



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2024 – 06:57 AM EDT

PDB ID : 4WIM  
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](mailto: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>.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

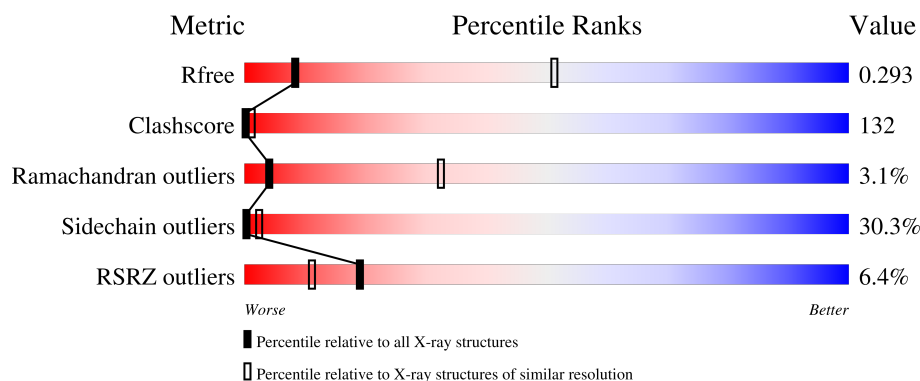
# 1 Overall quality at a glance

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))
$R_{free}$	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (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  $\geq 3$ , 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	
1	B	568	

## 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

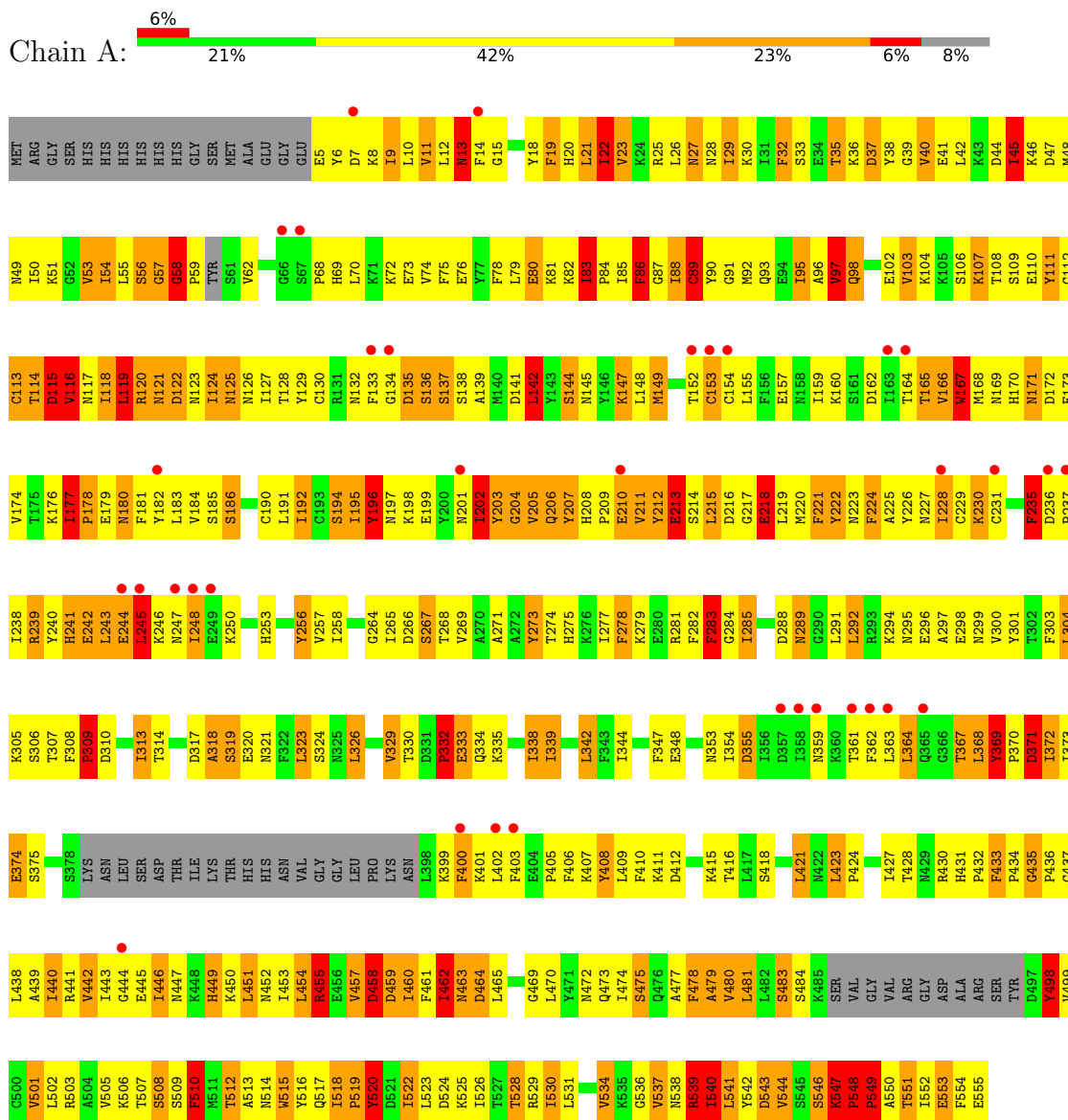
- Molecule 2 is water.

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

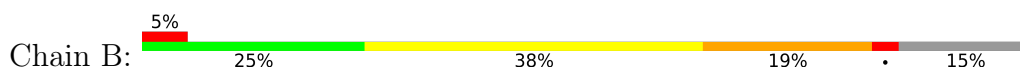
### 3 Residue-property plots

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, $\alpha$ , $\beta$ , $\gamma$	43.45Å 68.55Å 102.08Å 101.11° 99.17° 93.71°	Depositor
Resolution (Å)	49.30 – 3.60 49.31 – 3.60	Depositor EDS
% Data completeness (in resolution range)	89.4 (49.30-3.60) 89.7 (49.31-3.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.67 (at 3.57Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.281 , 0.293 0.282 , 0.293	Depositor DCC
$R_{free}$ test set	595 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	125.1	Xtriage
Anisotropy	0.434	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.21 , 150.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	7304	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	1.84	56/4017 (1.4%)	1.64	86/5449 (1.6%)
1	B	1.47	23/3394 (0.7%)	1.41	47/4633 (1.0%)
All	All	1.68	79/7411 (1.1%)	1.54	133/10082 (1.3%)

