



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:32 PM GMT

PDB ID : 1KPK  
Title : Crystal Structure of the ClC Chloride Channel from E. coli  
Authors : Dutzler, R.; Campbell, E.B.; Cadene, M.; Chait, B.T.; MacKinnon, R.  
Deposited on : 2001-12-31  
Resolution : 3.50 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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

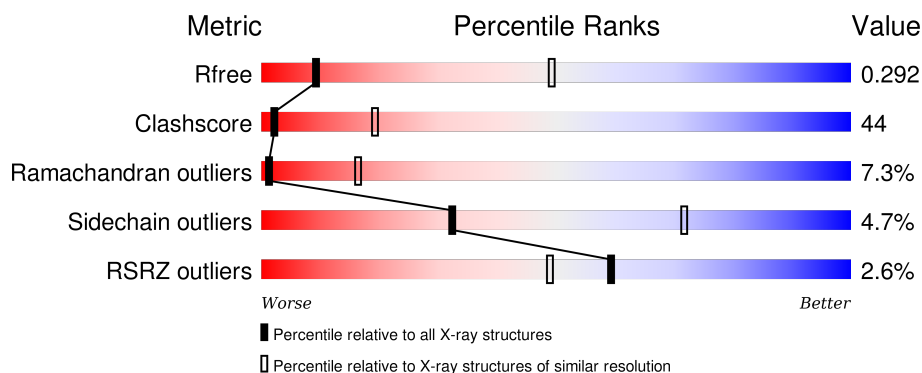
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 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.



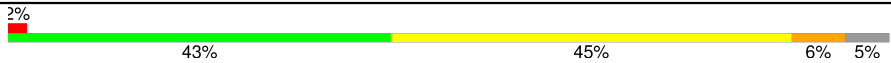
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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	473	
1	B	473	
1	C	473	
1	D	473	
1	E	473	

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Mol	Chain	Length	Quality of chain
1	F	473	 A horizontal bar chart showing the quality of chain F. The bar is divided into five segments: a small red segment at the beginning labeled '2%', followed by a green segment labeled '43%', a yellow segment labeled '45%', an orange segment labeled '6%', and a small grey segment at the end labeled '5%'.

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 20274 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.

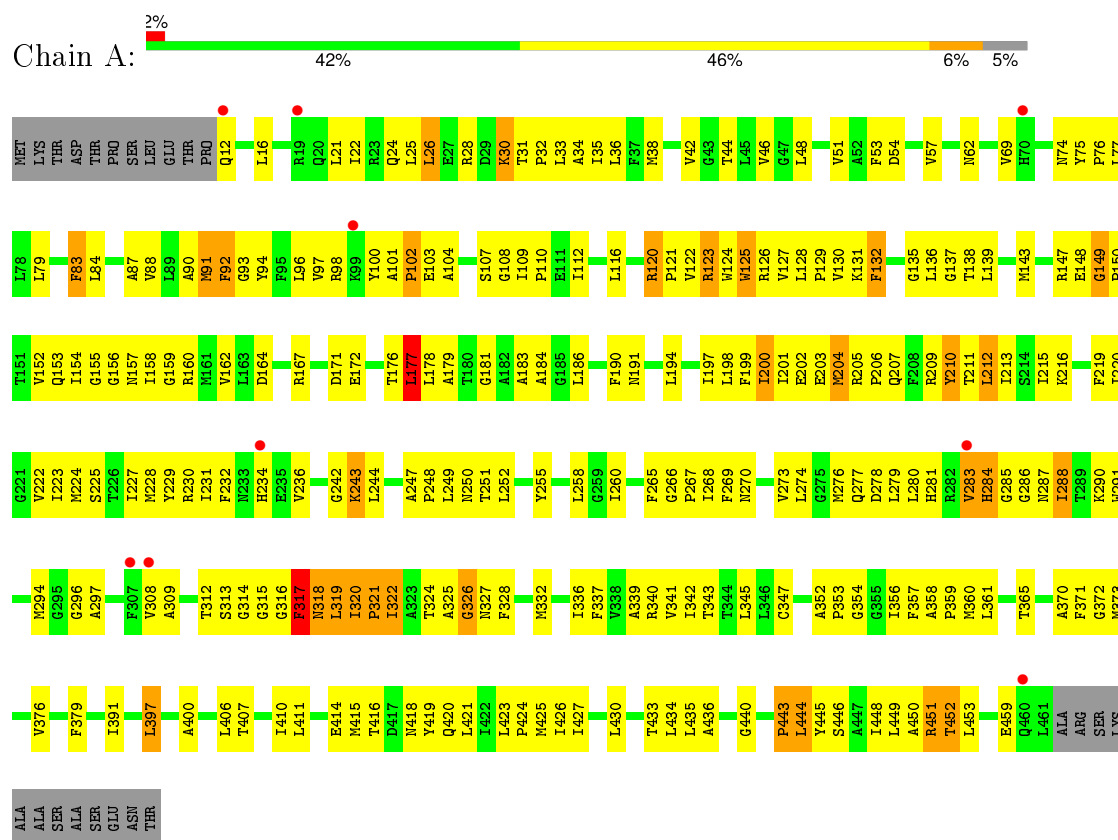
- Molecule 1 is a protein called putative channel transporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	450	Total	C	N	O	S	0	0	0
			3379	2219	570	570	20			
1	B	450	Total	C	N	O	S	0	0	0
			3379	2219	570	570	20			
1	C	450	Total	C	N	O	S	0	0	0
			3379	2219	570	570	20			
1	D	450	Total	C	N	O	S	0	0	0
			3379	2219	570	570	20			
1	E	450	Total	C	N	O	S	0	0	0
			3379	2219	570	570	20			
1	F	450	Total	C	N	O	S	0	0	0
			3379	2219	570	570	20			

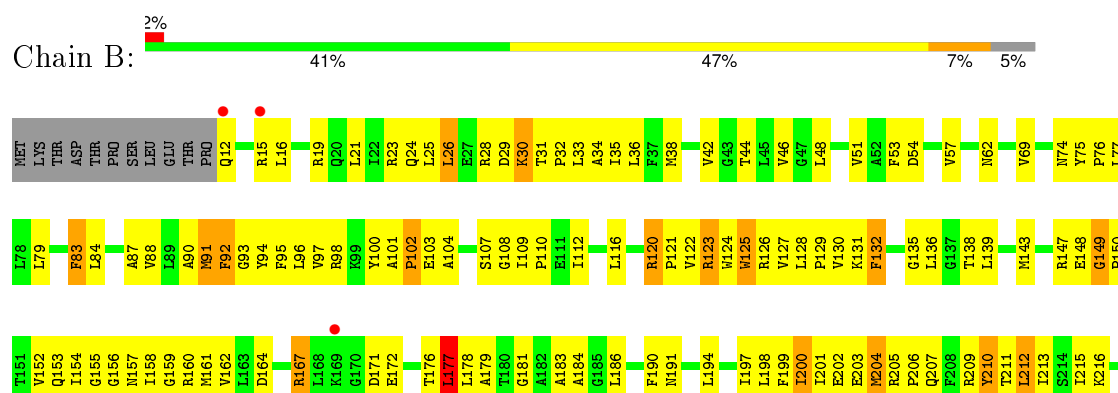
### 3 Residue-property plots

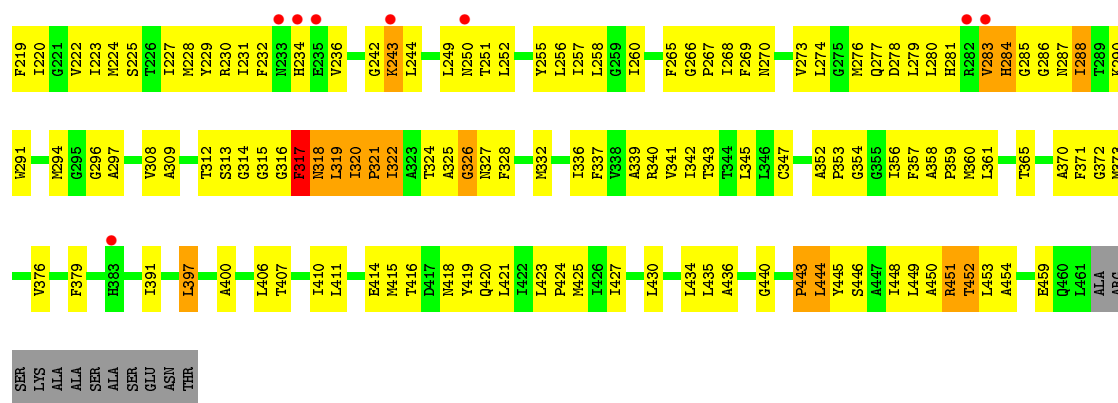
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: putative channel transporter

