



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 27, 2016 – 05:08 PM EDT

PDB ID : 5ELP  
Title : Ketosynthase from module 1 of the bacillaene synthase from *Bacillus amyloliquefaciens* FZB42  
Authors : Wagner, D.T.; Gay, D.C.; Keatinge-Clay, A.T.; Zogzas, C.E.  
Deposited on : 2015-11-04  
Resolution : 2.93 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

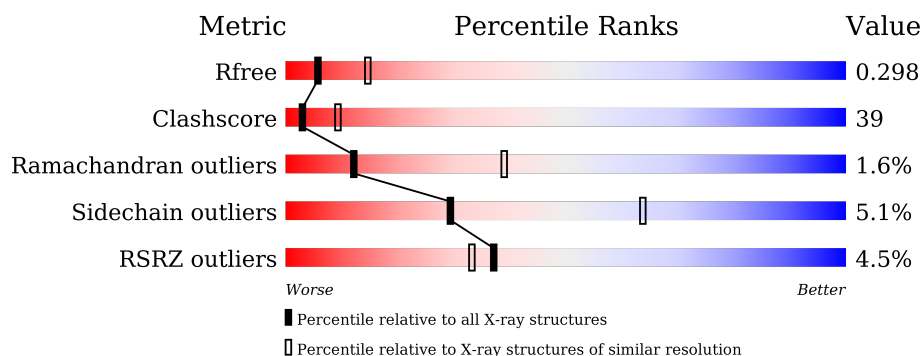
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.93 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))
$R_{free}$	91344	2057 (2.98-2.90)
Clashscore	102246	2308 (2.98-2.90)
Ramachandran outliers	100387	2245 (2.98-2.90)
Sidechain outliers	100360	2247 (2.98-2.90)
RSRZ outliers	91569	2065 (2.98-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	622	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 36%, green 47%, grey 16%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>47%</span> <span>36%</span> <span>• • 13%</span> </div> </div>
1	B	622	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 4%, orange 1%, yellow 41%, green 43%, grey 11%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>4%</span> <span>43%</span> <span>41%</span> <span>• 12%</span> </div> </div>
1	C	622	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 4%, orange 1%, yellow 35%, green 47%, grey 13%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>4%</span> <span>47%</span> <span>35%</span> <span>5% • 10%</span> </div> </div>
1	D	622	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 6%, orange 1%, yellow 38%, green 40%, grey 15%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>6%</span> <span>40%</span> <span>38%</span> <span>6% • 16%</span> </div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 16749 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 NRPS/PKS protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	557	Total	C	N	O	S	0	0	0
			4317	2757	722	821	17			
1	A	540	Total	C	N	O	S	0	0	0
			4169	2656	704	792	17			
1	B	547	Total	C	N	O	S	0	0	0
			4213	2691	699	806	17			
1	D	523	Total	C	N	O	S	0	0	0
			4050	2591	677	766	16			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-16	MET	-	initiating methionine	UNP Q1RS73
C	-15	GLY	-	expression tag	UNP Q1RS73
C	-14	SER	-	expression tag	UNP Q1RS73
C	-13	SER	-	expression tag	UNP Q1RS73
C	-12	HIS	-	expression tag	UNP Q1RS73
C	-11	HIS	-	expression tag	UNP Q1RS73
C	-10	HIS	-	expression tag	UNP Q1RS73
C	-9	HIS	-	expression tag	UNP Q1RS73
C	-8	HIS	-	expression tag	UNP Q1RS73
C	-7	HIS	-	expression tag	UNP Q1RS73
C	-6	SER	-	expression tag	UNP Q1RS73
C	-5	SER	-	expression tag	UNP Q1RS73
C	-4	GLY	-	expression tag	UNP Q1RS73
C	-3	LEU	-	expression tag	UNP Q1RS73
C	-2	VAL	-	expression tag	UNP Q1RS73
C	-1	PRO	-	expression tag	UNP Q1RS73
C	0	ARG	-	expression tag	UNP Q1RS73
C	1	GLY	-	expression tag	UNP Q1RS73
C	2	SER	-	expression tag	UNP Q1RS73
C	3	SER	-	expression tag	UNP Q1RS73
A	-16	MET	-	initiating methionine	UNP Q1RS73

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	GLY	-	expression tag	UNP Q1RS73
A	-14	SER	-	expression tag	UNP Q1RS73
A	-13	SER	-	expression tag	UNP Q1RS73
A	-12	HIS	-	expression tag	UNP Q1RS73
A	-11	HIS	-	expression tag	UNP Q1RS73
A	-10	HIS	-	expression tag	UNP Q1RS73
A	-9	HIS	-	expression tag	UNP Q1RS73
A	-8	HIS	-	expression tag	UNP Q1RS73
A	-7	HIS	-	expression tag	UNP Q1RS73
A	-6	SER	-	expression tag	UNP Q1RS73
A	-5	SER	-	expression tag	UNP Q1RS73
A	-4	GLY	-	expression tag	UNP Q1RS73
A	-3	LEU	-	expression tag	UNP Q1RS73
A	-2	VAL	-	expression tag	UNP Q1RS73
A	-1	PRO	-	expression tag	UNP Q1RS73
A	0	ARG	-	expression tag	UNP Q1RS73
A	1	GLY	-	expression tag	UNP Q1RS73
A	2	SER	-	expression tag	UNP Q1RS73
A	3	SER	-	expression tag	UNP Q1RS73
B	-16	MET	-	initiating methionine	UNP Q1RS73
B	-15	GLY	-	expression tag	UNP Q1RS73
B	-14	SER	-	expression tag	UNP Q1RS73
B	-13	SER	-	expression tag	UNP Q1RS73
B	-12	HIS	-	expression tag	UNP Q1RS73
B	-11	HIS	-	expression tag	UNP Q1RS73
B	-10	HIS	-	expression tag	UNP Q1RS73
B	-9	HIS	-	expression tag	UNP Q1RS73
B	-8	HIS	-	expression tag	UNP Q1RS73
B	-7	HIS	-	expression tag	UNP Q1RS73
B	-6	SER	-	expression tag	UNP Q1RS73
B	-5	SER	-	expression tag	UNP Q1RS73
B	-4	GLY	-	expression tag	UNP Q1RS73
B	-3	LEU	-	expression tag	UNP Q1RS73
B	-2	VAL	-	expression tag	UNP Q1RS73
B	-1	PRO	-	expression tag	UNP Q1RS73
B	0	ARG	-	expression tag	UNP Q1RS73
B	1	GLY	-	expression tag	UNP Q1RS73
B	2	SER	-	expression tag	UNP Q1RS73
B	3	SER	-	expression tag	UNP Q1RS73
D	-16	MET	-	initiating methionine	UNP Q1RS73
D	-15	GLY	-	expression tag	UNP Q1RS73
D	-14	SER	-	expression tag	UNP Q1RS73

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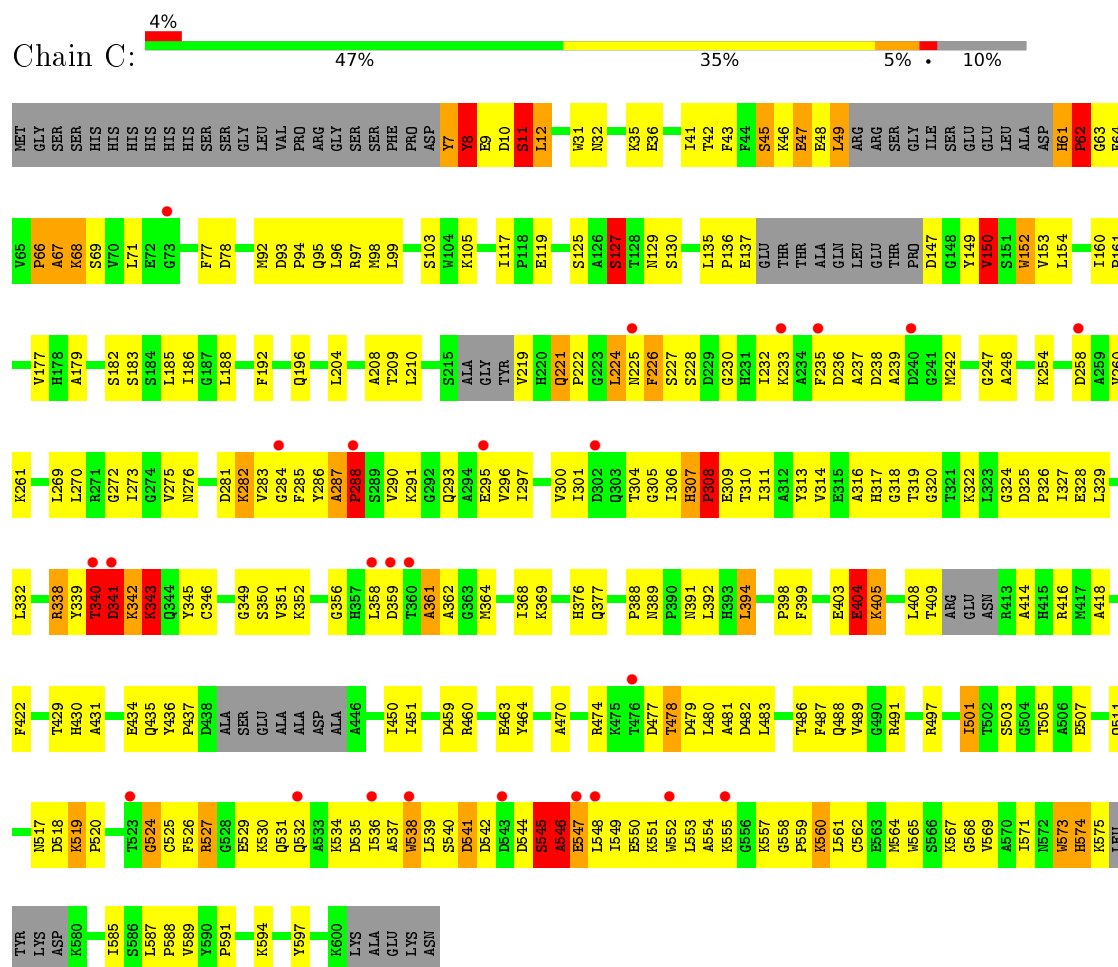
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-13	SER	-	expression tag	UNP Q1RS73
D	-12	HIS	-	expression tag	UNP Q1RS73
D	-11	HIS	-	expression tag	UNP Q1RS73
D	-10	HIS	-	expression tag	UNP Q1RS73
D	-9	HIS	-	expression tag	UNP Q1RS73
D	-8	HIS	-	expression tag	UNP Q1RS73
D	-7	HIS	-	expression tag	UNP Q1RS73
D	-6	SER	-	expression tag	UNP Q1RS73
D	-5	SER	-	expression tag	UNP Q1RS73
D	-4	GLY	-	expression tag	UNP Q1RS73
D	-3	LEU	-	expression tag	UNP Q1RS73
D	-2	VAL	-	expression tag	UNP Q1RS73
D	-1	PRO	-	expression tag	UNP Q1RS73
D	0	ARG	-	expression tag	UNP Q1RS73
D	1	GLY	-	expression tag	UNP Q1RS73
D	2	SER	-	expression tag	UNP Q1RS73
D	3	SER	-	expression tag	UNP Q1RS73

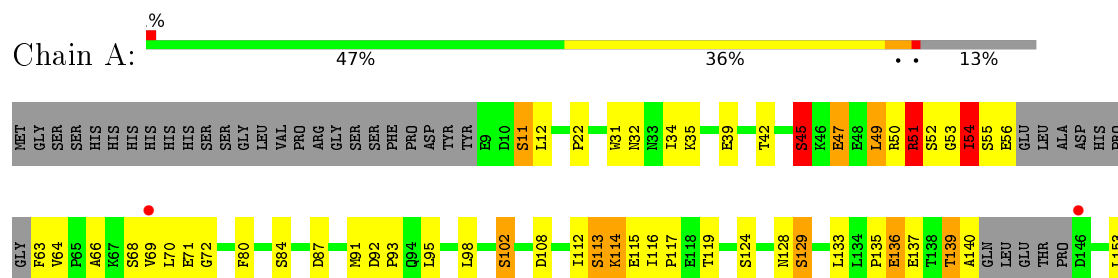
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

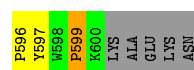
#### • Molecule 1: NRPS/PKS protein



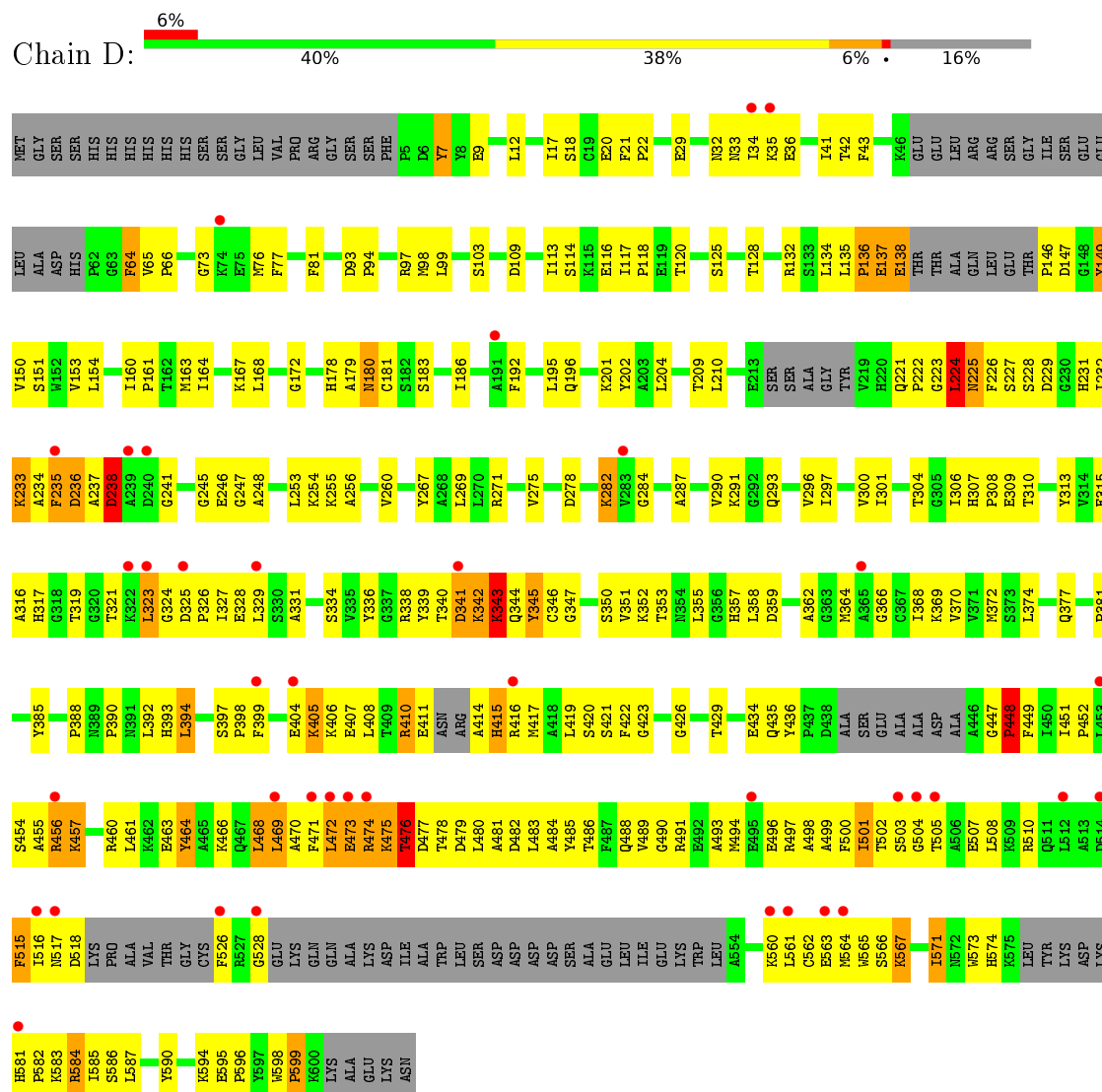
#### • Molecule 1: NRPS/PKS protein







- Molecule 1: NRPS/PKS protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.62Å 99.95Å 100.84Å 91.93° 88.18° 96.04°	Depositor
Resolution (Å)	99.35 – 2.93 53.01 – 2.93	Depositor EDS
% Data completeness (in resolution range)	94.9 (99.35-2.93) 68.8 (53.01-2.93)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.80 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, $R_{free}$	0.270 , 0.303 0.269 , 0.298	Depositor DCC
$R_{free}$ test set	2426 reflections (5.24%)	DCC
Wilson B-factor (Å <sup>2</sup> )	64.1	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 43.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	16749	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% 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	0.63	1/4264 (0.0%)	0.97	17/5749 (0.3%)
1	B	0.56	1/4311 (0.0%)	0.86	15/5813 (0.3%)
1	C	0.68	3/4421 (0.1%)	1.09	58/5968 (1.0%)
1	D	0.62	6/4148 (0.1%)	1.01	35/5595 (0.6%)
All	All	0.62	11/17144 (0.1%)	0.98	125/23125 (0.5%)

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	3
1	B	0	3
1	C	0	4
1	D	0	1
All	All	0	11

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	308	PRO	N-CD	13.48	1.66	1.47
1	A	309	THR	CB-OG1	12.87	1.69	1.43
1	C	288	PRO	N-CD	10.09	1.61	1.47
1	D	414	ALA	CA-C	6.99	1.71	1.52
1	D	414	ALA	N-CA	-6.51	1.33	1.46
1	C	66	PRO	N-CD	6.41	1.56	1.47
1	D	448	PRO	N-CD	6.09	1.56	1.47
1	D	136	PRO	N-CD	6.07	1.56	1.47
1	B	326	PRO	N-CD	5.58	1.55	1.47
1	D	415	HIS	N-CA	-5.23	1.35	1.46
1	D	415	HIS	CA-C	5.06	1.66	1.52

