN:O	1:A:133:PHE:CG	2.30	0.85
1:A:183:LEU:CD1	1:A:192:ILE:CD1	2.55	0.85
1:A:543:ASP:CB	1:B:541:LEU:HD22	1.99	0.85
1:A:132:ASN:O	1:A:133:PHE:CD1	2.29	0.85
1:B:212:TYR:HD1	1:B:213:GLU:N	1.75	0.85
1:B:500:CYS:SG	1:B:501:VAL:O	2.35	0.85
1:A:116:VAL:HG12	1:A:164:THR:C	2.01	0.84
1:A:205:VAL:HB	1:A:207:TYR:HE1	1.40	0.84
1:B:22:ILE:HG12	1:B:210:GLU:CB	2.07	0.84
1:B:518:ILE:HG21	1:B:523:LEU:CD2	2.05	0.84
1:A:515:TRP:O	1:A:515:TRP:CG	2.29	0.84
1:B:154:CYS:CB	1:B:203:TYR:OH	2.25	0.84
1:B:308:PHE:HA	1:B:311:MET:CE	2.07	0.84
1:A:548:PRO:HA	1:A:549:PRO:C	2.00	0.84
1:B:406:PHE:O	1:B:406:PHE:CD1	2.30	0.84
1:A:300:VAL:O	1:A:304:LEU:HD12	1.77	0.84
1:A:347:PHE:CZ	1:A:363:LEU:HD11	2.11	0.84
1:B:403:PHE:CD2	1:B:404:GLU:O	2.30	0.84
1:B:526:ILE:O	1:B:530:ILE:HD13	1.77	0.84
1:A:196:TYR:O	1:A:196:TYR:CG	2.29	0.84
1:A:211:VAL:HG11	1:A:213:GLU:HB2	1.57	0.84
1:A:27:ASN:OD1	1:A:28:ASN:N	2.11	0.84
1:A:461:PHE:HD1	1:A:462:ILE:HD12	1.41	0.84
1:A:512:THR:HG22	1:A:547:LYS:NZ	1.72	0.84
1:B:321:ASN:O	1:B:324:SER:HB2	1.78	0.84
1:B:534:VAL:HG12	1:B:535:LYS:H	1.28	0.84
1:A:273:TYR:HD1	1:A:421:LEU:HD11	1.41	0.84
1:A:238:ILE:O	1:A:241:HIS:ND1	2.11	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:531:LEU:HD22	1:B:549:PRO:HG3	1.59	0.84
1:A:292:LEU:O	1:A:455:ARG:CG	2.24	0.83
1:B:294:LYS:C	1:B:296:GLU:H	1.87	0.83
1:B:269:VAL:HG12	1:B:270:ALA:N	1.93	0.83
1:B:465:LEU:C	1:B:471:TYR:CB	2.51	0.83
1:B:166:VAL:HG11	1:B:214:SER:CB	2.07	0.83
1:B:289:ASN:O	1:B:291:LEU:N	2.12	0.83
1:B:465:LEU:O	1:B:471:TYR:HB3	1.78	0.83
1:B:515:TRP:CG	1:B:515:TRP:O	2.28	0.83
1:B:221:PHE:O	1:B:225:ALA:HB3	1.79	0.83
1:B:520:TYR:CD1	1:B:520:TYR:O	2.32	0.83
1:A:138:SER:O	1:A:141:ASP:OD1	1.95	0.83
1:A:57:GLY:HA3	1:A:90:TYR:HB3	1.61	0.82
1:A:181:PHE:HE1	1:A:195:ILE:CB	1.89	0.82
1:A:478:PHE:HD1	1:A:480:VAL:HG23	1.43	0.82
1:A:258:ILE:CG1	1:A:361:THR:HG21	2.09	0.82
1:A:400:PHE:N	1:A:400:PHE:CD1	2.42	0.82
1:B:499:VAL:HG12	1:B:500:CYS:N	1.93	0.82
1:A:95:ILE:HD12	1:A:202:ILE:HD13	1.60	0.82
1:A:273:TYR:OH	2:A:603:HOH:O	1.96	0.82
1:A:478:PHE:CE1	1:A:480:VAL:CG2	2.62	0.82
1:A:165:THR:O	1:A:166:VAL:HG22	1.79	0.82
1:A:205:VAL:CG2	1:A:207:TYR:CE1	2.61	0.82
1:A:120:ARG:HG3	1:A:123:ASN:OD1	1.79	0.82
1:A:271:ALA:HA	1:A:274:THR:HG22	1.61	0.82
1:A:460:ILE:HG22	1:A:461:PHE:N	1.92	0.81
1:A:516:TYR:CD1	1:A:517:GLN:O	2.33	0.81
1:A:92:MET:HA	1:A:95:ILE:HG21	0.83	0.81
1:A:116:VAL:N	1:A:164:THR:O	2.13	0.81
1:A:313:ILE:CD1	1:A:313:ILE:H	1.93	0.81
1:A:329:VAL:O	1:A:329:VAL:HG13	1.80	0.81
1:B:554:PHE:C	1:B:554:PHE:CD1	2.55	0.81
1:A:181:PHE:CE1	1:A:195:ILE:C	2.58	0.81
1:B:313:ILE:O	1:B:313:ILE:CD1	2.29	0.81
1:B:499:VAL:HG12	1:B:500:CYS:H	1.43	0.81
1:A:198:LYS:O	1:A:198:LYS:CG	2.29	0.81
1:A:449:HIS:ND1	1:A:450:LYS:N	2.29	0.81
1:B:297:ALA:CA	1:B:300:VAL:HG11	1.92	0.81
1:B:219:LEU:O	1:B:219:LEU:CD1	2.29	0.81
1:A:444:GLY:O	1:A:446:ILE:CD1	2.29	0.81
1:B:436:PRO:HG3	1:B:440:ILE:HG23	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:480:VAL:CG2	1:B:501:VAL:CB	2.58	0.81
1:A:452:ASN:HA	1:A:455:ARG:HH21	1.45	0.81
1:B:431:HIS:N	1:B:431:HIS:CD2	2.40	0.81
1:B:537:VAL:O	1:B:537:VAL:CG2	2.29	0.81
1:A:443:ILE:O	1:A:483:SER:OG	1.99	0.81
1:B:46:LYS:C	1:B:48:MET:HG2	2.04	0.81
1:B:296:GLU:O	1:B:300:VAL:CG1	2.29	0.81
1:B:326:LEU:O	1:B:446:ILE:HB	1.80	0.81
1:A:531:LEU:HD22	1:B:549:PRO:CG	2.12	0.80
1:B:133:PHE:CE2	1:B:191:LEU:HD12	2.15	0.80
1:B:201:ASN:O	1:B:203:TYR:CD1	2.34	0.80
1:B:526:ILE:O	1:B:530:ILE:CD1	2.29	0.80
1:A:35:THR:O	1:A:36:LYS:CG	2.30	0.80
1:A:210:GLU:O	1:A:211:VAL:CG2	2.29	0.80
1:A:452:ASN:CA	1:A:455:ARG:HH21	1.92	0.80
1:B:261:MET:SD	1:B:271:ALA:HB2	2.20	0.80
1:B:321:ASN:OD1	1:B:322:PHE:N	2.14	0.80
1:A:291:LEU:O	1:A:292:LEU:CD1	2.29	0.80
1:A:450:LYS:O	1:A:453:ILE:CG1	2.30	0.80
1:A:178:PRO:O	1:A:178:PRO:CG	2.29	0.80
1:A:499:VAL:O	1:A:499:VAL:CG2	2.29	0.80
1:B:245:LEU:O	1:B:248:ILE:CG1	2.29	0.80
1:B:342:LEU:O	1:B:345:GLU:CB	2.30	0.80
1:B:52:GLY:N	1:B:228:ILE:HG23	1.95	0.80
1:B:120:ARG:O	1:B:124:ILE:CB	2.30	0.80
1:A:478:PHE:CE1	1:A:480:VAL:HG23	2.17	0.80
1:B:219:LEU:CD1	1:B:223:ASN:HB2	2.03	0.80
1:A:46:LYS:O	1:A:47:ASP:CB	2.29	0.80
1:B:60:TYR:CD2	1:B:66:GLY:O	2.34	0.80
1:B:244:GLU:O	1:B:248:ILE:CG1	2.30	0.80
1:A:44:ASP:OD1	2:A:604:HOH:O	1.99	0.80
1:B:29:ILE:CG2	1:B:30:LYS:O	2.30	0.80
1:B:163:ILE:CG2	1:B:164:THR:N	2.42	0.80
1:B:436:PRO:CG	1:B:436:PRO:O	2.30	0.80
1:A:114:THR:CG2	1:A:115:ASP:O	2.30	0.80
1:A:320:GLU:O	1:A:323:LEU:CD2	2.29	0.80
1:A:517:GLN:O	1:A:518:ILE:CD1	2.29	0.80
1:B:518:ILE:CG2	1:B:518:ILE:O	2.30	0.80
1:A:120:ARG:CG	1:A:123:ASN:OD1	2.30	0.79
1:A:166:VAL:HG11	1:A:207:TYR:CB	2.12	0.79
1:A:205:VAL:HB	1:A:207:TYR:CE1	2.16	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:VAL:O	1:A:304:LEU:CD1	2.29	0.79
1:B:165:THR:O	1:B:166:VAL:CG1	2.30	0.79
1:B:470:LEU:O	1:B:473:GLN:CB	2.29	0.79
1:A:126:ASN:O	1:A:127:ILE:C	2.19	0.79
1:A:442:VAL:O	1:A:442:VAL:CG1	2.30	0.79
1:A:147:LYS:O	1:A:148:LEU:CD1	2.30	0.79
1:B:294:LYS:C	1:B:296:GLU:N	2.35	0.79
1:A:444:GLY:O	1:A:446:ILE:HD12	1.82	0.79
1:B:22:ILE:HG12	1:B:210:GLU:HB2	1.64	0.79
1:B:294:LYS:O	1:B:297:ALA:N	2.13	0.79
1:B:297:ALA:O	1:B:300:VAL:CG1	2.30	0.79
1:A:192:ILE:HD12	1:A:192:ILE:C	2.04	0.79
1:A:434:PRO:HG2	1:A:553:GLU:CD	2.07	0.79
1:B:308:PHE:CB	1:B:311:MET:HE3	2.11	0.79
1:B:436:PRO:HB2	1:B:439:ALA:N	1.97	0.79
1:A:123:ASN:ND2	1:A:126:ASN:ND2	2.30	0.79
1:A:155:LEU:O	1:A:155:LEU:CD2	2.29	0.79
1:A:224:PHE:HA	1:A:228:ILE:CD1	2.11	0.79
1:A:465:LEU:CD2	1:A:474:ILE:HD12	2.13	0.79
1:B:55:LEU:HB2	1:B:87:GLY:HA2	1.64	0.79
1:B:313:ILE:O	1:B:313:ILE:HG23	1.83	0.79
1:B:505:VAL:CG1	1:B:513:ALA:HB1	2.13	0.79
1:A:478:PHE:CE1	1:A:503:ARG:HB3	2.18	0.79
1:A:531:LEU:HD11	1:A:540:ILE:HG22	1.65	0.79
1:A:121:ASN:O	1:A:124:ILE:CB	2.30	0.79
1:A:516:TYR:HD1	1:A:517:GLN:O	1.64	0.79
1:B:94:GLU:OE1	1:B:95:ILE:CA	2.29	0.79
1:B:166:VAL:HG11	1:B:214:SER:HB3	1.64	0.79
1:A:454:LEU:O	1:A:454:LEU:CD1	2.30	0.79
1:B:238:ILE:HG22	1:B:239:ARG:N	1.96	0.79
1:A:369:TYR:CB	1:A:370:PRO:HD3	2.01	0.78
1:B:295:ASN:CA	1:B:298:GLU:CG	2.61	0.78
1:B:297:ALA:O	1:B:300:VAL:CG2	2.30	0.78
1:B:534:VAL:CG1	1:B:535:LYS:O	2.30	0.78
1:A:241:HIS:CE1	1:A:242:GLU:HG3	2.19	0.78
1:B:70:LEU:HD13	1:B:94:GLU:OE2	1.72	0.78
1:B:292:LEU:CD1	1:B:293:ARG:H	1.95	0.78
1:A:14:PHE:HD1	1:A:38:TYR:HB3	1.47	0.78
1:A:97:VAL:O	1:A:97:VAL:CG1	2.29	0.78
1:A:120:ARG:HH21	1:A:162:ASP:CG	1.91	0.78
1:A:177:ILE:O	1:A:177:ILE:CG1	2.29	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:ILE:HG22	1:A:239:ARG:N	1.97	0.78
1:A:367:THR:O	1:A:367:THR:HG22	1.82	0.78
1:A:408:TYR:O	1:A:409:LEU:CD1	2.30	0.78
1:B:406:PHE:CD1	1:B:406:PHE:C	2.62	0.78
1:A:215:LEU:N	1:A:215:LEU:CD1	2.28	0.78
1:A:369:TYR:O	1:A:372:ILE:HG22	1.84	0.78
1:B:52:GLY:HA3	1:B:228:ILE:HD13	1.66	0.78
1:B:326:LEU:CB	1:B:446:ILE:HB	2.14	0.78
1:B:411:LYS:O	1:B:415:LYS:HG3	1.84	0.78
1:A:363:LEU:O	1:A:364:LEU:CD1	2.29	0.77
1:A:463:ASN:C	1:A:463:ASN:OD1	2.28	0.77
1:B:17:GLN:HG2	1:B:18:TYR:N	1.98	0.77
1:B:184:VAL:O	1:B:184:VAL:CG1	2.30	0.77
1:B:436:PRO:O	1:B:436:PRO:CD	2.29	0.77
1:A:179:GLU:HG2	1:A:180:ASN:N	1.99	0.77
1:A:5:GLU:C	1:A:6:TYR:HD1	1.91	0.77
1:A:369:TYR:O	1:A:372:ILE:CG2	2.33	0.77
1:A:470:LEU:CD1	1:A:470:LEU:H	1.93	0.77
1:B:194:SER:O	1:B:195:ILE:CD1	2.29	0.77
1:A:118:ILE:O	1:A:118:ILE:CG2	2.30	0.77
1:A:111:TYR:HD2	1:A:112:GLY:H	1.26	0.77
1:A:537:VAL:HG23	1:A:537:VAL:O	1.85	0.77
1:B:52:GLY:HA3	1:B:228:ILE:CG2	2.13	0.77
1:B:25:ARG:NH2	1:B:212:TYR:HB2	2.00	0.77
1:B:246:LYS:C	1:B:246:LYS:CD	2.43	0.77
1:B:292:LEU:HD12	1:B:293:ARG:N	1.96	0.77
1:B:423:LEU:CB	1:B:424:PRO:CD	2.63	0.77
1:B:181:PHE:CE1	1:B:199:GLU:HG3	2.19	0.76
1:B:307:THR:O	1:B:309:PRO:HD3	1.84	0.76
1:B:525:LYS:HD2	1:B:528:THR:HG21	1.66	0.76
1:A:166:VAL:CG1	1:A:207:TYR:HB2	2.15	0.76
1:A:181:PHE:CD1	1:A:195:ILE:C	2.64	0.76
1:B:245:LEU:CA	1:B:248:ILE:CG1	2.63	0.76
1:B:520:TYR:CD1	1:B:520:TYR:C	2.61	0.76
1:A:166:VAL:HG11	1:A:207:TYR:HD2	0.74	0.76
1:A:454:LEU:HD12	1:A:455:ARG:N	2.00	0.76
1:A:109:SER:OG	1:A:170:HIS:O	2.03	0.76
1:A:235:PHE:CD1	1:A:235:PHE:C	2.62	0.76
1:B:245:LEU:C	1:B:245:LEU:CD1	2.37	0.76