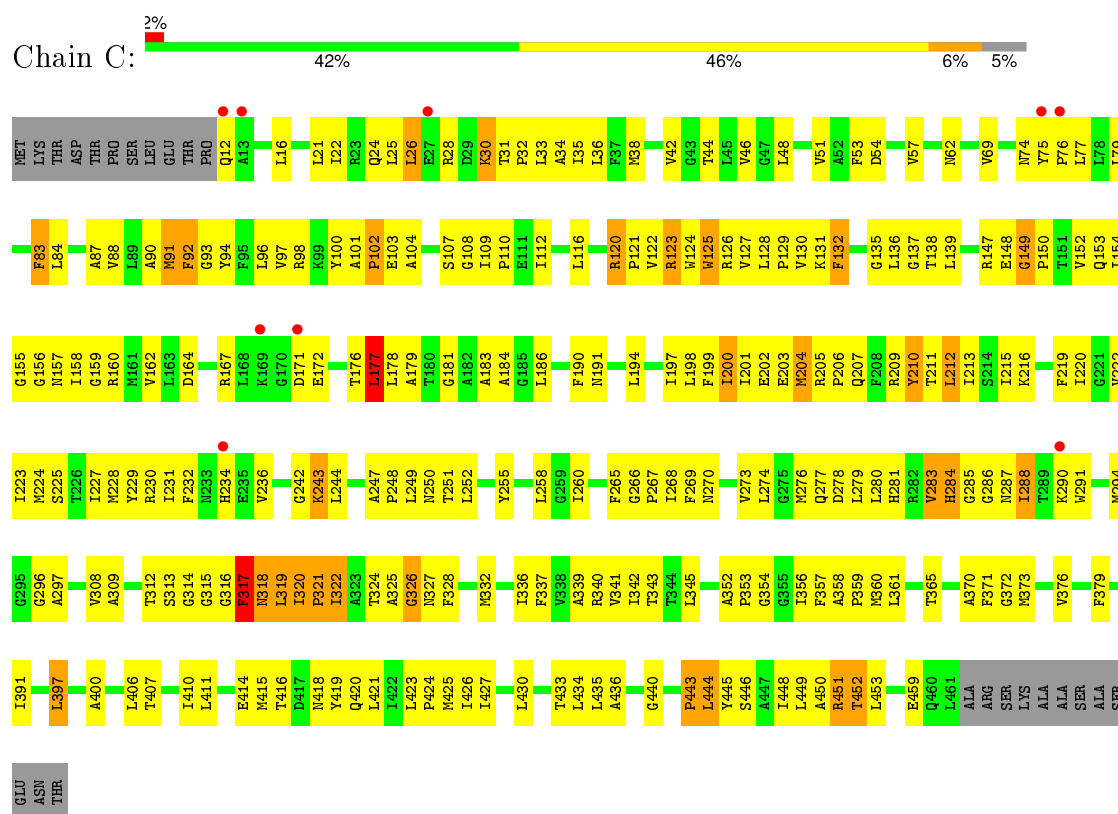


- Molecule 1: putative channel transporter

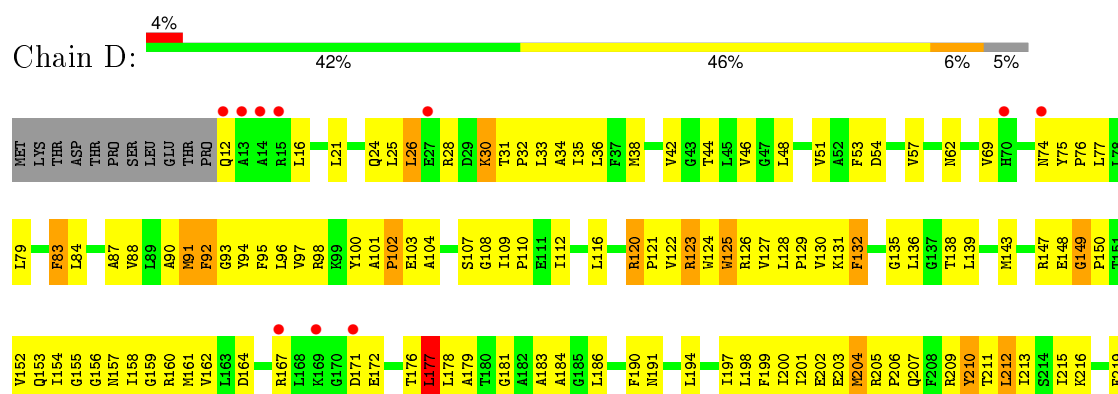


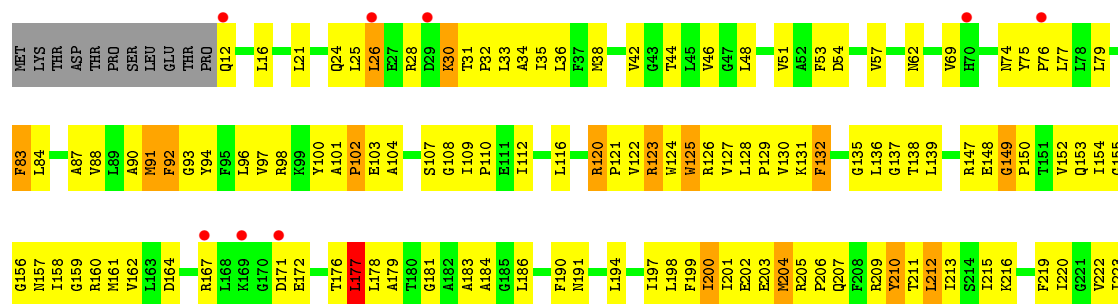


• Molecule 1: putative channel transporter



• Molecule 1: putative channel transporter





M224	V308	A400
S225	A309	L406
T226		T407
T227		
M228	T312	T410
Y229	S313	L411
P230	G314	
T231	G315	E414
F232	G316	M415
M233	F317	T416
M234	N318	D417
E235	L319	M418
V236	L320	Y419
	P321	Q420
	I322	L421
G242	A323	L422
E243	T324	L423
L244	A325	P424
	G326	M425
L249	N327	L426
N250	F328	T427
T251		
L252	M332	L430
L255		L434
	I336	L435
	F337	A436
L258	V338	
G259	A339	G440
T260	R340	
	V341	P443
F265	I342	L444
G266	T343	Y445
P267	T344	S446
L268	L345	L447
F269		T448
N270		L449
	A352	A450
	P353	R451
V273	G354	T452
L274	G355	L453
G275	I356	A454
M276	F357	
Q277	A358	E459
D278	P359	Q460
L279	M360	L461
L280	L361	ALA
H281		ARG
R282	T365	SER
V283		LYS
H284	A370	ALA
G285	F371	ALA
G286	G372	SER
N287	M373	ALA
I288		SER
T289	V376	ALA
K290		SER
H291	F379	GLU
		ASN
	I391	THR
M294		
G295		
G296		
A297		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.66 Å   152.53 Å   263.06 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	20.00 – 3.50 19.97 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (20.00-3.50) 99.4 (19.97-3.50)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.58 (at 3.52 Å)	Xtriage
Refinement program	CNS 0.3	Depositor
R, $R_{free}$	0.290   ,   0.301 0.285   ,   0.292	Depositor DCC
$R_{free}$ test set	5321 reflections (9.90%)	DCC
Wilson B-factor (Å <sup>2</sup> )	125.9	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 55.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 53763 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	20274	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.85% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.49	0/3451	0.76	2/4683 (0.0%)
1	B	0.49	0/3451	0.76	2/4683 (0.0%)
1	C	0.49	0/3451	0.76	2/4683 (0.0%)
1	D	0.49	0/3451	0.76	2/4683 (0.0%)
1	E	0.49	0/3451	0.76	2/4683 (0.0%)
1	F	0.49	0/3451	0.76	2/4683 (0.0%)
All	All	0.49	0/20706	0.76	12/28098 (0.0%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	320	ILE	N-CA-C	5.97	127.11	111.00
1	F	320	ILE	N-CA-C	5.97	127.11	111.00
1	A	320	ILE	N-CA-C	5.96	127.10	111.00
1	C	320	ILE	N-CA-C	5.95	127.06	111.00
1	B	320	ILE	N-CA-C	5.95	127.06	111.00
1	E	320	ILE	N-CA-C	5.94	127.05	111.00
1	F	327	ASN	N-CA-C	5.88	126.87	111.00
1	B	327	ASN	N-CA-C	5.88	126.87	111.00
1	A	327	ASN	N-CA-C	5.87	126.85	111.00
1	C	327	ASN	N-CA-C	5.87	126.85	111.00
1	E	327	ASN	N-CA-C	5.87	126.84	111.00
1	D	327	ASN	N-CA-C	5.86	126.82	111.00

There are no chirality outliers.

There are no planarity outliers.

### 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	3379	0	3537	338	0
1	B	3379	0	3537	336	52
1	C	3379	0	3537	336	1
1	D	3379	0	3537	337	4
1	E	3379	0	3537	332	49
1	F	3379	0	3537	335	0
All	All	20274	0	21222	1844	53

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 44.