All (125) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	309	THR	CA-CB-OG1	24.69	160.85	109.00
1	A	565	SER	CB-CA-C	16.56	141.57	110.10
1	B	57	GLU	CB-CA-C	16.45	143.30	110.40
1	A	45	SER	C-N-CA	16.14	162.05	121.70
1	C	477	ASP	CB-CA-C	-15.74	78.93	110.40
1	D	475	LYS	N-CA-CB	-15.47	82.75	110.60
1	D	447	GLY	C-N-CD	-14.26	89.24	120.60
1	C	547	GLU	N-CA-CB	14.25	136.26	110.60
1	A	45	SER	N-CA-C	13.79	148.22	111.00
1	A	309	THR	OG1-CB-CG2	-13.65	78.61	110.00
1	C	569	VAL	N-CA-C	13.59	147.69	111.00
1	C	569	VAL	CB-CA-C	-13.20	86.32	111.40
1	A	563	MET	CB-CA-C	-12.70	85.00	110.40
1	D	405	LYS	N-CA-CB	-12.20	88.63	110.60
1	D	474	ARG	N-CA-C	-11.56	79.78	111.00
1	D	475	LYS	CB-CA-C	11.43	133.25	110.40
1	B	154	LEU	CB-CA-C	-11.40	88.54	110.20
1	C	150	VAL	N-CA-C	11.18	141.19	111.00
1	C	150	VAL	N-CA-CB	-10.88	87.55	111.50
1	C	477	ASP	N-CA-CB	-9.96	92.68	110.60
1	D	476	THR	N-CA-C	-9.90	84.27	111.00
1	C	340	THR	CB-CA-C	-9.74	85.30	111.60
1	B	57	GLU	N-CA-C	-9.58	85.14	111.00
1	C	547	GLU	N-CA-C	-9.39	85.66	111.00
1	C	307	HIS	C-N-CD	-9.33	100.08	120.60
1	D	138	GLU	N-CA-C	-9.29	85.91	111.00
1	D	235	PHE	CB-CA-C	-9.12	92.17	110.40
1	B	222	PRO	N-CA-C	-9.04	88.60	112.10
1	C	341	ASP	N-CA-C	-8.65	87.65	111.00
1	C	478	THR	N-CA-C	-8.58	87.83	111.00
1	D	323	LEU	CB-CA-C	-8.58	93.90	110.20
1	C	9	GLU	N-CA-C	-8.49	88.07	111.00
1	C	285	PHE	N-CA-CB	-8.36	95.56	110.60
1	B	54	ILE	N-CA-C	-8.28	88.65	111.00
1	D	137	GLU	N-CA-C	-8.06	89.25	111.00
1	D	574	HIS	N-CA-C	8.02	132.65	111.00
1	D	137	GLU	CB-CA-C	7.89	126.19	110.40
1	D	473	GLU	N-CA-C	-7.87	89.75	111.00
1	B	155	ALA	N-CA-C	-7.77	90.02	111.00
1	B	56	GLU	N-CA-C	7.73	131.88	111.00
1	A	213	SER	N-CA-C	-7.73	90.13	111.00
1	C	340	THR	N-CA-C	-7.71	90.17	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	414	ALA	N-CA-CB	7.67	120.84	110.10
1	C	307	HIS	CB-CA-C	7.65	125.71	110.40
1	C	68	LYS	N-CA-CB	-7.63	96.86	110.60
1	C	530	LYS	N-CA-C	-7.60	90.48	111.00
1	A	49	LEU	CA-CB-CG	-7.57	97.88	115.30
1	C	530	LYS	CB-CA-C	-7.54	95.31	110.40
1	D	472	LEU	CB-CA-C	-7.49	95.97	110.20
1	A	225	PHE	N-CA-C	-7.48	90.81	111.00
1	A	179	ASN	CB-CA-C	-7.46	95.47	110.40
1	B	599	PRO	CB-CA-C	-7.44	93.40	112.00
1	C	45	SER	CB-CA-C	7.30	123.97	110.10
1	D	404	GLU	N-CA-C	-7.29	91.33	111.00
1	A	564	TRP	CB-CA-C	-7.13	96.13	110.40
1	D	180	ASN	N-CA-C	7.11	130.19	111.00
1	D	468	LEU	CB-CA-C	-7.11	96.70	110.20
1	D	154	LEU	CA-CB-CG	7.10	131.63	115.30
1	C	208	ALA	CB-CA-C	-7.08	99.47	110.10
1	C	308	PRO	CA-N-CD	-7.08	101.59	111.50
1	C	8	TYR	N-CA-C	-7.06	91.94	111.00
1	B	399	PHE	CB-CA-C	-6.96	96.47	110.40
1	C	11	SER	CB-CA-C	-6.95	96.91	110.10
1	C	67	ALA	CB-CA-C	-6.93	99.70	110.10
1	C	546	ALA	N-CA-CB	6.87	119.72	110.10
1	D	469	LEU	N-CA-C	-6.86	92.49	111.00
1	C	524	GLY	N-CA-C	-6.81	96.07	113.10
1	A	45	SER	CB-CA-C	-6.78	97.21	110.10
1	B	325	ASP	CB-CA-C	-6.74	96.92	110.40
1	C	67	ALA	N-CA-CB	-6.72	100.69	110.10
1	C	574	HIS	N-CA-C	6.70	129.08	111.00
1	C	285	PHE	N-CA-C	6.69	129.07	111.00
1	B	548	LEU	CA-CB-CG	-6.52	100.30	115.30
1	C	288	PRO	CA-N-CD	-6.51	102.38	111.50
1	C	12	LEU	N-CA-CB	-6.51	97.39	110.40
1	D	414	ALA	N-CA-C	-6.49	93.47	111.00
1	D	226	PHE	CB-CA-C	-6.48	97.44	110.40
1	C	545	SER	N-CA-C	-6.47	93.54	111.00
1	A	412	ARG	CB-CA-C	-6.46	97.48	110.40
1	D	138	GLU	N-CA-CB	6.42	122.16	110.60
1	C	546	ALA	N-CA-C	6.14	127.59	111.00
1	C	288	PRO	N-CA-CB	6.07	110.59	103.30
1	D	468	LEU	N-CA-C	6.07	127.39	111.00
1	D	468	LEU	O-C-N	-6.04	113.04	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	282	LYS	N-CA-C	-6.03	94.73	111.00
1	D	180	ASN	CB-CA-C	-6.02	98.36	110.40
1	B	524	GLY	N-CA-C	-6.01	98.08	113.10
1	C	541	ASP	N-CA-C	-5.99	94.84	111.00
1	D	341	ASP	O-C-N	5.97	132.25	122.70
1	C	149	TYR	CB-CA-C	5.94	122.28	110.40
1	C	287	ALA	CB-CA-C	5.92	118.98	110.10
1	D	253	LEU	CB-CA-C	-5.91	98.97	110.20
1	D	415	HIS	N-CA-CB	5.88	121.18	110.60
1	B	153	VAL	CB-CA-C	-5.87	100.25	111.40
1	C	519	LYS	C-N-CD	5.85	140.69	128.40
1	C	11	SER	O-C-N	-5.83	113.38	122.70
1	C	531	GLN	CB-CA-C	-5.81	98.77	110.40
1	D	405	LYS	N-CA-C	5.73	126.47	111.00
1	C	61	HIS	C-N-CD	5.68	140.34	128.40
1	C	47	GLU	N-CA-CB	-5.62	100.48	110.60
1	D	476	THR	N-CA-CB	5.62	120.98	110.30
1	C	404	GLU	N-CA-C	5.60	126.11	111.00
1	C	477	ASP	N-CA-C	-5.55	96.01	111.00
1	D	515	PHE	N-CA-CB	5.53	120.55	110.60
1	C	12	LEU	N-CA-C	5.52	125.91	111.00
1	B	518	ASP	N-CA-C	5.49	125.81	111.00
1	A	51	ARG	CB-CA-C	5.38	121.16	110.40
1	C	394	LEU	CB-CA-C	-5.35	100.04	110.20
1	C	68	LYS	N-CA-C	5.28	125.26	111.00
1	A	54	ILE	N-CA-C	5.28	125.26	111.00
1	C	8	TYR	O-C-N	-5.24	114.31	122.70
1	D	341	ASP	CB-CG-OD2	5.24	123.01	118.30
1	C	127	SER	CB-CA-C	5.23	120.03	110.10
1	C	62	PRO	CA-N-CD	-5.18	104.24	111.50
1	C	147	ASP	CB-CG-OD2	5.18	122.96	118.30
1	C	477	ASP	CB-CG-OD2	5.16	122.94	118.30
1	C	149	TYR	N-CA-C	5.14	124.89	111.00
1	A	557	GLY	C-N-CD	5.12	139.16	128.40
1	D	414	ALA	O-C-N	5.12	130.89	122.70
1	A	556	LYS	N-CA-C	5.11	124.80	111.00
1	C	66	PRO	CA-N-CD	-5.11	104.35	111.50
1	B	457	LYS	N-CA-CB	5.10	119.78	110.60
1	C	538	TRP	N-CA-C	5.09	124.74	111.00
1	C	361	ALA	CB-CA-C	-5.06	102.52	110.10
1	D	236	ASP	N-CA-C	-5.05	97.36	111.00

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	45	SER	Peptide
1	A	51	ARG	Peptide
1	A	516	ASN	Peptide
1	B	154	LEU	Peptide
1	B	517	ASN	Peptide
1	B	599	PRO	Mainchain
1	C	11	SER	Mainchain
1	C	546	ALA	Peptide
1	C	568	GLY	Peptide
1	C	8	TYR	Mainchain
1	D	468	LEU	Mainchain

## 5.2 Too-close contacts [i](#)

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	4169	0	4098	248	1
1	B	4213	0	4124	331	6
1	C	4317	0	4213	330	4
1	D	4050	0	3958	391	3
All	All	16749	0	16393	1294	7

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 39.