1:B:300:VAL:HG22	1:B:301:TYR:H	1.48	0.76
1:A:54:ILE:HG23	1:A:54:ILE:O	1.80	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:PHE:CD2	1:B:191:LEU:CD1	2.67	0.76
1:B:517:GLN:HG3	1:B:518:ILE:O	1.84	0.76
1:A:54:ILE:CG2	1:A:54:ILE:O	2.30	0.76
1:A:462:ILE:CD1	1:A:462:ILE:N	2.46	0.76
1:B:165:THR:C	1:B:166:VAL:HG22	2.11	0.76
1:B:324:SER:C	1:B:326:LEU:N	2.37	0.76
1:B:440:ILE:HD12	1:B:441:ARG:HA	1.68	0.76
1:A:283:PHE:N	1:A:283:PHE:HD1	1.83	0.76
1:A:347:PHE:HZ	1:A:363:LEU:HD13	1.51	0.76
1:A:478:PHE:O	1:A:478:PHE:HD1	1.66	0.76
1:B:420:GLU:O	1:B:421:LEU:CD2	2.30	0.76
1:A:465:LEU:HD11	1:A:474:ILE:HD12	1.67	0.75
1:A:82:LYS:C	1:A:83:ILE:HD12	2.11	0.75
1:B:52:GLY:CA	1:B:228:ILE:CG2	2.65	0.75
1:B:291:LEU:CD1	1:B:437:GLY:C	1.85	0.75
1:B:66:GLY:O	1:B:67:SER:C	2.24	0.75
1:B:92:MET:O	1:B:95:ILE:CG1	2.30	0.75
1:A:321:ASN:C	1:A:321:ASN:OD1	2.29	0.75
1:A:216:ASP:O	1:A:219:LEU:HB2	1.87	0.75
1:B:90:TYR:CE1	1:B:94:GLU:HB3	2.21	0.75
1:A:242:GLU:O	1:A:243:LEU:HD23	1.86	0.75
1:A:525:LYS:O	1:A:528:THR:HG23	1.86	0.75
1:B:82:LYS:O	1:B:82:LYS:HG3	1.85	0.75
1:B:498:TYR:CD1	1:B:536:GLY:O	2.39	0.75
1:B:515:TRP:CH2	1:B:544:VAL:HG13	2.22	0.75
1:B:171:ASN:OD1	1:B:172:ASP:CG	2.29	0.75
1:A:369:TYR:O	1:A:369:TYR:CD1	2.39	0.75
1:A:431:HIS:CE1	1:A:477:ALA:N	2.55	0.75
1:A:27:ASN:OD1	1:A:27:ASN:C	2.30	0.74
1:A:117:ASN:OD1	1:A:118:ILE:HG22	1.85	0.74
1:B:18:TYR:O	1:B:22:ILE:HG13	1.87	0.74
1:B:498:TYR:HD1	1:B:536:GLY:O	1.70	0.74
1:A:83:ILE:N	1:A:83:ILE:CD1	2.48	0.74
1:A:85:ILE:O	1:A:86:PHE:CD1	2.38	0.74
1:A:88:ILE:O	1:A:89:CYS:C	2.30	0.74
1:B:312:ASN:ND2	1:B:312:ASN:N	2.30	0.74
1:A:317:ASP:C	1:A:317:ASP:OD1	2.30	0.74
1:B:91:GLY:O	1:B:95:ILE:CG2	2.30	0.74
1:B:163:ILE:HG23	1:B:164:THR:H	1.53	0.74
1:B:515:TRP:CZ3	1:B:544:VAL:HG13	2.22	0.74
1:A:452:ASN:HA	1:A:455:ARG:CZ	2.18	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:TYR:O	1:B:111:TYR:HD1	1.70	0.74
1:A:503:ARG:HD3	1:A:543:ASP:OD1	1.87	0.74
1:B:106:SER:OG	1:B:171:ASN:O	2.06	0.74
1:A:326:LEU:CG	1:A:338:ILE:HD12	2.17	0.74
1:A:264:GLY:HA2	1:A:430:ARG:NH1	2.01	0.74
1:B:313:ILE:O	1:B:313:ILE:CG1	2.29	0.74
1:B:473:GLN:OE1	1:B:473:GLN:HA	1.86	0.74
1:A:196:TYR:HD1	1:A:203:TYR:CD2	2.06	0.73
1:B:160:LYS:O	1:B:161:SER:C	2.30	0.73
1:B:240:TYR:HB3	1:B:408:TYR:CD2	2.23	0.73
1:A:32:PHE:CD1	1:A:33:SER:O	2.41	0.73
1:A:243:LEU:O	1:A:244:GLU:C	2.30	0.73
1:B:291:LEU:CG	1:B:292:LEU:H	1.99	0.73
1:A:123:ASN:CG	1:A:126:ASN:HD21	1.93	0.73
1:A:179:GLU:CG	1:A:180:ASN:H	1.89	0.73
1:A:421:LEU:HB3	1:A:423:LEU:HD13	1.69	0.73
1:B:181:PHE:CZ	1:B:202:ILE:HD12	2.23	0.73
1:A:12:LEU:O	1:A:56:SER:OG	2.05	0.73
1:A:32:PHE:HD1	1:A:33:SER:N	1.85	0.73
1:A:258:ILE:CD1	1:A:361:THR:HG21	2.17	0.73
1:B:103:VAL:HG13	1:B:173:GLU:O	1.88	0.73
1:A:11:VAL:CA	1:A:54:ILE:CG2	2.62	0.73
1:A:181:PHE:CD1	1:A:195:ILE:HG22	2.23	0.73
1:A:329:VAL:O	1:A:329:VAL:HG22	1.84	0.73
1:A:461:PHE:HD2	1:A:502:LEU:HD21	1.47	0.73
1:B:94:GLU:CG	1:B:95:ILE:N	2.50	0.73
1:B:308:PHE:CA	1:B:311:MET:CE	2.65	0.73
1:B:88:ILE:O	1:B:89:CYS:C	2.29	0.73
1:A:230:LYS:O	1:A:231:CYS:C	2.28	0.73
1:A:257:VAL:HG12	1:A:282:PHE:CB	2.18	0.73
1:A:547:LYS:HB3	1:A:548:PRO:HD3	1.71	0.73
1:B:196:TYR:CE1	1:B:197:ASN:C	2.67	0.73
1:B:436:PRO:O	1:B:436:PRO:HG2	1.89	0.73
1:A:88:ILE:O	1:A:89:CYS:O	2.06	0.73
1:A:179:GLU:CG	1:A:180:ASN:N	2.48	0.72
1:A:238:ILE:O	1:A:241:HIS:CE1	2.42	0.72
1:B:440:ILE:CG1	1:B:441:ARG:N	2.52	0.72
1:B:127:ILE:HG13	1:B:129:TYR:H	1.54	0.72
1:A:305:LYS:HG2	1:A:306:SER:H	1.50	0.72
1:A:13:ASN:C	1:A:13:ASN:OD1	2.28	0.72
1:A:458:ASP:C	1:A:458:ASP:OD1	2.29	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:LYS:O	1:B:47:ASP:C	2.30	0.72
1:B:462:ILE:HG23	1:B:471:TYR:CE2	2.23	0.72
1:A:79:LEU:O	1:A:80:GLU:C	2.29	0.72
1:A:114:THR:HG21	1:A:168:MET:CE	2.19	0.72
1:A:166:VAL:HG11	1:A:207:TYR:HB2	1.71	0.72
1:A:215:LEU:H	1:A:215:LEU:CD1	1.72	0.72
1:A:237:PRO:HG2	1:A:238:ILE:H	1.53	0.72
1:B:46:LYS:O	1:B:48:MET:CG	2.27	0.72
1:A:116:VAL:CG1	1:A:164:THR:HB	2.19	0.72
1:A:205:VAL:HG21	1:A:207:TYR:CE1	2.21	0.72
1:A:441:ARG:NH1	1:A:478:PHE:HB2	2.04	0.72
1:B:13:ASN:OD1	1:B:13:ASN:C	2.29	0.72
1:B:291:LEU:HD12	1:B:438:LEU:N	1.95	0.72
1:B:294:LYS:HG2	1:B:295:ASN:H	1.53	0.72
1:A:116:VAL:HG13	1:A:164:THR:HB	1.71	0.72
1:A:478:PHE:HE1	1:A:480:VAL:HG21	1.55	0.72
1:B:39:GLY:O	1:B:41:GLU:HG3	1.90	0.72
1:B:462:ILE:CG2	1:B:471:TYR:HE2	2.02	0.72
1:A:241:HIS:ND1	1:A:242:GLU:N	2.36	0.72
1:A:256:TYR:CE1	1:A:281:ARG:NH1	2.58	0.72
1:A:457:VAL:O	1:A:457:VAL:HG12	1.82	0.72
1:B:313:ILE:HD12	1:B:314:THR:O	1.89	0.72
1:A:309:PRO:CG	1:A:310:ASP:H	1.96	0.72
1:B:291:LEU:HD12	1:B:437:GLY:CA	1.05	0.72
1:B:112:GLY:HA2	1:B:168:MET:H	1.54	0.72
1:A:38:TYR:C	1:A:40:VAL:HG12	2.15	0.71
1:B:89:CYS:O	1:B:92:MET:HB3	1.89	0.71
1:B:300:VAL:HG23	1:B:301:TYR:N	2.05	0.71
1:A:11:VAL:HG22	1:A:54:ILE:HG21	1.71	0.71
1:B:306:SER:OG	2:B:602:HOH:O	2.08	0.71
1:A:256:TYR:HE1	1:A:281:ARG:HH11	1.35	0.71
1:A:465:LEU:HD11	1:A:474:ILE:HD13	1.71	0.71
1:B:499:VAL:HG11	1:B:539:ARG:O	1.85	0.71
1:B:518:ILE:HG21	1:B:523:LEU:CG	2.20	0.71
1:A:301:TYR:CE1	1:A:313:ILE:CG2	2.55	0.71
1:B:518:ILE:CG2	1:B:523:LEU:CG	2.68	0.71
1:A:400:PHE:O	1:A:401:LYS:C	2.32	0.71
1:A:155:LEU:HD21	1:A:220:MET:HE3	1.71	0.71
1:A:470:LEU:O	1:A:474:ILE:N	2.21	0.71
1:A:38:TYR:O	1:A:40:VAL:HG12	1.89	0.71
1:A:192:ILE:O	1:A:192:ILE:CD1	2.30	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:ILE:H	1:A:313:ILE:HD13	1.55	0.71
1:B:90:TYR:O	1:B:91:GLY:C	2.27	0.71
1:B:465:LEU:O	1:B:471:TYR:CB	2.39	0.71
1:A:301:TYR:CA	1:A:304:LEU:HD12	2.21	0.71
1:B:133:PHE:CE2	1:B:191:LEU:HB2	2.23	0.71
1:B:212:TYR:CD1	1:B:212:TYR:O	2.44	0.71
1:A:517:GLN:C	1:A:518:ILE:HD13	2.15	0.71
1:B:29:ILE:O	1:B:31:ILE:CG2	2.29	0.71
1:B:294:LYS:H	1:B:294:LYS:CD	2.04	0.71
1:B:94:GLU:CD	1:B:95:ILE:N	2.49	0.70
1:B:309:PRO:HG2	1:B:310:ASP:N	2.04	0.70
1:B:518:ILE:HG23	1:B:518:ILE:O	1.91	0.70
1:B:35:THR:CB	1:B:376:LYS:HB3	2.21	0.70
1:B:334:GLN:O	1:B:335:LYS:C	2.29	0.70
1:B:423:LEU:CB	1:B:424:PRO:HD3	2.21	0.70
1:A:248:ILE:HG23	1:A:248:ILE:O	1.89	0.70
1:A:512:THR:HG21	1:A:547:LYS:HZ1	1.44	0.70
1:A:38:TYR:O	1:A:40:VAL:CG1	2.39	0.70
1:A:118:ILE:HG13	1:A:119:LEU:H	1.56	0.70
1:A:362:PHE:O	1:A:364:LEU:CD1	2.40	0.70
1:A:441:ARG:HG3	1:A:480:VAL:HG22	1.74	0.70
1:B:91:GLY:O	1:B:95:ILE:HD13	1.90	0.70
1:B:211:VAL:HG13	1:B:212:TYR:H	1.53	0.70
1:A:116:VAL:HG13	1:A:116:VAL:O	1.90	0.70
1:A:22:ILE:HG22	1:A:23:VAL:N	2.04	0.70
1:A:95:ILE:CD1	1:A:202:ILE:HD13	2.22	0.70
1:A:106:SER:OG	1:A:173:GLU:CB	2.39	0.70
1:A:470:LEU:HB3	1:A:474:ILE:HD11	1.74	0.70
1:A:478:PHE:CE1	1:A:480:VAL:HG21	2.26	0.70
1:B:112:GLY:CA	1:B:168:MET:H	2.04	0.70
1:B:403:PHE:O	1:B:405:PRO:CD	2.38	0.70
1:B:517:GLN:HG3	1:B:518:ILE:N	2.05	0.70
1:A:439:ALA:CA	1:A:442:VAL:HG12	2.22	0.69
1:A:517:GLN:O	1:A:518:ILE:HD13	1.92	0.69
1:B:289:ASN:CB	1:B:319:SER:CB	2.70	0.69
1:A:32:PHE:CE1	1:A:33:SER:O	2.44	0.69
1:A:106:SER:HG	1:A:173:GLU:HB2	1.55	0.69
1:B:219:LEU:CD1	1:B:223:ASN:H	2.02	0.69
1:B:238:ILE:HG23	1:B:239:ARG:N	2.02	0.69
1:B:505:VAL:HG11	1:B:513:ALA:HB1	1.74	0.69
1:B:94:GLU:HG3	1:B:95:ILE:N	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:SER:CB	1:A:428:THR:HG22	2.23	0.69
1:A:457:VAL:O	1:A:457:VAL:CG1	2.37	0.69
1:B:89:CYS:SG	2:B:605:HOH:O	2.50	0.69
1:B:153:CYS:CB	1:B:184:VAL:HG21	2.22	0.69
1:B:475:SER:OG	1:B:505:VAL:O	2.10	0.69
1:B:537:VAL:O	1:B:537:VAL:HG23	1.91	0.69
1:A:37:ASP:O	1:A:40:VAL:CG1	2.40	0.69
1:A:120:ARG:CD	1:A:123:ASN:OD1	2.40	0.69
1:A:240:TYR:O	1:A:241:HIS:C	2.29	0.69
1:A:132:ASN:C	1:A:133:PHE:CD1	2.69	0.69
1:A:174:VAL:O	1:A:174:VAL:HG13	1.91	0.69
1:A:418:SER:HB3	1:A:428:THR:HG22	1.74	0.69
1:A:5:GLU:C	1:A:6:TYR:CD1	2.71	0.69
1:A:51:LYS:HG3	1:A:229:CYS:HB2	1.75	0.69
1:A:470:LEU:CB	1:A:474:ILE:HD11	2.23	0.69
1:B:274:THR:O	1:B:277:ILE:CG1	2.40	0.69
1:A:465:LEU:CG	1:A:474:ILE:HD12	2.23	0.69
1:A:184:VAL:C	1:A:185:SER:OG	2.32	0.69
1:A:205:VAL:CB	1:A:207:TYR:CE1	2.75	0.69
1:A:550:ALA:O	1:A:552:ILE:N	2.26	0.69
1:B:332:PRO:O	1:B:333:GLU:C	2.30	0.69
1:A:512:THR:HG23	1:A:547:LYS:NZ	2.03	0.68
1:B:512:THR:O	2:B:601:HOH:O	2.09	0.68
1:B:513:ALA:CB	1:B:552:ILE:HD11	2.23	0.68