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 (79) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	332	PRO	N-CD	-20.41	1.19	1.47
1	A	190	CYS	CB-SG	-9.98	1.65	1.82
1	A	54	ILE	CA-CB	-9.14	1.33	1.54
1	A	153	CYS	CB-SG	-8.87	1.67	1.82
1	B	519	PRO	N-CD	-8.46	1.35	1.47
1	A	80	GLU	CG-CD	-8.25	1.39	1.51
1	A	498	TYR	CD2-CE2	-8.19	1.27	1.39
1	A	462	ILE	CA-CB	-7.96	1.36	1.54
1	B	553	GLU	CG-CD	-7.53	1.40	1.51
1	A	501	VAL	CA-CB	-7.48	1.39	1.54
1	A	480	VAL	CA-CB	-7.38	1.39	1.54
1	B	130	CYS	CB-SG	-7.38	1.69	1.82
1	A	522	ILE	CA-CB	-7.17	1.38	1.54
1	A	520	TYR	CE2-CZ	-7.11	1.29	1.38
1	A	408	TYR	CD2-CE2	-7.06	1.28	1.39
1	B	89	CYS	CB-SG	-6.98	1.70	1.82
1	A	542	TYR	CE1-CZ	-6.95	1.29	1.38
1	A	537	VAL	CB-CG2	-6.94	1.38	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	221	PHE	CD2-CE2	-6.88	1.25	1.39
1	B	515	TRP	CB-CG	-6.87	1.37	1.50
1	A	498	TYR	CE2-CZ	-6.78	1.29	1.38
1	A	118	ILE	CA-CB	-6.76	1.39	1.54
1	A	89	CYS	CB-SG	-6.70	1.70	1.82
1	A	408	TYR	CD1-CE1	-6.34	1.29	1.39
1	A	221	PHE	CD1-CE1	-6.23	1.26	1.39
1	B	515	TRP	CG-CD1	-6.19	1.28	1.36
1	A	212	TYR	CE2-CZ	-6.17	1.30	1.38
1	B	90	TYR	CD2-CE2	-6.14	1.30	1.39
1	A	116	VAL	CA-CB	-6.05	1.42	1.54
1	A	157	GLU	CG-CD	-6.04	1.42	1.51
1	A	408	TYR	CE2-CZ	-5.94	1.30	1.38
1	B	553	GLU	CD-OE1	-5.94	1.19	1.25
1	A	53	VAL	CA-CB	-5.82	1.42	1.54
1	A	519	PRO	CA-C	-5.82	1.41	1.52
1	A	534	VAL	CB-CG1	-5.75	1.40	1.52
1	B	468	TYR	CE1-CZ	-5.74	1.31	1.38
1	B	520	TYR	CD1-CE1	-5.73	1.30	1.39
1	A	408	TYR	CG-CD1	-5.73	1.31	1.39
1	A	520	TYR	CD2-CE2	-5.72	1.30	1.39
1	B	265	ILE	CA-CB	-5.68	1.41	1.54
1	A	515	TRP	CG-CD1	-5.67	1.28	1.36
1	A	103	VAL	CA-CB	-5.64	1.43	1.54
1	B	517	GLN	CA-C	-5.62	1.38	1.52
1	A	212	TYR	CD2-CE2	-5.56	1.31	1.39
1	A	369	TYR	CD2-CE2	-5.56	1.31	1.39
1	A	56	SER	CA-CB	-5.49	1.44	1.52
1	A	478	PHE	C-O	-5.48	1.12	1.23
1	A	284	GLY	C-O	-5.47	1.14	1.23
1	B	468	TYR	CD1-CE1	-5.47	1.31	1.39
1	A	479	ALA	CA-CB	-5.46	1.41	1.52
1	A	111	TYR	CE1-CZ	-5.45	1.31	1.38
1	A	213	GLU	CG-CD	-5.44	1.43	1.51
1	B	552	ILE	CA-CB	-5.40	1.42	1.54
1	A	549	PRO	N-CD	5.40	1.55	1.47
1	A	278	PHE	CD1-CE1	-5.36	1.28	1.39
1	B	514	ASN	C-O	5.34	1.33	1.23
1	A	369	TYR	CG-CD1	-5.31	1.32	1.39
1	A	501	VAL	CB-CG1	-5.29	1.41	1.52
1	A	515	TRP	CB-CG	-5.20	1.40	1.50
1	A	242	GLU	CG-CD	-5.20	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	196	TYR	CB-CG	-5.20	1.43	1.51
1	B	374	GLU	CG-CD	-5.18	1.44	1.51
1	A	9	ILE	CA-CB	-5.17	1.43	1.54
1	A	339	ILE	CA-CB	-5.17	1.43	1.54
1	B	344	ILE	CA-CB	-5.15	1.43	1.54
1	A	278	PHE	CD2-CE2	-5.12	1.29	1.39
1	A	498	TYR	CD1-CE1	-5.11	1.31	1.39
1	A	484	SER	CA-CB	-5.11	1.45	1.52
1	B	240	TYR	CD1-CE1	-5.11	1.31	1.39
1	B	542	TYR	C-O	-5.10	1.13	1.23
1	A	433	PHE	CD2-CE2	-5.08	1.29	1.39
1	A	318	ALA	CA-CB	-5.08	1.41	1.52
1	B	468	TYR	CE2-CZ	-5.06	1.31	1.38
1	A	548	PRO	N-CD	5.05	1.54	1.47
1	A	13	ASN	CB-CG	-5.03	1.39	1.51
1	B	77	TYR	CE1-CZ	-5.03	1.32	1.38
1	B	129	TYR	CD1-CE1	-5.03	1.31	1.39
1	A	235	PHE	CD2-CE2	-5.02	1.29	1.39
1	B	554	PHE	CB-CG	-5.02	1.42	1.51

All (133) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	332	PRO	N-CA-CB	-11.21	89.84	103.30
1	A	332	PRO	CA-N-CD	11.11	127.26	111.70
1	B	112	GLY	N-CA-C	10.99	140.58	113.10
1	A	167	TRP	N-CA-C	-10.99	81.33	111.00
1	A	87	GLY	N-CA-C	-9.73	88.77	113.10
1	A	421	LEU	CB-CG-CD2	-9.72	94.48	111.00
1	B	159	ILE	N-CA-C	-9.60	85.07	111.00
1	A	364	LEU	CA-CB-CG	-9.51	93.42	115.30
1	A	549	PRO	CA-N-CD	-9.28	98.51	111.50
1	B	531	LEU	CA-CB-CG	8.98	135.96	115.30
1	A	243	LEU	CA-CB-CG	-8.86	94.92	115.30
1	A	118	ILE	CB-CA-C	-8.81	93.99	111.60
1	B	67	SER	N-CA-C	-8.34	88.47	111.00
1	A	279	LYS	N-CA-C	8.24	133.25	111.00
1	B	265	ILE	CB-CA-C	-8.21	95.18	111.60
1	B	204	GLY	N-CA-C	-8.16	92.70	113.10
1	A	202	ILE	CB-CA-C	-8.02	95.57	111.60
1	A	58	GLY	N-CA-C	-7.99	93.12	113.10
1	A	329	VAL	CB-CA-C	-7.92	96.36	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	113	CYS	N-CA-C	-7.87	89.75	111.00
1	A	369	TYR	CB-CA-C	-7.84	94.72	110.40
1	B	103	VAL	CB-CA-C	-7.81	96.56	111.40
1	A	57	GLY	N-CA-C	-7.80	93.59	113.10
1	A	116	VAL	CB-CA-C	-7.67	96.83	111.40
1	B	30	LYS	N-CA-C	-7.60	90.48	111.00
1	A	342	LEU	CA-CB-CG	-7.49	98.08	115.30
1	A	86	PHE	N-CA-C	-7.44	90.92	111.00
1	B	523	LEU	CB-CG-CD1	-7.33	98.54	111.00
1	B	437	GLY	N-CA-C	-7.28	94.90	113.10
1	A	142	LEU	CA-CB-CG	-7.23	98.67	115.30
1	A	539	ARG	NE-CZ-NH2	7.18	123.89	120.30
1	B	549	PRO	N-CA-C	7.12	130.61	112.10
1	A	526	ILE	CB-CA-C	-7.12	97.37	111.60
1	A	338	ILE	CB-CA-C	-7.09	97.42	111.60
1	B	174	VAL	N-CA-C	-6.97	92.17	111.00
1	A	166	VAL	N-CA-C	-6.96	92.22	111.00
1	B	161	SER	N-CA-C	-6.95	92.23	111.00
1	A	22	ILE	CB-CA-C	-6.94	97.72	111.60
1	A	29	ILE	N-CA-C	-6.92	92.31	111.00
1	A	244	GLU	N-CA-C	-6.83	92.57	111.00
1	A	204	GLY	N-CA-C	6.78	130.05	113.10
1	A	54	ILE	N-CA-C	-6.68	92.96	111.00
1	B	15	GLY	N-CA-C	6.68	129.80	113.10
1	B	332	PRO	N-CA-C	6.68	129.46	112.10
1	A	540	ILE	CB-CA-C	6.60	124.81	111.60
1	A	319	SER	N-CA-C	6.59	128.80	111.00
1	A	11	VAL	CB-CA-C	-6.59	98.87	111.40
1	A	191	LEU	N-CA-C	6.55	128.69	111.00
1	A	285	ILE	CB-CA-C	-6.35	98.90	111.60
1	B	500	CYS	N-CA-C	6.31	128.04	111.00
1	B	29	ILE	CB-CA-C	-6.25	99.10	111.60
1	A	267	SER	N-CA-CB	-6.22	101.16	110.50
1	A	196	TYR	N-CA-C	6.21	127.78	111.00
1	A	353	ASN	N-CA-C	-6.21	94.23	111.00
1	A	539	ARG	NE-CZ-NH1	-6.18	117.21	120.30
1	B	524	ASP	CB-CG-OD1	-6.18	112.74	118.30
1	B	436	PRO	N-CA-C	-6.10	96.24	112.10
1	A	124	ILE	N-CA-C	-6.08	94.57	111.00
1	A	371	ASP	CB-CG-OD1	6.07	123.76	118.30
1	A	292	LEU	CB-CG-CD1	-6.07	100.69	111.00
1	A	522	ILE	CB-CA-C	-6.05	99.49	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	292	LEU	CA-CB-CG	-6.05	101.38	115.30
1	A	530	ILE	CB-CA-C	-6.05	99.50	111.60
1	A	45	ILE	N-CA-C	-6.04	94.70	111.00
1	A	88	ILE	CB-CA-C	-6.04	99.52	111.60
1	A	442	VAL	N-CA-C	-6.03	94.73	111.00
1	A	267	SER	N-CA-C	6.01	127.24	111.00
1	A	481	LEU	N-CA-C	5.99	127.16	111.00
1	A	224	PHE	C-N-CA	-5.96	106.79	121.70
1	B	219	LEU	C-N-CA	-5.96	106.79	121.70
1	A	326	LEU	CA-CB-CG	-5.94	101.65	115.30
1	A	354	ILE	N-CA-C	-5.92	95.01	111.00
1	B	427	ILE	CG1-CB-CG2	-5.87	98.49	111.40
1	B	91	GLY	N-CA-C	-5.85	98.47	113.10
1	B	518	ILE	N-CA-C	-5.85	95.22	111.00
1	B	126	ASN	N-CA-C	5.83	126.73	111.00
1	A	171	ASN	N-CA-C	-5.82	95.30	111.00
1	B	552	ILE	CB-CA-C	-5.80	100.00	111.60
1	B	334	GLN	C-N-CA	-5.76	107.31	121.70
1	A	547	LYS	C-N-CD	5.74	140.46	128.40
1	A	153	CYS	N-CA-C	5.74	126.49	111.00
1	B	278	PHE	N-CA-C	5.73	126.47	111.00
1	A	8	LYS	N-CA-C	5.72	126.43	111.00
1	A	283	PHE	N-CA-C	5.69	126.37	111.00
1	A	119	LEU	N-CA-C	5.67	126.32	111.00
1	A	457	VAL	CB-CA-C	-5.66	100.65	111.40
1	B	272	ALA	C-N-CA	-5.66	107.55	121.70
1	B	433	PHE	N-CA-C	-5.63	95.79	111.00
1	B	11	VAL	N-CA-C	-5.63	95.80	111.00
1	A	541	LEU	N-CA-C	-5.62	95.83	111.00
1	B	514	ASN	N-CA-C	-5.62	95.84	111.00
1	B	523	LEU	CA-CB-CG	5.59	128.17	115.30
1	A	45	ILE	CG1-CB-CG2	-5.56	99.16	111.40
1	A	458	ASP	N-CA-C	-5.51	96.12	111.00
1	B	541	LEU	CA-CB-CG	-5.51	102.63	115.30
1	A	435	GLY	C-N-CD	-5.50	108.51	120.60
1	B	431	HIS	N-CA-CB	-5.46	100.77	110.60
1	A	88	ILE	CG1-CB-CG2	-5.45	99.42	111.40
1	A	480	VAL	CB-CA-C	-5.43	101.08	111.40
1	A	53	VAL	N-CA-C	-5.34	96.58	111.00
1	A	455	ARG	N-CA-C	-5.34	96.59	111.00
1	A	9	ILE	CB-CA-C	-5.33	100.94	111.60
1	B	553	GLU	N-CA-C	-5.32	96.64	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	277	ILE	CB-CA-C	-5.29	101.01	111.60
1	A	245	LEU	N-CA-C	5.29	125.28	111.00
1	A	56	SER	CB-CA-C	-5.28	100.08	110.10
1	B	70	LEU	CA-CB-CG	5.28	127.44	115.30
1	A	115	ASP	N-CA-C	-5.26	96.79	111.00
1	A	177	ILE	CB-CA-C	-5.25	101.09	111.60
1	A	508	SER	N-CA-C	-5.24	96.85	111.00
1	A	309	PRO	N-CA-C	5.23	125.69	112.10
1	B	47	ASP	N-CA-C	-5.22	96.91	111.00
1	A	353	ASN	N-CA-CB	5.21	119.97	110.60
1	B	535	LYS	N-CA-C	-5.21	96.94	111.00
1	B	21	LEU	N-CA-C	-5.19	96.98	111.00
1	B	515	TRP	CB-CA-C	-5.19	100.01	110.40
1	B	540	ILE	CG1-CB-CG2	-5.19	99.99	111.40
1	B	427	ILE	N-CA-C	-5.18	97.01	111.00
1	A	202	ILE	CG1-CB-CG2	-5.17	100.04	111.40
1	A	218	GLU	N-CA-C	-5.13	97.16	111.00
1	A	97	VAL	CB-CA-C	-5.12	101.67	111.40
1	B	404	GLU	N-CA-C	-5.11	97.22	111.00
1	A	56	SER	N-CA-CB	-5.10	102.85	110.50
1	B	520	TYR	N-CA-C	5.10	124.76	111.00
1	B	66	GLY	N-CA-C	-5.08	100.41	113.10
1	A	21	LEU	CB-CA-C	5.07	119.83	110.20
1	A	83	ILE	C-N-CD	-5.06	109.46	120.60
1	A	421	LEU	CB-CA-C	-5.06	100.58	110.20
1	A	541	LEU	CB-CG-CD1	-5.06	102.40	111.00
1	A	510	PHE	CB-CG-CD1	5.03	124.32	120.80
1	A	203	TYR	CB-CA-C	-5.02	100.35	110.40
1	B	53	VAL	CB-CA-C	-5.01	101.87	111.40
1	A	37	ASP	CB-CG-OD1	5.01	122.81	118.30