All (1294) 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:309:THR:OG1	1:A:309:THR:CB	1.69	1.37
1:D:308:PRO:O	1:D:345:TYR:OH	1.54	1.23
1:D:345:TYR:N	1:D:398:PRO:O	1.78	1.15
1:D:340:THR:HA	1:D:341:ASP:HB2	1.18	1.14
1:D:342:LYS:HD3	1:D:342:LYS:H	1.13	1.13
1:D:340:THR:OG1	1:D:342:LYS:HB3	1.49	1.12
1:C:541:ASP:HB2	1:C:545:SER:CB	1.81	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:570:ILE:O	1:A:572:TRP:N	1.83	1.10
1:A:309:THR:OG1	1:A:309:THR:CG2	1.99	1.09
1:A:309:THR:HG21	1:A:415:ARG:HE	0.93	1.08
1:C:553:LEU:HG	1:C:574:HIS:HB2	1.28	1.08
1:C:288:PRO:HG2	1:C:327:ILE:HD12	1.35	1.06
1:A:309:THR:CG2	1:A:415:ARG:HE	1.71	1.03
1:C:541:ASP:CB	1:C:545:SER:HB3	1.90	1.01
1:A:570:ILE:HG22	1:A:572:TRP:HB2	1.37	1.00
1:C:541:ASP:HB2	1:C:545:SER:HB3	1.02	0.99
1:C:307:HIS:CE1	1:C:340:THR:OG1	2.18	0.96
1:A:309:THR:HG21	1:A:415:ARG:NE	1.79	0.96
1:B:482:ASP:OD1	1:B:582:PRO:HB2	1.66	0.96
1:D:340:THR:HB	1:D:342:LYS:N	1.80	0.95
1:D:308:PRO:HG2	1:D:339:TYR:CD2	2.01	0.95
1:A:309:THR:OG1	1:A:309:THR:HG21	1.65	0.94
1:D:598:TRP:CD1	1:D:599:PRO:HD2	2.01	0.94
1:C:541:ASP:CB	1:C:545:SER:CB	2.45	0.94
1:B:386:LYS:HG3	1:B:387:GLU:HG2	1.50	0.94
1:C:48:GLU:N	1:C:48:GLU:OE2	2.01	0.94
1:C:553:LEU:CG	1:C:574:HIS:HB2	1.97	0.94
1:D:340:THR:CA	1:D:341:ASP:HB2	1.98	0.93
1:D:342:LYS:CA	1:D:343:LYS:HE3	1.98	0.93
1:C:478:THR:HG22	1:C:479:ASP:H	1.32	0.93
1:C:474:ARG:NH2	1:A:339:THR:HA	1.84	0.93
1:D:34:ILE:HD13	1:D:369:LYS:HG3	1.49	0.92
1:D:381:PRO:HD3	1:D:405:LYS:HG2	1.47	0.92
1:D:502:THR:HG22	1:D:503:SER:H	1.33	0.91
1:B:416:ARG:HG2	1:B:434:GLU:OE1	1.70	0.91
1:C:12:LEU:HD12	1:C:270:LEU:HD23	1.52	0.91
1:D:561:LEU:HG	1:D:563:GLU:CB	2.00	0.91
1:D:342:LYS:HA	1:D:343:LYS:HE3	1.53	0.91
1:D:377:GLN:OE1	1:D:435:GLN:NE2	2.03	0.90
1:B:511:GLN:NE2	1:B:523:THR:HA	1.87	0.90
1:D:561:LEU:HG	1:D:563:GLU:HB2	1.51	0.90
1:B:310:THR:HG21	1:B:416:ARG:HE	1.35	0.90
1:D:344:GLN:H	1:D:398:PRO:HA	1.37	0.89
1:B:480:LEU:O	1:B:484:ALA:N	2.05	0.89
1:D:310:THR:HG21	1:D:416:ARG:HH11	1.36	0.89
1:C:307:HIS:HE1	1:C:340:THR:OG1	1.54	0.89
1:C:552:TRP:CD1	1:C:557:LYS:CE	2.56	0.88
1:C:529:GLU:O	1:C:567:LYS:HD3	1.72	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:245:GLY:C	1:D:358:LEU:HD23	1.93	0.88
1:A:315:ALA:HB1	1:A:327:GLU:OE2	1.73	0.88
1:B:486:THR:O	1:B:489:VAL:O	1.90	0.88
1:C:545:SER:OG	1:C:549:ILE:HG21	1.72	0.88
1:A:338:TYR:O	1:A:339:THR:OG1	1.91	0.88
1:B:192:PHE:CE2	1:B:196:GLN:NE2	2.41	0.88
1:B:551:LYS:HD3	1:B:552:TRP:CZ3	2.08	0.87
1:A:341:LYS:HD3	1:A:395:ASP:OD1	1.75	0.87
1:B:307:HIS:NE2	1:B:340:THR:HB	1.89	0.87
1:D:317:HIS:N	1:D:328:GLU:OE2	2.07	0.87
1:B:75:GLU:OE1	1:B:75:GLU:N	2.05	0.87
1:B:480:LEU:HA	1:B:483:LEU:HB3	1.55	0.86
1:A:496:ARG:HD2	1:A:565:SER:O	1.74	0.86
1:C:290:VAL:HG22	1:C:327:ILE:HG23	1.55	0.86
1:D:561:LEU:CD1	1:D:563:GLU:HB2	2.06	0.86
1:B:58:LEU:CD1	1:B:62:PRO:HB3	2.04	0.86
1:C:233:LYS:HD3	1:C:238:ASP:O	1.74	0.86
1:D:209:THR:C	1:D:210:LEU:HD23	1.96	0.86
1:D:340:THR:HB	1:D:341:ASP:C	1.95	0.86
1:D:232:ILE:HG23	1:D:353:THR:HA	1.57	0.85
1:D:473:GLU:C	1:D:474:ARG:O	1.90	0.85
1:D:499:ALA:C	1:D:500:PHE:HD1	1.79	0.85
1:B:277:ASN:OD1	1:B:427:THR:OG1	1.95	0.84
1:D:232:ILE:CG2	1:D:353:THR:HA	2.07	0.84
1:D:136:PRO:O	1:D:137:GLU:C	2.15	0.84
1:B:504:GLY:O	1:B:507:GLU:HB3	1.76	0.84
1:D:515:PHE:HE1	1:D:518:ASP:OD1	1.61	0.84
1:B:447:GLY:O	1:B:503:SER:OG	1.94	0.83
1:B:296:VAL:O	1:B:300:VAL:HG23	1.79	0.83
1:C:185:LEU:CD2	1:C:429:THR:OG1	2.25	0.83
1:B:495:GLU:OE1	1:B:495:GLU:N	2.11	0.83
1:A:508:LYS:O	1:A:512:ALA:N	2.10	0.83
1:D:278:ASP:OD1	1:D:426:GLY:O	1.96	0.83
1:C:11:SER:HB2	1:C:270:LEU:O	1.79	0.83
1:C:486:THR:O	1:C:489:VAL:O	1.94	0.83
1:D:357:HIS:CD2	1:D:359:ASP:OD1	2.32	0.82
1:C:546:ALA:O	1:C:550:GLU:HB2	1.79	0.82
1:C:552:TRP:CD1	1:C:557:LYS:HE2	2.14	0.82
1:A:289:VAL:HG22	1:A:326:ILE:HG23	1.59	0.82
1:B:112:TYR:CE1	1:B:584:ARG:NH1	2.47	0.82
1:D:293:GLN:O	1:D:296:VAL:HG12	1.79	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:394:LEU:O	1:B:397:SER:HB3	1.78	0.82
1:B:58:LEU:HD12	1:B:62:PRO:HB3	1.59	0.82
1:C:273:ILE:HG12	1:C:431:ALA:HB2	1.62	0.82
1:B:194:SER:CB	1:B:199:GLU:OE2	2.27	0.82
1:C:403:GLU:C	1:C:404:GLU:HG3	1.99	0.82
1:A:564:TRP:O	1:A:564:TRP:CD2	2.33	0.82
1:C:389:ASN:OD1	1:C:391:ASN:N	2.12	0.82
1:C:288:PRO:HG2	1:C:327:ILE:CD1	2.09	0.81
1:D:456:ARG:NH1	1:D:494:MET:SD	2.53	0.81
1:D:561:LEU:CG	1:D:563:GLU:HB2	2.09	0.81
1:B:584:ARG:O	1:B:585:ILE:HD13	1.80	0.81
1:B:93:ASP:OD1	1:B:94:PRO:HD2	1.80	0.81
1:B:511:GLN:HE22	1:B:523:THR:HA	1.45	0.81
1:C:288:PRO:O	1:C:327:ILE:HD13	1.81	0.81
1:D:309:GLU:HA	1:D:345:TYR:CZ	2.16	0.81
1:C:306:ILE:HG22	1:C:307:HIS:O	1.80	0.80
1:C:546:ALA:N	1:C:549:ILE:HG22	1.96	0.80
1:A:221:PRO:HG3	1:A:227:SER:HA	1.62	0.80
1:A:388:ASN:HB3	1:A:391:LEU:HG	1.61	0.80
1:D:342:LYS:HE2	1:D:342:LYS:O	1.80	0.80
1:A:308:GLU:OE2	1:A:339:THR:HG21	1.80	0.80
1:D:246:GLU:N	1:D:358:LEU:CD2	2.45	0.80
1:D:357:HIS:HD2	1:D:359:ASP:OD1	1.64	0.80
1:A:316:HIS:O	1:A:351:LYS:HE2	1.81	0.80
1:A:98:LEU:O	1:A:102:SER:OG	1.98	0.80
1:C:332:LEU:HG	1:C:399:PHE:HZ	1.47	0.80
1:C:185:LEU:HD22	1:C:429:THR:OG1	1.82	0.80
1:B:564:MET:O	1:B:568:GLY:HA3	1.82	0.80
1:C:553:LEU:HG	1:C:574:HIS:CB	2.10	0.79
1:D:515:PHE:HE1	1:D:518:ASP:CG	1.85	0.79
1:A:506:GLU:O	1:A:510:GLN:HG3	1.82	0.79
1:B:497:ARG:O	1:B:528:GLY:HA3	1.83	0.79
1:B:76:MET:SD	1:B:596:PRO:HB3	2.23	0.79
1:C:392:LEU:HB2	1:C:394:LEU:HG	1.63	0.79
1:D:32:ASN:HA	1:D:35:LYS:HG2	1.64	0.79
1:B:389:ASN:HB3	1:B:392:LEU:HG	1.64	0.79
1:C:222:PRO:HG3	1:C:228:SER:HA	1.64	0.79
1:B:96:LEU:HD13	1:B:160:ILE:HA	1.64	0.79
1:B:271:ARG:NH1	1:B:271:ARG:HB3	1.99	0.78
1:B:282:LYS:HG2	1:B:287:ALA:HB1	1.64	0.78
1:C:332:LEU:HG	1:C:399:PHE:CZ	2.17	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:523:THR:OG1	1:B:525:CYS:HB2	1.84	0.78
1:C:552:TRP:CD1	1:C:557:LYS:HE3	2.18	0.78
1:C:10:ASP:O	1:C:196:GLN:OE1	2.01	0.78
1:D:209:THR:O	1:D:210:LEU:HD23	1.83	0.78
1:B:42:THR:HG22	1:B:68:LYS:O	1.82	0.78
1:B:462:LYS:NZ	1:B:518:ASP:OD1	2.15	0.78
1:D:344:GLN:HA	1:D:398:PRO:C	2.03	0.78
1:A:136:GLU:C	1:A:137:GLU:HG3	2.03	0.78
1:D:304:THR:HB	1:D:306:ILE:HG13	1.65	0.78
1:B:595:GLU:OE1	1:B:597:TYR:OH	2.00	0.78
1:D:321:THR:HG22	1:D:323:LEU:H	1.48	0.78
1:A:457:LYS:O	1:A:461:LYS:HG3	1.83	0.77
1:D:300:VAL:O	1:D:304:THR:HG23	1.84	0.77
1:D:227:SER:HB2	1:D:241:GLY:O	1.84	0.77
1:D:598:TRP:CG	1:D:599:PRO:HD2	2.18	0.77
1:B:43:PHE:CD1	1:B:67:ALA:HB2	2.19	0.77
1:C:307:HIS:ND1	1:C:309:GLU:HG2	1.99	0.77
1:B:111:GLY:O	1:B:584:ARG:NH2	2.17	0.77
1:D:479:ASP:OD1	1:D:481:ALA:N	2.16	0.77
1:C:281:ASP:C	1:C:282:LYS:O	2.11	0.77
1:B:194:SER:HB2	1:B:199:GLU:OE2	1.85	0.77
1:C:338:ARG:HG3	1:C:338:ARG:HH11	1.49	0.77
1:A:136:GLU:O	1:A:137:GLU:HG3	1.85	0.76
1:B:482:ASP:OD1	1:B:582:PRO:CB	2.33	0.76
1:B:484:ALA:O	1:B:488:GLN:HG3	1.85	0.76
1:C:270:LEU:HD21	1:C:273:ILE:HD12	1.67	0.76
1:C:233:LYS:HB2	1:C:239:ALA:HA	1.66	0.76
1:C:549:ILE:O	1:C:552:TRP:HB2	1.85	0.76
1:D:201:LYS:HG2	1:D:202:TYR:CE1	2.20	0.76
1:D:342:LYS:N	1:D:342:LYS:HD3	1.94	0.76
1:D:310:THR:HG21	1:D:416:ARG:NH1	1.99	0.76
1:B:513:ALA:O	1:B:517:ASN:HB2	1.85	0.76
1:B:547:GLU:O	1:B:548:LEU:CD2	2.34	0.76
1:B:231:HIS:O	1:B:233:LYS:HD2	1.86	0.76
1:C:105:LYS:HG2	1:C:589:VAL:HG21	1.66	0.76
1:C:535:ASP:O	1:C:539:LEU:HB2	1.86	0.76
1:D:394:LEU:O	1:D:397:SER:OG	2.03	0.75
1:B:523:THR:OG1	1:B:525:CYS:CB	2.34	0.75
1:D:499:ALA:O	1:D:500:PHE:HD1	1.70	0.75
1:D:502:THR:HG22	1:D:503:SER:N	2.01	0.75
1:C:41:ILE:CD1	1:C:69:SER:HB2	2.16	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:488:GLN:OE1	1:C:575:LYS:NZ	2.16	0.75
1:D:466:LYS:O	1:D:470:ALA:HB3	1.86	0.75
1:D:366:GLY:O	1:D:370:VAL:HG23	1.87	0.75
1:D:474:ARG:NH1	1:D:587:LEU:HD23	2.01	0.75
1:C:341:ASP:OD2	1:C:398:PRO:HG3	1.87	0.75
1:B:282:LYS:HG2	1:B:287:ALA:CB	2.17	0.74
1:C:553:LEU:CD1	1:C:574:HIS:HB2	2.15	0.74
1:D:310:THR:CG2	1:D:416:ARG:HD2	2.16	0.74
1:D:499:ALA:C	1:D:500:PHE:CD1	2.59	0.74
1:D:340:THR:HA	1:D:341:ASP:CB	2.07	0.74
1:A:306:HIS:O	1:A:309:THR:HB	1.87	0.74
1:B:245:GLY:C	1:B:358:LEU:HD23	2.08	0.74
1:C:288:PRO:CG	1:C:327:ILE:HD12	2.15	0.74
1:C:541:ASP:HB3	1:C:545:SER:HB2	1.69	0.74
1:B:456:ARG:HA	1:B:495:GLU:OE2	1.88	0.74
1:B:547:GLU:O	1:B:548:LEU:HG	1.88	0.74
1:C:179:ALA:O	1:C:183:SER:OG	2.05	0.74
1:C:332:LEU:CD2	1:C:399:PHE:CZ	2.71	0.74
1:A:586:LEU:HB3	1:A:587:PRO:HD2	1.69	0.74
1:B:394:LEU:HA	1:B:397:SER:HB3	1.68	0.74
1:A:482:LEU:HD23	1:A:486:PHE:HD2	1.52	0.74
1:D:308:PRO:C	1:D:345:TYR:OH	2.26	0.73
1:B:352:LYS:NZ	1:B:357:HIS:ND1	2.32	0.73
1:C:152:TRP:O	1:C:153:VAL:HG22	1.87	0.73
1:C:49:LEU:N	1:C:49:LEU:HD23	2.03	0.73
1:C:552:TRP:HD1	1:C:557:LYS:HE2	1.52	0.73
1:D:471:PHE:O	1:D:473:GLU:N	2.21	0.73
1:B:497:ARG:O	1:B:528:GLY:CA	2.37	0.73
1:D:501:ILE:HG21	1:D:560:LYS:HD3	1.69	0.73
1:B:547:GLU:O	1:B:548:LEU:HD23	1.89	0.73
1:C:541:ASP:O	1:C:541:ASP:OD1	2.06	0.73
1:D:342:LYS:C	1:D:343:LYS:HE3	2.07	0.73
1:C:254:LYS:HE2	1:C:258:ASP:O	1.89	0.73
1:C:11:SER:CB	1:C:270:LEU:O	2.36	0.73
1:C:343:LYS:O	1:C:345:TYR:HD1	1.72	0.73
1:D:346:CYS:HB3	1:D:399:PHE:CD1	2.23	0.73
1:A:481:ASP:HB3	1:A:584:ILE:CG1	2.19	0.73
1:A:390:ASN:O	1:A:392:HIS:CE1	2.42	0.73
1:D:469:LEU:HD23	1:D:472:LEU:HB2	1.70	0.73
1:A:482:LEU:HD23	1:A:482:LEU:O	1.89	0.72
1:C:478:THR:HG22	1:C:479:ASP:N	2.03	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:541:ASP:CB	1:C:545:SER:HB2	2.17	0.72
1:B:308:PRO:HB3	1:B:336:TYR:CD2	2.24	0.72
1:C:233:LYS:O	1:C:320:GLY:HA2	1.88	0.72
1:B:414:ALA:HB3	1:B:435:GLN:HB3	1.70	0.72
1:C:224:LEU:HD23	1:C:224:LEU:O	1.89	0.72
1:D:151:SER:CA	1:D:153:VAL:HG13	2.20	0.72
1:A:11:SER:HB2	1:A:269:LEU:O	1.89	0.72
1:A:281:LYS:HD2	1:A:286:ALA:O	1.89	0.72
1:D:201:LYS:HE3	1:D:254:LYS:HE3	1.72	0.72
1:A:582:LYS:HE3	1:A:584:ILE:HD11	1.70	0.72
1:D:224:LEU:HD12	1:D:224:LEU:N	2.04	0.72
1:D:317:HIS:O	1:D:352:LYS:CE	2.37	0.72
1:A:80:PHE:CD1	1:A:455:ARG:HG3	2.24	0.71
1:B:394:LEU:HA	1:B:397:SER:CB	2.19	0.71
1:C:273:ILE:HG12	1:C:431:ALA:CB	2.19	0.71
1:D:235:PHE:O	1:D:385:TYR:HE1	1.73	0.71
1:D:515:PHE:CE1	1:D:518:ASP:CB	2.72	0.71
1:B:310:THR:HG21	1:B:416:ARG:NE	2.06	0.71
1:C:559:PRO:O	1:C:562:CYS:N	2.24	0.71
1:D:394:LEU:HA	1:D:397:SER:OG	1.90	0.71
1:B:125:SER:HB3	1:B:177:VAL:O	1.90	0.71
1:B:181:CYS:HB2	1:B:423:GLY:HA2	1.72	0.71
1:B:511:GLN:O	1:B:514:ASP:HB2	1.91	0.71
1:D:34:ILE:CD1	1:D:369:LYS:HG3	2.21	0.71
1:B:511:GLN:HA	1:B:514:ASP:HB2	1.71	0.71
1:D:515:PHE:CE1	1:D:518:ASP:CG	2.64	0.71
1:B:551:LYS:HD3	1:B:552:TRP:HZ3	1.51	0.70
1:D:224:LEU:O	1:D:225:ASN:HB2	1.90	0.70
1:C:340:THR:O	1:C:340:THR:OG1	1.96	0.70
1:C:511:GLN:NE2	1:C:524:GLY:HA3	2.06	0.70
1:D:293:GLN:HG2	1:D:422:PHE:CE2	2.27	0.70
1:C:474:ARG:HH21	1:A:339:THR:HA	1.54	0.70
1:C:553:LEU:C	1:C:555:LYS:H	1.94	0.70
1:D:507:GLU:O	1:D:510:ARG:HB2	1.91	0.70
1:A:390:ASN:O	1:A:392:HIS:ND1	2.25	0.70
1:C:537:ALA:HA	1:C:540:SER:OG	1.92	0.70
1:D:271:ARG:HB3	1:D:271:ARG:HH11	1.56	0.70
1:C:487:PHE:HD1	1:C:491:ARG:HG3	1.57	0.70
1:A:292:GLN:HG2	1:A:421:PHE:CZ	2.27	0.70
1:D:474:ARG:HH12	1:D:587:LEU:HD23	1.56	0.70
1:D:76:MET:SD	1:D:594:LYS:HB3	2.32	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:ILE:C	1:A:450:ILE:HD13	2.11	0.70
1:A:484:TYR:O	1:A:488:VAL:HG22	1.91	0.70
1:D:466:LYS:O	1:D:470:ALA:CB	2.39	0.70
1:B:528:GLY:O	1:B:566:SER:O	2.10	0.70
1:A:51:ARG:HG2	1:A:52:SER:H	1.55	0.69
1:C:405:LYS:O	1:C:405:LYS:HG2	1.92	0.69
1:D:344:GLN:N	1:D:398:PRO:HA	2.07	0.69
1:B:547:GLU:C	1:B:548:LEU:HG	2.13	0.69
1:B:379:ILE:HB	1:B:406:LYS:HB2	1.73	0.69
1:B:511:GLN:NE2	1:B:523:THR:HG22	2.06	0.69
1:D:421:SER:HB3	1:D:429:THR:OG1	1.91	0.69
1:D:410:ARG:O	1:D:411:GLU:HG3	1.91	0.69
1:C:209:THR:OG1	1:C:359:ASP:HB2	1.92	0.69
1:C:474:ARG:NH2	1:A:339:THR:CA	2.55	0.69
1:D:358:LEU:O	1:D:362:ALA:N	2.26	0.69
1:A:564:TRP:CG	1:A:564:TRP:O	2.43	0.69
1:A:583:ARG:O	1:A:584:ILE:HD13	1.93	0.69
1:D:342:LYS:CD	1:D:342:LYS:H	1.98	0.69
1:C:317:HIS:O	1:C:352:LYS:HE2	1.92	0.69
1:D:227:SER:HB2	1:D:241:GLY:C	2.13	0.69
1:D:340:THR:CB	1:D:342:LYS:HB3	2.23	0.69
1:D:394:LEU:HA	1:D:397:SER:CB	2.23	0.69
1:B:104:TRP:NE1	1:B:108:GLU:OE2	2.25	0.68
1:B:502:THR:HG21	1:B:508:LEU:HA	1.74	0.68
1:D:271:ARG:NH1	1:D:271:ARG:HB3	2.08	0.68
1:B:293:GLN:O	1:B:297:ILE:HG13	1.93	0.68
1:B:480:LEU:HA	1:B:483:LEU:CB	2.22	0.68
1:D:343:LYS:N	1:D:343:LYS:HD2	2.08	0.68
1:C:236:ASP:OD1	1:C:237:ALA:N	2.27	0.68
1:B:317:HIS:N	1:B:328:GLU:OE2	2.22	0.68
1:B:495:GLU:H	1:B:495:GLU:CD	1.95	0.68
1:C:338:ARG:CG	1:C:338:ARG:HH11	2.07	0.68
1:D:341:ASP:N	1:D:342:LYS:HD3	2.07	0.68
1:D:480:LEU:HD11	1:D:505:THR:HB	1.74	0.68
1:C:316:ALA:HB1	1:C:328:GLU:OE2	1.94	0.68
1:D:35:LYS:HG3	1:D:36:GLU:N	2.08	0.68
1:D:501:ILE:CG2	1:D:560:LYS:HD3	2.23	0.68
1:D:293:GLN:HG2	1:D:422:PHE:CZ	2.29	0.68
1:D:132:ARG:NH1	1:D:153:VAL:HG22	2.09	0.68
1:B:228:SER:HB3	1:B:240:ASP:OD2	1.95	0.67
1:C:518:ASP:C	1:C:520:PRO:HD3	2.14	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:529:GLU:O	1:C:567:LYS:CD	2.41	0.67
1:D:309:GLU:HA	1:D:345:TYR:OH	1.93	0.67
1:C:127:SER:HG	1:C:209:THR:CB	2.07	0.67
1:A:11:SER:CB	1:A:269:LEU:O	2.43	0.67
1:C:270:LEU:HD11	1:C:273:ILE:HG13	1.77	0.67
1:C:416:ARG:NH1	1:C:434:GLU:OE1	2.28	0.67
1:C:185:LEU:HD23	1:C:429:THR:OG1	1.94	0.67
1:A:34:ILE:HD12	1:A:368:LYS:HG3	1.77	0.67
1:C:338:ARG:HG3	1:C:338:ARG:NH1	2.07	0.67
1:A:457:LYS:CG	1:A:495:GLU:OE1	2.43	0.67
1:C:358:LEU:HD23	1:C:361:ALA:CB	2.25	0.67
1:C:532:GLN:HB3	1:C:535:ASP:HB3	1.75	0.67
1:D:331:ALA:O	1:D:334:SER:OG	2.13	0.67
1:D:340:THR:C	1:D:342:LYS:HD3	2.14	0.67
1:D:394:LEU:CA	1:D:397:SER:OG	2.42	0.67
1:A:485:THR:O	1:A:488:VAL:O	2.11	0.67
1:C:497:ARG:NH2	1:C:565:TRP:O	2.26	0.67
1:D:475:LYS:HB3	1:D:477:ASP:HB2	1.77	0.67
1:A:12:LEU:HD11	1:A:191:PHE:HA	1.75	0.66
1:A:277:ASP:N	1:A:425:GLY:O	2.18	0.66
1:C:270:LEU:HD21	1:C:273:ILE:CD1	2.26	0.66
1:C:358:LEU:HB3	1:C:362:ALA:N	2.10	0.66
1:A:95:LEU:HD13	1:A:159:ILE:HA	1.77	0.66
1:B:120:THR:O	1:B:172:GLY:HA3	1.96	0.66
1:D:482:ASP:OD1	1:D:483:LEU:N	2.29	0.66
1:B:160:ILE:O	1:B:164:ILE:HG13	1.95	0.66