All (1844) 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:D:200:ILE:HD13	1:D:204:MET:HG3	1.38	1.06
1:F:200:ILE:HD13	1:F:204:MET:HG3	1.38	1.05
1:B:200:ILE:HD13	1:B:204:MET:HG3	1.38	1.05
1:E:200:ILE:HD13	1:E:204:MET:HG3	1.38	1.05
1:F:322:ILE:HD12	1:F:322:ILE:N	1.74	1.03
1:C:322:ILE:HD12	1:C:322:ILE:N	1.74	1.02
1:A:322:ILE:N	1:A:322:ILE:HD12	1.74	1.01
1:A:200:ILE:HD13	1:A:204:MET:HG3	1.38	1.01
1:D:322:ILE:N	1:D:322:ILE:HD12	1.74	1.01
1:E:322:ILE:HD12	1:E:322:ILE:N	1.74	1.01
1:B:322:ILE:HD12	1:B:322:ILE:N	1.74	1.01
1:C:200:ILE:HD13	1:C:204:MET:HG3	1.38	1.01
1:A:120:ARG:HB3	1:A:120:ARG:NH1	1.80	0.96
1:E:120:ARG:HB3	1:E:120:ARG:NH1	1.80	0.96
1:F:322:ILE:H	1:F:322:ILE:HD12	1.30	0.96
1:C:120:ARG:HB3	1:C:120:ARG:NH1	1.80	0.96
1:F:120:ARG:HH11	1:F:120:ARG:HB3	1.31	0.95
1:B:120:ARG:NH1	1:B:120:ARG:HB3	1.80	0.95
1:F:120:ARG:NH1	1:F:120:ARG:HB3	1.80	0.95
1:D:120:ARG:HB3	1:D:120:ARG:NH1	1.80	0.95
1:B:322:ILE:H	1:B:322:ILE:HD12	1.29	0.94
1:E:430:LEU:HD21	1:F:220:ILE:HG12	1.48	0.94
1:C:322:ILE:H	1:C:322:ILE:HD12	1.29	0.93
1:C:430:LEU:HD21	1:D:220:ILE:HG12	1.48	0.93
1:D:322:ILE:H	1:D:322:ILE:HD12	1.30	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:120:ARG:HB3	1:E:120:ARG:HH11	1.31	0.93
1:B:120:ARG:HH11	1:B:120:ARG:HB3	1.31	0.93
1:D:120:ARG:HB3	1:D:120:ARG:HH11	1.31	0.93
1:A:430:LEU:HD21	1:B:220:ILE:HG12	1.48	0.93
1:A:322:ILE:H	1:A:322:ILE:HD12	1.29	0.92
1:A:120:ARG:HB3	1:A:120:ARG:HH11	1.31	0.92
1:E:104:ALA:HB1	1:E:131:LYS:HD3	1.52	0.92
1:C:104:ALA:HB1	1:C:131:LYS:HD3	1.52	0.91
1:F:104:ALA:HB1	1:F:131:LYS:HD3	1.52	0.91
1:D:123:ARG:HH11	1:D:123:ARG:H	0.91	0.91
1:C:120:ARG:HB3	1:C:120:ARG:HH11	1.31	0.91
1:A:104:ALA:HB1	1:A:131:LYS:HD3	1.52	0.91
1:B:123:ARG:HH11	1:B:123:ARG:H	0.91	0.91
1:B:104:ALA:HB1	1:B:131:LYS:HD3	1.52	0.90
1:E:322:ILE:HD12	1:E:322:ILE:H	1.29	0.89
1:D:104:ALA:HB1	1:D:131:LYS:HD3	1.52	0.89
1:F:451:ARG:HH11	1:F:451:ARG:HB3	1.38	0.89
1:F:123:ARG:HH11	1:F:123:ARG:H	0.91	0.88
1:B:451:ARG:HB3	1:B:451:ARG:HH11	1.38	0.88
1:D:451:ARG:HH11	1:D:451:ARG:HB3	1.38	0.88
1:C:317:PHE:HA	1:C:321:PRO:CD	2.03	0.88
1:C:451:ARG:HH11	1:C:451:ARG:HB3	1.38	0.88
1:E:337:PHE:O	1:E:341:VAL:HG23	1.74	0.88
1:A:317:PHE:HA	1:A:321:PRO:CD	2.04	0.88
1:C:123:ARG:H	1:C:123:ARG:HH11	0.91	0.88
1:F:317:PHE:HA	1:F:321:PRO:CD	2.04	0.87
1:A:123:ARG:H	1:A:123:ARG:HH11	0.91	0.87
1:C:337:PHE:O	1:C:341:VAL:HG23	1.74	0.87
1:A:451:ARG:HB3	1:A:451:ARG:HH11	1.38	0.87
1:D:317:PHE:HA	1:D:321:PRO:CD	2.04	0.87
1:B:317:PHE:HA	1:B:321:PRO:CD	2.04	0.87
1:F:337:PHE:O	1:F:341:VAL:HG23	1.74	0.87
1:A:337:PHE:O	1:A:341:VAL:HG23	1.74	0.87
1:E:451:ARG:HH11	1:E:451:ARG:HB3	1.38	0.86
1:E:317:PHE:HA	1:E:321:PRO:CD	2.04	0.86
1:E:123:ARG:HH11	1:E:123:ARG:H	0.91	0.86
1:E:31:THR:HG21	1:E:36:LEU:HD21	1.58	0.86
1:F:87:ALA:O	1:F:91:MET:HG2	1.76	0.86
1:D:337:PHE:O	1:D:341:VAL:HG23	1.74	0.86
1:B:337:PHE:O	1:B:341:VAL:HG23	1.74	0.85
1:D:87:ALA:O	1:D:91:MET:HG2	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:THR:HG21	1:A:36:LEU:HD21	1.58	0.85
1:C:87:ALA:O	1:C:91:MET:HG2	1.76	0.85
1:E:87:ALA:O	1:E:91:MET:HG2	1.76	0.85
1:E:183:ALA:HB2	1:E:200:ILE:HG13	1.59	0.85
1:F:31:THR:HG21	1:F:36:LEU:HD21	1.58	0.85
1:F:183:ALA:HB2	1:F:200:ILE:HG13	1.59	0.85
1:B:87:ALA:O	1:B:91:MET:HG2	1.76	0.85
1:C:31:THR:HG21	1:C:36:LEU:HD21	1.58	0.84
1:E:317:PHE:HA	1:E:321:PRO:HD3	1.60	0.84
1:D:421:LEU:O	1:D:425:MET:HG3	1.77	0.84
1:A:87:ALA:O	1:A:91:MET:HG2	1.76	0.84
1:F:421:LEU:O	1:F:425:MET:HG3	1.77	0.84
1:B:421:LEU:O	1:B:425:MET:HG3	1.77	0.84
1:A:183:ALA:HB2	1:A:200:ILE:HG13	1.59	0.84
1:E:421:LEU:O	1:E:425:MET:HG3	1.77	0.84
1:C:183:ALA:HB2	1:C:200:ILE:HG13	1.59	0.84
1:C:421:LEU:O	1:C:425:MET:HG3	1.77	0.84
1:F:317:PHE:HA	1:F:321:PRO:HD3	1.60	0.83
1:C:317:PHE:HA	1:C:321:PRO:HD3	1.60	0.83
1:A:421:LEU:O	1:A:425:MET:HG3	1.77	0.83
1:B:183:ALA:HB2	1:B:200:ILE:HG13	1.59	0.83
1:D:183:ALA:HB2	1:D:200:ILE:HG13	1.59	0.83
1:A:317:PHE:HA	1:A:321:PRO:HD3	1.60	0.83
1:D:31:THR:HG21	1:D:36:LEU:HD21	1.58	0.83
1:E:336:ILE:O	1:E:340:ARG:HG3	1.79	0.82
1:B:31:THR:HG21	1:B:36:LEU:HD21	1.58	0.82
1:D:336:ILE:O	1:D:340:ARG:HG3	1.79	0.82
1:F:336:ILE:O	1:F:340:ARG:HG3	1.79	0.82
1:E:123:ARG:HH11	1:E:123:ARG:N	1.76	0.82
1:B:336:ILE:O	1:B:340:ARG:HG3	1.79	0.82
1:C:211:THR:HG22	1:C:212:LEU:H	1.44	0.82
1:A:211:THR:HG22	1:A:212:LEU:H	1.45	0.81
1:C:336:ILE:O	1:C:340:ARG:HG3	1.79	0.81
1:D:317:PHE:HA	1:D:321:PRO:HD3	1.60	0.81
1:A:336:ILE:O	1:A:340:ARG:HG3	1.79	0.81
1:E:211:THR:HG22	1:E:212:LEU:H	1.45	0.81
1:B:317:PHE:HA	1:B:321:PRO:HD3	1.60	0.81
1:B:211:THR:HG22	1:B:212:LEU:H	1.45	0.81
1:B:98:ARG:HH21	1:B:102:PRO:HB3	1.46	0.80
1:D:211:THR:HG22	1:D:212:LEU:H	1.45	0.80
1:F:98:ARG:HH21	1:F:102:PRO:HB3	1.46	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:98:ARG:HH21	1:D:102:PRO:HB3	1.46	0.80
1:B:123:ARG:NH1	1:B:123:ARG:H	1.77	0.80
1:A:123:ARG:N	1:A:123:ARG:HH11	1.76	0.80
1:F:211:THR:HG22	1:F:212:LEU:H	1.44	0.80
1:C:98:ARG:HH21	1:C:102:PRO:HB3	1.46	0.79
1:D:123:ARG:NH1	1:D:123:ARG:H	1.77	0.79
1:C:123:ARG:N	1:C:123:ARG:HH11	1.76	0.79
1:A:98:ARG:HH21	1:A:102:PRO:HB3	1.46	0.79
1:E:123:ARG:NH1	1:E:123:ARG:H	1.77	0.79
1:A:322:ILE:H	1:A:322:ILE:CD1	1.96	0.78
1:E:98:ARG:HH21	1:E:102:PRO:HB3	1.46	0.78
1:C:322:ILE:CD1	1:C:322:ILE:H	1.96	0.78
1:A:227:ILE:O	1:A:231:ILE:HG12	1.84	0.78
1:E:227:ILE:O	1:E:231:ILE:HG12	1.84	0.78
1:C:227:ILE:O	1:C:231:ILE:HG12	1.84	0.78
1:D:227:ILE:O	1:D:231:ILE:HG12	1.84	0.78
1:F:123:ARG:N	1:F:123:ARG:HH11	1.76	0.78
1:B:227:ILE:O	1:B:231:ILE:HG12	1.84	0.78
1:E:322:ILE:CD1	1:E:322:ILE:H	1.96	0.77
1:E:430:LEU:HD22	1:F:223:ILE:HD12	1.66	0.77