1:A:181:PHE:CD2	1:A:197:ASN:CB	2.65	0.68
1:B:158:ASN:O	1:B:159:ILE:C	2.29	0.68
1:B:291:LEU:CD1	1:B:437:GLY:HA3	0.26	0.68
1:B:437:GLY:O	1:B:438:LEU:CD1	2.29	0.68
1:A:470:LEU:HB3	1:A:474:ILE:HG13	1.75	0.68
1:B:313:ILE:CD1	1:B:315:LYS:CG	2.70	0.68
1:A:11:VAL:HA	1:A:54:ILE:HG21	1.74	0.68
1:A:517:GLN:O	1:A:518:ILE:HD12	1.92	0.68
1:A:531:LEU:CD2	1:B:549:PRO:CG	2.70	0.68
1:B:194:SER:C	1:B:195:ILE:HD13	2.18	0.68
1:B:326:LEU:CB	1:B:446:ILE:CD1	2.68	0.68
1:A:266:ASP:OD1	1:A:368:LEU:HD21	1.93	0.68
1:B:188:GLU:O	1:B:188:GLU:HG2	1.93	0.68
1:A:525:LYS:HA	1:A:528:THR:CG2	2.23	0.68
1:B:46:LYS:CA	1:B:48:MET:HG3	2.23	0.68
1:B:245:LEU:C	1:B:248:ILE:CG1	2.67	0.68
1:A:118:ILE:HG13	1:A:119:LEU:N	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:PHE:CB	1:A:197:ASN:CB	2.72	0.68
1:A:470:LEU:HB3	1:A:474:ILE:CD1	2.24	0.68
1:A:38:TYR:HD1	1:A:39:GLY:N	1.90	0.68
1:B:291:LEU:HD11	1:B:437:GLY:CA	1.17	0.68
1:A:332:PRO:CG	1:A:333:GLU:N	2.42	0.68
1:B:153:CYS:O	1:B:154:CYS:C	2.33	0.68
1:A:114:THR:CB	1:A:168:MET:HE2	2.24	0.67
1:A:88:ILE:HG23	1:A:89:CYS:N	2.09	0.67
1:A:445:GLU:HG2	1:A:445:GLU:O	1.95	0.67
1:A:174:VAL:O	1:A:174:VAL:CG1	2.42	0.67
1:A:253:HIS:O	1:A:281:ARG:NH2	2.27	0.67
1:A:273:TYR:CD1	1:A:421:LEU:HD11	2.26	0.67
1:A:288:ASP:OD1	1:A:289:ASN:N	2.27	0.67
1:B:513:ALA:HB2	1:B:552:ILE:HD11	1.75	0.67
1:B:518:ILE:HG21	1:B:523:LEU:HG	1.75	0.67
1:A:88:ILE:O	1:A:91:GLY:N	2.27	0.67
1:A:461:PHE:HD1	1:A:462:ILE:CD1	2.06	0.67
1:A:534:VAL:O	1:A:534:VAL:CG1	2.30	0.67
1:B:418:SER:CB	1:B:427:ILE:HD12	2.25	0.67
1:A:227:ASN:HB2	1:A:228:ILE:HD12	1.74	0.67
1:A:530:ILE:O	1:A:534:VAL:HG12	1.94	0.67
1:A:9:ILE:HD12	1:A:26:LEU:CD2	2.24	0.67
1:B:471:TYR:CD1	1:B:471:TYR:O	2.46	0.67
1:B:518:ILE:CG1	1:B:523:LEU:HD23	2.24	0.67
1:A:524:ASP:O	1:A:528:THR:CG2	2.30	0.67
1:B:431:HIS:N	1:B:431:HIS:HD2	1.91	0.67
1:B:518:ILE:CG2	1:B:523:LEU:CD2	2.73	0.67
1:B:552:ILE:O	1:B:552:ILE:HG22	1.93	0.67
1:B:187:SER:OG	1:B:188:GLU:N	2.25	0.67
1:B:239:ARG:HG3	1:B:240:TYR:N	1.95	0.67
1:B:295:ASN:O	1:B:298:GLU:CG	2.43	0.67
1:B:430:ARG:C	1:B:431:HIS:HD2	2.03	0.67
1:B:515:TRP:CD1	1:B:515:TRP:H	2.12	0.67
1:A:166:VAL:HG13	1:A:207:TYR:CE2	2.28	0.67
1:A:213:GLU:OE1	1:A:213:GLU:CA	2.42	0.67
1:A:323:LEU:HG	1:A:324:SER:H	1.53	0.67
1:A:125:ASN:ND2	1:A:139:ALA:HB2	2.10	0.66
1:A:418:SER:HB3	1:A:428:THR:CG2	2.25	0.66
1:B:239:ARG:CG	1:B:240:TYR:N	2.55	0.66
1:A:120:ARG:NE	1:A:123:ASN:OD1	2.28	0.66
1:A:20:HIS:O	1:A:23:VAL:HG23	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:ASN:CB	1:A:455:ARG:HH21	2.04	0.66
1:B:243:LEU:HD23	1:B:243:LEU:O	1.93	0.66
1:B:243:LEU:HD23	1:B:247:ASN:ND2	2.07	0.66
1:A:214:SER:O	1:A:217:GLY:N	2.29	0.66
1:A:304:LEU:O	1:A:307:THR:OG1	2.13	0.66
1:B:52:GLY:CA	1:B:228:ILE:HG21	2.24	0.66
1:B:93:GLN:O	1:B:97:VAL:HG23	1.94	0.66
1:B:428:THR:OG1	1:B:429:ASN:N	2.29	0.66
1:A:6:TYR:CD1	1:A:6:TYR:N	2.59	0.66
1:A:32:PHE:CD1	1:A:33:SER:N	2.64	0.66
1:B:173:GLU:OE2	1:B:174:VAL:N	2.29	0.66
1:A:454:LEU:O	1:A:455:ARG:C	2.30	0.66
1:A:194:SER:CA	1:A:195:ILE:HD12	2.26	0.66
1:A:323:LEU:CG	1:A:324:SER:N	2.45	0.66
1:A:463:ASN:OD1	1:A:464:ASP:N	2.29	0.66
1:A:374:GLU:OE1	1:A:374:GLU:N	2.29	0.66
1:B:406:PHE:C	1:B:406:PHE:HD1	2.04	0.66
1:B:430:ARG:O	1:B:432:PRO:CD	2.44	0.66
1:B:436:PRO:O	1:B:437:GLY:C	2.30	0.66
1:A:117:ASN:OD1	1:A:118:ILE:N	2.29	0.65
1:A:268:THR:OG1	1:A:269:VAL:N	2.29	0.65
1:A:177:ILE:O	1:A:177:ILE:HG13	1.87	0.65
1:A:181:PHE:CB	1:A:197:ASN:HB2	2.25	0.65
1:A:206:GLN:NE2	1:A:206:GLN:O	2.29	0.65
1:B:291:LEU:HD12	1:B:438:LEU:HD12	1.77	0.65
1:B:295:ASN:OD1	1:B:295:ASN:N	2.28	0.65
1:B:29:ILE:CG2	1:B:30:LYS:H	2.09	0.65
1:B:89:CYS:O	1:B:92:MET:N	2.29	0.65
1:B:154:CYS:HB2	1:B:203:TYR:HH	1.61	0.65
1:B:190:CYS:O	1:B:191:LEU:C	2.37	0.65
1:B:196:TYR:HD1	1:B:196:TYR:O	1.78	0.65
1:A:213:GLU:N	1:A:213:GLU:OE1	2.29	0.65
1:B:29:ILE:O	1:B:30:LYS:C	2.36	0.65
1:A:121:ASN:ND2	1:A:122:ASP:OD1	2.30	0.65
1:B:241:HIS:ND1	1:B:241:HIS:O	2.29	0.65
1:A:125:ASN:ND2	1:A:125:ASN:O	2.30	0.65
1:B:173:GLU:OE2	1:B:173:GLU:CA	2.43	0.65
1:B:440:ILE:CD1	1:B:441:ARG:CA	2.60	0.65
1:B:512:THR:OG1	1:B:513:ALA:N	2.29	0.65
1:B:97:VAL:HG13	1:B:102:GLU:CD	2.21	0.65
1:B:294:LYS:CG	1:B:295:ASN:H	2.07	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:412:ASP:O	1:B:415:LYS:HB2	1.97	0.65
1:B:515:TRP:O	1:B:515:TRP:CD1	2.49	0.65
1:A:501:VAL:HG21	1:A:541:LEU:HD12	1.78	0.65
1:B:89:CYS:N	1:B:205:VAL:O	2.29	0.65
1:B:243:LEU:O	1:B:247:ASN:ND2	2.30	0.65
1:B:429:ASN:CB	1:B:472:ASN:CG	2.67	0.65
1:A:86:PHE:CD1	1:A:86:PHE:N	2.47	0.65
1:A:197:ASN:O	1:A:202:ILE:N	2.29	0.65
1:A:320:GLU:HG2	1:A:323:LEU:CD2	2.27	0.65
1:A:330:THR:O	1:A:330:THR:HG22	1.94	0.65
1:B:330:THR:O	1:B:330:THR:CG2	2.29	0.65
1:A:166:VAL:CG1	1:A:207:TYR:CG	2.62	0.65
1:A:465:LEU:CD1	1:A:474:ILE:CD1	2.74	0.65
1:B:181:PHE:HE1	1:B:199:GLU:CG	2.07	0.65
1:A:14:PHE:CD1	1:A:38:TYR:HB3	2.30	0.64
1:A:450:LYS:C	1:A:453:ILE:HG12	2.22	0.64
1:A:543:ASP:HA	1:B:541:LEU:HD22	1.69	0.64
1:A:25:ARG:HH21	1:A:211:VAL:H	1.35	0.64
1:A:68:PRO:O	1:A:90:TYR:CE1	2.50	0.64
1:A:123:ASN:CA	1:A:126:ASN:ND2	2.57	0.64
1:A:317:ASP:OD1	1:A:318:ALA:N	2.30	0.64
1:B:246:LYS:O	1:B:246:LYS:CD	2.38	0.64
1:B:309:PRO:CG	1:B:310:ASP:H	2.09	0.64
1:B:470:LEU:O	1:B:473:GLN:N	2.29	0.64
1:A:28:ASN:O	1:A:29:ILE:C	2.31	0.64
1:B:171:ASN:OD1	1:B:172:ASP:N	2.30	0.64
1:A:184:VAL:O	1:A:185:SER:OG	2.14	0.64
1:A:400:PHE:N	1:A:400:PHE:HD1	1.95	0.64
1:B:46:LYS:N	1:B:48:MET:CG	2.21	0.64
1:B:520:TYR:O	1:B:520:TYR:HD1	1.77	0.64
1:A:450:LYS:CG	1:A:451:LEU:N	2.48	0.64
1:A:224:PHE:CA	1:A:228:ILE:HD13	2.23	0.64
1:B:264:GLY:O	1:B:268:THR:HG23	1.97	0.64
1:A:9:ILE:HD12	1:A:26:LEU:HD21	1.79	0.64
1:A:321:ASN:HD21	1:A:342:LEU:HD21	1.61	0.64
1:A:465:LEU:CD1	1:A:474:ILE:HD12	2.28	0.64
1:B:46:LYS:C	1:B:48:MET:N	2.43	0.64
1:B:437:GLY:C	1:B:438:LEU:CD1	2.64	0.64
1:A:172:ASP:OD1	1:A:173:GLU:N	2.30	0.64
1:A:205:VAL:HG23	1:A:207:TYR:N	2.04	0.64
1:A:256:TYR:CE2	1:A:283:PHE:HZ	2.15	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:ALA:HA	1:A:442:VAL:HG12	1.80	0.64
1:B:29:ILE:HG22	1:B:30:LYS:C	2.20	0.64
1:A:478:PHE:CD1	1:A:480:VAL:CG2	2.77	0.64
1:B:240:TYR:HB3	1:B:408:TYR:HD2	1.63	0.64
1:A:164:THR:HG22	1:A:165:THR:O	1.98	0.64
1:A:427:ILE:CG2	1:A:428:THR:N	2.60	0.64
1:B:424:PRO:HD2	1:B:424:PRO:O	1.98	0.64
1:B:524:ASP:C	1:B:524:ASP:OD1	2.39	0.64
1:A:515:TRP:CD1	1:A:515:TRP:H	2.14	0.63
1:A:517:GLN:C	1:A:518:ILE:CD1	2.72	0.63
1:A:197:ASN:O	1:A:201:ASN:CA	2.46	0.63
1:A:237:PRO:HG2	1:A:238:ILE:N	2.11	0.63
1:A:355:ASP:N	1:A:355:ASP:OD1	2.30	0.63
1:B:518:ILE:HG12	1:B:523:LEU:HD23	1.79	0.63
1:A:127:ILE:HG23	1:A:129:TYR:H	1.63	0.63
1:A:211:VAL:HG13	1:A:212:TYR:H	1.61	0.63
1:B:185:SER:OG	1:B:186:SER:N	2.30	0.63
1:B:219:LEU:HD12	1:B:223:ASN:N	2.09	0.63
1:B:98:GLN:C	1:B:98:GLN:CD	2.64	0.63
1:B:522:ILE:CG1	1:B:523:LEU:N	2.58	0.63
1:A:412:ASP:O	1:A:415:LYS:HB3	1.98	0.63
1:B:97:VAL:O	1:B:98:GLN:C	2.37	0.63
1:B:112:GLY:H	1:B:168:MET:C	2.07	0.63
1:B:159:ILE:O	1:B:161:SER:N	2.28	0.63
1:B:462:ILE:HG23	1:B:471:TYR:HE2	1.61	0.63
1:A:123:ASN:CB	1:A:126:ASN:ND2	2.61	0.63
1:A:196:TYR:CD1	1:A:203:TYR:CE2	2.86	0.63
1:B:46:LYS:C	1:B:48:MET:CG	2.70	0.63
1:B:111:TYR:CA	1:B:168:MET:O	2.46	0.63
1:B:32:PHE:O	1:B:33:SER:OG	2.15	0.63
1:B:184:VAL:O	1:B:184:VAL:HG12	1.96	0.63
1:A:125:ASN:ND2	1:A:139:ALA:CB	2.62	0.63
1:A:423:LEU:CB	1:A:424:PRO:HD3	2.27	0.63
1:B:98:GLN:CD	1:B:98:GLN:O	2.42	0.63
1:B:130:CYS:O	1:B:133:PHE:HB2	1.98	0.63
1:B:238:ILE:HG22	1:B:239:ARG:H	1.62	0.63
1:A:214:SER:C	1:A:215:LEU:HD12	2.21	0.62
1:A:399:LYS:C	1:A:400:PHE:HD1	2.07	0.62
1:A:478:PHE:HE1	1:A:480:VAL:CG2	2.10	0.62
1:A:183:LEU:CD1	1:A:192:ILE:HD12	2.29	0.62
1:A:462:ILE:O	1:A:462:ILE:HG22	1.88	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:GLN:HG2	1:B:18:TYR:H	1.64	0.62
1:B:219:LEU:CD1	1:B:223:ASN:N	2.62	0.62
1:B:505:VAL:HG21	1:B:552:ILE:HG23	1.79	0.62
1:A:441:ARG:CD	1:A:479:ALA:O	2.42	0.62
1:A:38:TYR:O	1:A:40:VAL:N	2.29	0.62
1:A:95:ILE:HD11	1:A:202:ILE:HG21	1.80	0.62
1:A:291:LEU:C	1:A:292:LEU:HD13	2.22	0.62
1:A:292:LEU:N	1:A:292:LEU:HD13	2.14	0.62
1:A:515:TRP:H	1:A:515:TRP:HD1	1.48	0.62