1:C:41:ILE:HD13	1:C:69:SER:HB2	1.77	0.66
1:A:481:ASP:HB3	1:A:584:ILE:HG13	1.78	0.66
1:D:132:ARG:HH11	1:D:153:VAL:HG23	1.61	0.66
1:C:224:LEU:O	1:C:225:ASN:HB2	1.96	0.66
1:B:64:PHE:HE1	1:B:226:PHE:HB3	1.61	0.66
1:D:344:GLN:HA	1:D:398:PRO:O	1.96	0.66
1:D:344:GLN:CA	1:D:398:PRO:O	2.44	0.66
1:D:460:ARG:NH1	1:D:463:GLU:OE1	2.28	0.66
1:B:394:LEU:C	1:B:397:SER:HB3	2.16	0.65
1:B:571:ILE:HG13	1:B:571:ILE:O	1.96	0.65
1:D:132:ARG:NH1	1:D:153:VAL:CG2	2.59	0.65
1:B:58:LEU:HD11	1:B:62:PRO:HB3	1.79	0.65
1:A:235:ASP:OD1	1:A:236:ALA:N	2.29	0.65
1:B:112:TYR:CZ	1:B:584:ARG:NH1	2.63	0.65
1:B:310:THR:CG2	1:B:416:ARG:HE	2.09	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:497:ARG:HB3	1:D:565:TRP:CZ3	2.31	0.65
1:B:394:LEU:CA	1:B:397:SER:HB3	2.26	0.65
1:D:344:GLN:C	1:D:398:PRO:O	2.34	0.65
1:B:301:ILE:O	1:B:305:GLY:N	2.28	0.65
1:B:451:ILE:HD13	1:B:451:ILE:N	2.11	0.65
1:C:519:LYS:N	1:C:520:PRO:HD3	2.11	0.65
1:C:527:ARG:CG	1:C:527:ARG:HH11	2.10	0.65
1:C:553:LEU:O	1:C:555:LYS:N	2.29	0.65
1:D:103:SER:HB3	1:D:204:LEU:HD21	1.79	0.65
1:B:472:LEU:O	1:B:475:LYS:O	2.15	0.65
1:D:151:SER:HA	1:D:153:VAL:HG13	1.78	0.65
1:A:571:ASN:ND2	1:A:571:ASN:H	1.94	0.65
1:D:113:ILE:HD12	1:D:116:GLU:CD	2.17	0.65
1:D:485:TYR:OH	1:D:573:TRP:HZ3	1.80	0.65
1:A:519:PRO:HB2	1:A:521:VAL:HG23	1.78	0.64
1:B:290:VAL:HG22	1:B:327:ILE:HG23	1.77	0.64
1:B:526:PHE:CE2	1:B:562:CYS:HB2	2.32	0.64
1:C:296:VAL:O	1:C:300:VAL:HG23	1.96	0.64
1:D:515:PHE:CD1	1:D:518:ASP:HA	2.33	0.64
1:A:482:LEU:HD21	1:A:486:PHE:CE2	2.32	0.64
1:B:93:ASP:OD1	1:B:94:PRO:CD	2.44	0.64
1:C:291:LYS:O	1:C:295:GLU:HG3	1.98	0.64
1:C:342:LYS:O	1:C:343:LYS:HB3	1.95	0.64
1:C:358:LEU:CB	1:C:362:ALA:N	2.61	0.64
1:D:151:SER:C	1:D:153:VAL:HG13	2.18	0.64
1:D:98:MET:HE2	1:D:248:ALA:HB3	1.80	0.64
1:B:202:TYR:CE2	1:B:254:LYS:HE3	2.33	0.64
1:A:490:ARG:HG2	1:A:490:ARG:HH11	1.63	0.64
1:B:519:LYS:N	1:B:520:PRO:CD	2.60	0.64
1:B:526:PHE:CD2	1:B:562:CYS:HB2	2.33	0.64
1:D:310:THR:HG21	1:D:416:ARG:HD2	1.80	0.64
1:D:76:MET:HA	1:D:595:GLU:O	1.98	0.64
1:A:203:LEU:HD13	1:A:251:LEU:HD13	1.79	0.64
1:B:98:MET:HG3	1:B:210:LEU:HD11	1.78	0.64
1:C:392:LEU:HD13	1:C:394:LEU:HD21	1.80	0.64
1:D:321:THR:HG22	1:D:323:LEU:N	2.11	0.64
1:C:553:LEU:CD1	1:C:574:HIS:CB	2.76	0.63
1:D:486:THR:O	1:D:486:THR:HG22	1.97	0.63
1:A:12:LEU:HD22	1:A:194:LEU:CD1	2.27	0.63
1:B:112:TYR:OH	1:B:264:ASP:OD1	2.10	0.63
1:C:182:SER:O	1:C:186:ILE:HG12	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:536:ILE:O	1:C:540:SER:N	2.30	0.63
1:D:310:THR:HG22	1:D:416:ARG:HD2	1.80	0.63
1:A:45:SER:HB3	1:A:47:GLU:HG2	1.80	0.63
1:B:209:THR:O	1:B:210:LEU:HD23	1.98	0.63
1:B:282:LYS:CG	1:B:287:ALA:CB	2.75	0.63
1:C:233:LYS:HD2	1:C:239:ALA:HA	1.80	0.63
1:C:358:LEU:HD23	1:C:361:ALA:C	2.18	0.63
1:D:340:THR:HG1	1:D:342:LYS:HB3	1.62	0.63
1:C:558:GLY:O	1:C:561:LEU:HB3	1.98	0.63
1:C:98:MET:HE2	1:C:248:ALA:HB3	1.81	0.63
1:D:132:ARG:HH11	1:D:153:VAL:CG2	2.10	0.63
1:A:124:SER:HB3	1:A:176:VAL:O	1.99	0.63
1:C:318:GLY:HA3	1:C:350:SER:OG	1.98	0.63
1:B:517:ASN:O	1:B:520:PRO:HD3	1.99	0.63
1:B:129:ASN:HB2	1:B:212:THR:HG23	1.80	0.63
1:B:282:LYS:CG	1:B:287:ALA:HB1	2.29	0.63
1:B:396:ASP:O	1:B:398:PRO:HD3	1.99	0.63
1:C:587:LEU:HB3	1:C:588:PRO:HD2	1.81	0.63
1:D:293:GLN:O	1:D:296:VAL:CG1	2.47	0.63
1:D:293:GLN:O	1:D:297:ILE:HG13	1.99	0.63
1:C:358:LEU:HD23	1:C:361:ALA:O	1.99	0.62
1:D:308:PRO:HG2	1:D:339:TYR:HD2	1.63	0.62
1:D:476:THR:O	1:D:476:THR:HG22	1.99	0.62
1:A:564:TRP:O	1:A:564:TRP:CE3	2.52	0.62
1:C:358:LEU:HB2	1:C:362:ALA:HA	1.80	0.62
1:D:479:ASP:O	1:D:482:ASP:OD1	2.17	0.62
1:D:598:TRP:CG	1:D:599:PRO:CD	2.82	0.62
1:A:506:GLU:HG2	1:A:510:GLN:OE1	1.99	0.62
1:B:108:GLU:O	1:B:491:ARG:NH1	2.22	0.62
1:C:103:SER:HB3	1:C:204:LEU:HD21	1.82	0.62
1:C:358:LEU:HB2	1:C:362:ALA:CA	2.29	0.62
1:C:464:TYR:HD1	1:C:591:PRO:HD3	1.63	0.62
1:C:293:GLN:O	1:C:297:ILE:HG13	2.00	0.62
1:A:278:GLY:C	1:A:280:ASP:H	2.03	0.62
1:A:482:LEU:CD2	1:A:486:PHE:CD2	2.82	0.62
1:A:504:THR:HG22	1:A:508:LYS:HE2	1.81	0.62
1:A:479:LEU:HD11	1:A:504:THR:OG1	1.99	0.62
1:A:481:ASP:HB3	1:A:584:ILE:HG12	1.82	0.62
1:B:483:LEU:O	1:B:483:LEU:HD23	1.99	0.62
1:C:480:LEU:HD11	1:C:505:THR:HG22	1.81	0.62
1:C:41:ILE:HD12	1:C:69:SER:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:LEU:O	1:C:103:SER:OG	2.14	0.62
1:B:222:PRO:O	1:B:222:PRO:CD	2.38	0.61
1:D:326:PRO:HA	1:D:392:LEU:HD23	1.81	0.61
1:D:571:ILE:O	1:D:571:ILE:HG23	2.00	0.61
1:B:483:LEU:C	1:B:483:LEU:HD23	2.21	0.61
1:D:563:GLU:CG	1:D:564:MET:H	2.14	0.61
1:B:551:LYS:CA	1:B:552:TRP:HE3	2.12	0.61
1:A:407:LEU:HB3	1:A:414:HIS:CE1	2.35	0.61
1:C:152:TRP:O	1:C:153:VAL:CG2	2.48	0.61
1:C:332:LEU:CG	1:C:399:PHE:CZ	2.83	0.61
1:D:394:LEU:HA	1:D:397:SER:HB3	1.81	0.61
1:A:561:CYS:O	1:A:565:SER:N	2.34	0.61
1:B:406:LYS:HG3	1:B:407:GLU:H	1.64	0.61
1:C:527:ARG:HH11	1:C:527:ARG:HG2	1.65	0.61
1:A:482:LEU:HD23	1:A:486:PHE:CD2	2.35	0.61
1:C:594:LYS:HG3	1:C:594:LYS:O	2.00	0.61
1:D:246:GLU:C	1:D:358:LEU:HD22	2.20	0.61
1:D:469:LEU:O	1:D:469:LEU:HD23	2.00	0.61
1:D:499:ALA:H	1:D:526:PHE:N	1.99	0.61
1:B:348:ILE:HG23	1:B:399:PHE:CB	2.31	0.61
1:D:246:GLU:N	1:D:358:LEU:HD23	2.14	0.61
1:D:76:MET:CE	1:D:594:LYS:HD2	2.31	0.61
1:B:64:PHE:CE1	1:B:226:PHE:HB3	2.35	0.61
1:B:485:TYR:CG	1:B:582:PRO:HG2	2.36	0.61
1:D:326:PRO:HA	1:D:392:LEU:CD2	2.30	0.61
1:A:450:ILE:HD13	1:A:450:ILE:N	2.15	0.61
1:A:482:LEU:CD2	1:A:486:PHE:HD2	2.13	0.61
1:B:271:ARG:HH11	1:B:271:ARG:HB3	1.66	0.61
1:A:12:LEU:HD22	1:A:194:LEU:HD12	1.83	0.60
1:A:341:LYS:O	1:A:342:LYS:HG3	2.01	0.60
1:B:511:GLN:NE2	1:B:523:THR:CA	2.63	0.60
1:C:281:ASP:O	1:C:282:LYS:O	2.20	0.60
1:D:502:THR:CG2	1:D:503:SER:H	2.10	0.60
1:D:563:GLU:O	1:D:566:SER:HB2	2.01	0.60
1:A:228:ASP:OD2	1:A:232:LYS:HE3	2.01	0.60
1:B:562:CYS:O	1:B:566:SER:N	2.33	0.60
1:C:540:SER:O	1:C:541:ASP:C	2.39	0.60
1:D:368:ILE:O	1:D:372:MET:HG2	2.01	0.60
1:A:136:GLU:OE1	1:A:136:GLU:HA	2.02	0.60
1:C:364:MET:O	1:C:368:ILE:HG13	2.00	0.60
1:A:570:ILE:HG22	1:A:570:ILE:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:ASP:CG	1:B:342:LYS:H	2.03	0.60
1:B:547:GLU:O	1:B:548:LEU:CG	2.49	0.60
1:D:485:TYR:OH	1:D:573:TRP:CZ3	2.53	0.60
1:D:296:VAL:HG13	1:D:297:ILE:N	2.16	0.60
1:D:515:PHE:CE1	1:D:518:ASP:HB2	2.36	0.60
1:C:301:ILE:O	1:C:305:GLY:N	2.33	0.60
1:C:389:ASN:HB3	1:C:392:LEU:HG	1.83	0.60
1:D:98:MET:HE2	1:D:248:ALA:CB	2.32	0.60
1:D:374:LEU:HD22	1:D:435:GLN:HB2	1.84	0.60
1:D:501:ILE:HG21	1:D:560:LYS:CD	2.32	0.60
1:D:99:LEU:O	1:D:103:SER:OG	2.17	0.60
1:B:525:CYS:SG	1:B:526:PHE:N	2.74	0.59
1:C:550:GLU:O	1:C:553:LEU:N	2.34	0.59
1:D:278:ASP:OD1	1:D:426:GLY:CA	2.51	0.59
1:B:246:GLU:N	1:B:358:LEU:CD2	2.65	0.59
1:B:509:LYS:O	1:B:512:LEU:HB2	2.01	0.59
1:B:549:ILE:CG2	1:B:553:LEU:HD12	2.33	0.59
1:B:105:LYS:HG2	1:B:589:VAL:HG21	1.85	0.59
1:C:392:LEU:HB3	1:C:394:LEU:CD2	2.32	0.59
1:C:550:GLU:O	1:C:551:LYS:C	2.40	0.59
1:D:448:PRO:C	1:D:449:PHE:CD1	2.75	0.59
1:A:556:LYS:HG3	1:A:556:LYS:O	2.02	0.59
1:B:511:GLN:CA	1:B:514:ASP:HB2	2.33	0.59
1:C:392:LEU:CB	1:C:394:LEU:HG	2.32	0.59
1:C:474:ARG:NH2	1:A:339:THR:N	2.51	0.59
1:C:536:ILE:O	1:C:540:SER:OG	2.19	0.59
1:C:95:GLN:NE2	1:C:129:ASN:OD1	2.35	0.59
1:D:138:GLU:C	1:D:146:PRO:HD2	2.22	0.59
1:A:167:LEU:N	1:A:167:LEU:HD12	2.17	0.59
1:D:163:MET:O	1:D:167:LYS:HG2	2.02	0.59
1:A:484:TYR:HD1	1:A:575:LEU:HD12	1.66	0.59
1:B:136:PRO:O	1:B:138:GLU:OE1	2.21	0.59
1:D:35:LYS:O	1:D:405:LYS:HD3	2.03	0.59
1:D:410:ARG:C	1:D:411:GLU:HG3	2.23	0.59
1:D:41:ILE:HG22	1:D:42:THR:N	2.17	0.59
1:D:475:LYS:C	1:D:477:ASP:H	1.96	0.58
1:A:457:LYS:CE	1:A:495:GLU:OE1	2.51	0.58
1:A:53:GLY:C	1:A:54:ILE:HG23	2.23	0.58
1:B:504:GLY:O	1:B:507:GLU:CB	2.50	0.58
1:D:210:LEU:HD23	1:D:210:LEU:N	2.17	0.58
1:D:491:ARG:HG2	1:D:491:ARG:HH11	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:346:CYS:O	1:C:399:PHE:HA	2.03	0.58
1:B:192:PHE:HE2	1:B:196:GLN:HE22	1.48	0.58
1:A:32:ASN:HA	1:A:35:LYS:HE2	1.86	0.58
1:C:351:VAL:HB	1:C:369:LYS:HD2	1.85	0.58
1:A:316:HIS:O	1:A:351:LYS:CE	2.51	0.58
1:A:566:LYS:O	1:A:566:LYS:HG2	2.03	0.58
1:C:7:TYR:N	1:C:7:TYR:CD1	2.71	0.58
1:C:96:LEU:HD13	1:C:160:ILE:HA	1.86	0.58
1:C:288:PRO:HB2	1:C:293:GLN:HE22	1.67	0.58
1:C:341:ASP:CG	1:C:342:LYS:H	2.05	0.58
1:A:34:ILE:CD1	1:A:368:LYS:HG3	2.34	0.58
1:A:458:ASP:OD1	1:A:459:ARG:N	2.37	0.58
1:A:203:LEU:CD1	1:A:251:LEU:HD13	2.34	0.58
1:A:233:ALA:O	1:A:234:PHE:HB2	2.04	0.58
1:B:473:GLU:HB2	1:B:509:LYS:HE3	1.84	0.58
1:C:329:LEU:HD22	1:C:392:LEU:HD22	1.86	0.58
1:B:120:THR:HB	1:B:170:LEU:HD22	1.86	0.58
1:A:481:ASP:CB	1:A:584:ILE:HG13	2.34	0.57
1:A:80:PHE:HD1	1:A:455:ARG:HG3	1.69	0.57
1:A:482:LEU:HD23	1:A:482:LEU:C	2.24	0.57
1:B:414:ALA:N	1:B:434:GLU:OE2	2.37	0.57
1:C:403:GLU:O	1:C:404:GLU:HG3	2.04	0.57
1:D:343:LYS:O	1:D:344:GLN:HB3	2.04	0.57
1:A:570:ILE:C	1:A:572:TRP:N	2.53	0.57
1:D:246:GLU:CA	1:D:358:LEU:CD2	2.83	0.57
1:B:511:GLN:O	1:B:514:ASP:CB	2.53	0.57
1:C:185:LEU:HD23	1:C:429:THR:CB	2.35	0.57
1:B:325:ASP:HB2	1:B:326:PRO:HD3	1.86	0.57
1:C:408:LEU:O	1:C:409:THR:HB	2.04	0.57
1:A:309:THR:HG22	1:A:415:ARG:HG3	1.87	0.57
1:D:385:TYR:OH	1:D:388:PRO:HB3	2.04	0.57
1:C:546:ALA:N	1:C:549:ILE:CG2	2.68	0.57
1:D:342:LYS:O	1:D:343:LYS:HB3	2.05	0.57
1:B:223:GLY:O	1:B:224:LEU:HG	2.04	0.57
1:B:228:SER:CB	1:B:240:ASP:OD2	2.52	0.57
1:B:185:LEU:HD23	1:B:429:THR:HB	1.87	0.57
1:A:564:TRP:C	1:A:566:LYS:N	2.53	0.56
1:B:45:SER:C	1:B:46:LYS:HD3	2.25	0.56
1:C:233:LYS:CD	1:C:238:ASP:O	2.51	0.56
1:D:21:PHE:HB3	1:D:22:PRO:CD	2.35	0.56
1:D:232:ILE:HG21	1:D:353:THR:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:235:PHE:O	1:D:385:TYR:CE1	2.57	0.56
1:A:159:ILE:O	1:A:163:ILE:HG13	2.05	0.56
1:A:496:ARG:NH2	1:A:566:LYS:HA	2.20	0.56
1:C:152:TRP:C	1:C:153:VAL:HG22	2.24	0.56
1:C:551:LYS:O	1:C:555:LYS:HB2	2.05	0.56
1:C:532:GLN:CD	1:C:567:LYS:HG3	2.26	0.56
1:A:282:VAL:O	1:A:282:VAL:HG13	2.05	0.56
1:B:323:LEU:O	1:B:327:ILE:HG13	2.06	0.56
1:C:233:LYS:CB	1:C:239:ALA:HA	2.33	0.56
1:D:21:PHE:HB3	1:D:22:PRO:HD2	1.88	0.56
1:D:452:PRO:HB3	1:D:565:TRP:CZ2	2.40	0.56
1:A:487:GLN:HB3	1:A:571:ASN:HB2	1.87	0.56
1:B:192:PHE:O	1:B:196:GLN:HG3	2.05	0.56
1:B:549:ILE:CG2	1:B:553:LEU:CD1	2.83	0.56
1:C:93:ASP:OD1	1:C:94:PRO:HD2	2.04	0.56
1:D:301:ILE:HG23	1:D:306:ILE:O	2.04	0.56
1:C:32:ASN:O	1:C:36:GLU:HG2	2.05	0.56
1:C:480:LEU:CD1	1:C:505:THR:HG22	2.35	0.56
1:B:283:VAL:HG13	1:B:283:VAL:O	2.06	0.56
1:D:344:GLN:O	1:D:344:GLN:HG2	2.04	0.56
1:D:351:VAL:HB	1:D:369:LYS:HD2	1.87	0.56
1:B:482:ASP:OD1	1:B:583:LYS:N	2.38	0.56
1:C:311:ILE:HD12	1:C:311:ILE:N	2.21	0.56
1:D:151:SER:HA	1:D:153:VAL:CG1	2.35	0.56
1:A:32:ASN:OD1	1:A:35:LYS:NZ	2.30	0.56
1:B:39:GLU:OE1	1:B:231:HIS:CE1	2.59	0.56
1:D:317:HIS:CD2	1:D:319:THR:HG22	2.41	0.56
1:A:292:GLN:O	1:A:296:ILE:HG13	2.06	0.56
1:B:313:TYR:OH	1:B:349:GLY:HA3	2.06	0.56
1:C:544:ASP:O	1:C:546:ALA:N	2.39	0.56
1:D:325:ASP:O	1:D:392:LEU:HD21	2.06	0.56
1:B:111:GLY:O	1:B:490:GLY:HA3	2.06	0.56
1:C:464:TYR:CD1	1:C:591:PRO:HD3	2.41	0.56
1:D:564:MET:O	1:D:567:LYS:N	2.34	0.56
1:C:552:TRP:N	1:C:552:TRP:CD1	2.72	0.55
1:B:348:ILE:HG23	1:B:399:PHE:HB2	1.88	0.55
1:B:450:ILE:C	1:B:451:ILE:HD13	2.26	0.55
1:B:549:ILE:O	1:B:549:ILE:HG22	2.05	0.55
1:C:358:LEU:CG	1:C:361:ALA:HB3	2.37	0.55
1:B:341:ASP:O	1:B:342:LYS:HB2	2.07	0.55
1:C:553:LEU:C	1:C:555:LYS:N	2.60	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:469:LEU:CD2	1:D:472:LEU:HB2	2.35	0.55
1:B:434:GLU:HA	1:B:434:GLU:OE1	2.06	0.55
1:D:563:GLU:CG	1:D:564:MET:N	2.69	0.55
1:D:81:PHE:CE1	1:D:456:ARG:NH1	2.69	0.55
1:A:182:SER:OG	1:A:359:THR:HG23	2.07	0.55
1:C:358:LEU:O	1:C:362:ALA:HB2	2.07	0.55
1:D:448:PRO:C	1:D:449:PHE:HD1	2.08	0.55
1:D:584:ARG:O	1:D:585:ILE:HD13	2.06	0.55
1:A:128:ASN:O	1:A:129:SER:OG	2.24	0.55
1:A:393:LEU:HD21	1:A:400:VAL:HG23	1.88	0.55
1:C:63:GLY:C	1:C:64:PHE:CG	2.80	0.55
1:D:35:LYS:HE2	1:D:36:GLU:HG2	1.88	0.55
1:A:313:VAL:HG22	1:A:417:ALA:HB3	1.88	0.55
1:B:150:VAL:HG12	1:B:151:SER:N	2.21	0.55
1:B:523:THR:OG1	1:B:525:CYS:HB3	2.06	0.55
1:C:358:LEU:HD23	1:C:361:ALA:HB3	1.89	0.55
1:D:32:ASN:OD1	1:D:33:ASN:N	2.40	0.55
1:D:329:LEU:HD11	1:D:399:PHE:HD2	1.72	0.55
1:D:473:GLU:O	1:D:474:ARG:O	2.23	0.55
1:A:112:ILE:HG22	1:A:114:LYS:HG3	1.87	0.55
1:A:475:THR:O	1:A:477:THR:N	2.34	0.55
1:D:132:ARG:HH12	1:D:153:VAL:HG22	1.72	0.55
1:A:324:ASP:HB2	1:A:325:PRO:HD3	1.88	0.55
1:B:551:LYS:HA	1:B:552:TRP:CE3	2.41	0.55
1:C:63:GLY:O	1:C:64:PHE:CD1	2.60	0.55
1:D:500:PHE:N	1:D:500:PHE:CD1	2.74	0.55
1:A:568:VAL:O	1:A:569:ALA:HB3	2.06	0.55
1:C:239:ALA:O	1:C:322:LYS:HG2	2.07	0.55
1:B:138:GLU:OE1	1:B:138:GLU:N	2.40	0.54
1:C:93:ASP:OD2	1:C:95:GLN:NE2	2.40	0.54
1:A:488:VAL:HG11	1:A:572:TRP:CE2	2.41	0.54
1:A:69:VAL:HG12	1:A:70:LEU:N	2.21	0.54
1:C:48:GLU:C	1:C:49:LEU:HD23	2.28	0.54
1:C:63:GLY:O	1:C:64:PHE:CG	2.59	0.54
1:D:117:ILE:O	1:D:117:ILE:HG13	2.08	0.54
1:C:281:ASP:O	1:C:282:LYS:C	2.46	0.54
1:C:288:PRO:HG3	1:C:324:GLY:HA2	1.90	0.54
1:A:339:THR:CG2	1:A:340:ASP:H	2.21	0.54
1:D:340:THR:O	1:D:342:LYS:HD2	2.08	0.54
1:D:451:ILE:N	1:D:500:PHE:O	2.31	0.54
1:D:585:ILE:HG22	1:D:586:SER:N	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:288:PRO:O	1:C:327:ILE:HG21	2.06	0.54
1:D:232:ILE:O	1:D:232:ILE:HG23	2.07	0.54
1:D:329:LEU:HD11	1:D:399:PHE:CD2	2.42	0.54
1:D:410:ARG:O	1:D:411:GLU:CG	2.55	0.54
1:D:452:PRO:HB3	1:D:565:TRP:CH2	2.42	0.54
1:C:71:LEU:HD22	1:C:247:GLY:HA2	1.89	0.54
1:B:113:ILE:O	1:B:114:SER:C	2.44	0.54
1:B:35:LYS:HG3	1:B:36:GLU:HG2	1.89	0.54
1:B:306:ILE:HD13	1:B:416:ARG:HD2	1.90	0.54
1:A:468:LEU:HD22	1:A:515:ILE:HD11	1.90	0.54
1:A:490:ARG:HG2	1:A:490:ARG:NH1	2.22	0.54
1:B:501:ILE:HD13	1:B:560:LYS:HG3	1.90	0.54
1:D:321:THR:N	1:D:325:ASP:OD2	2.41	0.54
1:A:504:THR:O	1:A:507:LEU:N	2.40	0.54
1:A:64:VAL:O	1:A:64:VAL:HG23	2.07	0.54
1:D:113:ILE:HD12	1:D:116:GLU:OE2	2.08	0.54
1:B:569:VAL:O	1:B:569:VAL:HG13	2.06	0.54
1:B:43:PHE:CD1	1:B:67:ALA:CB	2.91	0.54
1:C:64:PHE:O	1:C:221:GLN:HG3	2.08	0.54
1:D:561:LEU:HD12	1:D:563:GLU:HB2	1.89	0.54
1:B:465:ALA:O	1:B:469:LEU:HB2	2.08	0.53
1:C:12:LEU:HD11	1:C:192:PHE:HD1	1.73	0.53