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	1001	1
1	B	3340	0	2831	832	1
2	A	14	0	0	4	0
2	B	9	0	0	4	0
All	All	7304	0	6460	1812	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 132.

All (1812) 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: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:B:70:LEU:CD1	1:B:94:GLU:CD	1.77	1.48
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: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:B:291:LEU:HD12	1:B:437:GLY:C	0.99	1.35
1:A:10:LEU:O	1:A:54:ILE:HG22	1.25	1.35
1:B:518:ILE:HD13	1:B:523:LEU:CD2	1.54	1.35
1:A:92:MET:C	1:A:95:ILE:HG23	1.46	1.35
1:A:92:MET:CA	1:A:95:ILE:CG2	2.02	1.34

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:454:LEU:C	1:A:454:LEU:HD12	1.50	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: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: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:A:363:LEU:C	1:A:364:LEU:HD12	1.56	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
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:243:LEU:HD23	1:B:243:LEU:C	1.58	1.22
1:B:297:ALA:C	1:B:300:VAL:HG13	1.56	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:440:ILE:HD12	1:B:440:ILE:C	1.55	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: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: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:85:ILE:C	1:A:86:PHE:HD1	1.48	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
1:A:451:LEU:HD23	1:A:451:LEU:C	1.58	1.14
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:242:GLU:C	1:A:243:LEU:HD23	1.66	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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: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: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:B:70:LEU:HD11	1:B:94:GLU:CD	1.69	1.08
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:534:VAL:HG12	1:B:535:LYS:N	1.64	1.08
1:B:70:LEU:HD12	1:B:94:GLU:CD	1.65	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:B:420:GLU:C	1:B:421:LEU:HD23	1.75	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:103:VAL:HG12	1:B:104:LYS:N	1.64	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: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
1:B:245:LEU:HD12	1:B:245:LEU:C	1.75	1.05
1:B:219:LEU:HD11	1:B:223:ASN:HB2	1.09	1.05
1:B:437:GLY:C	1:B:438:LEU:HD12	1.75	1.05
1:A:228:ILE:HD12	1:A:228:ILE:N	1.66	1.05
1:A:291:LEU:C	1:A:292:LEU:HD12	1.76	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:TYR:CD1	1:B:196:TYR:C	2.29	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:313:ILE:C	1:B:313:ILE:HD12	1.77	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: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: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
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: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:211:VAL:CG1	1:B:213:GLU:H	1.74	1.01
1:B:212:TYR:C	1:B:212:TYR:CD1	2.29	1.01
1:A:30:LYS:HG2	1:A:30:LYS:O	1.56	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:85:ILE:C	1:A:86:PHE:CD1	2.34	1.00
1:B:70:LEU:HD13	1:B:94:GLU:CD	1.79	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:92:MET:C	1:A:95:ILE:CG2	2.17	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: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: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:B:246:LYS:HD2	1:B:246:LYS:C	1.82	0.98
1:A:91:GLY:O	1:A:95:ILE:CG2	2.11	0.98
1:B:70:LEU:HD11	1:B:94:GLU:CG	1.92	0.98
1:A:222:TYR:O	1:A:222:TYR:HD1	1.47	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:294:LYS:HG3	1:B:295:ASN:OD1	1.63	0.97
1:A:451:LEU:C	1:A:451:LEU:CD2	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:194:SER:C	1:A:195:ILE:HD12	1.86	0.96
1:B:312:ASN:H	1:B:312:ASN:HD22	1.13	0.96
1:A:320:GLU:C	1:A:323:LEU:HD23	1.84	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:B:103:VAL:HG12	1:B:104:LYS:H	0.79	0.95
1:A:363:LEU:C	1:A:364:LEU:CD1	2.33	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
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:A:222:TYR:HD1	1:A:222:TYR:C	1.70	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:291:LEU:C	1:A:292:LEU:CD1	2.36	0.94
1:B:211:VAL:CG1	1:B:212:TYR:N	2.30	0.94
1:A:222:TYR:C	1:A:222:TYR:CD1	2.37	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:A:454:LEU:C	1:A:454:LEU:CD1	2.31	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
1:A:431:HIS:CE1	1:A:477:ALA:H	1.86	0.93
1:B:212:TYR:C	1:B:212:TYR:HD1	1.69	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: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:B:440:ILE:CD1	1:B:440:ILE:C	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:94:GLU:CD	1:B:94:GLU:C	2.27	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:B:196:TYR:C	1:B:196:TYR:HD1	1.70	0.91
1:A:470:LEU:C	1:A:474:ILE:HG13	1.90	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:B:166:VAL:CG1	1:B:214:SER:CA	2.47	0.90
1:B:297:ALA:C	1:B:300:VAL:CG1	2.38	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: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: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
1:A:165:THR:C	1:A:166:VAL:CG2	2.40	0.90
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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:194:SER:C	1:B:195:ILE:HD12	1.93	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:N	1:B:228:ILE:CG2	2.36	0.88
1:B:52:GLY:HA3	1:B:228:ILE:HG21	1.56	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:A:10:LEU:O	1:A:54:ILE:CG2	2.20	0.87
1:A:439:ALA:C	1:A:442:VAL:HG12	1.95	0.87
1:B:465:LEU:C	1:B:471:TYR:HB2	1.95	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: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: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: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:196:TYR:CD1	1:B:197:ASN:N	2.43	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: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:B:90:TYR:CD1	1:B:90:TYR:C	2.45	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:445:GLU:C	1:A:446:ILE:HD12	1.96	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:408:TYR:C	1:A:409:LEU:HD12	1.95	0.86
1:A:118:ILE:HG12	1:A:119:LEU:N	1.91	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:B:471:TYR:CD1	1:B:471:TYR:C	2.44	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:A:25:ARG:HH22	1:A:211:VAL:H	1.22	0.85
1:A:91:GLY:C	1:A:95:ILE:HG22	1.95	0.85
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: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:A:123:ASN:CG	1:A:126:ASN:ND2	2.30	0.85
1:A:423:LEU:CB	1:A:424:PRO:CD	2.48	0.85
1:B:98:GLN:C	1:B:98:GLN:NE2	2.30	0.85
1:B:471:TYR:C	1:B:471:TYR:HD1	1.80	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:B:324:SER:C	1:B:326:LEU:H	1.77	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: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:194:SER:C	1:B:195:ILE:CD1	2.45	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:A:531:LEU:HD22	1:B:549:PRO:HG3	1.59	0.84
1:B:499:VAL:HG12	1:B:500:CYS:N	1.93	0.84
1:A:155:LEU:HD21	1:A:220:MET:HE3	1.59	0.83
1:A:292:LEU:O	1:A:455:ARG:CG	2.24	0.83
1:B:269:VAL:HG12	1:B:270:ALA:N	1.93	0.83
1:A:165:THR:C	1:A:166:VAL:HG23	1.96	0.83
1:B:70:LEU:HD13	1:B:94:GLU:OE2	1.72	0.83
1:B:166:VAL:HG11	1:B:214:SER:CB	2.07	0.83
1:B:308:PHE:HA	1:B:311:MET:HE2	1.58	0.83
1:B:90:TYR:C	1:B:90:TYR:HD1	1.81	0.83
1:B:289:ASN:O	1:B:291:LEU:N	2.12	0.83
1:B:313:ILE:C	1:B:313:ILE:CD1	2.44	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:A:95:ILE:HD12	1:A:202:ILE:HD13	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:116:VAL:CG1	1:A:164:THR:C	2.48	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:291:LEU:HD12	1:B:438:LEU:N	1.95	0.81
1:B:51:LYS:C	1:B:228:ILE:HG23	2.00	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:A:54:ILE:HG23	1:A:54:ILE:O	1.80	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
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:A:548:PRO:HA	1:A:549:PRO:C	2.00	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:A:181:PHE:HB3	1:A:197:ASN:CG	2.01	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:ASN:OD1	1:B:322:PHE:N	2.14	0.80
1:B:554:PHE:HD1	1:B:554:PHE:C	1.82	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:B:241:HIS:C	1:B:241:HIS:ND1	2.34	0.80
1:A:178:PRO:O	1:A:178:PRO:CG	2.29	0.80
1:A:457:VAL:O	1:A:457:VAL:HG12	1.82	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:116:VAL:HG12	1:A:164:THR:C	2.01	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:194:SER:O	1:B:195:ILE:CD1	2.29	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:54:ILE:CG2	1:A:54:ILE:O	2.30	0.79
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
1:B:184:VAL:O	1:B:184:VAL:CG1	2.30	0.79
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:PHE:CA	1:B:311:MET:HE2	2.12	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:159:ILE:C	1:B:161:SER:H	1.82	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:B:294:LYS:C	1:B:296:GLU:H	1.87	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:292:LEU:CD1	1:B:293:ARG:H	1.95	0.78
1:B:465:LEU:C	1:B:471:TYR:CB	2.51	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:177:ILE:O	1:A:177:ILE:CG1	2.29	0.78