1:A:103:VAL:HG12	1:A:104:LYS:N	2.13	0.62
1:A:444:GLY:O	1:A:446:ILE:HD11	1.98	0.62
1:B:68:PRO:CG	1:B:68:PRO:O	2.47	0.62
1:A:123:ASN:ND2	1:A:126:ASN:HD22	1.97	0.62
1:A:155:LEU:CD2	1:A:220:MET:HE3	2.30	0.62
1:A:194:SER:HB2	1:A:204:GLY:O	2.00	0.62
1:B:419:ARG:HH12	1:B:422:ASN:CG	2.06	0.62
1:A:27:ASN:O	1:A:28:ASN:C	2.42	0.62
1:A:153:CYS:O	1:A:153:CYS:SG	2.57	0.62
1:A:369:TYR:H	1:A:370:PRO:HD2	1.63	0.62
1:B:52:GLY:CA	1:B:228:ILE:HG23	2.28	0.62
1:B:195:ILE:CD1	1:B:195:ILE:N	2.61	0.62
1:B:222:TYR:O	1:B:225:ALA:HB3	1.99	0.62
1:A:431:HIS:HE1	1:A:477:ALA:HB3	1.65	0.62
1:B:68:PRO:O	1:B:68:PRO:HG2	2.00	0.62
1:B:243:LEU:CD2	1:B:244:GLU:HA	2.28	0.62
1:B:317:ASP:OD1	1:B:317:ASP:N	2.32	0.62
1:B:534:VAL:HG12	1:B:535:LYS:C	2.22	0.62
1:A:552:ILE:HG13	1:A:553:GLU:N	2.13	0.61
1:B:267:SER:OG	1:B:268:THR:N	2.28	0.61
1:A:501:VAL:HG22	1:A:541:LEU:HD12	1.80	0.61
1:A:301:TYR:HA	1:A:304:LEU:CD1	2.29	0.61
1:A:320:GLU:CB	1:A:323:LEU:CD2	2.77	0.61
1:A:462:ILE:HD12	1:A:462:ILE:N	2.12	0.61
1:A:520:TYR:O	1:A:520:TYR:HD1	1.82	0.61
1:B:97:VAL:HG11	1:B:102:GLU:OE1	1.96	0.61
1:B:243:LEU:CG	1:B:247:ASN:HD21	2.12	0.61
1:B:412:ASP:OD1	1:B:412:ASP:N	2.30	0.61
1:A:164:THR:HG22	1:A:165:THR:N	2.15	0.61
1:B:465:LEU:C	1:B:471:TYR:HB3	2.24	0.61
1:A:462:ILE:N	1:A:462:ILE:HD13	2.15	0.61
1:A:256:TYR:HE1	1:A:281:ARG:NH1	1.93	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:ARG:HD2	1:A:218:GLU:HB2	1.82	0.61
1:A:120:ARG:HE	1:A:123:ASN:CG	2.08	0.61
1:A:271:ALA:O	1:A:274:THR:HG22	2.00	0.61
1:B:91:GLY:C	1:B:95:ILE:HD13	2.26	0.61
1:B:112:GLY:O	1:B:166:VAL:O	2.18	0.61
1:B:226:TYR:O	1:B:229:CYS:N	2.28	0.61
1:B:406:PHE:O	1:B:406:PHE:HD1	1.79	0.61
1:A:236:ASP:OD1	1:A:237:PRO:CD	2.30	0.61
1:A:503:ARG:CD	1:A:543:ASP:OD1	2.48	0.61
1:A:516:TYR:CD1	1:A:518:ILE:CD1	2.83	0.61
1:B:419:ARG:NH1	1:B:422:ASN:CG	2.58	0.61
1:B:326:LEU:O	1:B:446:ILE:O	2.19	0.60
1:B:472:ASN:O	1:B:472:ASN:ND2	2.29	0.60
1:A:214:SER:O	1:A:217:GLY:CA	2.49	0.60
1:B:166:VAL:HG13	1:B:214:SER:HA	1.80	0.60
1:B:291:LEU:CD1	1:B:438:LEU:N	2.60	0.60
1:B:498:TYR:CD1	1:B:498:TYR:N	2.68	0.60
1:A:205:VAL:CG2	1:A:207:TYR:N	2.56	0.60
1:A:122:ASP:OD1	1:A:122:ASP:N	2.29	0.60
1:A:499:VAL:HA	1:A:539:ARG:O	2.01	0.60
1:B:93:GLN:HE21	1:B:172:ASP:CB	2.11	0.60
1:B:159:ILE:C	1:B:161:SER:N	2.50	0.60
1:A:194:SER:CB	1:A:204:GLY:O	2.50	0.60
1:A:438:LEU:O	1:A:442:VAL:HG12	2.01	0.60
1:A:520:TYR:O	1:A:520:TYR:CD1	2.54	0.60
1:A:137:SER:O	1:A:138:SER:C	2.40	0.60
1:A:167:TRP:O	1:A:208:HIS:HB2	2.02	0.60
1:A:181:PHE:HD1	1:A:195:ILE:HG22	1.64	0.60
1:A:464:ASP:N	1:A:464:ASP:OD1	2.30	0.60
1:A:120:ARG:NH2	1:A:162:ASP:CG	2.56	0.60
1:A:243:LEU:N	1:A:243:LEU:CD2	2.30	0.60
1:A:438:LEU:HD23	1:A:454:LEU:HD21	1.84	0.60
1:B:90:TYR:HE1	1:B:94:GLU:HB3	1.65	0.60
1:B:436:PRO:CG	1:B:440:ILE:HG23	2.30	0.60
1:B:462:ILE:CG2	1:B:471:TYR:CE2	2.84	0.59
1:B:323:LEU:O	1:B:326:LEU:CB	2.50	0.59
1:A:520:TYR:CD1	1:A:520:TYR:C	2.79	0.59
1:A:294:LYS:H	1:A:455:ARG:HG2	1.68	0.59
1:B:243:LEU:CD2	1:B:244:GLU:CA	2.72	0.59
1:B:518:ILE:CG1	1:B:523:LEU:CD2	2.79	0.59
1:A:215:LEU:C	1:A:217:GLY:N	2.51	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:GLY:CA	1:A:430:ARG:CZ	2.78	0.59
1:B:39:GLY:O	1:B:40:VAL:C	2.40	0.59
1:A:195:ILE:CD1	1:A:195:ILE:H	2.15	0.59
1:B:291:LEU:HB2	1:B:438:LEU:HD13	1.84	0.59
1:B:470:LEU:C	1:B:473:GLN:HB3	2.26	0.59
1:A:159:ILE:HD13	1:A:159:ILE:N	2.16	0.59
1:A:181:PHE:HB3	1:A:197:ASN:OD1	2.02	0.59
1:A:309:PRO:CG	1:A:310:ASP:N	2.51	0.59
1:A:369:TYR:C	1:A:372:ILE:HG22	2.26	0.59
1:A:411:LYS:NZ	1:A:432:PRO:HG3	2.12	0.59
1:B:68:PRO:CD	1:B:68:PRO:O	2.51	0.59
1:B:107:LYS:C	1:B:108:THR:OG1	2.46	0.59
1:B:244:GLU:HA	1:B:247:ASN:HD22	1.67	0.59
1:A:10:LEU:HB2	1:A:50:ILE:HD11	1.85	0.59
1:A:123:ASN:CG	1:A:126:ASN:HD22	2.11	0.59
1:A:330:THR:O	1:A:330:THR:CG2	2.48	0.59
1:A:13:ASN:OD1	1:A:15:GLY:N	2.27	0.58
1:A:347:PHE:CZ	1:A:363:LEU:HD13	2.29	0.58
1:A:431:HIS:O	1:A:432:PRO:C	2.42	0.58
1:A:439:ALA:HA	1:A:442:VAL:CG1	2.33	0.58
1:B:87:GLY:O	1:B:204:GLY:HA2	2.03	0.58
1:B:436:PRO:O	1:B:436:PRO:HD2	2.01	0.58
1:A:196:TYR:HD1	1:A:203:TYR:CE2	2.22	0.58
1:B:353:ASN:O	1:B:354:ILE:C	2.45	0.58
1:A:10:LEU:C	1:A:54:ILE:HG22	2.18	0.58
1:A:214:SER:O	1:A:217:GLY:HA3	2.02	0.58
1:A:462:ILE:O	1:A:462:ILE:CG2	2.41	0.58
1:B:68:PRO:CD	1:B:90:TYR:CZ	2.78	0.58
1:A:11:VAL:O	1:A:11:VAL:CG1	2.29	0.58
1:A:442:VAL:CG2	1:A:450:LYS:CE	2.81	0.58
1:A:531:LEU:CD2	1:B:549:PRO:HG3	2.31	0.58
1:B:188:GLU:O	1:B:188:GLU:CG	2.51	0.58
1:B:219:LEU:O	1:B:220:MET:C	2.33	0.58
1:B:419:ARG:NH1	1:B:422:ASN:CA	2.63	0.58
1:B:291:LEU:HD13	1:B:437:GLY:CA	1.06	0.58
1:B:29:ILE:C	1:B:30:LYS:O	2.41	0.58
1:B:37:ASP:O	1:B:38:TYR:C	2.40	0.58
1:B:153:CYS:CB	1:B:184:VAL:CG2	2.81	0.58
1:A:110:GLU:C	1:A:111:TYR:CD1	2.82	0.58
1:A:320:GLU:HG2	1:A:323:LEU:HD22	1.85	0.58
1:A:470:LEU:CB	1:A:474:ILE:HG13	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:PHE:HA	1:B:22:ILE:CD1	2.26	0.58
1:B:462:ILE:O	1:B:462:ILE:HG22	2.03	0.57
1:A:427:ILE:HG23	1:A:428:THR:N	2.15	0.57
1:A:436:PRO:HB2	1:A:440:ILE:HG23	1.86	0.57
1:B:93:GLN:O	1:B:97:VAL:CG2	2.52	0.57
1:B:501:VAL:HA	1:B:541:LEU:O	2.04	0.57
1:B:515:TRP:H	1:B:515:TRP:HD1	1.50	0.57
1:A:469:GLY:C	1:A:470:LEU:HD12	2.27	0.57
1:B:68:PRO:HD3	1:B:90:TYR:CZ	2.38	0.57
1:A:62:VAL:O	1:A:62:VAL:HG22	2.05	0.57
1:A:503:ARG:HD3	1:A:543:ASP:CG	2.29	0.57
1:A:141:ASP:HA	1:A:144:SER:OG	2.04	0.57
1:B:73:GLU:H	1:B:73:GLU:CD	2.12	0.57
1:B:525:LYS:O	1:B:526:ILE:C	2.41	0.57
1:A:5:GLU:O	1:A:6:TYR:HD1	1.86	0.57
1:A:181:PHE:CD1	1:A:195:ILE:CG2	2.88	0.57
1:A:195:ILE:HD12	1:A:195:ILE:H	1.60	0.57
1:B:272:ALA:O	1:B:273:TYR:C	2.39	0.57
1:A:35:THR:C	1:A:36:LYS:HG2	2.29	0.57
1:A:83:ILE:HD12	1:A:83:ILE:N	2.14	0.57
1:A:42:LEU:HD12	1:A:45:ILE:HB	1.87	0.56
1:A:503:ARG:NH2	1:A:505:VAL:HG22	2.20	0.56
1:A:538:ASN:OD1	1:B:550:ALA:HB2	2.05	0.56
1:B:103:VAL:HG13	1:B:174:VAL:CA	2.29	0.56
1:B:307:THR:O	1:B:309:PRO:CD	2.52	0.56
1:B:313:ILE:CD1	1:B:314:THR:O	2.53	0.56
1:A:410:PHE:O	1:A:411:LYS:C	2.47	0.56
1:B:61:SER:C	1:B:67:SER:OG	2.48	0.56
1:B:295:ASN:C	1:B:298:GLU:CG	2.78	0.56
1:B:450:LYS:O	1:B:453:ILE:HG22	2.05	0.56
1:B:465:LEU:CA	1:B:471:TYR:HB2	2.35	0.56
1:A:35:THR:O	1:A:36:LYS:CD	2.53	0.56
1:A:40:VAL:HG23	1:A:41:GLU:O	2.06	0.56
1:A:257:VAL:O	1:A:282:PHE:HA	2.05	0.56
1:A:531:LEU:HD11	1:A:540:ILE:CG2	2.35	0.56
1:B:85:ILE:HG22	1:B:86:PHE:N	2.20	0.56
1:B:525:LYS:HA	1:B:528:THR:HG23	1.84	0.56
1:A:224:PHE:O	1:A:225:ALA:C	2.41	0.56
1:A:551:THR:O	1:A:551:THR:OG1	2.20	0.56
1:B:17:GLN:OE1	1:B:17:GLN:N	2.30	0.56
1:B:29:ILE:H	1:B:29:ILE:HD12	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:LYS:O	1:B:297:ALA:HB3	2.06	0.56
1:B:443:ILE:HD12	1:B:483:SER:HB3	1.86	0.56
1:A:205:VAL:CB	1:A:207:TYR:CD1	2.81	0.56
1:A:224:PHE:O	1:A:228:ILE:HD13	2.06	0.56
1:B:90:TYR:C	1:B:92:MET:N	2.55	0.56
1:B:312:ASN:HD22	1:B:312:ASN:N	1.91	0.56
1:B:403:PHE:O	1:B:404:GLU:C	2.45	0.56
1:A:123:ASN:CB	1:A:126:ASN:HD22	2.18	0.56
1:B:70:LEU:CD1	1:B:94:GLU:OE1	2.46	0.56
1:B:111:TYR:HA	1:B:168:MET:O	2.06	0.56
1:B:135:ASP:O	1:B:136:SER:HB2	2.06	0.56
1:B:184:VAL:O	1:B:184:VAL:HG13	2.04	0.56
1:A:155:LEU:O	1:A:155:LEU:CG	2.49	0.56
1:A:271:ALA:CA	1:A:274:THR:HG22	2.33	0.56
1:B:94:GLU:CD	1:B:94:GLU:O	2.48	0.56
1:A:29:ILE:HD13	1:A:222:TYR:HA	1.88	0.56
1:A:32:PHE:HD1	1:A:33:SER:O	1.89	0.56
1:A:211:VAL:CG1	1:A:213:GLU:N	2.30	0.56
1:A:82:LYS:C	1:A:83:ILE:CD1	2.77	0.56
1:B:98:GLN:NE2	1:B:99:MET:N	2.53	0.56
1:B:208:HIS:ND1	1:B:210:GLU:OE1	2.39	0.56
1:B:424:PRO:CD	1:B:424:PRO:O	2.50	0.56
1:A:72:LYS:NZ	1:A:76:GLU:OE2	2.39	0.55
1:B:97:VAL:CG1	1:B:102:GLU:CD	2.76	0.55
1:B:211:VAL:HG12	1:B:214:SER:H	1.70	0.55
1:A:132:ASN:C	1:A:133:PHE:CG	2.83	0.55
1:B:505:VAL:HG11	1:B:552:ILE:HD13	1.87	0.55
1:B:62:VAL:N	1:B:67:SER:OG	2.40	0.55
1:B:291:LEU:HD11	1:B:437:GLY:HA3	0.90	0.55
1:A:38:TYR:C	1:A:40:VAL:N	2.63	0.55
1:A:520:TYR:HD1	1:A:520:TYR:C	2.15	0.55
1:B:294:LYS:O	1:B:297:ALA:CB	2.54	0.55
1:A:112:GLY:O	1:A:167:TRP:HA	2.06	0.55
1:A:114:THR:HG21	1:A:168:MET:HE1	1.89	0.55
1:A:506:LYS:N	1:A:514:ASN:O	2.36	0.55
1:B:515:TRP:CH2	1:B:544:VAL:CG1	2.89	0.55
1:A:9:ILE:CD1	1:A:26:LEU:HD21	2.37	0.55