1:B:123:ARG:HH11	1:B:123:ARG:N	1.76	0.77
1:F:227:ILE:O	1:F:231:ILE:HG12	1.84	0.77
1:F:123:ARG:NH1	1:F:123:ARG:H	1.77	0.77
1:D:138:THR:HG21	1:D:352:ALA:HB1	1.65	0.77
1:B:322:ILE:H	1:B:322:ILE:CD1	1.96	0.77
1:C:430:LEU:HD22	1:D:223:ILE:HD12	1.66	0.77
1:D:322:ILE:H	1:D:322:ILE:CD1	1.96	0.77
1:D:123:ARG:HH11	1:D:123:ARG:N	1.76	0.77
1:C:138:THR:HG21	1:C:352:ALA:HB1	1.65	0.77
1:A:138:THR:HG21	1:A:352:ALA:HB1	1.65	0.77
1:B:138:THR:HG21	1:B:352:ALA:HB1	1.65	0.76
1:F:322:ILE:H	1:F:322:ILE:CD1	1.96	0.76
1:F:138:THR:HG21	1:F:352:ALA:HB1	1.65	0.76
1:A:430:LEU:HD22	1:B:223:ILE:HD12	1.66	0.76
1:C:103:GLU:HB3	1:C:123:ARG:HH21	1.51	0.76
1:E:324:THR:C	1:E:326:GLY:H	1.89	0.76
1:A:103:GLU:HB3	1:A:123:ARG:HH21	1.51	0.76
1:E:116:LEU:HD23	1:E:178:LEU:HD23	1.68	0.76
1:E:138:THR:HG21	1:E:352:ALA:HB1	1.65	0.76
1:B:116:LEU:HD23	1:B:178:LEU:HD23	1.68	0.76
1:A:324:THR:C	1:A:326:GLY:H	1.89	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:GLU:HB3	1:B:123:ARG:HH21	1.51	0.75
1:F:260:ILE:HG23	1:F:435:LEU:HG	1.68	0.75
1:E:103:GLU:HB3	1:E:123:ARG:HH21	1.51	0.75
1:A:260:ILE:HG23	1:A:435:LEU:HG	1.68	0.75
1:D:103:GLU:HB3	1:D:123:ARG:HH21	1.51	0.75
1:D:260:ILE:HG23	1:D:435:LEU:HG	1.68	0.75
1:D:116:LEU:HD23	1:D:178:LEU:HD23	1.68	0.75
1:C:123:ARG:H	1:C:123:ARG:NH1	1.77	0.75
1:F:116:LEU:HD23	1:F:178:LEU:HD23	1.68	0.75
1:E:260:ILE:HG23	1:E:435:LEU:HG	1.69	0.75
1:C:260:ILE:HG23	1:C:435:LEU:HG	1.69	0.75
1:B:260:ILE:HG23	1:B:435:LEU:HG	1.68	0.75
1:C:200:ILE:CD1	1:C:204:MET:HG3	2.17	0.75
1:B:98:ARG:HA	1:B:98:ARG:HE	1.52	0.75
1:C:324:THR:C	1:C:326:GLY:H	1.89	0.74
1:F:103:GLU:HB3	1:F:123:ARG:HH21	1.51	0.74
1:D:98:ARG:HE	1:D:98:ARG:HA	1.52	0.74
1:A:116:LEU:HD23	1:A:178:LEU:HD23	1.68	0.74
1:C:220:ILE:HG12	1:D:430:LEU:HD21	1.69	0.74
1:E:28:ARG:CZ	1:F:207:GLN:HE22	2.01	0.74
1:C:28:ARG:CZ	1:D:207:GLN:HE22	2.01	0.74
1:C:116:LEU:HD23	1:C:178:LEU:HD23	1.68	0.74
1:C:450:ALA:CB	1:D:26:LEU:HD21	2.17	0.74
1:D:324:THR:C	1:D:326:GLY:H	1.89	0.74
1:F:98:ARG:HA	1:F:98:ARG:HE	1.52	0.74
1:E:98:ARG:HE	1:E:98:ARG:HA	1.52	0.74
1:A:220:ILE:HG12	1:B:430:LEU:HD21	1.69	0.74
1:E:223:ILE:HD12	1:F:430:LEU:HD22	1.69	0.74
1:E:450:ALA:CB	1:F:26:LEU:HD21	2.17	0.74
1:A:123:ARG:H	1:A:123:ARG:NH1	1.77	0.74
1:A:28:ARG:CZ	1:B:207:GLN:HE22	2.01	0.74
1:B:324:THR:C	1:B:326:GLY:H	1.89	0.74
1:E:220:ILE:HG12	1:F:430:LEU:HD21	1.69	0.74
1:A:450:ALA:CB	1:B:26:LEU:HD21	2.17	0.74
1:F:324:THR:C	1:F:326:GLY:H	1.89	0.74
1:D:322:ILE:N	1:D:322:ILE:CD1	2.42	0.74
1:C:98:ARG:HA	1:C:98:ARG:HE	1.52	0.73
1:A:98:ARG:HE	1:A:98:ARG:HA	1.52	0.73
1:F:92:PHE:O	1:F:96:LEU:HD23	1.88	0.73
1:D:92:PHE:O	1:D:96:LEU:HD23	1.88	0.73
1:B:92:PHE:O	1:B:96:LEU:HD23	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:92:PHE:O	1:E:96:LEU:HD23	1.88	0.73
1:A:92:PHE:O	1:A:96:LEU:HD23	1.88	0.73
1:A:223:ILE:CD1	1:B:430:LEU:HD22	2.19	0.73
1:E:223:ILE:CD1	1:F:430:LEU:HD22	2.19	0.72
1:C:223:ILE:CD1	1:D:430:LEU:HD22	2.19	0.72
1:A:223:ILE:HD12	1:B:430:LEU:HD22	1.69	0.72
1:C:223:ILE:HD12	1:D:430:LEU:HD22	1.69	0.72
1:C:92:PHE:O	1:C:96:LEU:HD23	1.88	0.72
1:C:207:GLN:HE22	1:D:28:ARG:CZ	2.01	0.72
1:E:207:GLN:HE22	1:F:28:ARG:CZ	2.01	0.72
1:A:207:GLN:HE22	1:B:28:ARG:CZ	2.01	0.72
1:F:200:ILE:CD1	1:F:204:MET:HG3	2.17	0.72
1:E:200:ILE:CD1	1:E:204:MET:HG3	2.17	0.71
1:E:211:THR:CG2	1:E:213:ILE:HG13	2.20	0.71
1:E:44:THR:O	1:E:48:LEU:HB2	1.91	0.71
1:F:148:GLU:OE1	1:F:357:PHE:HB3	1.91	0.71
1:B:44:THR:O	1:B:48:LEU:HB2	1.90	0.71
1:E:430:LEU:HD22	1:F:223:ILE:CD1	2.21	0.71
1:F:211:THR:CG2	1:F:213:ILE:HG13	2.20	0.71
1:D:211:THR:CG2	1:D:213:ILE:HG13	2.20	0.71
1:A:148:GLU:OE1	1:A:357:PHE:HB3	1.91	0.71
1:D:44:THR:O	1:D:48:LEU:HB2	1.90	0.71
1:B:211:THR:CG2	1:B:213:ILE:HG13	2.20	0.71
1:B:148:GLU:OE1	1:B:357:PHE:HB3	1.91	0.71
1:C:148:GLU:OE1	1:C:357:PHE:HB3	1.91	0.71
1:F:448:ILE:O	1:F:452:THR:HG22	1.91	0.70
1:A:44:THR:O	1:A:48:LEU:HB2	1.90	0.70
1:C:430:LEU:HD22	1:D:223:ILE:CD1	2.21	0.70
1:F:44:THR:O	1:F:48:LEU:HB2	1.91	0.70
1:D:148:GLU:OE1	1:D:357:PHE:HB3	1.91	0.70
1:C:211:THR:CG2	1:C:213:ILE:HG13	2.20	0.70
1:A:84:LEU:O	1:A:88:VAL:HG23	1.92	0.70
1:A:270:ASN:CG	1:A:444:LEU:HD23	2.12	0.70
1:C:270:ASN:CG	1:C:444:LEU:HD23	2.12	0.70
1:A:211:THR:CG2	1:A:213:ILE:HG13	2.20	0.70
1:C:84:LEU:O	1:C:88:VAL:HG23	1.92	0.70
1:C:44:THR:O	1:C:48:LEU:HB2	1.91	0.70
1:E:148:GLU:OE1	1:E:357:PHE:HB3	1.91	0.70
1:E:448:ILE:O	1:E:452:THR:HG22	1.91	0.70
1:A:430:LEU:HD22	1:B:223:ILE:CD1	2.21	0.70
1:A:200:ILE:CD1	1:A:204:MET:HG3	2.17	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:270:ASN:CG	1:E:444:LEU:HD23	2.12	0.70
1:A:317:PHE:C	1:A:319:LEU:H	1.96	0.70
1:C:317:PHE:C	1:C:319:LEU:H	1.96	0.70
1:D:448:ILE:O	1:D:452:THR:HG22	1.91	0.70
1:D:270:ASN:CG	1:D:444:LEU:HD23	2.12	0.69
1:F:317:PHE:C	1:F:319:LEU:H	1.96	0.69
1:E:451:ARG:HH11	1:E:451:ARG:CB	2.06	0.69
1:B:448:ILE:O	1:B:452:THR:HG22	1.91	0.69
1:F:84:LEU:O	1:F:88:VAL:HG23	1.92	0.69
1:B:84:LEU:O	1:B:88:VAL:HG23	1.92	0.69
1:B:244:LEU:HD12	1:B:244:LEU:N	2.08	0.69
1:C:244:LEU:HD12	1:C:244:LEU:N	2.08	0.69
1:A:448:ILE:O	1:A:452:THR:HG22	1.91	0.69
1:C:448:ILE:O	1:C:452:THR:HG22	1.91	0.69
1:F:270:ASN:CG	1:F:444:LEU:HD23	2.12	0.69
1:E:84:LEU:O	1:E:88:VAL:HG23	1.92	0.69
1:C:75:TYR:N	1:C:76:PRO:HD2	2.08	0.69
1:E:198:LEU:HD21	1:F:198:LEU:HD21	1.75	0.69
1:A:75:TYR:N	1:A:76:PRO:HD2	2.08	0.69
1:B:109:ILE:HD11	1:B:152:VAL:HG21	1.74	0.69
1:D:84:LEU:O	1:D:88:VAL:HG23	1.92	0.69
1:D:75:TYR:N	1:D:76:PRO:HD2	2.08	0.69
1:D:244:LEU:N	1:D:244:LEU:HD12	2.08	0.69
1:B:75:TYR:N	1:B:76:PRO:HD2	2.08	0.69
1:F:109:ILE:HD11	1:F:152:VAL:HG21	1.73	0.69
1:B:270:ASN:CG	1:B:444:LEU:HD23	2.12	0.69