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: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:364:LEU:HD12	1:A:364:LEU:N	1.73	0.77
1:A:363:LEU:O	1:A:364:LEU:CD1	2.29	0.77
1:B:17:GLN:HG2	1:B:18:TYR:N	1.98	0.77
1:B:436:PRO:O	1:B:436:PRO:CD	2.29	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:GLU:HG2	1:A:180:ASN:N	1.99	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:554:PHE:CD1	1:B:554:PHE:C	2.55	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:A:450:LYS:CG	1:A:451:LEU:N	2.48	0.77
1:B:25:ARG:NH2	1:B:212:TYR:HB2	2.00	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:A:181:PHE:CE1	1:A:195:ILE:C	2.58	0.76
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:B:245:LEU:CA	1:B:248:ILE:CG1	2.63	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:B:300:VAL:HG22	1:B:301:TYR:H	1.48	0.76
1:B:46:LYS:C	1:B:48:MET:HG2	2.04	0.76
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:462:ILE:CD1	1:A:462:ILE:N	2.46	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:B:52:GLY:CA	1:B:228:ILE:CG2	2.65	0.75
1:B:92:MET:O	1:B:95:ILE:CG1	2.30	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:294:LYS:C	1:B:296:GLU:N	2.35	0.75
1:B:498:TYR:CD1	1:B:536:GLY:O	2.39	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:515:TRP:CH2	1:B:544:VAL:HG13	2.22	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:126:ASN:O	1:A:127:ILE:C	2.19	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:434:PRO:HG2	1:A:553:GLU:CD	2.07	0.74
1:B:312:ASN:ND2	1:B:312:ASN:N	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
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: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:B:291:LEU:CG	1:B:292:LEU:H	1.99	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:B:245:LEU:C	1:B:245:LEU:CD1	2.37	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:120:ARG:HH21	1:A:162:ASP:CG	1.91	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:GLU:C	1:A:6:TYR:HD1	1.91	0.73
1:B:406:PHE:CD1	1:B:406:PHE:C	2.62	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: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:A:463:ASN:C	1:A:463:ASN:OD1	2.28	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:B:462:ILE:HG23	1:B:471:TYR:CE2	2.23	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: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: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:A:248:ILE:HG23	1:A:248:ILE:O	1.89	0.72
1:B:112:GLY:HA2	1:B:168:MET:H	1.54	0.72
1:B:89:CYS:O	1:B:92:MET:HB3	1.89	0.71
1:B:246:LYS:C	1:B:246:LYS:CD	2.43	0.71
1:B:300:VAL:HG23	1:B:301:TYR:N	2.05	0.71
1:B:520:TYR:CD1	1:B:520:TYR:C	2.61	0.71
1:A:11:VAL:HG22	1:A:54:ILE:HG21	1.71	0.71
1:A:177:ILE:O	1:A:177:ILE:HG13	1.87	0.71
1:A:235:PHE:CD1	1:A:235:PHE:C	2.62	0.71
1:A:256:TYR:HE1	1:A:281:ARG:HH11	1.35	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:165:THR:C	1:B:166:VAL:HG22	2.11	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
1:A:313:ILE:H	1:A:313:ILE:HD13	1.55	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:B:308:PHE:CB	1:B:311:MET:HE2	2.19	0.71
1:A:82:LYS:C	1:A:83:ILE:HD12	2.11	0.71
1:B:29:ILE:O	1:B:31:ILE:CG2	2.29	0.71
1:B:291:LEU:CD1	1:B:437:GLY:C	1.85	0.71
1:B:294:LYS:H	1:B:294:LYS:CD	2.04	0.71
1:B:66:GLY:O	1:B:67:SER:C	2.24	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:423:LEU:CB	1:B:424:PRO:HD3	2.21	0.70
1:A:106:SER:HG	1:A:173:GLU:HB2	1.54	0.70
1:A:321:ASN:C	1:A:321:ASN:OD1	2.29	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:181:PHE:CD1	1:A:195:ILE:C	2.64	0.70
1:A:362:PHE:O	1:A:364:LEU:CD1	2.40	0.70
1:B:171:ASN:OD1	1:B:172:ASP:CG	2.29	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:27:ASN:OD1	1:A:27:ASN:C	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:88:ILE:O	1:A:89:CYS:C	2.30	0.70
1:B:324:SER:C	1:B:326:LEU:N	2.37	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: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:A:123:ASN:CG	1:A:126:ASN:HD21	1.93	0.69
1:A:317:ASP:C	1:A:317:ASP:OD1	2.30	0.69
1:B:94:GLU:HG3	1:B:95:ILE:N	2.07	0.69
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: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:51:LYS:HG3	1:A:229:CYS:HB2	1.75	0.69
1:A:243:LEU:O	1:A:244:GLU:C	2.30	0.69
1:A:470:LEU:CB	1:A:474:ILE:HD11	2.23	0.69
1:B:160:LYS:O	1:B:161:SER:C	2.30	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: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:A:86:PHE:CD1	1:A:86:PHE:N	2.47	0.68
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:88:ILE:O	1:B:89:CYS:C	2.29	0.68
1:B:196:TYR:CE1	1:B:197:ASN:C	2.67	0.68
1:B:326:LEU:CB	1:B:446:ILE:CD1	2.68	0.68
1:A:230:LYS:O	1:A:231:CYS:C	2.28	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:A:118:ILE:HG13	1:A:119:LEU:N	2.08	0.68
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:13:ASN:C	1:A:13:ASN:OD1	2.28	0.68
1:A:332:PRO:CG	1:A:333:GLU:N	2.42	0.68
1:A:458:ASP:C	1:A:458:ASP:OD1	2.29	0.68
1:B:46:LYS:O	1:B:47:ASP:C	2.30	0.68
1:A:79:LEU:O	1:A:80:GLU:C	2.29	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:B:13:ASN:OD1	1:B:13:ASN:C	2.29	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:184:VAL:C	1:A:185:SER:OG	2.32	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:308:PHE:CB	1:B:311:MET:HE3	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:38:TYR:C	1:A:40:VAL:HG12	2.15	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:A:330:THR:O	1:A:330:THR:HG22	1.94	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: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:400:PHE:O	1:A:401:LYS:C	2.32	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
1:A:452:ASN:CB	1:A:455:ARG:HH21	2.04	0.66
1:B:90:TYR:O	1:B:91:GLY:C	2.27	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:B:291:LEU:HD12	1:B:438:LEU:HD12	1.77	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:A:517:GLN:C	1:A:518:ILE:HD13	2.15	0.66
1:B:428:THR:OG1	1:B:429:ASN:N	2.29	0.66
1:A:6:TYR:N	1:A:6:TYR:CD1	2.59	0.66
1:A:32:PHE:CD1	1:A:33:SER:N	2.64	0.66
1:B:94:GLU:CD	1:B:95:ILE:N	2.49	0.66
1:B:173:GLU:OE2	1:B:174:VAL:N	2.29	0.66
1:B:241:HIS:ND1	1:B:241:HIS:O	2.29	0.66
1:B:334:GLN:O	1:B:335:LYS:C	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:430:ARG:O	1:B:432:PRO:CD	2.44	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: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: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: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:46:LYS:C	1:B:48:MET:N	2.43	0.65
1:A:121:ASN:ND2	1:A:122:ASP:OD1	2.30	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:294:LYS:CG	1:B:295:ASN:H	2.07	0.65
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: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: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:240:TYR:O	1:A:241:HIS:C	2.29	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:A:509:SER:OG	1:A:510:PHE: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:237:PRO:HG2	1:A:238:ILE:N	2.11	0.64
1:B:171:ASN:OD1	1:B:172:ASP:N	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:ASN:C	1:A:133:PHE:CD1	2.69	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: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:332:PRO:O	1:B:333:GLU:C	2.30	0.64
1:A:165:THR:O	1:A:166:VAL:CG2	2.46	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
1:A:439:ALA:HA	1:A:442:VAL:HG12	1.80	0.64
1:A:5:GLU:C	1:A:6:TYR:CD1	2.71	0.64
1:A:478:PHE:CD1	1:A:480:VAL:CG2	2.77	0.64
1:B:158:ASN:O	1:B:159:ILE:C	2.29	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:A:197:ASN:O	1:A:201:ASN:CA	2.46	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:245:LEU:C	1:B:248:ILE:CG1	2.67	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: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:111:TYR:CA	1:B:168:MET:O	2.46	0.63
1:B:153:CYS:O	1:B:154:CYS:C	2.33	0.63
1:B:194:SER:C	1:B:195:ILE:HD13	2.18	0.63
1:B:32:PHE:O	1:B:33:SER:OG	2.15	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:478:PHE:HE1	1:A:480:VAL:CG2	2.10	0.62
1:A:83:ILE:N	1:A:83:ILE:HD12	2.14	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
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:B:219:LEU:O	1:B:220:MET:C	2.33	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:292:LEU:N	1:A:292:LEU:HD13	2.14	0.62
1:A:515:TRP:HD1	1:A:515:TRP:H	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:B:317:ASP:OD1	1:B:317:ASP:N	2.32	0.62
1:A:123:ASN:ND2	1:A:126:ASN:HD22	1.97	0.62
1:A:194:SER:HB2	1:A:204:GLY:O	2.00	0.62
1:A:153:CYS:O	1:A:153:CYS:SG	2.57	0.62
1:B:430:ARG:C	1:B:431:HIS:HD2	2.03	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:A:330:THR:O	1:A:330:THR:CG2	2.48	0.61
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:454:LEU:O	1:A:455:ARG:C	2.30	0.61
1:A:462:ILE:N	1:A:462:ILE:HD13	2.15	0.61
1:B:406:PHE:C	1:B:406:PHE:HD1	2.04	0.61
1:A:256:TYR:HE1	1:A:281:ARG:NH1	1.93	0.61
1:A:25:ARG:HD2	1:A:218:GLU:HB2	1.82	0.61
1:A:427:ILE:HG23	1:A:428:THR:N	2.15	0.61
1:B:436:PRO:O	1:B:437:GLY:C	2.30	0.61
1:A:271:ALA:O	1:A:274:THR:HG22	2.00	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:190:CYS:O	1:B:191:LEU:C	2.37	0.60
1:B:326:LEU:O	1:B:446:ILE:O	2.19	0.60