1:A:173:GLU:CD	1:A:174:VAL:O	2.50	0.55
1:A:243:LEU:O	1:A:247:ASN:ND2	2.29	0.55
1:A:480:VAL:CG1	1:A:481:LEU:N	2.60	0.55
1:B:29:ILE:HD12	1:B:29:ILE:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:TYR:CD1	1:B:111:TYR:C	2.83	0.55
1:B:196:TYR:HE1	1:B:197:ASN:C	2.15	0.55
1:B:214:SER:HB2	1:B:217:GLY:HA3	1.89	0.55
1:B:316:ILE:O	1:B:316:ILE:HG22	2.07	0.55
1:A:289:ASN:C	1:A:291:LEU:H	2.13	0.55
1:A:457:VAL:O	1:A:458:ASP:C	2.46	0.55
1:B:370:PRO:O	1:B:374:GLU:HG3	2.06	0.55
1:A:543:ASP:OD1	1:A:543:ASP:C	2.49	0.55
1:A:117:ASN:OD1	1:A:118:ILE:CG2	2.54	0.55
1:A:166:VAL:HG12	1:A:207:TYR:HB2	1.86	0.55
1:A:181:PHE:CB	1:A:197:ASN:CA	2.85	0.54
1:A:30:LYS:O	1:A:30:LYS:CG	2.30	0.54
1:A:453:ILE:HG13	1:A:454:LEU:N	2.22	0.54
1:B:196:TYR:HD1	1:B:197:ASN:N	1.96	0.54
1:A:194:SER:HA	1:A:195:ILE:HD12	1.88	0.54
1:A:308:PHE:HB3	1:A:309:PRO:HD2	1.88	0.54
1:A:450:LYS:HG2	1:A:451:LEU:H	1.72	0.54
1:B:62:VAL:C	1:B:64:GLU:H	2.13	0.54
1:B:525:LYS:HA	1:B:528:THR:HG22	1.87	0.54
1:A:215:LEU:O	1:A:216:ASP:C	2.48	0.54
1:A:362:PHE:O	1:A:364:LEU:HD13	2.08	0.54
1:B:98:GLN:C	1:B:98:GLN:HE21	2.13	0.54
1:B:195:ILE:O	1:B:203:TYR:HA	2.07	0.54
1:B:499:VAL:CG1	1:B:500:CYS:N	2.67	0.54
1:A:35:THR:O	1:A:36:LYS:HD3	2.08	0.54
1:A:114:THR:CG2	1:A:168:MET:CE	2.85	0.54
1:B:294:LYS:CG	1:B:295:ASN:N	2.53	0.54
1:A:53:VAL:HG12	1:A:54:ILE:N	2.22	0.54
1:B:42:LEU:HG	1:B:74:VAL:HG22	1.90	0.54
1:B:439:ALA:O	1:B:442:VAL:HG22	2.08	0.54
1:A:56:SER:HA	1:A:88:ILE:CG2	2.37	0.54
1:A:103:VAL:CG1	1:A:104:LYS:N	2.71	0.54
1:A:181:PHE:HB3	1:A:197:ASN:CA	2.37	0.54
1:B:27:ASN:HA	1:B:31:ILE:CG1	2.38	0.54
1:B:88:ILE:O	1:B:91:GLY:N	2.40	0.54
1:B:530:ILE:H	1:B:530:ILE:HD13	1.67	0.54
1:A:127:ILE:HD11	1:A:186:SER:HB2	1.89	0.54
1:A:141:ASP:OD1	1:A:141:ASP:N	2.41	0.54
1:A:166:VAL:CG1	1:A:207:TYR:CB	2.79	0.54
1:A:520:TYR:HD2	1:B:517:GLN:HB2	1.73	0.54
1:B:46:LYS:H	1:B:48:MET:HG3	0.52	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:435:GLY:O	1:B:436:PRO:C	2.45	0.54
1:B:515:TRP:HD1	1:B:546:SER:HB3	1.72	0.54
1:A:57:GLY:O	1:A:89:CYS:HB3	2.08	0.54
1:A:516:TYR:CE1	1:A:518:ILE:CD1	2.91	0.53
1:B:62:VAL:HA	1:B:67:SER:CB	2.33	0.53
1:B:153:CYS:O	1:B:156:PHE:N	2.41	0.53
1:A:502:LEU:CD1	1:A:540:ILE:CG1	2.84	0.53
1:B:30:LYS:C	1:B:31:ILE:HG23	2.34	0.53
1:A:69:HIS:ND1	1:A:98:GLN:OE1	2.42	0.53
1:A:442:VAL:HG21	1:A:450:LYS:CE	2.39	0.53
1:B:51:LYS:C	1:B:228:ILE:CG2	2.74	0.53
1:B:160:LYS:C	1:B:161:SER:O	2.46	0.53
1:B:534:VAL:HG13	1:B:535:LYS:H	1.69	0.53
1:B:35:THR:HG1	1:B:376:LYS:CG	2.22	0.53
1:B:117:ASN:N	1:B:117:ASN:OD1	2.41	0.53
1:B:219:LEU:O	1:B:219:LEU:CG	2.56	0.53
1:B:403:PHE:CE2	1:B:404:GLU:O	2.61	0.53
1:B:470:LEU:C	1:B:473:GLN:H	2.16	0.53
1:A:89:CYS:N	1:A:205:VAL:O	2.42	0.53
1:A:126:ASN:O	1:A:128:THR:OG1	2.26	0.53
1:A:436:PRO:HB2	1:A:440:ILE:CG2	2.37	0.53
1:A:446:ILE:CD1	1:A:446:ILE:H	2.17	0.53
1:B:20:HIS:HA	1:B:23:VAL:HG13	1.91	0.53
1:B:201:ASN:O	1:B:203:TYR:HE1	1.88	0.53
1:A:473:GLN:O	1:A:473:GLN:HG2	2.08	0.53
1:A:516:TYR:CD1	1:A:518:ILE:HD13	2.44	0.53
1:A:14:PHE:HD1	1:A:38:TYR:CB	2.19	0.53
1:A:239:ARG:O	1:A:243:LEU:HG	2.09	0.53
1:A:480:VAL:HG11	1:A:554:PHE:CD2	2.44	0.53
1:B:171:ASN:OD1	1:B:171:ASN:N	2.33	0.53
1:B:497:ASP:C	1:B:498:TYR:CD1	2.87	0.53
1:A:125:ASN:O	1:A:126:ASN:C	2.51	0.53
1:B:95:ILE:HG12	1:B:96:ALA:N	2.24	0.53
1:B:116:VAL:O	1:B:164:THR:O	2.26	0.53
1:B:200:TYR:O	1:B:201:ASN:HB2	2.08	0.53
1:B:291:LEU:HD13	1:B:437:GLY:HA3	0.86	0.53
1:A:228:ILE:H	1:A:228:ILE:HD13	1.64	0.52
1:A:320:GLU:CG	1:A:323:LEU:CD2	2.87	0.52
1:B:173:GLU:OE2	1:B:173:GLU:HA	2.07	0.52
1:A:215:LEU:C	1:A:217:GLY:H	2.17	0.52
1:A:470:LEU:CB	1:A:474:ILE:CG1	2.84	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:TYR:C	1:B:225:ALA:HB3	2.34	0.52
1:A:369:TYR:CD1	1:A:369:TYR:C	2.74	0.52
1:B:470:LEU:O	1:B:473:GLN:CA	2.57	0.52
1:B:498:TYR:CE1	1:B:536:GLY:HA2	2.44	0.52
1:A:112:GLY:O	1:A:113:CYS:C	2.46	0.52
1:B:294:LYS:CD	1:B:294:LYS:N	2.73	0.52
1:B:373:ILE:O	1:B:374:GLU:C	2.45	0.52
1:A:83:ILE:N	1:A:83:ILE:HD13	2.25	0.52
1:A:109:SER:CB	1:A:170:HIS:O	2.57	0.52
1:A:502:LEU:HD12	1:A:540:ILE:CG1	2.36	0.52
1:B:460:ILE:O	1:B:463:ASN:HB3	2.09	0.52
1:A:55:LEU:HD21	1:A:70:LEU:HD11	1.92	0.52
1:A:537:VAL:O	1:A:537:VAL:CG2	2.50	0.52
1:B:90:TYR:HD1	1:B:90:TYR:O	1.76	0.52
1:B:326:LEU:CB	1:B:446:ILE:CB	2.86	0.52
1:A:172:ASP:OD1	1:A:172:ASP:C	2.49	0.52
1:A:177:ILE:O	1:A:178:PRO:C	2.44	0.52
1:A:241:HIS:HE1	1:A:242:GLU:HG3	1.71	0.52
1:A:538:ASN:OD1	1:A:538:ASN:O	2.28	0.52
1:A:538:ASN:OD1	1:B:550:ALA:CB	2.58	0.52
1:B:52:GLY:HA2	1:B:84:PRO:O	2.10	0.52
1:B:122:ASP:OD1	1:B:122:ASP:N	2.29	0.52
1:B:419:ARG:O	1:B:419:ARG:HG3	2.10	0.52
1:A:120:ARG:H	1:A:123:ASN:HB2	1.75	0.51
1:A:320:GLU:HG2	1:A:323:LEU:HD21	1.92	0.51
1:A:543:ASP:OD1	1:A:543:ASP:O	2.28	0.51
1:B:37:ASP:O	1:B:40:VAL:HG22	2.09	0.51
1:A:123:ASN:HA	1:A:126:ASN:CG	2.35	0.51
1:A:197:ASN:O	1:A:201:ASN:HA	2.09	0.51
1:B:17:GLN:HA	1:B:511:MET:HB2	1.92	0.51
1:B:244:GLU:HA	1:B:247:ASN:ND2	2.25	0.51
1:B:434:PRO:HD2	1:B:434:PRO:O	2.10	0.51
1:A:265:ILE:O	1:A:269:VAL:CG2	2.45	0.51
1:A:470:LEU:CB	1:A:474:ILE:CD1	2.86	0.51
1:B:434:PRO:O	1:B:434:PRO:CD	2.57	0.51
1:A:38:TYR:O	1:A:40:VAL:HG13	2.10	0.51
1:A:84:PRO:CB	1:A:86:PHE:HE1	2.24	0.51
1:A:181:PHE:HE1	1:A:195:ILE:O	1.45	0.51
1:A:184:VAL:HG21	1:A:196:TYR:HB3	1.93	0.51
1:A:370:PRO:O	1:A:373:ILE:N	2.43	0.51
1:A:516:TYR:CE1	1:A:518:ILE:HD11	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:GLY:O	1:B:291:LEU:HB3	2.10	0.51
1:B:440:ILE:CD1	1:B:441:ARG:HA	2.36	0.51
1:A:441:ARG:HG3	1:A:480:VAL:CA	2.30	0.51
1:B:94:GLU:OE1	1:B:95:ILE:N	2.43	0.51
1:B:153:CYS:C	1:B:155:LEU:N	2.61	0.51
1:B:351:VAL:HG12	1:B:352:ASN:N	2.16	0.51
1:A:84:PRO:HB2	1:A:86:PHE:HE1	1.76	0.51
1:A:181:PHE:HE1	1:A:195:ILE:C	2.10	0.51
1:B:97:VAL:C	1:B:99:MET:N	2.64	0.51
1:B:425:GLU:HG3	1:B:426:GLU:N	2.25	0.51
1:B:542:TYR:CD1	1:B:543:ASP:N	2.78	0.51
1:A:141:ASP:O	1:A:144:SER:OG	2.28	0.51
1:B:443:ILE:CD1	1:B:483:SER:HB3	2.41	0.51
1:A:25:ARG:NH2	1:A:209:PRO:O	2.44	0.51
1:A:196:TYR:CD1	1:A:203:TYR:CD2	2.94	0.51
1:A:321:ASN:HD21	1:A:342:LEU:CD2	2.23	0.51
1:A:111:TYR:CG	1:A:112:GLY:N	2.69	0.51
1:A:461:PHE:CD1	1:A:462:ILE:HD12	2.32	0.51
1:A:463:ASN:OD1	1:A:464:ASP:OD1	2.29	0.51
1:A:531:LEU:HD22	1:B:549:PRO:HG2	1.92	0.51
1:B:98:GLN:NE2	1:B:98:GLN:O	2.44	0.51
1:A:515:TRP:O	1:A:515:TRP:CD2	2.64	0.51
1:A:38:TYR:CD1	1:A:38:TYR:C	2.89	0.50
1:A:42:LEU:HG	1:A:42:LEU:O	2.10	0.50
1:A:210:GLU:C	1:A:211:VAL:HG23	2.28	0.50
1:A:320:GLU:CB	1:A:323:LEU:HD21	2.40	0.50
1:A:370:PRO:O	1:A:371:ASP:C	2.51	0.50
1:A:438:LEU:O	1:A:442:VAL:CG1	2.59	0.50
1:A:438:LEU:O	1:A:442:VAL:N	2.44	0.50
1:B:241:HIS:O	1:B:242:GLU:C	2.52	0.50
1:A:173:GLU:OE1	1:A:174:VAL:O	2.30	0.50
1:A:449:HIS:ND1	1:A:449:HIS:C	2.68	0.50
1:A:478:PHE:O	1:A:479:ALA:C	2.48	0.50
1:A:516:TYR:CE1	1:A:517:GLN:O	2.65	0.50
1:B:226:TYR:C	1:B:228:ILE:H	2.19	0.50
1:B:324:SER:O	1:B:326:LEU:C	2.54	0.50
1:B:471:TYR:HD1	1:B:472:ASN:N	2.08	0.50
1:B:499:VAL:CG1	1:B:500:CYS:H	2.20	0.50
1:A:399:LYS:C	1:A:400:PHE:CD1	2.86	0.50
1:A:300:VAL:C	1:A:304:LEU:HD12	2.35	0.50
1:A:438:LEU:O	1:A:442:VAL:HB	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:ILE:O	1:B:89:CYS:O	2.29	0.50
1:B:111:TYR:C	1:B:168:MET:O	2.53	0.50
1:B:191:LEU:HD23	1:B:192:ILE:HG12	1.92	0.50
1:B:275:HIS:O	1:B:278:PHE:O	2.30	0.50
1:A:362:PHE:HB3	1:A:403:PHE:HB3	1.92	0.50
1:A:465:LEU:CG	1:A:474:ILE:CD1	2.89	0.50
1:B:118:ILE:HG12	1:B:119:LEU:H	1.77	0.50
1:B:173:GLU:OE1	1:B:190:CYS:HA	2.12	0.50
1:B:538:ASN:OD1	1:B:538:ASN:O	2.30	0.50
1:A:44:ASP:OD1	1:A:44:ASP:O	2.30	0.50
1:A:116:VAL:CG2	1:A:117:ASN:H	2.22	0.50
1:A:173:GLU:OE2	1:A:174:VAL:O	2.30	0.50
1:B:94:GLU:OE2	1:B:94:GLU:O	2.30	0.50
1:B:95:ILE:CG1	1:B:96:ALA:N	2.74	0.50
1:B:97:VAL:HG12	1:B:102:GLU:OE1	2.01	0.50
1:B:289:ASN:C	1:B:291:LEU:H	2.20	0.50
1:B:304:LEU:O	1:B:307:THR:OG1	2.30	0.50
1:A:117:ASN:OD1	1:A:118:ILE:O	2.29	0.50
1:A:194:SER:HA	1:A:204:GLY:O	2.12	0.50
1:A:32:PHE:CD1	1:A:32:PHE:C	2.89	0.49
1:A:321:ASN:O	1:A:324:SER:OG	2.30	0.49
1:A:438:LEU:O	1:A:442:VAL:CB	2.60	0.49
1:B:30:LYS:C	1:B:31:ILE:CG2	2.84	0.49
1:B:107:LYS:O	1:B:108:THR:C	2.54	0.49