1:F:75:TYR:N	1:F:76:PRO:HD2	2.08	0.69
1:A:244:LEU:HD12	1:A:244:LEU:N	2.08	0.69
1:F:244:LEU:N	1:F:244:LEU:HD12	2.08	0.69
1:C:109:ILE:HD11	1:C:152:VAL:HG21	1.74	0.69
1:D:109:ILE:HD11	1:D:152:VAL:HG21	1.74	0.69
1:E:281:HIS:HA	1:E:284:HIS:NE2	2.09	0.68
1:A:451:ARG:HH11	1:A:451:ARG:CB	2.05	0.68
1:C:451:ARG:HH11	1:C:451:ARG:CB	2.05	0.68
1:D:281:HIS:HA	1:D:284:HIS:NE2	2.09	0.68
1:A:281:HIS:HA	1:A:284:HIS:NE2	2.09	0.68
1:A:109:ILE:HD11	1:A:152:VAL:HG21	1.74	0.68
1:B:281:HIS:HA	1:B:284:HIS:NE2	2.09	0.68
1:F:281:HIS:HA	1:F:284:HIS:NE2	2.09	0.68
1:D:317:PHE:C	1:D:319:LEU:H	1.96	0.68
1:E:75:TYR:N	1:E:76:PRO:HD2	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:200:ILE:CD1	1:D:204:MET:HG3	2.17	0.68
1:C:281:HIS:HA	1:C:284:HIS:NE2	2.09	0.68
1:D:451:ARG:CB	1:D:451:ARG:HH11	2.06	0.68
1:D:251:THR:HG22	1:D:255:TYR:HE1	1.59	0.68
1:E:98:ARG:HH21	1:E:102:PRO:CB	2.07	0.68
1:F:451:ARG:HH11	1:F:451:ARG:CB	2.05	0.68
1:B:451:ARG:CB	1:B:451:ARG:HH11	2.05	0.68
1:C:251:THR:HG22	1:C:255:TYR:HE1	1.59	0.68
1:E:244:LEU:N	1:E:244:LEU:HD12	2.08	0.68
1:C:30:LYS:NZ	1:C:30:LYS:HB3	2.09	0.68
1:B:200:ILE:CD1	1:B:204:MET:HG3	2.17	0.68
1:A:98:ARG:HH21	1:A:102:PRO:CB	2.07	0.68
1:A:30:LYS:HB3	1:A:30:LYS:NZ	2.09	0.68
1:B:98:ARG:HH21	1:B:102:PRO:CB	2.07	0.68
1:F:98:ARG:HH21	1:F:102:PRO:CB	2.07	0.68
1:D:98:ARG:HH21	1:D:102:PRO:CB	2.07	0.68
1:C:98:ARG:HH21	1:C:102:PRO:CB	2.07	0.68
1:E:30:LYS:NZ	1:E:30:LYS:HB3	2.09	0.68
1:B:30:LYS:HB3	1:B:30:LYS:NZ	2.09	0.68
1:E:251:THR:HG22	1:E:255:TYR:HE1	1.59	0.68
1:D:30:LYS:HB3	1:D:30:LYS:NZ	2.09	0.68
1:E:109:ILE:HD11	1:E:152:VAL:HG21	1.74	0.67
1:B:251:THR:HG22	1:B:255:TYR:HE1	1.59	0.67
1:F:30:LYS:NZ	1:F:30:LYS:HB3	2.09	0.67
1:C:198:LEU:HD21	1:D:198:LEU:HD21	1.75	0.67
1:A:251:THR:HG22	1:A:255:TYR:HE1	1.59	0.67
1:B:317:PHE:C	1:B:319:LEU:H	1.96	0.67
1:A:198:LEU:HD21	1:B:198:LEU:HD21	1.75	0.67
1:F:251:THR:HG22	1:F:255:TYR:HE1	1.59	0.67
1:E:317:PHE:C	1:E:319:LEU:H	1.96	0.67
1:D:211:THR:HG22	1:D:212:LEU:N	2.11	0.67
1:C:120:ARG:CB	1:C:120:ARG:HH11	2.07	0.66
1:B:211:THR:HG22	1:B:212:LEU:N	2.11	0.66
1:F:317:PHE:O	1:F:319:LEU:N	2.29	0.66
1:A:120:ARG:CB	1:A:120:ARG:HH11	2.07	0.66
1:D:211:THR:HG22	1:D:213:ILE:HG13	1.78	0.66
1:E:223:ILE:O	1:E:227:ILE:HG13	1.96	0.66
1:E:211:THR:HG22	1:E:213:ILE:HG13	1.78	0.66
1:E:211:THR:HG22	1:E:212:LEU:N	2.11	0.66
1:B:211:THR:HG22	1:B:213:ILE:HG13	1.78	0.66
1:E:317:PHE:O	1:E:319:LEU:N	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:THR:HG22	1:A:212:LEU:N	2.10	0.65
1:F:273:VAL:HA	1:F:345:LEU:HD22	1.78	0.65
1:C:211:THR:HG22	1:C:212:LEU:N	2.10	0.65
1:D:212:LEU:HD12	1:D:212:LEU:N	2.11	0.65
1:F:223:ILE:O	1:F:227:ILE:HG13	1.96	0.65
1:D:317:PHE:O	1:D:319:LEU:N	2.29	0.65
1:C:273:VAL:HA	1:C:345:LEU:HD22	1.78	0.65
1:B:32:PRO:HD2	1:B:35:ILE:HD12	1.79	0.65
1:D:32:PRO:HD2	1:D:35:ILE:HD12	1.79	0.65
1:F:120:ARG:CB	1:F:120:ARG:HH11	2.07	0.65
1:B:317:PHE:O	1:B:319:LEU:N	2.29	0.65
1:B:223:ILE:O	1:B:227:ILE:HG13	1.96	0.65
1:F:212:LEU:HD12	1:F:212:LEU:N	2.11	0.65
1:E:32:PRO:HD2	1:E:35:ILE:HD12	1.79	0.65
1:A:223:ILE:O	1:A:227:ILE:HG13	1.96	0.65
1:C:223:ILE:O	1:C:227:ILE:HG13	1.96	0.65
1:E:317:PHE:HA	1:E:321:PRO:HD2	1.79	0.65
1:B:212:LEU:HD12	1:B:212:LEU:N	2.11	0.65
1:C:126:ARG:O	1:C:130:VAL:HG23	1.97	0.65
1:F:211:THR:HG22	1:F:213:ILE:HG13	1.78	0.65
1:A:126:ARG:O	1:A:130:VAL:HG23	1.97	0.65
1:A:212:LEU:N	1:A:212:LEU:HD12	2.11	0.65
1:B:273:VAL:HA	1:B:345:LEU:HD22	1.78	0.65
1:D:317:PHE:HA	1:D:321:PRO:HD2	1.79	0.64
1:D:223:ILE:O	1:D:227:ILE:HG13	1.96	0.64
1:D:273:VAL:HA	1:D:345:LEU:HD22	1.78	0.64
1:C:317:PHE:O	1:C:319:LEU:N	2.29	0.64
1:C:324:THR:HG22	1:C:328:PHE:CE2	2.32	0.64
1:A:317:PHE:O	1:A:319:LEU:N	2.29	0.64
1:A:273:VAL:HA	1:A:345:LEU:HD22	1.79	0.64
1:D:324:THR:HG22	1:D:328:PHE:CE2	2.33	0.64
1:B:317:PHE:HA	1:B:321:PRO:HD2	1.79	0.64
1:C:212:LEU:N	1:C:212:LEU:HD12	2.11	0.64
1:C:211:THR:HG22	1:C:213:ILE:HG13	1.78	0.64
1:E:450:ALA:HB3	1:F:26:LEU:HD21	1.79	0.64
1:C:194:LEU:HD13	1:D:410:ILE:HD11	1.79	0.64
1:B:324:THR:HG22	1:B:328:PHE:CE2	2.32	0.64
1:A:211:THR:HG22	1:A:213:ILE:HG13	1.78	0.64
1:A:324:THR:HG22	1:A:328:PHE:CE2	2.33	0.64
1:A:207:GLN:NE2	1:B:28:ARG:CZ	2.61	0.64
1:E:120:ARG:CB	1:E:120:ARG:HH11	2.08	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:ARG:CB	1:B:120:ARG:HH11	2.07	0.64
1:F:211:THR:HG22	1:F:212:LEU:N	2.10	0.64
1:A:32:PRO:HD2	1:A:35:ILE:HD12	1.79	0.64
1:C:317:PHE:HA	1:C:321:PRO:HD2	1.79	0.64
1:A:317:PHE:HA	1:A:321:PRO:HD2	1.79	0.64
1:C:207:GLN:NE2	1:D:28:ARG:CZ	2.61	0.64
1:F:32:PRO:HD2	1:F:35:ILE:HD12	1.79	0.64
1:E:212:LEU:HD12	1:E:212:LEU:N	2.11	0.64
1:C:32:PRO:HD2	1:C:35:ILE:HD12	1.79	0.64
1:E:273:VAL:HA	1:E:345:LEU:HD22	1.79	0.64
1:F:324:THR:HG22	1:F:328:PHE:CE2	2.33	0.64
1:E:28:ARG:CZ	1:F:207:GLN:NE2	2.61	0.64
1:E:126:ARG:O	1:E:130:VAL:HG23	1.97	0.64
1:A:194:LEU:HD13	1:B:410:ILE:HD11	1.80	0.64
1:F:126:ARG:O	1:F:130:VAL:HG23	1.97	0.64
1:D:123:ARG:HD3	1:D:123:ARG:N	2.13	0.64
1:F:317:PHE:HA	1:F:321:PRO:HD2	1.79	0.63
1:D:120:ARG:CB	1:D:120:ARG:HH11	2.07	0.63
1:C:154:ILE:O	1:C:158:ILE:HG12	1.98	0.63
1:B:123:ARG:HD3	1:B:123:ARG:N	2.13	0.63
1:E:324:THR:HG22	1:E:328:PHE:CE2	2.33	0.63
1:A:123:ARG:HD3	1:A:123:ARG:N	2.13	0.63
1:A:450:ALA:HB3	1:B:26:LEU:HD21	1.79	0.63
1:E:434:LEU:HD23	1:F:216:LYS:HD3	1.81	0.63
1:E:123:ARG:HD3	1:E:123:ARG:N	2.13	0.63
1:F:123:ARG:HD3	1:F:123:ARG:N	2.13	0.63
1:A:154:ILE:O	1:A:158:ILE:HG12	1.98	0.63
1:C:123:ARG:HD3	1:C:123:ARG:N	2.13	0.63
1:E:194:LEU:HD13	1:F:410:ILE:HD11	1.79	0.63
1:C:434:LEU:HD23	1:D:216:LYS:HD3	1.81	0.63
1:E:154:ILE:O	1:E:158:ILE:HG12	1.98	0.63
1:F:154:ILE:O	1:F:158:ILE:HG12	1.98	0.63