1:C:534:LYS:O	1:C:538:TRP:CD2	2.61	0.53
1:D:310:THR:O	1:D:310:THR:HG22	2.08	0.53
1:C:341:ASP:C	1:C:342:LYS:HG3	2.29	0.53
1:B:246:GLU:C	1:B:358:LEU:HD22	2.29	0.53
1:D:323:LEU:O	1:D:327:ILE:HG13	2.07	0.53
1:D:483:LEU:HA	1:D:587:LEU:HD11	1.90	0.53
1:B:214:SER:O	1:B:215:SER:OG	2.23	0.53
1:B:108:GLU:C	1:B:491:ARG:HH12	2.08	0.53
1:C:487:PHE:CD1	1:C:491:ARG:HG3	2.39	0.53
1:D:528:GLY:C	1:D:566:SER:O	2.46	0.53
1:A:309:THR:CG2	1:A:415:ARG:NE	2.55	0.53
1:A:481:ASP:OD2	1:A:582:LYS:CE	2.56	0.53
1:D:160:ILE:HB	1:D:161:PRO:CD	2.38	0.53
1:D:343:LYS:CD	1:D:343:LYS:N	2.71	0.53
1:A:113:SER:OG	1:A:167:LEU:HB3	2.09	0.53
1:A:473:ARG:CG	1:A:474:LYS:N	2.72	0.53
1:B:456:ARG:HD3	1:B:495:GLU:OE2	2.09	0.53
1:B:504:GLY:O	1:B:507:GLU:N	2.42	0.53
1:C:534:LYS:O	1:C:538:TRP:CG	2.62	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:VAL:HG23	1:A:260:LYS:HG2	1.91	0.53
1:C:537:ALA:CA	1:C:540:SER:OG	2.56	0.53
1:D:498:ALA:HB1	1:D:500:PHE:CE1	2.43	0.53
1:B:456:ARG:O	1:B:457:LYS:HG3	2.08	0.53
1:D:485:TYR:O	1:D:489:VAL:HG22	2.09	0.53
1:A:39:GLU:OE2	1:A:230:HIS:HD2	1.92	0.53
1:B:113:ILE:HB	1:B:116:GLU:HG3	1.90	0.53
1:B:42:THR:CG2	1:B:68:LYS:O	2.53	0.53
1:C:478:THR:CG2	1:C:479:ASP:H	2.12	0.53
1:C:545:SER:C	1:C:549:ILE:CG2	2.77	0.53
1:D:304:THR:CB	1:D:306:ILE:HG13	2.37	0.52
1:B:367:CYS:O	1:B:371:VAL:HG23	2.09	0.52
1:C:269:LEU:HD13	1:C:436:TYR:HB2	1.90	0.52
1:C:42:THR:OG1	1:C:68:LYS:O	2.22	0.52
1:D:563:GLU:HG2	1:D:564:MET:N	2.23	0.52
1:C:460:ARG:NH1	1:C:463:GLU:OE1	2.42	0.52
1:B:271:ARG:HE	1:B:416:ARG:NH1	2.08	0.52
1:A:292:GLN:O	1:A:295:VAL:HG22	2.09	0.52
1:A:340:ASP:O	1:A:342:LYS:HG3	2.09	0.52
1:B:307:HIS:HD2	1:B:309:GLU:H	1.58	0.52
1:C:95:GLN:OE1	1:C:127:SER:O	2.27	0.52
1:C:501:ILE:HG23	1:C:501:ILE:O	2.09	0.52
1:A:11:SER:HB3	1:A:270:ARG:HA	1.90	0.52
1:A:482:LEU:HD21	1:A:486:PHE:CD2	2.44	0.52
1:A:51:ARG:HG2	1:A:52:SER:N	2.24	0.52
1:B:328:GLU:HG3	1:B:422:PHE:HE2	1.74	0.52
1:C:474:ARG:HH22	1:A:339:THR:N	2.07	0.52
1:D:282:LYS:CE	1:D:284:GLY:O	2.58	0.52
1:A:485:THR:O	1:A:485:THR:HG22	2.09	0.52
1:A:561:CYS:O	1:A:565:SER:HB2	2.09	0.52
1:B:150:VAL:CG1	1:B:151:SER:N	2.72	0.52
1:B:317:HIS:CD2	1:B:422:PHE:H	2.27	0.52
1:A:457:LYS:HG2	1:A:495:GLU:OE1	2.09	0.52
1:A:513:ASP:O	1:A:519:PRO:HG3	2.10	0.52
1:B:346:CYS:O	1:B:399:PHE:HB3	2.10	0.52
1:C:332:LEU:HD21	1:C:399:PHE:CZ	2.45	0.52
1:C:63:GLY:C	1:C:64:PHE:CD2	2.83	0.52
1:D:278:ASP:OD1	1:D:426:GLY:C	2.48	0.52
1:D:419:LEU:HD12	1:D:420:SER:H	1.75	0.52
1:B:41:ILE:HG22	1:B:42:THR:N	2.25	0.52
1:B:587:LEU:HB3	1:B:588:PRO:HD2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:95:GLN:HG2	1:C:210:LEU:HB2	1.92	0.52
1:D:12:LEU:HD13	1:D:192:PHE:CD2	2.45	0.52
1:D:419:LEU:HD12	1:D:420:SER:N	2.24	0.52
1:D:76:MET:HE3	1:D:594:LYS:HD2	1.92	0.52
1:A:570:ILE:HG23	1:A:572:TRP:HD1	1.75	0.52
1:C:388:PRO:HB3	1:C:394:LEU:HD12	1.92	0.52
1:D:449:PHE:N	1:D:449:PHE:CD1	2.76	0.52
1:A:457:LYS:HG3	1:A:495:GLU:OE1	2.10	0.51
1:D:325:ASP:N	1:D:326:PRO:CD	2.73	0.51
1:D:326:PRO:HD2	1:D:327:ILE:H	1.75	0.51
1:D:81:PHE:CD1	1:D:456:ARG:HD2	2.45	0.51
1:B:321:THR:O	1:B:325:ASP:OD2	2.28	0.51
1:C:559:PRO:O	1:C:561:LEU:N	2.42	0.51
1:D:116:GLU:O	1:D:118:PRO:HD2	2.10	0.51
1:B:549:ILE:HG21	1:B:553:LEU:CD1	2.40	0.51
1:B:526:PHE:HZ	1:B:560:LYS:HD3	1.74	0.51
1:C:43:PHE:HA	1:C:67:ALA:CB	2.40	0.51
1:D:282:LYS:HD2	1:D:287:ALA:O	2.10	0.51
1:D:246:GLU:C	1:D:358:LEU:CD2	2.78	0.51
1:D:491:ARG:NH1	1:D:491:ARG:HG2	2.25	0.51
1:B:153:VAL:HG12	1:B:153:VAL:O	2.10	0.51
1:B:93:ASP:OD1	1:B:94:PRO:N	2.42	0.51
1:C:389:ASN:OD1	1:C:391:ASN:HB2	2.11	0.51
1:D:136:PRO:O	1:D:138:GLU:N	2.42	0.51
1:D:515:PHE:CE1	1:D:518:ASP:OD1	2.52	0.51
1:A:292:GLN:HG2	1:A:421:PHE:CE1	2.44	0.51
1:B:277:ASN:HA	1:B:426:GLY:O	2.09	0.51
1:C:343:LYS:O	1:C:345:TYR:CD1	2.60	0.51
1:D:181:CYS:HB2	1:D:423:GLY:HA2	1.91	0.51
1:D:338:ARG:O	1:D:338:ARG:HG2	2.10	0.51
1:D:475:LYS:HB3	1:D:477:ASP:CB	2.40	0.51
1:B:31:TRP:O	1:B:34:ILE:HG12	2.10	0.51
1:B:511:GLN:C	1:B:514:ASP:HB2	2.30	0.51
1:C:36:GLU:HA	1:C:36:GLU:OE1	2.10	0.51
1:C:518:ASP:CG	1:C:518:ASP:O	2.48	0.51
1:C:559:PRO:O	1:C:560:LYS:C	2.49	0.51
1:D:147:ASP:C	1:D:149:TYR:H	2.14	0.51
1:D:317:HIS:O	1:D:352:LYS:HE2	2.09	0.51
1:D:246:GLU:N	1:D:358:LEU:HD21	2.24	0.51
1:B:194:SER:HA	1:B:199:GLU:OE2	2.11	0.51
1:B:515:PHE:C	1:B:515:PHE:CD1	2.84	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:286:TYR:O	1:C:287:ALA:HB2	2.10	0.51
1:C:377:GLN:O	1:C:408:LEU:HB2	2.11	0.51
1:D:221:GLN:HG3	1:D:221:GLN:O	2.11	0.51
1:D:501:ILE:HG21	1:D:560:LYS:CG	2.41	0.51
1:A:162:MET:O	1:A:166:LYS:HG2	2.09	0.51
1:A:309:THR:HG1	1:A:309:THR:CB	2.12	0.51
1:D:300:VAL:HG12	1:D:304:THR:HG21	1.92	0.51
1:D:345:TYR:C	1:D:345:TYR:CD1	2.84	0.51
1:B:549:ILE:HG22	1:B:553:LEU:CD1	2.41	0.50
1:C:127:SER:OG	1:C:209:THR:CB	2.59	0.50
1:D:113:ILE:O	1:D:116:GLU:HB2	2.12	0.50
1:A:163:ILE:O	1:A:167:LEU:HD13	2.11	0.50
1:A:227:SER:HB3	1:A:239:ASP:OD2	2.10	0.50
1:A:92:ASP:OD1	1:A:93:PRO:HD2	2.12	0.50
1:C:209:THR:OG1	1:C:359:ASP:CB	2.58	0.50
1:C:358:LEU:HB2	1:C:362:ALA:N	2.26	0.50
1:D:246:GLU:CA	1:D:358:LEU:HD22	2.42	0.50
1:D:405:LYS:O	1:D:406:LYS:HG2	2.11	0.50
1:B:307:HIS:O	1:B:310:THR:HB	2.12	0.50
1:B:480:LEU:O	1:B:484:ALA:CB	2.59	0.50
1:C:339:TYR:O	1:C:340:THR:C	2.47	0.50
1:C:519:LYS:N	1:C:520:PRO:CD	2.71	0.50
1:C:540:SER:O	1:C:542:ASP:N	2.44	0.50
1:D:300:VAL:HG12	1:D:304:THR:CG2	2.41	0.50
1:A:289:VAL:CG2	1:A:326:ILE:HG23	2.34	0.50
1:C:11:SER:HB3	1:C:270:LEU:O	2.12	0.50
1:C:314:VAL:HG22	1:C:418:ALA:HB3	1.92	0.50
1:D:561:LEU:HG	1:D:563:GLU:HB3	1.91	0.50
1:A:506:GLU:O	1:A:510:GLN:CG	2.57	0.50
1:A:564:TRP:O	1:A:565:SER:C	2.48	0.50
1:B:282:LYS:CG	1:B:287:ALA:HB3	2.40	0.50
1:B:323:LEU:C	1:B:326:PRO:HD2	2.32	0.50
1:A:509:ARG:HG3	1:A:510:GLN:N	2.27	0.50
1:C:153:VAL:HG23	1:C:153:VAL:O	2.12	0.50
1:C:32:ASN:HA	1:C:35:LYS:HG2	1.93	0.50
1:A:31:TRP:CD1	1:A:371:MET:HB3	2.47	0.50
1:B:549:ILE:HG22	1:B:553:LEU:HD12	1.92	0.50
1:B:351:VAL:HB	1:B:369:LYS:HD2	1.94	0.50
1:D:461:LEU:O	1:D:464:TYR:CB	2.59	0.50
1:D:490:GLY:O	1:D:491:ARG:NH1	2.43	0.50
1:A:341:LYS:O	1:A:342:LYS:CG	2.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:484:TYR:HD1	1:A:575:LEU:CD1	2.25	0.50
1:A:517:ASP:OD1	1:A:518:LYS:HG3	2.12	0.50
1:B:223:GLY:C	1:B:224:LEU:HG	2.32	0.49
1:B:480:LEU:HD11	1:B:505:THR:HG22	1.94	0.49
1:C:117:ILE:HG13	1:C:117:ILE:O	2.13	0.49
1:D:390:PRO:O	1:D:393:HIS:CD2	2.65	0.49
1:D:461:LEU:O	1:D:464:TYR:HB3	2.12	0.49
1:D:77:PHE:CD1	1:D:97:ARG:HB3	2.47	0.49
1:B:114:SER:O	1:B:116:GLU:N	2.45	0.49
1:B:150:VAL:CG1	1:B:151:SER:H	2.25	0.49
1:B:282:LYS:HG3	1:B:283:VAL:N	2.27	0.49
1:D:98:MET:CE	1:D:248:ALA:HB3	2.40	0.49
1:D:34:ILE:HD11	1:D:369:LYS:NZ	2.27	0.49
1:A:239:ASP:OD1	1:A:239:ASP:N	2.42	0.49
1:A:295:VAL:HG23	1:A:296:ILE:N	2.27	0.49
1:C:545:SER:C	1:C:549:ILE:HG21	2.33	0.49
1:C:483:LEU:HG	1:C:587:LEU:HD13	1.94	0.49
1:A:341:LYS:HD3	1:A:395:ASP:CG	2.31	0.49
1:A:71:GLU:HG2	1:A:72:GLY:N	2.27	0.49
1:B:339:TYR:O	1:B:341:ASP:N	2.45	0.49
1:B:471:PHE:CD1	1:B:471:PHE:C	2.85	0.49
1:C:571:ILE:HG23	1:C:571:ILE:O	2.13	0.49
1:D:515:PHE:CE1	1:D:518:ASP:HA	2.46	0.49
1:B:514:ASP:HB3	1:B:523:THR:CG2	2.42	0.49
1:C:47:GLU:N	1:C:48:GLU:OE2	2.45	0.49
1:D:497:ARG:HD2	1:D:565:TRP:O	2.11	0.49
1:B:43:PHE:CE1	1:B:67:ALA:HB2	2.47	0.49
1:C:539:LEU:O	1:C:540:SER:C	2.51	0.49
1:D:282:LYS:HE3	1:D:284:GLY:O	2.13	0.49
1:D:34:ILE:HD12	1:D:351:VAL:HG23	1.93	0.49
1:D:501:ILE:HG21	1:D:560:LYS:HG2	1.93	0.49
1:D:64:PHE:CD1	1:D:64:PHE:C	2.85	0.49
1:A:516:ASN:O	1:A:519:PRO:HD2	2.13	0.49
1:B:194:SER:CA	1:B:199:GLU:OE2	2.61	0.49
1:B:245:GLY:C	1:B:358:LEU:CD2	2.77	0.49
1:A:108:ASP:OD2	1:A:266:TYR:OH	2.23	0.49
1:A:11:SER:HB3	1:A:269:LEU:O	2.13	0.49
1:C:364:MET:HA	1:C:364:MET:CE	2.42	0.49
1:D:179:ALA:O	1:D:180:ASN:HB2	2.13	0.49
1:B:448:PRO:O	1:B:449:PHE:CD1	2.65	0.49
1:B:468:LEU:O	1:B:471:PHE:HB3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:209:THR:HG23	1:C:209:THR:O	2.12	0.49
1:C:542:ASP:HB3	1:C:544:ASP:OD2	2.13	0.49
1:C:546:ALA:O	1:C:550:GLU:CB	2.57	0.49
1:D:17:ILE:HG22	1:D:18:SER:N	2.28	0.49
1:B:234:ALA:O	1:B:235:PHE:HB2	2.13	0.49
1:B:291:LYS:O	1:B:295:GLU:HG3	2.12	0.49
1:B:64:PHE:HA	1:B:66:PRO:CD	2.43	0.49
1:C:283:VAL:O	1:C:284:GLY:C	2.50	0.49
1:D:515:PHE:HD1	1:D:518:ASP:HA	1.75	0.49
1:D:456:ARG:HB2	1:D:590:TYR:OH	2.13	0.49
1:A:473:ARG:HG3	1:A:474:LYS:N	2.28	0.48
1:B:115:LYS:HB3	1:B:115:LYS:HE3	1.61	0.48
1:B:222:PRO:O	1:B:222:PRO:HD2	2.12	0.48
1:B:325:ASP:N	1:B:326:PRO:CD	2.76	0.48
1:C:137:GLU:HA	1:C:137:GLU:OE1	2.13	0.48
1:D:415:HIS:O	1:D:435:GLN:N	2.30	0.48
1:A:102:SER:HB3	1:A:203:LEU:HD21	1.95	0.48
1:C:392:LEU:CD1	1:C:394:LEU:HD21	2.43	0.48
1:D:120:THR:O	1:D:172:GLY:HA3	2.13	0.48
1:D:502:THR:HB	1:D:508:LEU:HD12	1.95	0.48
1:A:268:LEU:HD13	1:A:435:TYR:HB2	1.96	0.48
1:A:570:ILE:CG2	1:A:572:TRP:HB2	2.28	0.48
1:C:260:VAL:HG23	1:C:261:LYS:N	2.28	0.48
1:D:120:THR:HG23	1:D:202:TYR:HB2	1.95	0.48
1:A:339:THR:CG2	1:A:340:ASP:N	2.76	0.48
1:A:341:LYS:CD	1:A:395:ASP:OD1	2.54	0.48
1:B:64:PHE:HA	1:B:66:PRO:N	2.27	0.48
1:C:227:SER:OG	1:C:230:GLY:HA2	2.13	0.48
1:C:548:LEU:O	1:C:552:TRP:CD1	2.67	0.48
1:D:316:ALA:HB1	1:D:328:GLU:OE2	2.12	0.48
1:C:317:HIS:CD2	1:C:319:THR:CG2	2.95	0.48
1:A:341:LYS:C	1:A:342:LYS:HG3	2.34	0.48
1:B:317:HIS:HD2	1:B:421:SER:HA	1.79	0.48
1:B:458:LYS:HG2	1:B:496:GLU:CG	2.43	0.48
1:D:231:HIS:O	1:D:233:LYS:HE3	2.14	0.48
1:D:309:GLU:CA	1:D:345:TYR:OH	2.62	0.48
1:A:11:SER:CB	1:A:270:ARG:HA	2.44	0.48
1:A:446:GLY:O	1:A:502:SER:HA	2.14	0.48
1:A:69:VAL:CG1	1:A:70:LEU:N	2.77	0.48
1:B:458:LYS:HG2	1:B:496:GLU:HG2	1.95	0.48
1:C:483:LEU:HA	1:C:587:LEU:HD11	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:573:TRP:O	1:C:573:TRP:CD1	2.67	0.48
1:C:71:LEU:HD23	1:C:210:LEU:HD21	1.96	0.48
1:D:336:TYR:C	1:D:338:ARG:H	2.16	0.48
1:A:519:PRO:O	1:A:520:ALA:HB3	2.13	0.48
1:A:525:PHE:N	1:A:525:PHE:CD1	2.81	0.48
1:B:246:GLU:C	1:B:358:LEU:CD2	2.82	0.48
1:B:337:GLY:HA2	1:B:341:ASP:OD2	2.14	0.48
1:C:325:ASP:O	1:C:329:LEU:HD13	2.14	0.48
1:D:293:GLN:CG	1:D:422:PHE:CE2	2.96	0.48
1:D:300:VAL:O	1:D:304:THR:CG2	2.59	0.48
1:D:32:ASN:CA	1:D:35:LYS:HG2	2.39	0.48
1:B:66:PRO:HD2	1:B:67:ALA:H	1.78	0.48
1:C:503:SER:OG	1:C:507:GLU:HG3	2.14	0.48
1:D:224:LEU:CD1	1:D:225:ASN:H	2.26	0.48
1:B:526:PHE:CD2	1:B:562:CYS:CB	2.96	0.47
1:D:501:ILE:O	1:D:502:THR:OG1	2.31	0.47
1:A:256:SER:O	1:A:259:VAL:CG2	2.62	0.47
1:A:259:VAL:HG23	1:A:260:LYS:N	2.29	0.47
1:A:380:PRO:HD3	1:A:404:LYS:HB3	1.95	0.47
1:B:268:ALA:HB3	1:B:371:VAL:HG13	1.96	0.47
1:C:392:LEU:HD12	1:C:394:LEU:HD11	1.95	0.47
1:D:394:LEU:C	1:D:397:SER:OG	2.53	0.47
1:D:93:ASP:OD1	1:D:94:PRO:HD2	2.12	0.47
1:A:84:SER:O	1:A:87:ASP:HB2	2.14	0.47
1:B:22:PRO:HD3	1:B:246:GLU:O	2.15	0.47
1:B:348:ILE:O	1:B:348:ILE:HG13	2.13	0.47
1:C:358:LEU:HG	1:C:361:ALA:HB3	1.95	0.47
1:D:290:VAL:HG13	1:D:291:LYS:N	2.29	0.47
1:A:272:ILE:O	1:A:272:ILE:HG23	2.14	0.47
1:B:351:VAL:HG22	1:B:351:VAL:O	2.13	0.47
1:B:392:LEU:CD1	1:B:394:LEU:HD21	2.44	0.47
1:D:484:ALA:O	1:D:488:GLN:HG3	2.14	0.47
1:A:112:ILE:HG23	1:A:491:GLU:HG3	1.95	0.47
1:A:564:TRP:HD1	1:A:568:VAL:O	1.98	0.47
1:B:307:HIS:CE1	1:B:340:THR:HB	2.49	0.47
1:C:332:LEU:HD23	1:C:399:PHE:CE2	2.49	0.47
1:C:450:ILE:HB	1:C:488:GLN:HE21	1.80	0.47
1:C:460:ARG:CZ	1:C:463:GLU:OE1	2.63	0.47
1:D:29:GLU:O	1:D:32:ASN:OD1	2.32	0.47
1:A:278:GLY:O	1:A:280:ASP:N	2.47	0.47
1:A:393:LEU:O	1:A:396:SER:OG	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:LEU:HD22	1:A:515:ILE:CD1	2.45	0.47
1:B:551:LYS:CB	1:B:552:TRP:HE3	2.28	0.47
1:D:336:TYR:CD1	1:D:336:TYR:N	2.81	0.47
1:D:381:PRO:HD3	1:D:405:LYS:CG	2.34	0.47
1:D:517:ASN:O	1:D:518:ASP:C	2.53	0.47
1:D:504:GLY:O	1:D:508:LEU:CB	2.62	0.47
1:C:450:ILE:C	1:C:451:ILE:HD13	2.35	0.47
1:D:340:THR:C	1:D:342:LYS:CD	2.81	0.47
1:C:536:ILE:O	1:C:540:SER:CA	2.63	0.47
1:D:275:VAL:HG22	1:D:429:THR:HG22	1.96	0.47
1:D:293:GLN:CD	1:D:422:PHE:CE2	2.89	0.47
1:A:373:LEU:HD22	1:A:434:GLN:HB2	1.97	0.47
1:A:84:SER:OG	1:A:87:ASP:CG	2.52	0.47
1:B:239:ALA:O	1:B:322:LYS:HG2	2.15	0.47
1:B:317:HIS:CD2	1:B:421:SER:HA	2.50	0.47
1:B:436:TYR:HA	1:B:437:PRO:HD3	1.51	0.47
1:B:58:LEU:HD12	1:B:62:PRO:CB	2.39	0.47
1:C:42:THR:O	1:C:67:ALA:HB1	2.15	0.47
1:D:160:ILE:O	1:D:164:ILE:HG13	2.15	0.47
1:D:515:PHE:HE1	1:D:518:ASP:CB	2.20	0.47
1:A:115:GLU:C	1:A:117:PRO:HD3	2.35	0.47
1:A:213:SER:O	1:A:214:SER:CB	2.63	0.47
1:A:276:ASN:HA	1:A:426:THR:HA	1.97	0.47
1:A:482:LEU:HD21	1:A:486:PHE:HE2	1.79	0.47
1:B:519:LYS:N	1:B:520:PRO:HD2	2.30	0.47
1:B:94:PRO:HD3	1:B:131:TYR:CE1	2.50	0.47
1:A:139:THR:O	1:A:140:ALA:O	2.33	0.46
1:B:454:SER:HB2	1:B:494:MET:HB2	1.97	0.46
1:D:364:MET:O	1:D:368:ILE:HG13	2.15	0.46
1:D:493:ALA:HB1	1:D:497:ARG:HE	1.80	0.46
1:D:483:LEU:HG	1:D:587:LEU:HD13	1.97	0.46
1:A:332:GLN:HG3	1:A:397:PRO:HD2	1.97	0.46
1:B:259:ALA:HA	1:B:264:ASP:OD2	2.15	0.46
1:A:322:LEU:HD12	1:A:322:LEU:H	1.79	0.46
1:A:454:ALA:HB3	1:A:460:LEU:HB2	1.96	0.46
1:B:306:ILE:CD1	1:B:432:ILE:HG21	2.45	0.46
1:B:304:THR:C	1:B:306:ILE:H	2.18	0.46
1:B:480:LEU:CD1	1:B:505:THR:HG22	2.46	0.46
1:B:471:PHE:CE2	1:B:588:PRO:HD3	2.50	0.46
1:C:49:LEU:N	1:C:49:LEU:CD2	2.72	0.46
1:D:317:HIS:O	1:D:352:LYS:HE3	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:457:LYS:HE2	1:D:457:LYS:HB3	1.60	0.46
1:D:507:GLU:O	1:D:510:ARG:N	2.39	0.46
1:D:515:PHE:CD1	1:D:515:PHE:O	2.69	0.46
1:A:276:ASN:HA	1:A:425:GLY:O	2.16	0.46
1:B:138:GLU:HB3	1:B:151:SER:OG	2.15	0.46
1:C:479:ASP:OD2	1:C:481:ALA:HB3	2.16	0.46
1:D:153:VAL:HG23	1:D:153:VAL:O	2.16	0.46
1:D:504:GLY:O	1:D:508:LEU:N	2.46	0.46
1:A:297:GLN:NE2	1:A:338:TYR:OH	2.46	0.46
1:B:337:GLY:C	1:B:339:TYR:H	2.18	0.46
1:B:527:ARG:O	1:B:566:SER:OG	2.34	0.46
1:C:219:VAL:O	1:C:219:VAL:HG12	2.15	0.46
1:C:526:PHE:CD1	1:C:526:PHE:N	2.84	0.46
1:D:326:PRO:CD	1:D:327:ILE:H	2.29	0.46
1:B:293:GLN:O	1:B:296:VAL:HG22	2.16	0.46
1:C:276:ASN:CG	1:C:296:VAL:HG13	2.36	0.46
1:C:553:LEU:HD12	1:C:574:HIS:CB	2.44	0.46
1:B:395:GLU:HG3	1:B:396:ASP:N	2.30	0.46
1:C:308:PRO:HA	1:C:311:ILE:HD13	1.96	0.46