1:B:171:ASN:OD1	1:B:172:ASP:OD1	2.30	0.49
1:B:95:ILE:HG12	1:B:96:ALA:H	1.76	0.49
1:B:246:LYS:HG3	1:B:247:ASN:N	2.26	0.49
1:B:434:PRO:O	1:B:436:PRO:HD2	2.12	0.49
1:B:524:ASP:O	1:B:524:ASP:OD1	2.30	0.49
1:A:14:PHE:HE2	1:A:91:GLY:HA2	1.77	0.49
1:A:407:LYS:O	1:A:408:TYR:HD1	1.92	0.49
1:B:171:ASN:OD1	1:B:172:ASP:OD2	2.30	0.49
1:B:518:ILE:CG2	1:B:523:LEU:HD21	2.29	0.49
1:B:527:THR:HG22	1:B:528:THR:N	2.20	0.49
1:B:540:ILE:C	1:B:541:LEU:HG	2.37	0.49
1:A:45:ILE:HG23	1:A:46:LYS:N	2.23	0.49
1:A:56:SER:HA	1:A:88:ILE:HG22	1.93	0.49
1:A:116:VAL:CG1	1:A:164:THR:CB	2.90	0.49
1:A:222:TYR:CD1	1:A:222:TYR:O	2.39	0.49
1:A:246:LYS:O	1:A:250:LYS:CE	2.60	0.49
1:A:295:ASN:O	1:A:299:ASN:OD1	2.29	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:519:PRO:HB2	1:B:522:ILE:HG23	1.94	0.49
1:A:458:ASP:OD1	1:A:458:ASP:O	2.30	0.49
1:A:117:ASN:OD1	1:A:117:ASN:C	2.52	0.49
1:A:430:ARG:O	1:A:432:PRO:HD3	2.11	0.49
1:B:265:ILE:O	1:B:266:ASP:C	2.53	0.49
1:A:120:ARG:CG	1:A:123:ASN:CG	2.86	0.49
1:A:303:PHE:O	1:A:307:THR:HG23	2.12	0.49
1:A:320:GLU:O	1:A:321:ASN:C	2.54	0.49
1:A:321:ASN:OD1	1:A:321:ASN:O	2.30	0.49
1:A:515:TRP:CD1	1:A:515:TRP:N	2.77	0.49
1:B:94:GLU:OE2	1:B:94:GLU:C	2.53	0.49
1:B:224:PHE:O	1:B:228:ILE:CG1	2.29	0.49
1:A:92:MET:CA	1:A:95:ILE:HG23	1.91	0.49
1:B:104:LYS:O	1:B:173:GLU:O	2.30	0.49
1:B:237:PRO:HG2	1:B:238:ILE:H	1.78	0.49
1:A:57:GLY:CA	1:A:90:TYR:HB3	2.39	0.49
1:A:205:VAL:HG22	1:A:207:TYR:H	1.67	0.49
1:A:194:SER:CA	1:A:204:GLY:O	2.61	0.48
1:A:278:PHE:O	1:A:278:PHE:CG	2.66	0.48
1:A:449:HIS:O	1:A:453:ILE:HG23	2.13	0.48
1:A:454:LEU:HD12	1:A:455:ARG:CA	2.43	0.48
1:B:13:ASN:OD1	1:B:14:PHE:N	2.45	0.48
1:B:103:VAL:HG12	1:B:104:LYS:O	2.13	0.48
1:B:470:LEU:HA	1:B:473:GLN:HB2	1.95	0.48
1:A:159:ILE:O	1:A:160:LYS:HB3	2.12	0.48
1:A:258:ILE:O	1:A:364:LEU:HD13	2.14	0.48
1:B:498:TYR:C	1:B:499:VAL:CG2	2.86	0.48
1:B:22:ILE:CG1	1:B:210:GLU:HB2	2.40	0.48
1:B:537:VAL:O	1:B:537:VAL:HG22	2.11	0.48
1:A:372:ILE:HG23	1:A:373:ILE:N	2.27	0.48
1:A:528:THR:O	1:A:529:ARG:C	2.53	0.48
1:B:30:LYS:O	1:B:31:ILE:CG2	2.60	0.48
1:A:116:VAL:HG11	1:A:164:THR:HB	1.95	0.48
1:A:256:TYR:CD1	1:A:281:ARG:NH1	2.79	0.48
1:B:270:ALA:O	1:B:274:THR:OG1	2.30	0.48
1:A:116:VAL:O	1:A:164:THR:O	2.32	0.48
1:A:211:VAL:HG12	1:A:212:TYR:C	2.29	0.48
1:A:214:SER:O	1:A:214:SER:OG	2.29	0.48
1:A:374:GLU:OE2	1:A:510:PHE:HE2	1.97	0.48
1:A:512:THR:HG23	1:A:547:LYS:HZ1	1.66	0.48
1:A:9:ILE:HD12	1:A:26:LEU:HD22	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:ASN:OD1	1:A:299:ASN:N	2.45	0.48
1:A:321:ASN:ND2	1:A:342:LEU:CD2	2.77	0.48
1:B:412:ASP:CG	1:B:413:ASP:H	2.21	0.48
1:A:170:HIS:HB2	1:A:206:GLN:OE1	2.14	0.48
1:A:408:TYR:C	1:A:409:LEU:CD1	2.80	0.48
1:B:196:TYR:CD1	1:B:197:ASN:CA	2.97	0.48
1:B:440:ILE:CD1	1:B:441:ARG:H	2.14	0.48
1:A:74:VAL:O	1:A:78:PHE:CG	2.67	0.48
1:A:121:ASN:OD1	1:A:149:MET:O	2.32	0.48
1:B:289:ASN:C	1:B:291:LEU:N	2.72	0.48
1:A:148:LEU:O	1:A:149:MET:CB	2.58	0.47
1:B:166:VAL:HG11	1:B:214:SER:HB2	1.93	0.47
1:A:11:VAL:CA	1:A:54:ILE:HG21	2.39	0.47
1:A:121:ASN:C	1:A:124:ILE:H	2.22	0.47
1:A:442:VAL:HG11	1:A:446:ILE:HG23	1.96	0.47
1:A:515:TRP:O	1:A:515:TRP:CD1	2.64	0.47
1:B:17:GLN:C	1:B:19:PHE:N	2.71	0.47
1:A:114:THR:CB	1:A:168:MET:CE	2.92	0.47
1:A:152:THR:O	1:A:152:THR:OG1	2.30	0.47
1:B:518:ILE:O	1:B:518:ILE:HG22	2.10	0.47
1:A:196:TYR:CE1	1:A:203:TYR:CE2	3.02	0.47
1:A:253:HIS:O	1:A:281:ARG:CZ	2.62	0.47
1:A:271:ALA:HA	1:A:274:THR:CG2	2.38	0.47
1:A:518:ILE:HA	1:A:519:PRO:HD3	1.82	0.47
1:A:550:ALA:C	1:A:552:ILE:N	2.72	0.47
1:B:414:VAL:HG12	1:B:415:LYS:N	2.23	0.47
1:A:285:ILE:O	1:A:285:ILE:HG22	2.07	0.47
1:A:301:TYR:HE1	1:A:313:ILE:HG22	1.64	0.47
1:A:427:ILE:O	1:A:427:ILE:HG12	2.13	0.47
1:A:499:VAL:HB	1:A:539:ARG:O	2.14	0.47
1:B:41:GLU:HB2	1:B:43:LYS:NZ	2.28	0.47
1:B:159:ILE:O	1:B:160:LYS:CB	2.63	0.47
1:A:142:LEU:O	1:A:145:ASN:HB3	2.13	0.47
1:A:285:ILE:HA	1:A:314:THR:HG1	1.73	0.47
1:A:320:GLU:CG	1:A:323:LEU:HD22	2.45	0.47
1:A:374:GLU:OE1	1:A:374:GLU:CA	2.63	0.47
1:A:418:SER:CB	1:A:428:THR:CG2	2.89	0.47
1:B:86:PHE:C	1:B:86:PHE:CD1	2.93	0.47
1:A:120:ARG:HE	1:A:123:ASN:ND2	2.12	0.47
1:A:230:LYS:HD2	1:A:230:LYS:HA	1.22	0.47
1:A:548:PRO:HA	1:A:550:ALA:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:ASN:O	1:B:14:PHE:HD1	1.98	0.47
1:B:294:LYS:O	1:B:296:GLU:N	2.47	0.47
1:B:296:GLU:C	1:B:300:VAL:CG1	2.87	0.47
1:B:321:ASN:CG	1:B:322:PHE:N	2.73	0.47
1:B:498:TYR:C	1:B:499:VAL:HG23	2.39	0.47
1:A:62:VAL:O	1:A:62:VAL:CG2	2.63	0.47
1:A:125:ASN:HD21	1:A:139:ALA:HB2	1.80	0.47
1:A:178:PRO:O	1:A:178:PRO:CD	2.62	0.47
1:A:344:ILE:O	1:A:348:GLU:HG3	2.15	0.47
1:A:441:ARG:HE	1:A:441:ARG:HB2	1.24	0.47
1:A:509:SER:OG	1:A:510:PHE:N	2.30	0.47
1:A:14:PHE:HA	1:A:38:TYR:HD2	1.79	0.47
1:A:38:TYR:CG	1:A:39:GLY:N	2.76	0.47
1:A:197:ASN:HB3	1:A:202:ILE:HB	1.97	0.47
1:A:369:TYR:O	1:A:372:ILE:HG23	2.14	0.47
1:A:441:ARG:CG	1:A:441:ARG:O	2.63	0.47
1:A:271:ALA:C	1:A:274:THR:HG22	2.40	0.46
1:A:434:PRO:HG2	1:A:553:GLU:OE2	2.15	0.46
1:B:417:LEU:HD23	1:B:417:LEU:HA	1.44	0.46
1:B:30:LYS:O	1:B:31:ILE:HG22	2.14	0.46
1:B:332:PRO:C	1:B:334:GLN:N	2.66	0.46
1:A:440:ILE:C	1:A:442:VAL:N	2.71	0.46
1:A:515:TRP:CE3	1:A:544:VAL:HA	2.50	0.46
1:B:311:MET:HE3	1:B:311:MET:HB2	1.46	0.46
1:A:227:ASN:HB2	1:A:228:ILE:CD1	2.45	0.46
1:B:376:LYS:HA	1:B:376:LYS:HD3	1.58	0.46
1:A:320:GLU:O	1:A:324:SER:OG	2.29	0.46
1:A:332:PRO:O	1:A:335:LYS:N	2.49	0.46
1:A:470:LEU:HB2	1:A:474:ILE:HD11	1.94	0.46
1:B:171:ASN:CG	1:B:172:ASP:N	2.73	0.46
1:B:185:SER:HB3	1:B:194:SER:HB2	1.97	0.46
1:B:291:LEU:CG	1:B:292:LEU:N	2.73	0.46
1:B:308:PHE:CB	1:B:311:MET:HE2	2.32	0.46
1:A:296:GLU:O	1:A:297:ALA:C	2.52	0.46
1:A:513:ALA:O	1:A:547:LYS:N	2.49	0.46
1:A:531:LEU:CD1	1:A:540:ILE:CG2	2.93	0.46
1:B:17:GLN:CB	1:B:512:THR:HG22	2.46	0.46
1:B:418:SER:CB	1:B:427:ILE:CD1	2.93	0.46
1:A:88:ILE:O	1:A:88:ILE:HG22	2.15	0.46
1:A:258:ILE:HD11	1:A:361:THR:HG21	1.94	0.46
1:A:364:LEU:N	1:A:364:LEU:HD13	2.26	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:GLN:N	1:B:93:GLN:OE1	2.49	0.46
1:B:121:ASN:HA	1:B:124:ILE:CB	2.45	0.46
1:B:207:TYR:O	1:B:209:PRO:HD3	2.16	0.46
1:A:18:TYR:O	1:A:19:PHE:C	2.58	0.46
1:A:238:ILE:C	1:A:240:TYR:N	2.68	0.46
1:A:367:THR:HG22	1:A:406:PHE:O	2.16	0.46
1:B:133:PHE:HE2	1:B:191:LEU:CB	2.19	0.46
1:A:461:PHE:CD1	1:A:462:ILE:CD1	2.94	0.46
1:A:546:SER:O	1:A:549:PRO:HB2	2.16	0.46
1:A:32:PHE:HE1	1:A:33:SER:O	1.96	0.46
1:A:478:PHE:CD1	1:A:478:PHE:C	2.94	0.46
1:A:531:LEU:CD2	1:B:549:PRO:HG2	2.46	0.46
1:B:66:GLY:C	1:B:67:SER:O	2.47	0.46
1:B:128:THR:O	1:B:128:THR:OG1	2.30	0.46
1:A:89:CYS:O	1:A:90:TYR:C	2.55	0.45
1:A:214:SER:OG	1:A:217:GLY:HA3	2.16	0.45
1:A:282:PHE:C	1:A:283:PHE:HD1	2.24	0.45
1:A:435:GLY:C	1:A:437:GLY:N	2.70	0.45
1:A:459:ASP:O	1:A:460:ILE:C	2.50	0.45
1:A:461:PHE:CD1	1:A:461:PHE:C	2.95	0.45
1:B:35:THR:HB	1:B:376:LYS:HB3	1.98	0.45
1:B:201:ASN:O	1:B:203:TYR:HD1	1.96	0.45
1:A:54:ILE:HG22	1:A:54:ILE:O	2.15	0.45
1:A:498:TYR:O	1:A:537:VAL:HA	2.17	0.45
1:B:471:TYR:C	1:B:473:GLN:N	2.69	0.45
1:B:527:THR:O	1:B:527:THR:HG23	2.17	0.45
1:A:117:ASN:C	1:A:118:ILE:O	2.53	0.45
1:A:208:HIS:C	1:A:210:GLU:H	2.23	0.45
1:A:531:LEU:CD1	1:A:540:ILE:HG22	2.43	0.45
1:A:264:GLY:C	1:A:267:SER:OG	2.48	0.45
1:A:372:ILE:O	1:A:375:SER:OG	2.30	0.45
1:B:51:LYS:HB3	1:B:228:ILE:O	2.16	0.45
1:B:92:MET:N	1:B:95:ILE:HD13	2.31	0.45
1:B:421:LEU:HD23	1:B:421:LEU:N	2.09	0.45
1:A:14:PHE:CD1	1:A:38:TYR:CB	2.98	0.45
1:A:50:ILE:O	1:A:50:ILE:HG23	2.16	0.45
1:A:164:THR:CG2	1:A:165:THR:N	2.77	0.45
1:A:181:PHE:HD1	1:A:195:ILE:C	2.21	0.45
1:A:435:GLY:C	1:A:437:GLY:H	2.23	0.45
1:B:20:HIS:NE2	1:B:510:PHE:CB	2.80	0.45
1:B:61:SER:O	1:B:64:GLU:O	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:GLN:HE21	1:B:99:MET:N	2.14	0.45
1:B:296:GLU:C	1:B:300:VAL:HG12	2.32	0.45
1:A:111:TYR:HB3	1:A:169:ASN:HA	1.98	0.45
1:A:462:ILE:HD13	1:A:462:ILE:H	1.80	0.45
1:B:17:GLN:C	1:B:19:PHE:H	2.25	0.45
1:B:29:ILE:HG23	1:B:30:LYS:H	1.81	0.45
1:B:62:VAL:C	1:B:64:GLU:N	2.73	0.45
1:B:471:TYR:C	1:B:473:GLN:H	2.24	0.45
1:A:107:LYS:HA	1:A:107:LYS:HD2	1.75	0.45
1:A:265:ILE:O	1:A:266:ASP:C	2.58	0.45