1:C:450:ALA:HB3	1:D:26:LEU:HD21	1.79	0.63
1:A:434:LEU:HD23	1:B:216:LYS:HD3	1.81	0.63
1:F:278:ASP:C	1:F:280:LEU:H	2.03	0.63
1:E:207:GLN:NE2	1:F:28:ARG:CZ	2.61	0.62
1:D:126:ARG:O	1:D:130:VAL:HG23	1.97	0.62
1:B:126:ARG:O	1:B:130:VAL:HG23	1.97	0.62
1:A:320:ILE:O	1:A:324:THR:HG23	1.99	0.62
1:D:320:ILE:O	1:D:324:THR:HG23	1.99	0.62
1:B:320:ILE:O	1:B:324:THR:HG23	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:THR:HG23	1:D:228:MET:CE	2.30	0.62
1:C:320:ILE:O	1:C:324:THR:HG23	1.99	0.62
1:D:154:ILE:O	1:D:158:ILE:HG12	1.98	0.62
1:B:44:THR:HG23	1:B:228:MET:CE	2.30	0.62
1:D:46:VAL:HG21	1:D:181:GLY:HA2	1.81	0.62
1:B:154:ILE:O	1:B:158:ILE:HG12	1.98	0.62
1:B:244:LEU:HD12	1:B:418:ASN:HD21	1.65	0.62
1:A:244:LEU:HD12	1:A:418:ASN:HD21	1.65	0.62
1:C:244:LEU:HD12	1:C:418:ASN:HD21	1.65	0.62
1:F:46:VAL:HG21	1:F:181:GLY:HA2	1.81	0.62
1:A:28:ARG:CZ	1:B:207:GLN:NE2	2.61	0.62
1:C:28:ARG:CZ	1:D:207:GLN:NE2	2.61	0.62
1:D:244:LEU:HD12	1:D:418:ASN:HD21	1.65	0.62
1:F:276:MET:O	1:F:280:LEU:HD23	2.00	0.62
1:A:276:MET:O	1:A:280:LEU:HD23	2.00	0.62
1:A:200:ILE:HG22	1:A:200:ILE:O	2.00	0.62
1:C:200:ILE:O	1:C:200:ILE:HG22	2.00	0.62
1:C:276:MET:O	1:C:280:LEU:HD23	2.00	0.62
1:E:320:ILE:O	1:E:324:THR:HG23	2.00	0.62
1:E:276:MET:O	1:E:280:LEU:HD23	1.99	0.62
1:C:131:LYS:NZ	1:C:153:GLN:NE2	2.48	0.61
1:C:46:VAL:HG21	1:C:181:GLY:HA2	1.81	0.61
1:B:131:LYS:NZ	1:B:153:GLN:NE2	2.48	0.61
1:B:46:VAL:HG21	1:B:181:GLY:HA2	1.81	0.61
1:F:200:ILE:O	1:F:200:ILE:HG22	2.00	0.61
1:E:131:LYS:NZ	1:E:153:GLN:NE2	2.48	0.61
1:D:131:LYS:NZ	1:D:153:GLN:NE2	2.48	0.61
1:D:276:MET:O	1:D:280:LEU:HD23	2.00	0.61
1:B:313:SER:OG	1:B:314:GLY:N	2.32	0.61
1:A:278:ASP:C	1:A:280:LEU:H	2.03	0.61
1:F:320:ILE:O	1:F:324:THR:HG23	1.99	0.61
1:E:46:VAL:HG21	1:E:181:GLY:HA2	1.81	0.61
1:A:131:LYS:NZ	1:A:153:GLN:NE2	2.48	0.61
1:F:244:LEU:HD12	1:F:418:ASN:HD21	1.65	0.61
1:A:44:THR:HG23	1:A:228:MET:CE	2.30	0.61
1:C:44:THR:HG23	1:C:228:MET:CE	2.30	0.61
1:B:200:ILE:HG22	1:B:200:ILE:O	2.00	0.61
1:E:203:GLU:CD	1:F:28:ARG:HH22	2.05	0.61
1:D:313:SER:OG	1:D:314:GLY:N	2.32	0.61
1:E:44:THR:HG23	1:E:228:MET:CE	2.30	0.61
1:E:278:ASP:C	1:E:280:LEU:H	2.03	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:MET:O	1:B:280:LEU:HD23	2.00	0.61
1:D:200:ILE:HG22	1:D:200:ILE:O	2.00	0.61
1:A:46:VAL:HG21	1:A:181:GLY:HA2	1.81	0.61
1:E:420:GLN:HG3	1:E:421:LEU:HG	1.83	0.61
1:F:44:THR:HG23	1:F:228:MET:CE	2.30	0.61
1:A:372:GLY:O	1:A:376:VAL:HG23	2.01	0.61
1:C:103:GLU:CB	1:C:123:ARG:HH21	2.14	0.61
1:A:103:GLU:CB	1:A:123:ARG:HH21	2.14	0.61
1:B:278:ASP:C	1:B:280:LEU:H	2.03	0.61
1:F:103:GLU:CB	1:F:123:ARG:HH21	2.14	0.60
1:F:420:GLN:HG3	1:F:421:LEU:HG	1.83	0.60
1:C:372:GLY:O	1:C:376:VAL:HG23	2.01	0.60
1:F:131:LYS:NZ	1:F:153:GLN:NE2	2.48	0.60
1:E:200:ILE:HG22	1:E:200:ILE:O	2.00	0.60
1:E:103:GLU:CB	1:E:123:ARG:HH21	2.14	0.60
1:B:103:GLU:CB	1:B:123:ARG:HH21	2.14	0.60
1:D:420:GLN:HG3	1:D:421:LEU:HG	1.83	0.60
1:C:278:ASP:C	1:C:280:LEU:H	2.03	0.60
1:D:278:ASP:C	1:D:280:LEU:H	2.03	0.60
1:D:103:GLU:CB	1:D:123:ARG:HH21	2.14	0.60
1:E:372:GLY:O	1:E:376:VAL:HG23	2.01	0.60
1:A:203:GLU:CD	1:B:28:ARG:HH22	2.04	0.60
1:E:433:THR:HG22	1:F:216:LYS:NZ	2.16	0.60
1:B:420:GLN:HG3	1:B:421:LEU:HG	1.83	0.60
1:C:203:GLU:CD	1:D:28:ARG:HH22	2.05	0.60
1:A:420:GLN:HG3	1:A:421:LEU:HG	1.83	0.60
1:B:372:GLY:O	1:B:376:VAL:HG23	2.01	0.60
1:A:433:THR:HG22	1:B:216:LYS:NZ	2.16	0.60
1:C:420:GLN:HG3	1:C:421:LEU:HG	1.83	0.60
1:E:198:LEU:HD21	1:F:198:LEU:CD2	2.32	0.60
1:A:313:SER:OG	1:A:314:GLY:N	2.32	0.60
1:C:433:THR:HG22	1:D:216:LYS:NZ	2.16	0.60
1:E:244:LEU:HD12	1:E:418:ASN:HD21	1.65	0.60
1:D:372:GLY:O	1:D:376:VAL:HG23	2.01	0.60
1:F:313:SER:OG	1:F:314:GLY:N	2.32	0.59
1:A:75:TYR:O	1:A:79:LEU:HG	2.03	0.59
1:F:372:GLY:O	1:F:376:VAL:HG23	2.01	0.59
1:F:44:THR:HG23	1:F:228:MET:HE2	1.83	0.59
1:C:75:TYR:O	1:C:79:LEU:HG	2.03	0.59
1:E:419:TYR:CE1	1:F:414:GLU:OE1	2.56	0.59
1:C:313:SER:OG	1:C:314:GLY:N	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:423:LEU:HB3	1:F:424:PRO:HD3	1.85	0.59
1:E:97:VAL:HG21	1:E:353:PRO:HD3	1.85	0.59
1:C:198:LEU:HD21	1:D:198:LEU:CD2	2.32	0.59
1:B:324:THR:C	1:B:326:GLY:N	2.56	0.59
1:D:97:VAL:HG21	1:D:353:PRO:HD3	1.85	0.59
1:E:423:LEU:HB3	1:E:424:PRO:HD3	1.85	0.58
1:F:148:GLU:CD	1:F:148:GLU:H	2.07	0.58
1:F:75:TYR:O	1:F:79:LEU:HG	2.03	0.58
1:B:423:LEU:HB3	1:B:424:PRO:HD3	1.85	0.58
1:C:423:LEU:HB3	1:C:424:PRO:HD3	1.85	0.58
1:B:75:TYR:O	1:B:79:LEU:HG	2.03	0.58
1:C:419:TYR:CE1	1:D:414:GLU:OE1	2.56	0.58
1:C:157:ASN:C	1:C:159:GLY:N	2.56	0.58
1:C:159:GLY:O	1:C:162:VAL:HG22	2.04	0.58
1:D:159:GLY:O	1:D:162:VAL:HG22	2.04	0.58
1:A:159:GLY:O	1:A:162:VAL:HG22	2.04	0.58
1:B:159:GLY:O	1:B:162:VAL:HG22	2.04	0.58
1:D:423:LEU:HB3	1:D:424:PRO:HD3	1.85	0.58
1:A:148:GLU:H	1:A:148:GLU:CD	2.07	0.58
1:F:97:VAL:HG21	1:F:353:PRO:HD3	1.85	0.58
1:D:324:THR:C	1:D:326:GLY:N	2.56	0.58
1:E:198:LEU:CD2	1:F:198:LEU:HD21	2.33	0.58
1:D:75:TYR:O	1:D:79:LEU:HG	2.03	0.58
1:A:198:LEU:HD21	1:B:198:LEU:CD2	2.32	0.58
1:A:419:TYR:CE1	1:B:414:GLU:OE1	2.56	0.58
1:A:203:GLU:OE1	1:B:28:ARG:NH2	2.36	0.58
1:E:157:ASN:C	1:E:159:GLY:N	2.56	0.58
1:E:75:TYR:O	1:E:79:LEU:HG	2.03	0.58
1:C:21:LEU:O	1:C:25:LEU:N	2.34	0.58
1:C:270:ASN:HA	1:C:273:VAL:CG1	2.34	0.58
1:A:157:ASN:C	1:A:159:GLY:N	2.56	0.58
1:B:148:GLU:H	1:B:148:GLU:CD	2.07	0.58
1:E:148:GLU:CD	1:E:148:GLU:H	2.07	0.58
1:B:97:VAL:HG21	1:B:353:PRO:HD3	1.85	0.58
1:C:203:GLU:OE1	1:D:28:ARG:NH2	2.36	0.58
1:A:423:LEU:HB3	1:A:424:PRO:HD3	1.85	0.58
1:C:198:LEU:CD2	1:D:198:LEU:HD21	2.33	0.58
1:B:234:HIS:O	1:B:236:VAL:HG23	2.04	0.58
1:D:234:HIS:O	1:D:236:VAL:HG23	2.04	0.58
1:A:270:ASN:HA	1:A:273:VAL:CG1	2.34	0.58