1:B:29:ILE:O	1:B:30:LYS:C	2.36	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:215:LEU:C	1:A:217:GLY:N	2.51	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:429:ASN:CB	1:B:472:ASN:CG	2.67	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:B:97:VAL:HG13	1:B:102:GLU:CD	2.21	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:450:LYS:C	1:A:453:ILE:HG12	2.22	0.60
1:A:464:ASP:N	1:A:464:ASP:OD1	2.30	0.60
1:A:222:TYR:O	1:A:222:TYR:CD1	2.39	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:28:ASN:O	1:A:29:ILE:C	2.31	0.59
1:B:462:ILE:CG2	1:B:471:TYR:CE2	2.84	0.59
1:B:524:ASP:C	1:B:524:ASP:OD1	2.39	0.59
1:B:323:LEU:O	1:B:326:LEU:CB	2.50	0.59
1:B:245:LEU:O	1:B:245:LEU:CD1	2.29	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:264:GLY:CA	1:A:430:ARG:CZ	2.78	0.59
1:A:537:VAL:O	1:A:537:VAL:CG2	2.50	0.59
1:A:195:ILE:CD1	1:A:195:ILE:H	2.15	0.59
1:B:29:ILE:HG22	1:B:30:LYS:C	2.20	0.59
1:B:62:VAL:HA	1:B:67:SER:HG	1.65	0.59
1:B:291:LEU:HB2	1:B:438:LEU:HD13	1.84	0.59
1:A:159:ILE:HD13	1:A:159:ILE:N	2.16	0.59
1:B:272:ALA:O	1:B:273:TYR:C	2.39	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: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: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: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: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:A:517:GLN:C	1:A:518:ILE:CD1	2.72	0.58
1:B:46:LYS:C	1:B:48:MET:CG	2.70	0.58
1:B:97:VAL:O	1:B:98:GLN:C	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:GLN:O	1:B:98:GLN:CD	2.42	0.58
1:B:188:GLU:O	1:B:188:GLU:CG	2.51	0.58
1:B:419:ARG:NH1	1:B:422:ASN:CA	2.63	0.58
1:A:214:SER:C	1:A:215:LEU:HD12	2.21	0.58
1:A:291:LEU:C	1:A:292:LEU:HD13	2.22	0.58
1:A:399:LYS:C	1:A:400:PHE:HD1	2.07	0.58
1:B:291:LEU:HD13	1:B:437:GLY:CA	1.06	0.58
1:B:153:CYS:CB	1:B:184:VAL:CG2	2.81	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
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:436:PRO:HB2	1:A:440:ILE:HG23	1.86	0.57
1:B:90:TYR:O	1:B:90:TYR:HD1	1.76	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:B:68:PRO:HD3	1:B:90:TYR:CZ	2.38	0.57
1:A:27:ASN:O	1:A:28:ASN:C	2.42	0.57
1:A:62:VAL:O	1:A:62:VAL:HG22	2.05	0.57
1:A:141:ASP:HA	1:A:144:SER:OG	2.04	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:37:ASP:O	1:B:38:TYR:C	2.40	0.57
1:A:480:VAL:CG1	1:A:481:LEU:N	2.60	0.57
1:B:534:VAL:HG12	1:B:535:LYS:C	2.22	0.57
1:B:243:LEU:C	1:B:243:LEU:CD2	2.31	0.57
1:B:437:GLY:C	1:B:438:LEU:CD1	2.64	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:ILE:HG22	1:B:86:PHE:N	2.20	0.56
1:B:308:PHE:HA	1:B:311:MET:HE1	1.86	0.56
1:B:465:LEU:C	1:B:471:TYR:HB3	2.24	0.56
1:B:525:LYS:HA	1:B:528:THR:HG23	1.84	0.56
1:A:120:ARG:HE	1:A:123:ASN:CG	2.08	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
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:91:GLY:C	1:B:95:ILE:HD13	2.26	0.56
1:B:159:ILE:C	1:B:161:SER:N	2.50	0.56
1:B:312:ASN:HD22	1:B:312:ASN:N	1.91	0.56
1:B:427:ILE:HG12	1:B:428:THR:N	2.12	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:B:419:ARG:NH1	1:B:422:ASN:CG	2.58	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: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:B:98:GLN:C	1:B:98:GLN:CD	2.64	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:211:VAL:HG12	1:B:214:SER:H	1.70	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: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:137:SER:O	1:A:138:SER:C	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:ILE:CD1	1:A:26:LEU:HD21	2.37	0.55
1:A:120:ARG:NH2	1:A:162:ASP:CG	2.56	0.55
1:A:243:LEU:O	1:A:247:ASN:ND2	2.29	0.55
1:B:29:ILE:HD12	1:B:29:ILE:N	2.21	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:B:370:PRO:O	1:B:374:GLU:HG3	2.06	0.55
1:B:419:ARG:HH12	1:B:422:ASN:CG	2.06	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:520:TYR:CD1	1:A:520:TYR:C	2.79	0.55
1:A:181:PHE:CB	1:A:197:ASN:CA	2.85	0.54
1:B:39:GLY:O	1:B:40:VAL:C	2.40	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:B:470:LEU:C	1:B:473:GLN:HB3	2.26	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:525:LYS:HA	1:B:528:THR:HG22	1.87	0.54
1:A:362:PHE:O	1:A:364:LEU:HD13	2.08	0.54
1:A:369:TYR:C	1:A:372:ILE:HG22	2.26	0.54
1:B:107:LYS:C	1:B:108:THR:OG1	2.46	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:A:123:ASN:CG	1:A:126:ASN:HD22	2.11	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:A:431:HIS:O	1:A:432:PRO:C	2.42	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:10:LEU:C	1:A:54:ILE:HG22	2.18	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:353:ASN:O	1:B:354:ILE: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: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:534:VAL:HG13	1:B:535:LYS:H	1.69	0.53
1:B:29:ILE:C	1:B:30:LYS:O	2.41	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:A:89:CYS:N	1:A:205:VAL:O	2.42	0.53
1:A:110:GLU:C	1:A:111:TYR:CD1	2.82	0.53
1:A:126:ASN:O	1:A:128:THR:OG1	2.26	0.53
1:B:525:LYS:O	1:B:526:ILE:C	2.41	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:469:GLY:C	1:A:470:LEU:HD12	2.27	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:73:GLU:H	1:B:73:GLU:CD	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:GLU:CG	1:A:323:LEU:CD2	2.87	0.52
1:A:503:ARG:HD3	1:A:543:ASP:CG	2.29	0.52
1:B:173:GLU:OE2	1:B:173:GLU:HA	2.07	0.52
1:A:470:LEU:CB	1:A:474:ILE:CG1	2.84	0.52
1:A:192:ILE:HD12	1:A:192:ILE:C	2.04	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:155:LEU:CD2	1:A:220:MET:HE3	2.34	0.52
1:A:35:THR:C	1:A:36:LYS:HG2	2.29	0.52
1:B:294:LYS:CD	1:B:294:LYS:N	2.73	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:90:TYR:C	1:B:92:MET:N	2.55	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:B:326:LEU:CB	1:B:446:ILE:CB	2.86	0.52
1:A:241:HIS:HE1	1:A:242:GLU:HG3	1.71	0.52
1:A:410:PHE:O	1:A:411:LYS:C	2.47	0.52
1:A:538:ASN:OD1	1:A:538:ASN:O	2.28	0.52
1:B:61:SER:C	1:B:67:SER:OG	2.48	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:224:PHE:O	1:A:225:ALA:C	2.41	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: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:403:PHE:O	1:B:404:GLU:C	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:112:GLY:H	1:B:168:MET:C	2.07	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: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:82:LYS:C	1:A:83:ILE:CD1	2.77	0.51
1:A:141:ASP:O	1:A:144:SER:OG	2.28	0.51
1:B:295:ASN:C	1:B:298:GLU:CG	2.78	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:42:LEU:HG	1:A:42:LEU:O	2.10	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:B:97:VAL:CG1	1:B:102:GLU:CD	2.76	0.51
1:A:111:TYR:CG	1:A:112:GLY:N	2.69	0.51
1:A:132:ASN:C	1:A:133:PHE:CG	2.83	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:C	1:A:40:VAL:N	2.63	0.50
1:A:289:ASN:C	1:A:291:LEU:H	2.13	0.50
1:A:320:GLU:CB	1:A:323:LEU:HD21	2.40	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:A:520:TYR:HD1	1:A:520:TYR:C	2.15	0.50
1:B:94:GLU:CD	1:B:94:GLU:O	2.48	0.50
1:A:173:GLU:OE1	1:A:174:VAL:O	2.30	0.50
1:A:516:TYR:CE1	1:A:517:GLN:O	2.65	0.50
1:B:196:TYR:HE1	1:B:197:ASN:C	2.15	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:B:111:TYR:CD1	1:B:111:TYR:C	2.83	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:LEU:O	1:A:442:VAL:HB	2.12	0.50
1:A:457:VAL:O	1:A:458:ASP:C	2.46	0.50
1:A:543:ASP:OD1	1:A:543:ASP:C	2.49	0.50
1:B:88:ILE:O	1:B:89:CYS:O	2.29	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:173:GLU:CD	1:A:174:VAL:O	2.50	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:A:480:VAL:HG12	1:A:481:LEU:N	2.20	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:62:VAL:C	1:B:64:GLU:H	2.13	0.50
1:B:97:VAL:HG12	1:B:102:GLU:OE1	2.01	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: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:171:ASN:OD1	1:B:172:ASP:OD1	2.30	0.49
1:A:215:LEU:O	1:A:216:ASP:C	2.48	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:51:LYS:C	1:B:228:ILE:CG2	2.74	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: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:246:LYS:O	1:A:250:LYS:CE	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:ASN:O	1:A:299:ASN:OD1	2.29	0.49
1:B:98:GLN:C	1:B:98:GLN:HE21	2.13	0.49
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:430:ARG:O	1:A:432:PRO:HD3	2.11	0.49
1:B:435:GLY:O	1:B:436:PRO:C	2.45	0.49
1:A:303:PHE:O	1:A:307:THR:HG23	2.12	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: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:114:THR:HB	1:A:168:MET:CE	2.43	0.49
1:A:205:VAL:HG22	1:A:207:TYR:H	1.67	0.49
1:B:306:SER:OG	2:B:602:HOH:O	2.08	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:30:LYS:C	1:B:31:ILE:HG23	2.34	0.48
1:B:103:VAL:HG12	1:B:104:LYS:O	2.13	0.48
1:A:45:ILE:O	1:A:45:ILE:HG22	2.13	0.48
1:A:114:THR:CG2	1:A:168:MET:HE2	2.43	0.48
1:B:160:LYS:C	1:B:161:SER:O	2.46	0.48
1:B:373:ILE:O	1:B:374:GLU:C	2.45	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:153:CYS:C	1:B:155:LEU:N	2.61	0.48
1:B:470:LEU:C	1:B:473:GLN:H	2.16	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: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:177:ILE:O	1:A:178:PRO:C	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:VAL:O	1:A:164:THR:O	2.32	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:B:497:ASP:C	1:B:498:TYR:CD1	2.87	0.48
1:A:9:ILE:HD12	1:A:26:LEU:HD22	1.94	0.48
1:A:125:ASN:O	1:A:126:ASN:C	2.51	0.48