1:A:431:HIS:HE1	1:A:477:ALA:CB	2.29	0.45
1:A:470:LEU:O	1:A:474:ILE:CB	2.63	0.45
1:A:120:ARG:HG3	1:A:123:ASN:CG	2.41	0.45
1:A:440:ILE:HD12	1:A:555:GLU:O	2.16	0.45
1:B:22:ILE:HG12	1:B:210:GLU:CG	2.47	0.45
1:B:46:LYS:CA	1:B:48:MET:CG	2.89	0.45
1:B:412:ASP:CG	1:B:413:ASP:N	2.75	0.45
1:A:21:LEU:O	1:A:22:ILE:C	2.56	0.45
1:A:342:LEU:N	1:A:342:LEU:CD1	2.66	0.45
1:A:518:ILE:HD12	1:A:518:ILE:HA	1.67	0.44
1:B:196:TYR:CD1	1:B:196:TYR:O	2.60	0.44
1:B:330:THR:O	1:B:330:THR:OG1	2.29	0.44
1:A:19:PHE:O	1:A:23:VAL:HG22	2.17	0.44
1:A:62:VAL:HG11	1:A:93:GLN:NE2	2.32	0.44
1:A:135:ASP:O	1:A:141:ASP:OD2	2.35	0.44
1:B:212:TYR:HD1	1:B:213:GLU:CA	2.29	0.44
1:B:372:ILE:HG12	1:B:373:ILE:N	2.31	0.44
1:A:48:MET:O	1:A:48:MET:CG	2.40	0.44
1:A:89:CYS:O	1:A:92:MET:N	2.50	0.44
1:A:92:MET:O	1:A:93:GLN:C	2.56	0.44
1:A:181:PHE:CD1	1:A:195:ILE:CB	2.99	0.44
1:A:336:ARG:O	1:A:337:LYS:C	2.55	0.44
1:A:45:ILE:O	1:A:45:ILE:HG22	2.13	0.44
1:A:164:THR:HG22	1:A:166:VAL:HG22	1.99	0.44
1:A:208:HIS:ND1	1:A:210:GLU:HG3	2.31	0.44
1:A:431:HIS:C	1:A:432:PRO:O	2.53	0.44
1:A:499:VAL:CA	1:A:539:ARG:O	2.64	0.44
1:B:85:ILE:CG2	1:B:86:PHE:N	2.79	0.44
1:B:450:LYS:HA	1:B:453:ILE:HG22	1.99	0.44
1:A:374:GLU:OE2	1:A:510:PHE:CE2	2.70	0.44
1:A:531:LEU:HD23	1:B:549:PRO:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:MET:C	1:B:95:ILE:CD1	2.88	0.44
1:A:27:ASN:OD1	1:A:28:ASN:CA	2.66	0.44
1:A:102:GLU:CB	1:A:176:LYS:HD3	2.47	0.44
1:B:408:TYR:CD1	1:B:408:TYR:N	2.80	0.44
1:A:10:LEU:O	1:A:54:ILE:N	2.51	0.44
1:A:222:TYR:O	1:A:226:TYR:HB2	2.16	0.44
1:B:112:GLY:HA2	1:B:168:MET:N	2.28	0.44
1:B:165:THR:O	1:B:166:VAL:CB	2.64	0.44
1:B:483:SER:O	1:B:483:SER:OG	2.29	0.44
1:B:52:GLY:HA3	1:B:228:ILE:CD1	2.44	0.44
1:B:68:PRO:HD3	1:B:90:TYR:CE2	2.52	0.44
1:B:94:GLU:HG3	1:B:95:ILE:H	1.79	0.44
1:B:127:ILE:O	1:B:127:ILE:HG23	2.17	0.44
1:B:313:ILE:HD12	1:B:314:THR:C	2.43	0.44
1:B:443:ILE:HG13	1:B:483:SER:N	2.32	0.44
1:A:109:SER:HB2	1:A:170:HIS:NE2	2.32	0.44
1:A:237:PRO:CG	1:A:238:ILE:N	2.78	0.44
1:A:332:PRO:C	1:A:334:GLN:N	2.72	0.44
1:B:120:ARG:HB3	1:B:121:ASN:H	1.70	0.44
1:B:309:PRO:CG	1:B:310:ASP:N	2.67	0.44
1:A:214:SER:CA	1:A:215:LEU:HD12	2.47	0.43
1:A:517:GLN:HG3	1:A:518:ILE:H	1.83	0.43
1:A:159:ILE:O	1:A:159:ILE:HG22	2.17	0.43
1:B:101:GLY:H	1:B:178:PRO:HA	1.83	0.43
1:B:123:ASN:O	1:B:126:ASN:CB	2.66	0.43
1:A:46:LYS:C	1:A:48:MET:N	2.73	0.43
1:A:114:THR:O	1:A:115:ASP:C	2.50	0.43
1:A:405:PRO:HD2	1:A:406:PHE:H	1.83	0.43
1:B:202:ILE:C	1:B:203:TYR:CD1	2.97	0.43
1:B:267:SER:O	1:B:268:THR:C	2.54	0.43
1:B:339:ILE:O	1:B:342:LEU:CB	2.65	0.43
1:B:515:TRP:CD1	1:B:546:SER:HB3	2.53	0.43
1:A:440:ILE:C	1:A:442:VAL:H	2.26	0.43
1:B:163:ILE:O	1:B:164:THR:OG1	2.30	0.43
1:B:164:THR:HG22	1:B:165:THR:N	2.33	0.43
1:B:222:TYR:O	1:B:226:TYR:CD2	2.70	0.43
1:B:240:TYR:CD2	1:B:408:TYR:CE2	3.05	0.43
1:B:303:PHE:O	1:B:304:LEU:C	2.59	0.43
1:B:427:ILE:HG12	1:B:428:THR:N	2.12	0.43
1:A:516:TYR:HD1	1:A:518:ILE:HD13	1.82	0.43
1:B:165:THR:O	1:B:166:VAL:HG22	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:GLU:CB	1:B:278:PHE:HE2	2.31	0.43
1:A:339:ILE:O	1:A:339:ILE:CG2	2.58	0.43
1:B:199:GLU:H	1:B:199:GLU:HG2	1.46	0.43
1:A:58:GLY:N	1:A:59:PRO:HD3	2.34	0.43
1:A:62:VAL:CG1	1:A:93:GLN:NE2	2.81	0.43
1:A:83:ILE:HA	1:A:84:PRO:HD2	1.76	0.43
1:A:114:THR:HG22	1:A:115:ASP:O	2.18	0.43
1:A:114:THR:CG2	1:A:168:MET:HE2	2.48	0.43
1:A:177:ILE:O	1:A:177:ILE:HG23	2.19	0.43
1:A:214:SER:C	1:A:217:GLY:H	2.26	0.43
1:A:224:PHE:C	1:A:228:ILE:HD13	2.43	0.43
1:B:440:ILE:CG1	1:B:441:ARG:H	2.28	0.43
1:B:506:LYS:O	1:B:514:ASN:O	2.37	0.43
1:A:45:ILE:HG23	1:A:45:ILE:HD13	1.65	0.43
1:A:95:ILE:HG12	1:A:96:ALA:N	2.34	0.43
1:A:153:CYS:O	1:A:155:LEU:N	2.49	0.43
1:A:369:TYR:N	1:A:370:PRO:HD2	2.30	0.43
1:A:14:PHE:HA	1:A:38:TYR:CD2	2.54	0.43
1:A:53:VAL:CG1	1:A:54:ILE:N	2.82	0.43
1:A:160:LYS:HB3	1:A:160:LYS:HE2	1.91	0.43
1:A:243:LEU:C	1:A:245:LEU:N	2.67	0.43
1:A:372:ILE:O	1:A:372:ILE:HG12	2.19	0.43
1:A:499:VAL:CB	1:A:539:ARG:O	2.67	0.43
1:B:16:SER:O	1:B:19:PHE:CB	2.67	0.43
1:B:338:ILE:O	1:B:339:ILE:C	2.59	0.43
1:A:94:GLU:O	1:A:95:ILE:C	2.55	0.43
1:A:129:TYR:CE1	1:A:186:SER:OG	2.62	0.43
1:A:208:HIS:ND1	1:A:210:GLU:CG	2.82	0.43
1:A:452:ASN:CG	1:A:455:ARG:HH21	2.26	0.43
1:B:61:SER:C	1:B:67:SER:HG	2.19	0.43
1:A:320:GLU:C	1:A:323:LEU:CD2	2.64	0.42
1:B:13:ASN:C	1:B:14:PHE:HD1	2.27	0.42
1:B:419:ARG:O	1:B:419:ARG:CG	2.67	0.42
1:A:283:PHE:O	1:A:284:GLY:C	2.59	0.42
1:A:528:THR:HG22	1:A:528:THR:H	1.48	0.42
1:B:112:GLY:N	1:B:168:MET:H	2.17	0.42
1:B:209:PRO:O	1:B:214:SER:OG	2.24	0.42
1:B:238:ILE:O	1:B:239:ARG:C	2.56	0.42
1:A:95:ILE:CD1	1:A:202:ILE:HG21	2.46	0.42
1:A:441:ARG:CZ	1:A:478:PHE:HB2	2.49	0.42
1:B:36:LYS:CB	1:B:40:VAL:HG11	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:ILE:CG2	1:A:10:LEU:N	2.75	0.42
1:B:29:ILE:C	1:B:31:ILE:HG23	2.28	0.42
1:B:211:VAL:HG11	1:B:213:GLU:CB	2.50	0.42
1:B:308:PHE:HA	1:B:309:PRO:HD2	1.91	0.42
1:A:125:ASN:CG	1:A:139:ALA:HB3	2.44	0.42
1:A:181:PHE:CB	1:A:197:ASN:HA	2.48	0.42
1:B:32:PHE:HD1	1:B:32:PHE:HA	1.57	0.42
1:B:498:TYR:O	1:B:499:VAL:HG22	2.19	0.42
1:A:498:TYR:HB2	1:A:536:GLY:O	2.19	0.42
1:B:173:GLU:OE1	1:B:190:CYS:C	2.63	0.42
1:B:196:TYR:CD1	1:B:197:ASN:C	2.97	0.42
1:A:227:ASN:O	1:A:228:ILE:C	2.61	0.42
1:A:342:LEU:N	1:A:342:LEU:HD12	2.16	0.42
1:A:480:VAL:HG12	1:A:481:LEU:N	2.20	0.42
1:B:184:VAL:HG23	1:B:196:TYR:HB2	2.02	0.42
1:B:305:LYS:O	1:B:306:SER:C	2.57	0.42
1:B:419:ARG:NH1	1:B:422:ASN:CB	2.83	0.42
1:B:439:ALA:O	1:B:442:VAL:HG13	2.20	0.42
1:A:19:PHE:O	1:A:22:ILE:HB	2.19	0.42
1:A:321:ASN:ND2	1:A:342:LEU:HD23	2.34	0.42
1:B:331:ASP:CB	1:B:334:GLN:HB2	2.50	0.42
1:A:32:PHE:HD1	1:A:32:PHE:C	2.26	0.42
1:A:245:LEU:HA	1:A:245:LEU:HD12	1.76	0.42
1:A:421:LEU:HD23	1:A:423:LEU:HD13	2.02	0.42
1:A:441:ARG:HG3	1:A:480:VAL:CG2	2.47	0.42
1:B:94:GLU:HG3	1:B:95:ILE:HG23	2.02	0.42
1:B:195:ILE:HD13	1:B:195:ILE:N	2.31	0.42
1:B:264:GLY:O	1:B:267:SER:CB	2.68	0.42
1:B:264:GLY:O	1:B:267:SER:OG	2.30	0.42
1:B:522:ILE:HG12	1:B:523:LEU:N	2.33	0.42
1:A:38:TYR:C	1:A:40:VAL:H	2.15	0.42
1:A:95:ILE:CG1	1:A:96:ALA:N	2.82	0.42
1:A:196:TYR:OH	1:A:198:LYS:HB2	2.19	0.42
1:A:294:LYS:C	1:A:296:GLU:H	2.28	0.42
1:B:46:LYS:O	1:B:48:MET:N	2.49	0.42
1:B:158:ASN:O	1:B:159:ILE:O	2.37	0.42
1:B:303:PHE:O	1:B:307:THR:OG1	2.29	0.42
1:B:374:GLU:HG3	1:B:374:GLU:H	1.52	0.42
1:A:20:HIS:O	1:A:23:VAL:CG2	2.67	0.41
1:A:455:ARG:HE	1:A:455:ARG:HB2	1.33	0.41
1:A:525:LYS:HA	1:A:528:THR:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:LYS:C	1:A:408:TYR:CD1	2.97	0.41
1:A:427:ILE:HG21	1:A:427:ILE:HD13	1.60	0.41
1:A:440:ILE:HD13	1:A:440:ILE:HG21	1.82	0.41
1:A:516:TYR:CD1	1:A:517:GLN:N	2.87	0.41
1:B:158:ASN:C	1:B:160:LYS:N	2.63	0.41
1:A:148:LEU:O	1:A:149:MET:HB2	2.20	0.41
1:A:230:LYS:O	1:A:231:CYS:O	2.36	0.41
1:A:335:LYS:O	1:A:339:ILE:HD12	2.19	0.41
1:A:513:ALA:O	1:A:547:LYS:CA	2.68	0.41
1:B:66:GLY:O	1:B:68:PRO:N	2.52	0.41
1:B:181:PHE:CZ	1:B:202:ILE:CD1	2.99	0.41
1:A:88:ILE:HD13	1:A:88:ILE:HG21	1.86	0.41
1:A:119:LEU:CD2	1:A:183:LEU:CD2	2.99	0.41
1:A:448:LYS:HZ3	1:A:448:LYS:HG2	1.69	0.41
1:A:480:VAL:HG11	1:A:554:PHE:HD2	1.85	0.41
1:B:107:LYS:C	1:B:108:THR:HG1	2.21	0.41
1:A:102:GLU:C	1:A:103:VAL:HG23	2.45	0.41
1:A:258:ILE:HB	1:A:363:LEU:HA	2.01	0.41
1:B:181:PHE:CE2	1:B:202:ILE:HD12	2.53	0.41
1:A:239:ARG:HH11	1:A:239:ARG:HG3	1.86	0.41
1:B:164:THR:CG2	1:B:165:THR:N	2.83	0.41
1:B:173:GLU:OE2	1:B:173:GLU:C	2.64	0.41
1:A:135:ASP:O	1:A:136:SER:CB	2.69	0.41
1:A:206:GLN:HE21	1:A:206:GLN:C	2.29	0.41
1:A:447:ASN:O	1:A:451:LEU:HB3	2.20	0.41
1:A:13:ASN:O	1:A:13:ASN:CG	2.52	0.41
1:A:22:ILE:HD13	1:A:22:ILE:HG21	1.65	0.41
1:A:177:ILE:HD11	1:A:181:PHE:H	1.85	0.41
1:B:35:THR:HG1	1:B:376:LYS:HG3	1.72	0.41
1:A:10:LEU:CD2	1:A:12:LEU:CG	2.98	0.41
1:A:25:ARG:HH22	1:A:211:VAL:N	2.00	0.41
1:A:106:SER:OG	1:A:173:GLU:N	2.54	0.41
1:A:147:LYS:HE3	1:A:147:LYS:HB3	1.14	0.41
1:A:170:HIS:CB	1:A:206:GLN:OE1	2.69	0.41
1:A:214:SER:HA	1:A:215:LEU:HD12	2.03	0.41
1:A:431:HIS:O	1:A:432:PRO:O	2.39	0.41
1:A:510:PHE:CD1	1:A:510:PHE:C	2.98	0.41
1:A:516:TYR:HD1	1:A:517:GLN:N	2.19	0.41
1:B:14:PHE:CD2	1:B:56:SER:O	2.73	0.41