1:C:329:LEU:HD12	1:C:329:LEU:N	2.31	0.46
1:D:301:ILE:CG2	1:D:306:ILE:O	2.64	0.46
1:A:115:GLU:O	1:A:117:PRO:HD3	2.16	0.46
1:A:324:ASP:HB2	1:A:325:PRO:CD	2.45	0.46
1:A:53:GLY:C	1:A:54:ILE:CG2	2.83	0.46
1:B:471:PHE:CD1	1:B:472:LEU:N	2.84	0.46
1:B:553:LEU:HD23	1:B:554:ALA:O	2.15	0.46
1:C:460:ARG:NH2	1:C:463:GLU:OE1	2.49	0.46
1:A:457:LYS:HE3	1:A:495:GLU:OE1	2.16	0.45
1:B:348:ILE:CG2	1:B:399:PHE:CB	2.94	0.45
1:B:41:ILE:HG22	1:B:42:THR:H	1.82	0.45
1:B:517:ASN:O	1:B:520:PRO:CD	2.62	0.45
1:C:527:ARG:CG	1:C:527:ARG:NH1	2.72	0.45
1:D:109:ASP:OD2	1:D:267:TYR:OH	2.31	0.45
1:D:336:TYR:N	1:D:336:TYR:HD1	2.13	0.45
1:A:178:ALA:O	1:A:182:SER:HB3	2.15	0.45
1:B:296:VAL:HG23	1:B:297:ILE:N	2.31	0.45
1:C:254:LYS:CE	1:C:258:ASP:O	2.61	0.45
1:C:185:LEU:HD23	1:C:429:THR:HB	1.98	0.45
1:D:315:GLU:OE2	1:D:350:SER:HA	2.16	0.45
1:D:581:HIS:CD2	1:D:581:HIS:O	2.69	0.45
1:A:281:LYS:HE3	1:A:283:GLY:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:562:GLU:O	1:A:565:SER:CB	2.64	0.45
1:B:584:ARG:O	1:B:585:ILE:CD1	2.59	0.45
1:C:232:ILE:HD12	1:C:352:LYS:O	2.16	0.45
1:C:376:HIS:O	1:C:377:GLN:HB2	2.17	0.45
1:C:470:ALA:O	1:C:474:ARG:HG2	2.16	0.45
1:C:573:TRP:HD1	1:C:573:TRP:O	1.99	0.45
1:D:516:ILE:CG2	1:D:517:ASN:N	2.79	0.45
1:D:581:HIS:O	1:D:581:HIS:CG	2.70	0.45
1:B:112:TYR:CD1	1:B:584:ARG:NH1	2.69	0.45
1:B:96:LEU:HB2	1:B:160:ILE:HG12	1.99	0.45
1:C:597:TYR:CD1	1:C:597:TYR:N	2.85	0.45
1:D:296:VAL:CG1	1:D:297:ILE:N	2.79	0.45
1:D:504:GLY:O	1:D:508:LEU:HB2	2.16	0.45
1:B:471:PHE:HD1	1:B:472:LEU:N	2.14	0.45
1:C:62:PRO:O	1:C:63:GLY:C	2.54	0.45
1:D:9:GLU:HG2	1:D:9:GLU:O	2.16	0.45
1:A:156:SER:HB3	1:A:175:PHE:CG	2.52	0.45
1:C:235:PHE:HD1	1:C:325:ASP:HB3	1.82	0.45
1:C:68:LYS:HE3	1:C:219:VAL:HB	1.99	0.45
1:D:471:PHE:C	1:D:473:GLU:N	2.69	0.45
1:D:479:ASP:OD1	1:D:480:LEU:N	2.50	0.45
1:A:116:ILE:O	1:A:116:ILE:HG13	2.17	0.45
1:A:91:MET:HG3	1:A:153:LEU:HD13	1.99	0.45
1:B:377:GLN:O	1:B:408:LEU:HB2	2.16	0.45
1:B:348:ILE:CG2	1:B:399:PHE:HB2	2.46	0.45
1:B:79:PRO:HD2	1:B:80:GLY:H	1.82	0.45
1:C:129:ASN:O	1:C:130:SER:C	2.53	0.45
1:C:188:LEU:HB3	1:C:273:ILE:CD1	2.46	0.45
1:C:317:HIS:N	1:C:328:GLU:OE2	2.42	0.45
1:C:358:LEU:CD2	1:C:361:ALA:HB3	2.46	0.45
1:D:256:ALA:O	1:D:260:VAL:HG22	2.16	0.45
1:A:42:THR:O	1:A:66:ALA:HA	2.17	0.45
1:B:358:LEU:O	1:B:362:ALA:N	2.50	0.45
1:D:192:PHE:O	1:D:196:GLN:HB2	2.16	0.45
1:D:454:SER:HB2	1:D:494:MET:H	1.82	0.45
1:A:372:SER:HB3	1:A:377:GLU:O	2.16	0.45
1:B:394:LEU:HA	1:B:397:SER:HB2	1.96	0.45
1:B:512:LEU:C	1:B:514:ASP:N	2.70	0.45
1:D:516:ILE:HG23	1:D:517:ASN:N	2.32	0.45
1:D:93:ASP:OD1	1:D:94:PRO:CD	2.65	0.45
1:A:278:GLY:C	1:A:280:ASP:N	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:456:ARG:O	1:B:457:LYS:CG	2.65	0.45
1:C:135:LEU:HA	1:C:136:PRO:HD3	1.86	0.45
1:C:535:ASP:OD1	1:C:539:LEU:HD12	2.16	0.45
1:D:317:HIS:O	1:D:352:LYS:HD2	2.17	0.45
1:A:128:ASN:C	1:A:129:SER:OG	2.55	0.44
1:A:68:SER:HB3	1:A:243:GLY:O	2.17	0.44
1:C:291:LYS:HA	1:C:291:LYS:HD2	1.68	0.44
1:C:538:TRP:CE3	1:C:539:LEU:HG	2.52	0.44
1:D:388:PRO:HB2	1:D:394:LEU:HD21	1.99	0.44
1:A:309:THR:HG22	1:A:309:THR:O	2.16	0.44
1:B:307:HIS:O	1:B:310:THR:CB	2.65	0.44
1:B:329:LEU:HD12	1:B:329:LEU:N	2.32	0.44
1:B:559:PRO:O	1:B:561:LEU:HG	2.16	0.44
1:C:125:SER:HB3	1:C:177:VAL:O	2.17	0.44
1:D:291:LYS:HA	1:D:291:LYS:HD3	1.72	0.44
1:D:324:GLY:C	1:D:326:PRO:CD	2.86	0.44
1:A:223:LEU:O	1:A:224:ASN:HB2	2.18	0.44
1:B:32:ASN:HA	1:B:35:LYS:HG2	1.99	0.44
1:B:34:ILE:HD12	1:B:369:LYS:HG3	1.99	0.44
1:B:497:ARG:HB3	1:B:565:TRP:CZ3	2.53	0.44
1:B:504:GLY:O	1:B:508:LEU:N	2.41	0.44
1:B:573:TRP:O	1:B:573:TRP:CE3	2.71	0.44
1:C:307:HIS:CE1	1:C:340:THR:HG1	2.30	0.44
1:D:329:LEU:CD1	1:D:399:PHE:CD2	3.00	0.44
1:D:473:GLU:O	1:D:474:ARG:C	2.53	0.44
1:B:114:SER:O	1:B:115:LYS:C	2.55	0.44
1:B:153:VAL:O	1:B:155:ALA:N	2.47	0.44
1:B:31:TRP:CE3	1:B:34:ILE:HD11	2.53	0.44
1:B:341:ASP:CG	1:B:342:LYS:N	2.69	0.44
1:C:233:LYS:CD	1:C:239:ALA:HA	2.47	0.44
1:D:269:LEU:HD13	1:D:436:TYR:HB2	1.99	0.44
1:D:313:TYR:HD1	1:D:347:GLY:O	1.99	0.44
1:A:167:LEU:CD1	1:A:167:LEU:N	2.80	0.44
1:A:292:GLN:HG2	1:A:421:PHE:CE2	2.52	0.44
1:B:337:GLY:C	1:B:339:TYR:N	2.70	0.44
1:B:346:CYS:O	1:B:399:PHE:CB	2.65	0.44
1:D:338:ARG:O	1:D:339:TYR:CD1	2.71	0.44
1:A:303:THR:HB	1:A:305:ILE:HG13	1.99	0.44
1:A:453:SER:HB2	1:A:493:MET:H	1.82	0.44
1:B:282:LYS:HB2	1:B:289:SER:HB3	2.00	0.44
1:B:282:LYS:HG3	1:B:287:ALA:CB	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:452:PRO:HD2	1:B:487:PHE:HB3	1.98	0.44
1:D:585:ILE:CG2	1:D:586:SER:N	2.81	0.44
1:A:31:TRP:CZ3	1:A:35:LYS:HD3	2.52	0.44
1:A:423:LEU:HA	1:A:423:LEU:HD12	1.84	0.44
1:B:43:PHE:CE1	1:B:67:ALA:CB	3.01	0.44
1:C:325:ASP:HB2	1:C:326:PRO:CD	2.48	0.44
1:C:541:ASP:HB3	1:C:545:SER:CB	2.30	0.44
1:C:61:HIS:CG	1:C:61:HIS:O	2.70	0.44
1:D:136:PRO:CD	1:D:138:GLU:OE2	2.65	0.44
1:A:274:VAL:HG22	1:A:428:THR:HG22	2.00	0.44
1:A:312:TYR:HB3	1:A:416:MET:HG2	1.98	0.44
1:B:39:GLU:HB2	1:B:383:ILE:HD12	1.98	0.44
1:B:526:PHE:CZ	1:B:560:LYS:HD3	2.52	0.44
1:C:548:LEU:O	1:C:551:LYS:HB2	2.18	0.44
1:D:254:LYS:HG2	1:D:255:LYS:N	2.32	0.44
1:D:390:PRO:O	1:D:393:HIS:HD2	2.00	0.44
1:B:308:PRO:HB3	1:B:336:TYR:CE2	2.52	0.43
1:B:373:SER:O	1:B:377:GLN:N	2.51	0.43
1:C:150:VAL:H	1:C:150:VAL:HG22	1.07	0.43
1:D:135:LEU:HB3	1:D:136:PRO:CD	2.48	0.43
1:D:224:LEU:HD13	1:D:225:ASN:H	1.83	0.43
1:D:346:CYS:HB3	1:D:399:PHE:HD1	1.78	0.43
1:D:595:GLU:HA	1:D:596:PRO:HD3	1.77	0.43
1:C:232:ILE:CD1	1:C:356:GLY:HA2	2.48	0.43
1:D:282:LYS:HE2	1:D:284:GLY:O	2.18	0.43
1:D:34:ILE:HD11	1:D:369:LYS:CE	2.48	0.43
1:D:408:LEU:HD23	1:D:408:LEU:HA	1.80	0.43
1:D:562:CYS:O	1:D:565:TRP:N	2.40	0.43
1:A:453:SER:CB	1:A:493:MET:H	2.31	0.43
1:B:385:TYR:OH	1:B:388:PRO:HB3	2.18	0.43
1:C:225:ASN:O	1:C:226:PHE:CG	2.70	0.43
1:C:585:ILE:HD13	1:C:585:ILE:HA	1.84	0.43
1:D:168:LEU:N	1:D:168:LEU:HD12	2.33	0.43
1:D:296:VAL:O	1:D:300:VAL:HG23	2.18	0.43
1:D:448:PRO:O	1:D:449:PHE:HD1	2.01	0.43
1:D:482:ASP:OD2	1:D:585:ILE:HG13	2.18	0.43
1:A:237:ASP:O	1:A:237:ASP:OD1	2.36	0.43
1:B:275:VAL:HG22	1:B:429:THR:HG22	2.01	0.43
1:C:311:ILE:CD1	1:C:311:ILE:N	2.80	0.43
1:C:414:ALA:HB1	1:C:435:GLN:HB3	2.00	0.43
1:D:336:TYR:O	1:D:338:ARG:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:570:ILE:O	1:A:572:TRP:HB2	2.18	0.43
1:A:56:GLU:C	1:A:63:PHE:N	2.72	0.43
1:B:64:PHE:HA	1:B:66:PRO:HD3	1.99	0.43
1:D:307:HIS:O	1:D:310:THR:HB	2.19	0.43
1:A:339:THR:HG22	1:A:340:ASP:N	2.32	0.43
1:B:480:LEU:CA	1:B:483:LEU:HB3	2.37	0.43
1:A:459:ARG:HA	1:A:459:ARG:HD3	1.74	0.43
1:B:282:LYS:HG2	1:B:287:ALA:HB3	1.97	0.43
1:C:332:LEU:HD23	1:C:399:PHE:CZ	2.53	0.43
1:D:344:GLN:CA	1:D:398:PRO:C	2.78	0.43
1:D:573:TRP:O	1:D:573:TRP:CG	2.71	0.43
1:A:22:PRO:HD3	1:A:245:GLU:O	2.19	0.43
1:B:68:LYS:HB3	1:B:68:LYS:HE3	1.74	0.43
1:C:548:LEU:HD22	1:C:551:LYS:HD2	2.00	0.43
1:D:324:GLY:C	1:D:326:PRO:HD2	2.39	0.43
1:D:336:TYR:C	1:D:338:ARG:N	2.71	0.43
1:D:455:ALA:HB3	1:D:461:LEU:HB2	2.00	0.43
1:A:119:THR:HG23	1:A:201:TYR:HB2	2.00	0.43
1:A:315:ALA:CB	1:A:327:GLU:OE2	2.57	0.43
1:B:232:ILE:HG13	1:B:243:ILE:HG22	2.00	0.43
1:B:271:ARG:CZ	1:B:271:ARG:HB3	2.47	0.43
1:B:551:LYS:HB3	1:B:552:TRP:HE3	1.83	0.43
1:D:150:VAL:O	1:D:150:VAL:HG12	2.18	0.43
1:A:481:ASP:OD2	1:A:582:LYS:HE2	2.19	0.43
1:A:483:ALA:O	1:A:487:GLN:HG3	2.19	0.43
1:A:504:THR:O	1:A:507:LEU:HB3	2.19	0.43
1:B:194:SER:O	1:B:199:GLU:HG2	2.18	0.43
1:C:270:LEU:HD11	1:C:273:ILE:CG1	2.47	0.43
1:C:545:SER:C	1:C:549:ILE:HG22	2.40	0.43
1:A:363:MET:O	1:A:367:ILE:HG13	2.19	0.42
1:C:233:LYS:O	1:C:320:GLY:CA	2.63	0.42
1:C:358:LEU:HD23	1:C:361:ALA:HB1	2.01	0.42
1:C:545:SER:OG	1:C:549:ILE:HD13	2.19	0.42
1:D:113:ILE:HD12	1:D:116:GLU:OE1	2.18	0.42
1:A:500:ILE:HG22	1:A:523:GLY:HA3	2.01	0.42
1:B:120:THR:O	1:B:172:GLY:CA	2.66	0.42
1:B:516:ILE:C	1:B:518:ASP:H	2.21	0.42
1:C:459:ASP:OD1	1:C:459:ASP:N	2.52	0.42
1:C:559:PRO:C	1:C:561:LEU:N	2.72	0.42
1:D:317:HIS:CB	1:D:328:GLU:OE2	2.67	0.42
1:D:313:TYR:HB3	1:D:417:MET:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:485:TYR:HB2	1:D:582:PRO:HB2	2.01	0.42
1:A:133:LEU:HD12	1:A:133:LEU:N	2.33	0.42
1:A:12:LEU:HD22	1:A:194:LEU:HD13	1.98	0.42
1:C:474:ARG:NH2	1:A:338:TYR:C	2.73	0.42
1:A:471:LEU:HA	1:A:471:LEU:HD23	1.76	0.42
1:B:318:GLY:HA3	1:B:350:SER:HB2	2.02	0.42
1:C:317:HIS:CD2	1:C:319:THR:HG23	2.54	0.42
1:C:482:ASP:HB3	1:C:585:ILE:CG1	2.49	0.42
1:D:201:LYS:HE3	1:D:254:LYS:CE	2.47	0.42
1:D:237:ALA:O	1:D:238:ASP:CB	2.66	0.42
1:B:346:CYS:O	1:B:399:PHE:CA	2.67	0.42
1:D:134:LEU:HB3	1:D:599:PRO:HG2	2.00	0.42
1:D:301:ILE:HA	1:D:304:THR:HG1	1.84	0.42
1:D:43:PHE:N	1:D:43:PHE:CD1	2.87	0.42
1:A:98:LEU:HA	1:A:98:LEU:HD23	1.86	0.42
1:B:257:SER:O	1:B:260:VAL:CG2	2.68	0.42
1:B:295:GLU:O	1:B:299:LYS:HB2	2.19	0.42
1:C:547:GLU:O	1:C:551:LYS:HG3	2.20	0.42
1:D:183:SER:O	1:D:186:ILE:HB	2.19	0.42
1:D:186:ILE:HD13	1:D:186:ILE:HA	1.89	0.42
1:D:234:ALA:O	1:D:235:PHE:C	2.57	0.42
1:B:233:LYS:O	1:B:239:ALA:HB2	2.19	0.42
1:B:246:GLU:CA	1:B:358:LEU:CD2	2.97	0.42
1:B:373:SER:HB3	1:B:378:GLU:O	2.19	0.42
1:B:414:ALA:CB	1:B:435:GLN:HB3	2.45	0.42
1:C:552:TRP:NE1	1:C:557:LYS:CE	2.83	0.42
1:D:7:TYR:CE1	1:D:434:GLU:OE2	2.72	0.42
1:C:464:TYR:HH	1:C:487:PHE:HE1	1.65	0.42
1:D:489:VAL:O	1:D:489:VAL:HG23	2.20	0.42
1:D:64:PHE:CG	1:D:65:VAL:N	2.86	0.42
1:B:397:SER:HA	1:B:398:PRO:HD2	1.84	0.42
1:D:307:HIS:O	1:D:310:THR:CB	2.68	0.42
1:A:570:ILE:HG23	1:A:572:TRP:CD1	2.54	0.42
1:A:68:SER:O	1:A:68:SER:OG	2.29	0.42
1:B:128:THR:O	1:B:128:THR:OG1	2.35	0.42
1:B:488:GLN:HB3	1:B:572:ASN:HB3	2.01	0.42
1:C:105:LYS:HG2	1:C:589:VAL:CG2	2.43	0.42
1:C:77:PHE:CD1	1:C:78:ASP:N	2.87	0.42
1:D:22:PRO:HD2	1:D:355:LEU:HD22	2.02	0.42
1:D:515:PHE:O	1:D:515:PHE:CG	2.72	0.42
1:D:561:LEU:HA	1:D:561:LEU:HD12	1.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:583:LYS:O	1:D:585:ILE:HG12	2.20	0.42
1:A:521:VAL:HB	1:A:522:THR:HG23	2.02	0.42
1:C:12:LEU:CD1	1:C:192:PHE:HD1	2.32	0.42
1:C:233:LYS:HD3	1:C:238:ASP:C	2.35	0.42
1:C:272:GLY:O	1:C:273:ILE:HG13	2.19	0.42
1:C:297:ILE:HG23	1:C:430:HIS:CD2	2.54	0.42
1:D:562:CYS:O	1:D:563:GLU:C	2.59	0.42
1:A:180:CYS:HB2	1:A:422:GLY:HA2	2.01	0.41
1:B:39:GLU:HB2	1:B:383:ILE:CD1	2.50	0.41
1:B:8:TYR:CZ	1:B:269:LEU:HD21	2.55	0.41
1:C:328:GLU:HG3	1:C:422:PHE:HE2	1.85	0.41
1:C:92:MET:HG2	1:C:96:LEU:HD23	2.02	0.41
1:D:340:THR:O	1:D:342:LYS:CD	2.68	0.41
1:A:39:GLU:OE2	1:A:230:HIS:CD2	2.72	0.41
1:B:223:GLY:O	1:B:224:LEU:CG	2.68	0.41
1:B:594:LYS:HE3	1:B:594:LYS:HB2	1.76	0.41
1:C:304:THR:O	1:C:305:GLY:C	2.58	0.41
1:D:136:PRO:O	1:D:138:GLU:HG3	2.20	0.41
1:D:474:ARG:NH1	1:D:586:SER:O	2.38	0.41
1:D:237:ALA:O	1:D:238:ASP:HB2	2.21	0.41
1:D:41:ILE:CG2	1:D:42:THR:N	2.83	0.41
1:D:497:ARG:HD3	1:D:565:TRP:CE3	2.56	0.41
1:A:156:SER:HB3	1:A:175:PHE:CD1	2.55	0.41
1:B:282:LYS:HG3	1:B:287:ALA:HB3	2.02	0.41
1:B:497:ARG:H	1:B:528:GLY:HA3	1.84	0.41
1:B:557:LYS:HD3	1:B:574:HIS:CB	2.50	0.41
1:C:392:LEU:HB3	1:C:394:LEU:HD21	2.01	0.41
1:D:73:GLY:HA3	1:D:76:MET:HE2	2.01	0.41
1:C:225:ASN:O	1:C:226:PHE:CB	2.69	0.41
1:C:351:VAL:HG22	1:C:351:VAL:O	2.19	0.41
1:D:313:TYR:HA	1:D:347:GLY:O	2.19	0.41
1:D:34:ILE:HG23	1:D:35:LYS:N	2.36	0.41
1:C:552:TRP:CZ3	1:C:564:MET:HG3	2.56	0.41
1:C:77:PHE:CD2	1:C:97:ARG:HD3	2.54	0.41
1:B:342:LYS:O	1:B:343:LYS:CB	2.69	0.41
1:B:374:LEU:HD22	1:B:435:GLN:HB2	2.02	0.41
1:B:501:ILE:HG23	1:B:501:ILE:O	2.20	0.41
1:C:77:PHE:CG	1:C:78:ASP:N	2.89	0.41
1:A:159:ILE:HB	1:A:160:PRO:CD	2.50	0.41
1:A:516:ASN:O	1:A:519:PRO:CD	2.68	0.41
1:B:386:LYS:HB3	1:B:386:LYS:HE2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:VAL:HG22	1:B:418:ALA:HB3	2.01	0.41
1:C:160:ILE:HB	1:C:161:PRO:CD	2.50	0.41
1:D:201:LYS:CG	1:D:202:TYR:CE1	2.98	0.41
1:A:388:ASN:O	1:A:391:LEU:HB2	2.21	0.41
1:A:456:LYS:O	1:A:459:ARG:HB2	2.20	0.41
1:B:456:ARG:CD	1:B:495:GLU:OE2	2.68	0.41
1:C:127:SER:OG	1:C:209:THR:HA	2.21	0.41
1:C:31:TRP:CH2	1:C:35:LYS:HE3	2.56	0.41
1:C:61:HIS:CD2	1:C:61:HIS:O	2.74	0.41
1:D:138:GLU:C	1:D:146:PRO:CD	2.89	0.41
1:D:486:THR:CG2	1:D:486:THR:O	2.68	0.41
1:B:342:LYS:O	1:B:343:LYS:CG	2.69	0.41
1:B:512:LEU:O	1:B:515:PHE:N	2.54	0.41
1:B:551:LYS:HB3	1:B:552:TRP:CE3	2.56	0.41
1:D:515:PHE:CE1	1:D:518:ASP:CA	3.04	0.41
1:B:246:GLU:CA	1:B:358:LEU:HD22	2.51	0.41
1:B:310:THR:O	1:B:310:THR:HG22	2.21	0.41
1:B:337:GLY:O	1:B:339:TYR:N	2.54	0.41
1:B:185:LEU:CD2	1:B:429:THR:HB	2.51	0.41
1:C:154:LEU:HA	1:C:154:LEU:HD23	1.81	0.41
1:C:553:LEU:HD12	1:C:574:HIS:O	2.20	0.41
1:D:229:ASP:OD1	1:D:233:LYS:HE2	2.21	0.41
1:D:278:ASP:OD1	1:D:426:GLY:HA2	2.21	0.41
1:D:236:ASP:HB2	1:D:385:TYR:CD1	2.56	0.41
1:C:571:ILE:CG2	1:C:571:ILE:O	2.69	0.40
1:D:160:ILE:HB	1:D:161:PRO:HD3	2.03	0.40
1:D:317:HIS:O	1:D:352:LYS:CD	2.68	0.40
1:D:64:PHE:CE1	1:D:66:PRO:HB3	2.56	0.40
1:B:202:TYR:CZ	1:B:254:LYS:HE3	2.55	0.40
1:B:258:ASP:O	1:B:262:ASP:HB2	2.20	0.40
1:B:483:LEU:CD2	1:B:483:LEU:C	2.89	0.40
1:B:587:LEU:CB	1:B:588:PRO:CD	2.99	0.40
1:B:286:TYR:CD1	1:B:286:TYR:N	2.89	0.40
1:B:66:PRO:CD	1:B:67:ALA:H	2.35	0.40
1:C:313:TYR:OH	1:C:349:GLY:HA3	2.22	0.40
1:C:341:ASP:CG	1:C:342:LYS:N	2.73	0.40
1:C:434:GLU:HG2	1:C:435:GLN:N	2.35	0.40
1:C:95:GLN:NE2	1:C:129:ASN:CG	2.75	0.40
1:D:317:HIS:CA	1:D:328:GLU:OE2	2.70	0.40
1:D:457:LYS:HA	1:D:496:GLU:OE1	2.21	0.40
1:A:51:ARG:CG	1:A:52:SER:N	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:SER:O	1:B:133:SER:HB2	2.22	0.40
1:B:493:ALA:HB1	1:B:497:ARG:NH1	2.37	0.40
1:C:316:ALA:HB1	1:C:328:GLU:CD	2.42	0.40
1:C:436:TYR:HA	1:C:437:PRO:HD3	1.87	0.40
1:C:511:GLN:NE2	1:C:524:GLY:CA	2.80	0.40
1:C:517:ASN:O	1:C:518:ASP:HB3	2.21	0.40
1:C:553:LEU:HD12	1:C:574:HIS:HB3	2.02	0.40
1:D:178:HIS:CE1	1:D:180:ASN:HA	2.56	0.40
1:D:290:VAL:HG23	1:D:331:ALA:HB2	2.03	0.40
1:D:247:GLY:N	1:D:358:LEU:HD22	2.36	0.40
1:A:391:LEU:HA	1:A:391:LEU:HD23	1.89	0.40
1:A:64:VAL:CG2	1:A:64:VAL:O	2.69	0.40
1:B:313:TYR:OH	1:B:349:GLY:CA	2.68	0.40
1:C:232:ILE:HD12	1:C:356:GLY:HA2	2.03	0.40
1:C:275:VAL:HG22	1:C:429:THR:HG22	2.03	0.40
1:D:222:PRO:HG3	1:D:228:SER:HA	2.03	0.40