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:A:170:HIS:HB2	1:A:206:GLN:OE1	2.14	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:222:TYR:C	1:B:225:ALA:HB3	2.34	0.48
1:A:148:LEU:O	1:A:149:MET:CB	2.58	0.47
1:A:369:TYR:CD1	1:A:369:TYR:C	2.74	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: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:A:112:GLY:O	1:A:113:CYS:C	2.46	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:ARG:HE	1:A:123:ASN:ND2	2.12	0.47
1:A:172:ASP:OD1	1:A:172:ASP:C	2.49	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
1:B:13:ASN:O	1:B:14:PHE:HD1	1.98	0.47
1:B:107:LYS:O	1:B:108:THR:OG1	2.29	0.47
1:B:294:LYS:O	1:B:296:GLU:N	2.47	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:14:PHE:HA	1:A:38:TYR:HD2	1.79	0.47
1:A:123:ASN:HA	1:A:126:ASN:CG	2.35	0.47
1:B:97:VAL:C	1:B:99:MET:N	2.64	0.47
1:B:421:LEU:HD23	1:B:421:LEU:N	2.09	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:B:522:ILE:HG13	1:B:523:LEU:N	2.19	0.47
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:A:530:ILE:HG22	1:A:531:LEU:N	2.20	0.46
1:B:30:LYS:O	1:B:31:ILE:HG22	2.14	0.46
1:B:61:SER:O	1:B:67:SER:OG	2.31	0.46
1:A:515:TRP:CE3	1:A:544:VAL:HA	2.50	0.46
1:A:181:PHE:HE1	1:A:195:ILE:C	2.10	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: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: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:A:13:ASN:O	1:A:13:ASN:CG	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:215:LEU:C	1:A:217:GLY:H	2.17	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:210:GLU:C	1:A:211:VAL:HG23	2.28	0.46
1:A:367:THR:HG22	1:A:406:PHE:O	2.16	0.46
1:A:370:PRO:O	1:A:371:ASP:C	2.51	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:478:PHE:O	1:A:479:ALA:C	2.48	0.46
1:A:546:SER:O	1:A:549:PRO:HB2	2.16	0.46
1:B:241:HIS:O	1:B:242:GLU:C	2.52	0.46
1:B:324:SER:O	1:B:326:LEU:C	2.54	0.46
1:A:32:PHE:HE1	1:A:33:SER:O	1.96	0.46
1:A:449:HIS:ND1	1:A:449:HIS:C	2.68	0.46
1:A:531:LEU:CD2	1:B:549:PRO:HG2	2.46	0.46
1:B:128:THR:O	1:B:128:THR:OG1	2.30	0.46
1:A:214:SER:OG	1:A:217:GLY:HA3	2.16	0.45
1:A:399:LYS:C	1:A:400:PHE:CD1	2.86	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:300:VAL:C	1:A:304:LEU:HD12	2.35	0.45
1:A:498:TYR:O	1:A:537:VAL:HA	2.17	0.45
1:B:111:TYR:C	1:B:168:MET:O	2.53	0.45
1:B:195:ILE:HD13	1:B:195:ILE:N	2.31	0.45
1:B:527:THR:O	1:B:527:THR:HG23	2.17	0.45
1:A:531:LEU:CD1	1:A:540:ILE:HG22	2.43	0.45
1:B:212:TYR:CD1	1:B:213:GLU:N	2.64	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: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: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
1:B:372:ILE:HG12	1:B:373:ILE:N	2.31	0.45
1:B:30:LYS:C	1:B:31:ILE:CG2	2.84	0.45
1:B:98:GLN:HE21	1:B:99:MET:N	2.14	0.45
1:B:289:ASN:C	1:B:291:LEU:H	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:PHE:CD1	1:A:32:PHE:C	2.89	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:29:ILE:HG23	1:B:30:LYS:H	1.81	0.45
1:B:107:LYS:O	1:B:108:THR:C	2.54	0.45
1:B:552:ILE:O	1:B:552:ILE:CG2	2.62	0.45
1:A:107:LYS:HA	1:A:107:LYS:HD2	1.75	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: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:540:ILE:C	1:B:541:LEU:HG	2.37	0.45
1:A:342:LEU:N	1:A:342:LEU:CD1	2.66	0.45
1:A:459:ASP:O	1:A:460:ILE:C	2.50	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:114:THR:HG21	1:A:168:MET:HE1	1.97	0.44
1:A:117:ASN:OD1	1:A:117:ASN:C	2.52	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: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:181:PHE:CD1	1:A:195:ILE:CB	2.99	0.44
1:B:46:LYS:O	1:B:48:MET:N	2.49	0.44
1:B:85:ILE:CG2	1:B:86:PHE:N	2.79	0.44
1:B:265:ILE:O	1:B:266:ASP:C	2.53	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:320:GLU:O	1:A:321:ASN:C	2.54	0.44
1:A:499:VAL:CA	1:A:539:ARG:O	2.64	0.44
1:B:94:GLU:OE2	1:B:94:GLU:C	2.53	0.44
1:B:450:LYS:HA	1:B:453:ILE:HG22	1.99	0.44
1:A:114:THR:CB	1:A:168:MET:HE3	2.47	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:408:TYR:CD1	1:B:408:TYR:N	2.80	0.44
1:B:414:VAL:O	1:B:414:VAL:HG13	2.18	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:17:GLN:C	1:B:19:PHE:N	2.71	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:443:ILE:HG13	1:B:483:SER:N	2.32	0.44
1:B:498:TYR:C	1:B:499:VAL:CG2	2.86	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: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:159:ILE:O	1:A:159:ILE:HG22	2.17	0.43
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:528:THR:O	1:A:529:ARG:C	2.53	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:405:PRO:HD2	1:A:406:PHE:H	1.83	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:21:LEU:O	1:A:22:ILE:C	2.56	0.43
1:A:28:ASN:C	1:A:29:ILE:O	2.42	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: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
1:B:249:GLU:CB	1:B:278:PHE:HE2	2.31	0.43
1:B:412:ASP:CG	1:B:413:ASP:H	2.21	0.43
1:A:230:LYS:O	1:A:231:CYS:O	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:177:ILE:O	1:A:177:ILE:HG23	2.19	0.43
1:A:181:PHE:HD1	1:A:195:ILE:C	2.21	0.43
1:B:289:ASN:C	1:B:291:LEU:N	2.72	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:9:ILE:HG22	1:A:10:LEU:N	2.27	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:B:70:LEU:HD11	1:B:94:GLU:OE1	2.15	0.43
1:B:226:TYR:C	1:B:228:ILE:H	2.19	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:121:ASN:C	1:A:124:ILE:H	2.22	0.43
1:A:160:LYS:HB3	1:A:160:LYS:HE2	1.91	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: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:408:TYR:C	1:A:409:LEU:CD1	2.80	0.42
1:B:419:ARG:O	1:B:419:ARG:CG	2.67	0.42
1:A:528:THR:HG22	1:A:528:THR:H	1.48	0.42
1:A:550:ALA:C	1:A:552:ILE:N	2.72	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: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
1:B:86:PHE:CD1	1:B:86:PHE:C	2.93	0.42
1:A:9:ILE:CG2	1:A:10:LEU:N	2.75	0.42
1:B:211:VAL:HG11	1:B:213:GLU:CB	2.50	0.42
1:B:296:GLU:C	1:B:300:VAL:CG1	2.87	0.42
1:B:308:PHE:HA	1:B:309:PRO:HD2	1.91	0.42
1:B:498:TYR:C	1:B:499:VAL:HG23	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:ASN:CG	1:B:322:PHE:N	2.73	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:A:342:LEU:N	1:A:342:LEU:HD12	2.16	0.42
1:B:184:VAL:HG23	1:B:196:TYR:HB2	2.02	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:114:THR:HG21	1:A:168:MET:HE2	2.01	0.42
1:A:117:ASN:C	1:A:118:ILE:O	2.53	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:435:GLY:C	1:A:437:GLY:N	2.70	0.42
1:A:441:ARG:HG3	1:A:480:VAL:CG2	2.47	0.42
1:B:62:VAL:C	1:B:64:GLU:N	2.73	0.42
1:B:94:GLU:HG3	1:B:95:ILE:HG23	2.02	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: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:296:GLU:O	1:A:297:ALA:C	2.52	0.42
1:B:158:ASN:O	1:B:159:ILE:O	2.37	0.42
1:B:332:PRO:C	1:B:334:GLN:N	2.66	0.42
1:B:374:GLU:HG3	1:B:374:GLU:H	1.52	0.42
1:B:527:THR:O	1:B:527:THR:CG2	2.59	0.42
1:A:20:HIS:O	1:A:23:VAL:CG2	2.67	0.41
1:A:116:VAL:CG1	1:A:116:VAL:O	2.59	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
1:B:154:CYS:HB2	1:B:203:TYR:HH	1.73	0.41
1:A:238:ILE:C	1:A:240:TYR:N	2.68	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:A:89:CYS:O	1:A:90:TYR:C	2.55	0.41
1:A:148:LEU:O	1:A:149:MET:HB2	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:GLY:O	1:B:68:PRO:N	2.52	0.41
1:B:171:ASN:CG	1:B:172:ASP:N	2.73	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:120:ARG:CG	1:A:123:ASN:CG	2.86	0.41
1:A:339:ILE:O	1:A:339:ILE:HG22	2.15	0.41
1:A:372:ILE:O	1:A:375:SER:OG	2.30	0.41
1:A:480:VAL:HG11	1:A:554:PHE:HD2	1.85	0.41
1:A:258:ILE:HB	1:A:363:LEU:HA	2.01	0.41
1:A:271:ALA:C	1:A:274:THR:HG22	2.40	0.41
1:B:181:PHE:CE2	1:B:202:ILE:HD12	2.53	0.41
1:A:18:TYR:O	1:A:19:PHE:C	2.58	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:241:HIS:CG	1:B:242:GLU:N	2.85	0.41
1:A:135:ASP:O	1:A:136:SER:CB	2.69	0.41
1:A:447:ASN:O	1:A:451:LEU:HB3	2.20	0.41
1:A:522:ILE:HG22	1:A:523:LEU:N	2.25	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:A:431:HIS:C	1:A:432:PRO:O	2.53	0.41
1:A:435:GLY:C	1:A:437:GLY:H	2.23	0.41
1:B:35:THR:HG1	1:B:376:LYS:HG3	1.72	0.41
1:B:66:GLY:C	1:B:67:SER:O	2.47	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:114:THR:HB	1:A:168:MET:HE2	2.02	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:461:PHE:CD1	1:A:461:PHE:C	2.95	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
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:470:LEU:HA	1:B:473:GLN:CB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:551:THR:OG1	1:B:552:ILE:N	2.53	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: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:264:GLY:C	1:A:267:SER:OG	2.48	0.40
1:A:332:PRO:C	1:A:334:GLN:N	2.72	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:A:205:VAL:O	1:A:205:VAL:HG22	2.16	0.40
1:A:239:ARG:HD2	1:A:239:ARG:HA	1.45	0.40
1:B:296:GLU:C	1:B:300:VAL:HG12	2.32	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: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:B:287:ILE:O	1:B:288:ASP:CB	2.70	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 [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	512/568 (90%)	460 (90%)	39 (8%)	13 (2%)	5	36
1	B	466/568 (82%)	405 (87%)	44 (9%)	17 (4%)	3	29
All	All	978/1136 (86%)	865 (88%)	83 (8%)	30 (3%)	4	32