1:C:148:GLU:CD	1:C:148:GLU:H	2.07	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:LEU:CD2	1:B:198:LEU:HD21	2.33	0.58
1:E:203:GLU:OE1	1:F:28:ARG:NH2	2.36	0.58
1:F:324:THR:C	1:F:326:GLY:N	2.56	0.58
1:C:97:VAL:HG21	1:C:353:PRO:HD3	1.85	0.58
1:F:159:GLY:O	1:F:162:VAL:HG22	2.04	0.58
1:F:270:ASN:HA	1:F:273:VAL:CG1	2.34	0.58
1:D:332:MET:O	1:D:336:ILE:HG13	2.04	0.58
1:E:419:TYR:OH	1:F:414:GLU:OE1	2.19	0.58
1:A:184:ALA:HB1	1:A:225:SER:HB2	1.86	0.58
1:E:270:ASN:HA	1:E:273:VAL:CG1	2.34	0.57
1:C:324:THR:C	1:C:326:GLY:N	2.56	0.57
1:E:159:GLY:O	1:E:162:VAL:HG22	2.04	0.57
1:A:88:VAL:O	1:A:91:MET:HB2	2.04	0.57
1:B:332:MET:O	1:B:336:ILE:HG13	2.04	0.57
1:B:44:THR:HG23	1:B:228:MET:HE3	1.86	0.57
1:F:34:ALA:O	1:F:38:MET:HB2	2.05	0.57
1:E:234:HIS:O	1:E:236:VAL:HG23	2.04	0.57
1:C:184:ALA:HB1	1:C:225:SER:HB2	1.86	0.57
1:F:157:ASN:C	1:F:159:GLY:N	2.56	0.57
1:A:332:MET:O	1:A:336:ILE:HG13	2.04	0.57
1:C:430:LEU:HD13	1:D:219:PHE:CD2	2.39	0.57
1:C:88:VAL:O	1:C:91:MET:HB2	2.04	0.57
1:D:148:GLU:H	1:D:148:GLU:CD	2.07	0.57
1:A:97:VAL:HG21	1:A:353:PRO:HD3	1.85	0.57
1:E:34:ALA:O	1:E:38:MET:HB2	2.05	0.57
1:C:332:MET:O	1:C:336:ILE:HG13	2.04	0.57
1:A:324:THR:C	1:A:326:GLY:N	2.56	0.57
1:A:430:LEU:HD13	1:B:219:PHE:CD2	2.39	0.57
1:A:446:SER:O	1:A:449:LEU:N	2.38	0.57
1:C:446:SER:O	1:C:449:LEU:N	2.38	0.57
1:C:128:LEU:HB2	1:C:129:PRO:CD	2.35	0.57
1:F:128:LEU:HB2	1:F:129:PRO:CD	2.35	0.57
1:B:128:LEU:HB2	1:B:129:PRO:CD	2.35	0.57
1:B:446:SER:O	1:B:449:LEU:N	2.38	0.57
1:D:446:SER:O	1:D:449:LEU:N	2.38	0.57
1:E:132:PHE:O	1:E:136:LEU:HB2	2.05	0.57
1:F:184:ALA:HB1	1:F:225:SER:HB2	1.86	0.57
1:E:313:SER:OG	1:E:314:GLY:N	2.32	0.57
1:E:430:LEU:HD13	1:F:219:PHE:CD2	2.39	0.57
1:A:128:LEU:HB2	1:A:129:PRO:CD	2.35	0.57
1:F:446:SER:O	1:F:449:LEU:N	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:270:ASN:HA	1:D:273:VAL:CG1	2.34	0.57
1:D:184:ALA:HB1	1:D:225:SER:HB2	1.86	0.57
1:B:184:ALA:HB1	1:B:225:SER:HB2	1.86	0.57
1:A:426:ILE:HG22	1:B:223:ILE:HD11	1.87	0.57
1:D:128:LEU:HB2	1:D:129:PRO:CD	2.35	0.57
1:D:127:VAL:HB	1:D:157:ASN:ND2	2.20	0.57
1:F:88:VAL:O	1:F:91:MET:HB2	2.04	0.57
1:B:88:VAL:O	1:B:91:MET:HB2	2.04	0.57
1:D:98:ARG:HA	1:D:98:ARG:NE	2.20	0.57
1:C:234:HIS:O	1:C:236:VAL:HG23	2.04	0.57
1:E:127:VAL:HB	1:E:157:ASN:ND2	2.20	0.57
1:B:127:VAL:HB	1:B:157:ASN:ND2	2.20	0.57
1:B:270:ASN:HA	1:B:273:VAL:CG1	2.34	0.57
1:A:132:PHE:O	1:A:136:LEU:HB2	2.05	0.57
1:B:132:PHE:O	1:B:136:LEU:HB2	2.05	0.57
1:F:332:MET:O	1:F:336:ILE:HG13	2.04	0.57
1:A:270:ASN:ND2	1:A:444:LEU:HD23	2.20	0.57
1:C:270:ASN:ND2	1:C:444:LEU:HD23	2.20	0.57
1:D:131:LYS:HZ2	1:D:153:GLN:NE2	2.03	0.57
1:A:234:HIS:O	1:A:236:VAL:HG23	2.04	0.57
1:C:324:THR:HG22	1:C:328:PHE:CD2	2.40	0.56
1:C:426:ILE:HG22	1:D:223:ILE:HD11	1.87	0.56
1:E:128:LEU:HB2	1:E:129:PRO:CD	2.35	0.56
1:B:211:THR:HG21	1:B:213:ILE:HG13	1.87	0.56
1:C:132:PHE:O	1:C:136:LEU:HB2	2.05	0.56
1:E:270:ASN:ND2	1:E:444:LEU:HD23	2.20	0.56
1:A:317:PHE:C	1:A:319:LEU:N	2.58	0.56
1:A:324:THR:HG22	1:A:328:PHE:CD2	2.40	0.56
1:E:324:THR:HG22	1:E:328:PHE:CD2	2.40	0.56
1:E:332:MET:O	1:E:336:ILE:HG13	2.04	0.56
1:C:211:THR:HG21	1:C:213:ILE:HG13	1.87	0.56
1:F:270:ASN:ND2	1:F:444:LEU:HD23	2.20	0.56
1:D:88:VAL:O	1:D:91:MET:HB2	2.04	0.56
1:E:88:VAL:O	1:E:91:MET:HB2	2.04	0.56
1:B:98:ARG:NE	1:B:98:ARG:HA	2.20	0.56
1:F:234:HIS:O	1:F:236:VAL:HG23	2.04	0.56
1:C:34:ALA:O	1:C:38:MET:HB2	2.05	0.56
1:F:317:PHE:C	1:F:319:LEU:N	2.58	0.56
1:B:324:THR:HG22	1:B:328:PHE:CD2	2.40	0.56
1:D:211:THR:HG21	1:D:213:ILE:HG13	1.87	0.56
1:A:127:VAL:HB	1:A:157:ASN:ND2	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:THR:HG21	1:A:213:ILE:HG13	1.87	0.56
1:E:44:THR:HG23	1:E:228:MET:HE2	1.88	0.56
1:D:132:PHE:O	1:D:136:LEU:HB2	2.05	0.56
1:E:184:ALA:HB1	1:E:225:SER:HB2	1.86	0.56
1:D:44:THR:HG23	1:D:228:MET:HE3	1.87	0.56
1:A:83:PHE:C	1:A:83:PHE:CD1	2.79	0.56
1:F:324:THR:HG22	1:F:328:PHE:CD2	2.41	0.56
1:C:127:VAL:HB	1:C:157:ASN:ND2	2.20	0.56
1:D:270:ASN:ND2	1:D:444:LEU:HD23	2.20	0.56
1:A:34:ALA:O	1:A:38:MET:HB2	2.05	0.56
1:C:83:PHE:C	1:C:83:PHE:CD1	2.79	0.56
1:D:34:ALA:O	1:D:38:MET:HB2	2.05	0.56
1:C:317:PHE:C	1:C:319:LEU:N	2.58	0.56
1:D:324:THR:HG22	1:D:328:PHE:CD2	2.41	0.56
1:E:426:ILE:HG22	1:F:223:ILE:HD11	1.87	0.56
1:E:21:LEU:O	1:E:25:LEU:N	2.34	0.56
1:F:127:VAL:HB	1:F:157:ASN:ND2	2.20	0.56
1:D:116:LEU:CD2	1:D:178:LEU:HD23	2.36	0.56
1:F:360:MET:SD	1:F:397:LEU:HD12	2.46	0.56
1:F:132:PHE:O	1:F:136:LEU:HB2	2.05	0.56
1:B:360:MET:SD	1:B:397:LEU:HD12	2.46	0.56
1:B:34:ALA:O	1:B:38:MET:HB2	2.05	0.56
1:F:312:THR:HG22	1:F:339:ALA:CB	2.36	0.56
1:D:360:MET:SD	1:D:397:LEU:HD12	2.46	0.56
1:C:322:ILE:CD1	1:C:322:ILE:N	2.42	0.56
1:D:317:PHE:C	1:D:319:LEU:N	2.58	0.56
1:E:122:VAL:HB	1:E:160:ARG:CD	2.36	0.56
1:F:122:VAL:HB	1:F:160:ARG:CD	2.36	0.56
1:A:122:VAL:HB	1:A:160:ARG:CD	2.36	0.56
1:B:83:PHE:CD1	1:B:83:PHE:C	2.79	0.56
1:D:83:PHE:C	1:D:83:PHE:CD1	2.79	0.56
1:E:360:MET:SD	1:E:397:LEU:HD12	2.46	0.56
1:E:317:PHE:C	1:E:319:LEU:N	2.59	0.56
1:C:122:VAL:HB	1:C:160:ARG:CD	2.36	0.56
1:B:116:LEU:CD2	1:B:178:LEU:HD23	2.36	0.56
1:A:312:THR:HG22	1:A:339:ALA:CB	2.36	0.56
1:A:360:MET:SD	1:A:397:LEU:HD12	2.46	0.56
1:E:446:SER:O	1:E:449:LEU:N	2.38	0.55
1:D:312:THR:HG22	1:D:339:ALA:CB	2.36	0.55
1:C:360:MET:SD	1:C:397:LEU:HD12	2.46	0.55
1:B:288:ILE:O	1:B:288:ILE:HG22	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:116:LEU:CD2	1:F:178:LEU:HD23	2.36	0.55
1:A:116:LEU:CD2	1:A:178:LEU:HD23	2.36	0.55
1:C:312:THR:HG22	1:C:339:ALA:CB	2.36	0.55
1:E:312:THR:HG22	1:E:339:ALA:CB	2.36	0.55
1:F:321:PRO:N	1:F:322:ILE:HD12	2.22	0.55
1:E:324:THR:C	1:E:326:GLY:N	2.56	0.55