All (7) 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:155:GLN:OE1	1:D:128:THR:OG1[1_556]	1.71	0.49
1:C:284:GLY:O	1:B:166:HIS:CD2[1_565]	1.78	0.42
1:B:477:ASP:OD2	1:D:223:GLY:O[1_655]	1.95	0.25
1:C:284:GLY:C	1:B:166:HIS:NE2[1_565]	2.03	0.17
1:C:284:GLY:O	1:B:166:HIS:CE1[1_565]	2.06	0.14
1:C:284:GLY:CA	1:B:166:HIS:NE2[1_565]	2.11	0.09
1:B:87:LYS:CD	1:D:507:GLU:OE2[1_545]	2.15	0.05

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	526/622 (85%)	483 (92%)	34 (6%)	9 (2%)	11	37
1	B	529/622 (85%)	473 (89%)	48 (9%)	8 (2%)	13	41
1	C	543/622 (87%)	485 (89%)	48 (9%)	10 (2%)	11	36
1	D	505/622 (81%)	461 (91%)	38 (8%)	6 (1%)	16	47
All	All	2103/2488 (84%)	1902 (90%)	168 (8%)	33 (2%)	12	39

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	226	PHE
1	C	288	PRO
1	C	554	ALA
1	A	447	PRO
1	A	571	ASN
1	B	343	LYS
1	B	448	PRO
1	B	452	PRO
1	D	225	ASN
1	D	343	LYS
1	C	62	PRO
1	C	343	LYS
1	B	342	LYS
1	C	342	LYS
1	C	560	LYS
1	A	279	ALA
1	A	558	PRO
1	A	568	VAL
1	B	559	PRO
1	D	224	LEU
1	C	308	PRO
1	C	341	ASP
1	B	437	PRO
1	A	569	ALA
1	B	326	PRO
1	D	238	ASP
1	D	448	PRO
1	A	135	PRO
1	A	567	GLY
1	D	599	PRO
1	B	519	LYS
1	C	66	PRO
1	A	222	GLY