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
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%)	272 (70%)	115 (30%)	0	2
1	B	284/516 (55%)	196 (69%)	88 (31%)	0	2
All	All	671/1032 (65%)	468 (70%)	203 (30%)	0	2

All (203) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	19	PHE
1	A	22	ILE
1	A	23	VAL
1	A	27	ASN
1	A	32	PHE
1	A	35	THR
1	A	40	VAL
1	A	45	ILE
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	98	GLN
1	A	107	LYS
1	A	108	THR
1	A	114	THR
1	A	115	ASP
1	A	116	VAL
1	A	119	LEU
1	A	120	ARG
1	A	121	ASN
1	A	122	ASP
1	A	125	ASN
1	A	142	LEU

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Mol	Chain	Res	Type
1	A	144	SER
1	A	147	LYS
1	A	154	CYS
1	A	165	THR
1	A	167	TRP
1	A	171	ASN
1	A	177	ILE
1	A	178	PRO
1	A	180	ASN
1	A	182	TYR
1	A	186	SER
1	A	192	ILE
1	A	194	SER
1	A	195	ILE
1	A	196	TYR
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	228	ILE
1	A	230	LYS
1	A	235	PHE
1	A	239	ARG
1	A	241	HIS
1	A	245	LEU
1	A	248	ILE
1	A	256	TYR
1	A	273	TYR
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