1:B:173:GLU:OE2	1:B:174:VAL:O	2.39	0.41
1:B:219:LEU:O	1:B:219:LEU:HG	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:LEU:O	1:B:326:LEU:CA	2.69	0.41
1:B:323:LEU:O	1:B:326:LEU:N	2.52	0.41
1:B:343:PHE:O	1:B:344:ILE:C	2.61	0.41
1:B:470:LEU:HA	1:B:473:GLN:CB	2.50	0.41
1:B:551:THR:OG1	1:B:552:ILE:N	2.53	0.41
1:A:25:ARG:NH2	1:A:211:VAL:C	2.72	0.41
1:A:441:ARG:CD	1:A:480:VAL:HA	2.51	0.41
1:A:462:ILE:HD12	1:A:462:ILE:HA	1.50	0.41
1:A:530:ILE:O	1:A:531:LEU:C	2.57	0.41
1:B:93:GLN:NE2	1:B:172:ASP:HB2	2.15	0.41
1:A:50:ILE:O	1:A:50:ILE:CG2	2.70	0.40
1:A:104:LYS:O	1:A:173:GLU:O	2.39	0.40
1:A:116:VAL:HG23	1:A:117:ASN:N	2.30	0.40
1:A:211:VAL:HG12	1:A:213:GLU:H	0.70	0.40
1:A:436:PRO:CB	1:A:440:ILE:CG2	2.99	0.40
1:B:17:GLN:O	1:B:19:PHE:N	2.54	0.40
1:B:265:ILE:H	1:B:265:ILE:HG13	1.65	0.40
1:B:29:ILE:H	1:B:29:ILE:CD1	2.34	0.40
1:B:92:MET:HE1	1:B:192:ILE:HG22	2.04	0.40
1:A:239:ARG:HD2	1:A:239:ARG:HA	1.45	0.40
1:A:523:LEU:O	1:A:524:ASP:C	2.57	0.40
1:A:46:LYS:C	1:A:48:MET:H	2.24	0.40
1:A:205:VAL:HG22	1:A:207:TYR:O	2.21	0.40
1:A:361:THR:HG22	1:A:362:PHE:N	2.35	0.40
1:A:423:LEU:HB3	1:A:424:PRO:HD3	1.75	0.40
1:A:462:ILE:O	1:A:463:ASN:C	2.61	0.40
1:B:222:TYR:HA	1:B:225:ALA:HB3	2.04	0.40
1:B:243:LEU:HG	1:B:247:ASN:HD21	1.85	0.40
1:B:440:ILE:HG23	1:B:440:ILE:H	1.47	0.40
1:B:440:ILE:HG13	1:B:441:ARG:H	1.87	0.40
1:B:525:LYS:O	1:B:528:THR:HG23	2.21	0.40
1:A:116:VAL:HG13	1:A:164:THR:C	2.33	0.40
1:A:341:LYS:C	1:A:342:LEU:HD12	2.44	0.40
1:B:287:ILE:O	1:B:288:ASP:CB	2.70	0.40
1:B:538:ASN:OD1	1:B:538:ASN:C	2.63	0.40

All (1) 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:A:132:ASN:OD1	1:B:108:THR:CG2[1_545]	1.24	0.96

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	512/568 (90%)	460 (90%)	39 (8%)	13 (2%)	4	28
1	B	466/568 (82%)	405 (87%)	44 (9%)	17 (4%)	2	22
All	All	978/1136 (86%)	865 (88%)	83 (8%)	30 (3%)	3	25

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	89	CYS
1	A	136	SER
1	A	549	PRO
1	B	89	CYS
1	B	136	SER
1	B	163	ILE
1	B	178	PRO
1	B	290	GLY
1	B	291	LEU
1	B	292	LEU
1	B	325	ASN
1	A	137	SER
1	A	149	MET
1	A	211	VAL
1	A	332	PRO
1	A	547	LYS
1	B	31	ILE
1	B	120	ARG
1	B	293	ARG
1	A	548	PRO
1	B	324	SER
1	B	191	LEU
1	A	58	GLY
1	A	81	LYS
1	B	316	ILE

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Mol	Chain	Res	Type
1	A	369	TYR
1	B	103	VAL
1	A	277	ILE
1	B	166	VAL
1	B	211	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	387/516 (75%)	265 (68%)	122 (32%)	0	2
1	B	284/516 (55%)	180 (63%)	104 (37%)	0	1
All	All	671/1032 (65%)	445 (66%)	226 (34%)	0	2

All (226) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	TYR
1	A	13	ASN
1	A	20	HIS
1	A	22	ILE
1	A	23	VAL
1	A	27	ASN
1	A	35	THR
1	A	40	VAL
1	A	45	ILE
1	A	54	ILE
1	A	62	VAL
1	A	73	GLU
1	A	75	PHE
1	A	83	ILE
1	A	86	PHE
1	A	95	ILE
1	A	97	VAL
1	A	107	LYS

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Mol	Chain	Res	Type
1	A	108	THR
1	A	114	THR
1	A	115	ASP
1	A	116	VAL
1	A	118	ILE
1	A	119	LEU
1	A	121	ASN
1	A	122	ASP
1	A	125	ASN
1	A	127	ILE
1	A	142	LEU
1	A	144	SER
1	A	147	LYS
1	A	149	MET
1	A	159	ILE
1	A	163	ILE
1	A	165	THR
1	A	166	VAL
1	A	167	TRP
1	A	171	ASN
1	A	177	ILE
1	A	178	PRO
1	A	182	TYR
1	A	184	VAL
1	A	186	SER
1	A	192	ILE
1	A	195	ILE
1	A	199	GLU
1	A	202	ILE
1	A	205	VAL
1	A	206	GLN
1	A	207	TYR
1	A	210	GLU
1	A	213	GLU
1	A	215	LEU
1	A	218	GLU
1	A	221	PHE
1	A	222	TYR
1	A	223	ASN
1	A	228	ILE
1	A	230	LYS
1	A	235	PHE

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Mol	Chain	Res	Type
1	A	238	ILE
1	A	239	ARG
1	A	241	HIS
1	A	245	LEU
1	A	248	ILE
1	A	257	VAL
1	A	269	VAL
1	A	275	HIS
1	A	283	PHE
1	A	289	ASN
1	A	298	GLU
1	A	304	LEU
1	A	309	PRO
1	A	313	ILE
1	A	319	SER
1	A	323	LEU
1	A	329	VAL
1	A	333	GLU
1	A	342	LEU
1	A	355	ASP
1	A	359	ASN
1	A	367	THR
1	A	368	LEU
1	A	371	ASP
1	A	372	ILE
1	A	374	GLU
1	A	400	PHE
1	A	402	LEU
1	A	416	THR
1	A	423	LEU
1	A	427	ILE
1	A	438	LEU
1	A	440	ILE
1	A	446	ILE
1	A	449	HIS
1	A	451	LEU
1	A	452	ASN
1	A	454	LEU
1	A	455	ARG
1	A	458	ASP
1	A	459	ASP
1	A	460	ILE

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Mol	Chain	Res	Type
1	A	462	ILE
1	A	463	ASN
1	A	464	ASP
1	A	475	SER
1	A	480	VAL
1	A	483	SER
1	A	512	THR
1	A	517	GLN
1	A	518	ILE
1	A	520	TYR
1	A	523	LEU
1	A	528	THR
1	A	539	ARG
1	A	540	ILE
1	A	543	ASP
1	A	544	VAL
1	A	546	SER
1	A	549	PRO
1	A	551	THR
1	A	553	GLU
1	B	11	VAL
1	B	16	SER
1	B	23	VAL
1	B	40	VAL
1	B	41	GLU
1	B	48	MET
1	B	53	VAL
1	B	55	LEU
1	B	67	SER
1	B	68	PRO
1	B	69	HIS
1	B	70	LEU
1	B	82	LYS
1	B	85	ILE
1	B	90	TYR
1	B	93	GLN
1	B	94	GLU
1	B	95	ILE
1	B	97	VAL
1	B	98	GLN
1	B	103	VAL
1	B	104	LYS

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Mol	Chain	Res	Type
1	B	108	THR
1	B	111	TYR
1	B	117	ASN
1	B	122	ASP
1	B	127	ILE
1	B	129	TYR
1	B	136	SER
1	B	154	CYS
1	B	163	ILE
1	B	165	THR
1	B	166	VAL
1	B	172	ASP
1	B	173	GLU
1	B	182	TYR
1	B	184	VAL
1	B	191	LEU
1	B	194	SER
1	B	195	ILE
1	B	196	TYR
1	B	202	ILE
1	B	208	HIS
1	B	210	GLU
1	B	211	VAL
1	B	212	TYR
1	B	228	ILE
1	B	236	ASP
1	B	239	ARG
1	B	241	HIS
1	B	243	LEU
1	B	245	LEU
1	B	246	LYS
1	B	262	SER
1	B	268	THR
1	B	269	VAL
1	B	274	THR
1	B	275	HIS
1	B	291	LEU
1	B	295	ASN
1	B	300	VAL
1	B	312	ASN
1	B	313	ILE
1	B	314	THR

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Mol	Chain	Res	Type
1	B	317	ASP
1	B	321	ASN
1	B	329	VAL
1	B	339	ILE
1	B	344	ILE
1	B	347	PHE
1	B	348	GLU
1	B	351	VAL
1	B	372	ILE
1	B	376	LYS
1	B	404	GLU
1	B	414	VAL
1	B	416	THR
1	B	425	GLU
1	B	427	ILE
1	B	428	THR
1	B	440	ILE
1	B	443	ILE
1	B	459	ASP
1	B	463	ASN
1	B	471	TYR
1	B	472	ASN
1	B	474	ILE
1	B	484	SER
1	B	498	TYR
1	B	502	LEU
1	B	512	THR
1	B	519	PRO
1	B	522	ILE
1	B	523	LEU
1	B	525	LYS
1	B	526	ILE
1	B	527	THR
1	B	528	THR
1	B	530	ILE
1	B	537	VAL
1	B	540	ILE
1	B	546	SER
1	B	552	ILE
1	B	553	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	GLN
1	A	125	ASN
1	A	126	ASN
1	A	223	ASN
1	A	227	ASN
1	A	431	HIS
1	B	98	GLN
1	B	201	ASN
1	B	247	ASN
1	B	312	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	A	520/568 (91%)	0.71	61 (11%) 9 8	71, 106, 130, 151	0
1	B	480/568 (84%)	0.54	47 (9%) 13 10	74, 127, 155, 177	0
All	All	1000/1136 (88%)	0.63	108 (10%) 11 9	71, 116, 150, 177	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	231	CYS	8.0
1	A	248	ILE	6.5
1	A	237	PRO	6.3
1	A	66	GLY	5.7
1	B	476	GLN	5.1
1	A	153	CYS	4.9
1	B	482	LEU	4.8
1	A	210	GLU	4.6
1	B	11	VAL	4.5
1	A	218	GLU	4.5
1	A	261	MET	4.4
1	A	154	CYS	4.3
1	B	126	ASN	4.2
1	A	110	GLU	4.1
1	B	76	GLU	4.1
1	A	361	THR	4.0
1	B	414	VAL	4.0
1	A	414	VAL	3.9
1	A	362	PHE	3.9
1	B	484	SER	3.8
1	A	203	TYR	3.8
1	A	133	PHE	3.8
1	A	357	ASP	3.8
1	B	537	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	42	LEU	3.7
1	B	78	PHE	3.6
1	A	444	GLY	3.6
1	A	365	GLN	3.5
1	A	20	HIS	3.4
1	A	236	ASP	3.4
1	A	14	PHE	3.4
1	B	378	SER	3.4
1	A	363	LEU	3.3
1	B	549	PRO	3.2
1	A	535	LYS	3.2
1	A	182	TYR	3.2
1	A	29	ILE	3.2
1	B	22	ILE	3.1
1	B	527	THR	3.1
1	B	408	TYR	3.1
1	A	245	LEU	3.1
1	A	527	THR	3.0
1	A	200	TYR	3.0
1	A	410	PHE	3.0
1	A	50	ILE	2.9
1	A	522	ILE	2.9
1	B	63	THR	2.9
1	A	65	ALA	2.9
1	B	352	ASN	2.8
1	A	147	LYS	2.8
1	B	269	VAL	2.8
1	A	550	ALA	2.8
1	A	549	PRO	2.8
1	A	403	PHE	2.8
1	B	194	SER	2.7
1	B	225	ALA	2.7
1	A	526	ILE	2.7
1	A	151	GLU	2.7
1	B	65	ALA	2.7
1	A	164	THR	2.7
1	A	289	ASN	2.6
1	A	228	ILE	2.6
1	B	328	GLY	2.6
1	A	244	GLU	2.6
1	A	461	PHE	2.6
1	B	379	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	474	ILE	2.5
1	A	513	ALA	2.5
1	B	375	SER	2.5
1	A	19	PHE	2.5
1	B	479	ALA	2.5
1	B	516	TYR	2.4
1	B	57	GLY	2.4
1	B	10	LEU	2.4
1	A	536	GLY	2.4
1	A	542	TYR	2.4
1	A	407	LYS	2.4
1	B	334	GLN	2.3
1	B	9	ILE	2.3
1	A	135	ASP	2.3
1	A	67	SER	2.3
1	B	424	PRO	2.3
1	B	33	SER	2.3
1	B	164	THR	2.3
1	B	274	THR	2.3
1	B	268	THR	2.3
1	A	548	PRO	2.2
1	A	152	THR	2.2
1	A	174	VAL	2.2
1	A	340	GLY	2.2
1	A	500	CYS	2.2
1	B	73	GLU	2.2
1	B	69	HIS	2.2
1	A	327	GLN	2.2
1	B	416	THR	2.2
1	A	23	VAL	2.1
1	B	542	TYR	2.1
1	B	454	LEU	2.1
1	B	83	ILE	2.1
1	A	269	VAL	2.1
1	B	97	VAL	2.1
1	A	163	ILE	2.1
1	B	541	LEU	2.1
1	B	114	THR	2.1
1	B	128	THR	2.1
1	B	12	LEU	2.0
1	B	543	ASP	2.0
1	A	541	LEU	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.