### 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	439/506 (87%)	417 (95%)	22 (5%)	30	64
1	B	442/506 (87%)	426 (96%)	16 (4%)	42	76
1	C	453/506 (90%)	427 (94%)	26 (6%)	25	58
1	D	425/506 (84%)	399 (94%)	26 (6%)	23	55
All	All	1759/2024 (87%)	1669 (95%)	90 (5%)	29	64

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	7	TYR
1	C	8	TYR
1	C	11	SER
1	C	45	SER
1	C	46	LYS
1	C	49	LEU
1	C	62	PRO
1	C	119	GLU
1	C	127	SER
1	C	150	VAL
1	C	152	TRP
1	C	221	GLN
1	C	224	LEU
1	C	242	MET
1	C	308	PRO
1	C	310	THR
1	C	338	ARG
1	C	340	THR
1	C	343	LYS
1	C	404	GLU
1	C	405	LYS
1	C	501	ILE
1	C	525	CYS
1	C	527	ARG

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Mol	Chain	Res	Type
1	C	545	SER
1	C	573	TRP
1	A	11	SER
1	A	47	GLU
1	A	49	LEU
1	A	50	ARG
1	A	54	ILE
1	A	55	SER
1	A	102	SER
1	A	113	SER
1	A	114	LYS
1	A	129	SER
1	A	136	GLU
1	A	139	THR
1	A	275	ASN
1	A	367	ILE
1	A	436	PRO
1	A	459	ARG
1	A	463	TYR
1	A	473	ARG
1	A	510	GLN
1	A	565	SER
1	A	568	VAL
1	A	571	ASN
1	B	55	SER
1	B	57	GLU
1	B	114	SER
1	B	233	LYS
1	B	255	LYS
1	B	257	SER
1	B	308	PRO
1	B	343	LYS
1	B	399	PHE
1	B	406	LYS
1	B	407	GLU
1	B	464	TYR
1	B	471	PHE
1	B	476	THR
1	B	514	ASP
1	B	572	ASN
1	D	7	TYR
1	D	20	GLU

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Mol	Chain	Res	Type
1	D	64	PHE
1	D	114	SER
1	D	125	SER
1	D	149	TYR
1	D	195	LEU
1	D	224	LEU
1	D	233	LYS
1	D	238	ASP
1	D	282	LYS
1	D	342	LYS
1	D	343	LYS
1	D	345	TYR
1	D	394	LEU
1	D	407	GLU
1	D	410	ARG
1	D	456	ARG
1	D	457	LYS
1	D	464	TYR
1	D	476	THR
1	D	478	THR
1	D	501	ILE
1	D	567	LYS
1	D	571	ILE
1	D	584	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	95	GLN
1	C	221	GLN
1	C	307	HIS
1	C	317	HIS
1	C	511	GLN
1	C	581	HIS
1	A	230	HIS
1	A	297	GLN
1	A	375	HIS
1	A	466	GLN
1	A	571	ASN
1	A	580	HIS
1	B	178	HIS
1	B	196	GLN

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Mol	Chain	Res	Type
1	B	231	HIS
1	B	265	HIS
1	B	317	HIS
1	B	435	GLN
1	B	511	GLN
1	D	178	HIS
1	D	221	GLN
1	D	225	ASN
1	D	307	HIS
1	D	317	HIS
1	D	391	ASN
1	D	393	HIS
1	D	488	GLN
1	D	581	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	540/622 (86%)	0.07	9 (1%) 73 72	23, 48, 87, 109	0
1	B	547/622 (87%)	0.30	24 (4%) 38 34	24, 62, 100, 121	0
1	C	557/622 (89%)	0.32	25 (4%) 37 33	23, 55, 104, 162	0
1	D	523/622 (84%)	0.44	39 (7%) 17 13	24, 63, 108, 133	0
All	All	2167/2488 (87%)	0.28	97 (4%) 37 33	23, 57, 101, 162	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	548	LEU	8.3
1	D	503	SER	6.4
1	D	240	ASP	5.3
1	B	572	ASN	5.3
1	D	471	PHE	5.0
1	D	404	GLU	4.9
1	C	532	GLN	4.8
1	C	538	TRP	4.5
1	C	288	PRO	4.3
1	C	340	THR	4.3
1	C	341	ASP	4.3
1	D	505	THR	4.3
1	D	512	LEU	3.9
1	A	412	ARG	3.9
1	D	495	GLU	3.9
1	B	340	THR	3.7
1	B	509	LYS	3.7
1	D	474	ARG	3.5
1	A	69	VAL	3.5
1	D	473	GLU	3.5
1	C	476	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	517	ASN	3.4
1	C	235	PHE	3.4
1	C	555	LYS	3.3
1	C	233	LYS	3.2
1	D	560	LYS	3.2
1	B	329	LEU	3.2
1	D	528	GLY	3.1
1	D	469	LEU	3.1
1	C	225	ASN	3.1
1	D	239	ALA	3.0
1	D	516	ILE	3.0
1	B	519	LYS	3.0
1	D	235	PHE	2.9
1	C	359	ASP	2.9
1	D	34	ILE	2.9
1	D	329	LEU	2.9
1	D	563	GLU	2.9
1	D	341	ASP	2.9
1	B	154	LEU	2.8
1	C	523	THR	2.8
1	B	445	ALA	2.8
1	D	325	ASP	2.8
1	D	453	LEU	2.8
1	B	561	LEU	2.8
1	B	569	VAL	2.7
1	A	223	LEU	2.7
1	B	230	GLY	2.7
1	C	552	TRP	2.7
1	A	521	VAL	2.7
1	D	322	LYS	2.7
1	A	146	ASP	2.6
1	A	232	LYS	2.6
1	D	35	LYS	2.6
1	D	514	ASP	2.6
1	D	365	ALA	2.6
1	C	547	GLU	2.6
1	B	547	GLU	2.6
1	C	536	ILE	2.6
1	D	564	MET	2.5
1	A	578	ASP	2.5
1	B	253	LEU	2.5
1	B	319	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	517	ASN	2.5
1	B	568	GLY	2.5
1	C	543	ASP	2.4
1	D	581	HIS	2.4
1	D	283	VAL	2.4
1	C	258	ASP	2.4
1	C	73	GLY	2.4
1	B	480	LEU	2.4
1	D	416	ARG	2.4
1	C	360	THR	2.4
1	D	74	LYS	2.3
1	A	354	LEU	2.3
1	C	302	ASP	2.3
1	B	443	ALA	2.3
1	B	499	ALA	2.3
1	D	399	PHE	2.2
1	D	526	PHE	2.2
1	C	240	ASP	2.2
1	B	476	THR	2.2
1	C	295	GLU	2.2
1	D	323	LEU	2.2
1	D	191	ALA	2.1
1	B	515	PHE	2.1
1	C	358	LEU	2.1
1	D	472	LEU	2.1
1	D	504	GLY	2.1
1	D	561	LEU	2.1
1	B	278	ASP	2.1
1	B	224	LEU	2.0
1	B	317	HIS	2.0
1	A	574	LYS	2.0
1	C	284	GLY	2.0
1	B	348	ILE	2.0
1	D	456	ARG	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.