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Mol	Chain	Res	Type
1	A	319	SER
1	A	323	LEU
1	A	333	GLU
1	A	355	ASP
1	A	359	ASN
1	A	367	THR
1	A	368	LEU
1	A	369	TYR
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	433	PHE
1	A	440	ILE
1	A	446	ILE
1	A	449	HIS
1	A	451	LEU
1	A	454	LEU
1	A	455	ARG
1	A	458	ASP
1	A	459	ASP
1	A	460	ILE
1	A	462	ILE
1	A	463	ASN
1	A	464	ASP
1	A	472	ASN
1	A	475	SER
1	A	483	SER
1	A	498	TYR
1	A	508	SER
1	A	510	PHE
1	A	512	THR
1	A	518	ILE
1	A	520	TYR
1	A	528	THR
1	A	539	ARG
1	A	540	ILE
1	A	543	ASP
1	A	544	VAL

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Mol	Chain	Res	Type
1	A	546	SER
1	A	549	PRO
1	A	551	THR
1	A	553	GLU
1	B	16	SER
1	B	32	PHE
1	B	40	VAL
1	B	41	GLU
1	B	48	MET
1	B	67	SER
1	B	68	PRO
1	B	69	HIS
1	B	70	LEU
1	B	82	LYS
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	104	LYS
1	B	108	THR
1	B	111	TYR
1	B	117	ASN
1	B	122	ASP
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	187	SER
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

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Mol	Chain	Res	Type
1	B	212	TYR
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	274	THR
1	B	275	HIS
1	B	291	LEU
1	B	295	ASN
1	B	310	ASP
1	B	312	ASN
1	B	313	ILE
1	B	314	THR
1	B	317	ASP
1	B	321	ASN
1	B	329	VAL
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	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	484	SER
1	B	498	TYR
1	B	502	LEU
1	B	512	THR
1	B	522	ILE
1	B	523	LEU

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Mol	Chain	Res	Type
1	B	525	LYS
1	B	527	THR
1	B	528	THR
1	B	530	ILE
1	B	540	ILE
1	B	546	SER
1	B	552	ILE
1	B	554	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) 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	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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	520/568 (91%)	0.07	34 (6%)	18 11	71, 106, 130, 151	0
1	B	480/568 (84%)	-0.12	30 (6%)	20 11	74, 127, 155, 177	0
All	All	1000/1136 (88%)	-0.02	64 (6%)	19 11	71, 116, 150, 177	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	248	ILE	10.1
1	A	361	THR	7.6
1	A	66	GLY	6.8
1	A	237	PRO	5.7
1	A	182	TYR	5.5
1	A	210	GLU	5.4
1	B	476	GLN	5.3
1	A	362	PHE	5.3
1	A	245	LEU	5.2
1	B	35	THR	4.7
1	A	67	SER	4.7
1	A	402	LEU	4.5
1	B	164	THR	4.4
1	A	231	CYS	4.3
1	A	153	CYS	4.2
1	A	152	THR	3.9
1	B	14	PHE	3.8
1	A	236	ASP	3.7
1	B	375	SER	3.7
1	B	60	TYR	3.6
1	A	357	ASP	3.6
1	B	114	THR	3.6
1	A	154	CYS	3.4
1	A	133	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	228	ILE	3.4
1	A	7	ASP	3.4
1	B	378	SER	3.4
1	B	9	ILE	3.4
1	A	444	GLY	3.3
1	A	403	PHE	3.3
1	B	482	LEU	3.2
1	A	249	GLU	3.1
1	B	63	THR	2.9
1	B	33	SER	2.9
1	B	65	ALA	2.9
1	B	352	ASN	2.8
1	B	414	VAL	2.7
1	A	164	THR	2.7
1	A	358	ILE	2.7
1	B	481	LEU	2.7
1	A	363	LEU	2.7
1	B	162	ASP	2.6
1	A	359	ASN	2.6
1	A	14	PHE	2.6
1	B	201	ASN	2.5
1	B	76	GLU	2.5
1	B	416	THR	2.5
1	A	247	ASN	2.5
1	B	483	SER	2.5
1	B	11	VAL	2.4
1	A	400	PHE	2.3
1	A	201	ASN	2.3
1	B	132	ASN	2.2
1	A	134	GLY	2.2
1	A	365	GLN	2.2
1	A	163	ILE	2.2
1	B	328	GLY	2.2
1	B	66	GLY	2.1
1	B	131	ARG	2.1
1	A	244	GLU	2.1
1	B	318	ALA	2.1
1	B	413	ASP	2.1
1	B	475	SER	2.0
1	B	10	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 monosaccharides 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.