1:B:317:PHE:C	1:B:319:LEU:N	2.59	0.55
1:D:288:ILE:O	1:D:288:ILE:HG22	2.06	0.55
1:F:320:ILE:O	1:F:322:ILE:N	2.39	0.55
1:C:210:TYR:H	1:D:210:TYR:HB2	1.70	0.55
1:A:210:TYR:H	1:B:210:TYR:HB2	1.70	0.55
1:E:320:ILE:O	1:E:322:ILE:N	2.39	0.55
1:B:312:THR:HG22	1:B:339:ALA:CB	2.36	0.55
1:C:320:ILE:O	1:C:322:ILE:N	2.39	0.55
1:A:320:ILE:O	1:A:322:ILE:N	2.39	0.55
1:D:157:ASN:C	1:D:159:GLY:N	2.56	0.55
1:B:270:ASN:ND2	1:B:444:LEU:HD23	2.20	0.55
1:C:116:LEU:CD2	1:C:178:LEU:HD23	2.35	0.55
1:D:21:LEU:O	1:D:25:LEU:N	2.34	0.55
1:E:258:LEU:HD13	1:E:371:PHE:CG	2.42	0.55
1:B:157:ASN:C	1:B:159:GLY:N	2.56	0.55
1:A:210:TYR:HB2	1:B:210:TYR:H	1.71	0.55
1:F:258:LEU:HD13	1:F:371:PHE:CG	2.42	0.55
1:E:210:TYR:HB2	1:F:210:TYR:H	1.71	0.55
1:E:321:PRO:N	1:E:322:ILE:HD12	2.22	0.55
1:E:211:THR:HG21	1:E:213:ILE:HG13	1.87	0.55
1:C:171:ASP:HB2	1:C:212:LEU:HD22	1.89	0.55
1:B:98:ARG:NH2	1:B:102:PRO:HB3	2.21	0.55
1:E:370:ALA:O	1:E:373:MET:HB2	2.07	0.55
1:E:210:TYR:H	1:F:210:TYR:HB2	1.70	0.55
1:F:83:PHE:CD1	1:F:83:PHE:C	2.79	0.55
1:F:171:ASP:HB2	1:F:212:LEU:HD22	1.89	0.55
1:F:211:THR:HG21	1:F:213:ILE:HG13	1.87	0.55
1:B:122:VAL:HB	1:B:160:ARG:CD	2.36	0.55
1:D:98:ARG:NH2	1:D:102:PRO:HB3	2.21	0.55
1:C:258:LEU:HD13	1:C:371:PHE:CG	2.42	0.55
1:E:74:ASN:HD21	1:E:77:LEU:CB	2.20	0.55
1:B:320:ILE:O	1:B:322:ILE:N	2.39	0.55
1:A:288:ILE:O	1:A:288:ILE:HG22	2.07	0.55
1:F:370:ALA:O	1:F:373:MET:HB2	2.07	0.55
1:A:258:LEU:HD13	1:A:371:PHE:CG	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:ASN:HD21	1:B:77:LEU:CB	2.20	0.55
1:D:320:ILE:O	1:D:322:ILE:N	2.39	0.54
1:D:122:VAL:HB	1:D:160:ARG:CD	2.36	0.54
1:C:288:ILE:O	1:C:288:ILE:HG22	2.06	0.54
1:C:135:GLY:HA2	1:C:138:THR:OG1	2.08	0.54
1:C:74:ASN:HD21	1:C:77:LEU:CB	2.20	0.54
1:E:83:PHE:C	1:E:83:PHE:CD1	2.79	0.54
1:A:135:GLY:HA2	1:A:138:THR:OG1	2.08	0.54
1:E:116:LEU:CD2	1:E:178:LEU:HD23	2.36	0.54
1:F:244:LEU:CD1	1:F:418:ASN:ND2	2.70	0.54
1:D:74:ASN:HD21	1:D:77:LEU:CB	2.20	0.54
1:A:74:ASN:HD21	1:A:77:LEU:CB	2.20	0.54
1:D:258:LEU:HD13	1:D:371:PHE:CG	2.42	0.54
1:D:171:ASP:HB2	1:D:212:LEU:HD22	1.89	0.54
1:A:171:ASP:HB2	1:A:212:LEU:HD22	1.89	0.54
1:E:216:LYS:HD3	1:F:434:LEU:HD23	1.89	0.54
1:A:370:ALA:O	1:A:373:MET:HB2	2.07	0.54
1:C:74:ASN:HD21	1:C:77:LEU:HB2	1.73	0.54
1:A:74:ASN:HD21	1:A:77:LEU:HB2	1.73	0.54
1:B:258:LEU:HD13	1:B:371:PHE:CG	2.42	0.54
1:A:321:PRO:N	1:A:322:ILE:HD12	2.22	0.54
1:D:135:GLY:HA2	1:D:138:THR:OG1	2.08	0.54
1:C:44:THR:HG23	1:C:228:MET:HE3	1.89	0.54
1:C:210:TYR:HB2	1:D:210:TYR:H	1.71	0.54
1:E:410:ILE:HD11	1:F:194:LEU:HD13	1.89	0.54
1:C:321:PRO:N	1:C:322:ILE:HD12	2.22	0.54
1:C:98:ARG:HA	1:C:98:ARG:NE	2.20	0.54
1:B:21:LEU:O	1:B:25:LEU:N	2.34	0.54
1:A:54:ASP:OD1	1:A:147:ARG:NH1	2.40	0.54
1:B:54:ASP:OD1	1:B:147:ARG:NH1	2.40	0.54
1:F:322:ILE:CD1	1:F:322:ILE:N	2.42	0.54
1:D:321:PRO:N	1:D:322:ILE:HD12	2.22	0.54
1:C:433:THR:HG22	1:D:216:LYS:HZ3	1.73	0.54
1:F:135:GLY:HA2	1:F:138:THR:OG1	2.08	0.54
1:D:370:ALA:O	1:D:373:MET:HB2	2.07	0.54
1:F:74:ASN:HD21	1:F:77:LEU:CB	2.20	0.54
1:B:135:GLY:HA2	1:B:138:THR:OG1	2.08	0.54
1:C:370:ALA:O	1:C:373:MET:HB2	2.07	0.54
1:F:54:ASP:OD1	1:F:147:ARG:NH1	2.40	0.54
1:D:54:ASP:OD1	1:D:147:ARG:NH1	2.40	0.54
1:B:321:PRO:N	1:B:322:ILE:HD12	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:171:ASP:HB2	1:E:212:LEU:HD22	1.89	0.54
1:E:244:LEU:CD1	1:E:418:ASN:ND2	2.70	0.54
1:A:224:MET:O	1:A:228:MET:HG2	2.08	0.54
1:B:244:LEU:CD1	1:B:418:ASN:ND2	2.70	0.54
1:B:171:ASP:HB2	1:B:212:LEU:HD22	1.89	0.54
1:E:135:GLY:HA2	1:E:138:THR:OG1	2.08	0.54
1:D:224:MET:O	1:D:228:MET:HG2	2.08	0.54
1:C:244:LEU:CD1	1:C:418:ASN:ND2	2.70	0.54
1:D:244:LEU:CD1	1:D:418:ASN:ND2	2.70	0.54
1:A:244:LEU:CD1	1:A:418:ASN:ND2	2.70	0.54
1:E:54:ASP:OD1	1:E:147:ARG:NH1	2.40	0.54
1:C:54:ASP:OD1	1:C:147:ARG:NH1	2.40	0.54
1:A:216:LYS:HD3	1:B:434:LEU:HD23	1.89	0.53
1:A:28:ARG:NH2	1:B:207:GLN:HE22	2.05	0.53
1:C:28:ARG:NH2	1:D:207:GLN:HE22	2.05	0.53
1:F:98:ARG:HA	1:F:98:ARG:NE	2.20	0.53
1:B:224:MET:O	1:B:228:MET:HG2	2.08	0.53
1:C:224:MET:O	1:C:228:MET:HG2	2.08	0.53
1:B:370:ALA:O	1:B:373:MET:HB2	2.07	0.53
1:A:98:ARG:HA	1:A:98:ARG:NE	2.20	0.53
1:B:74:ASN:HD21	1:B:77:LEU:HB2	1.73	0.53
1:E:446:SER:OG	1:F:28:ARG:NH1	2.41	0.53
1:F:288:ILE:O	1:F:288:ILE:HG22	2.07	0.53
1:E:74:ASN:HD21	1:E:77:LEU:HB2	1.73	0.53
1:A:449:LEU:O	1:A:453:LEU:HB2	2.09	0.53
1:B:449:LEU:O	1:B:453:LEU:HB2	2.09	0.53
1:C:198:LEU:HD13	1:C:406:LEU:HG	1.89	0.53
1:C:410:ILE:HD11	1:D:194:LEU:HD13	1.89	0.53
1:A:446:SER:OG	1:B:28:ARG:NH1	2.41	0.53
1:C:446:SER:OG	1:D:28:ARG:NH1	2.41	0.53
1:C:28:ARG:NH1	1:D:446:SER:OG	2.42	0.53
1:C:219:PHE:CD2	1:D:430:LEU:HD13	2.44	0.53
1:D:74:ASN:HD21	1:D:77:LEU:HB2	1.73	0.53
1:F:74:ASN:HD21	1:F:77:LEU:HB2	1.73	0.53
1:A:410:ILE:HD11	1:B:194:LEU:HD13	1.89	0.53
1:C:449:LEU:O	1:C:453:LEU:HB2	2.09	0.53
1:A:433:THR:HG22	1:B:216:LYS:HZ3	1.74	0.53
1:D:449:LEU:O	1:D:453:LEU:HB2	2.09	0.53
1:E:98:ARG:NE	1:E:98:ARG:HA	2.20	0.53
1:A:219:PHE:CD2	1:B:430:LEU:HD13	2.44	0.53
1:C:216:LYS:HD3	1:D:434:LEU:HD23	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:224:MET:O	1:F:228:MET:HG2	2.08	0.53
1:C:244:LEU:HD13	1:C:418:ASN:ND2	2.24	0.53
1:F:198:LEU:HD13	1:F:406:LEU:HG	1.89	0.53
1:E:109:ILE:N	1:E:110:PRO:HD2	2.24	0.53
1:A:28:ARG:NH1	1:B:446:SER:OG	2.42	0.53
1:E:288:ILE:HG22	1:E:288:ILE:O	2.07	0.53
1:E:219:PHE:CD2	1:F:430:LEU:HD13	2.44	0.53
1:A:244:LEU:HD13	1:A:418:ASN:ND2	2.24	0.53
1:B:198:LEU:HD13	1:B:406:LEU:HG	1.89	0.53
1:C:110:PRO:O	1:C:449:LEU:HD13	2.09	0.53
1:F:109:ILE:N	1:F:110:PRO:HD2	2.24	0.53
1:F:191:ASN:HB2	1:F:229:TYR:CE2	2.44	0.53
1:C:288:ILE:N	1:C:288:ILE:HD12	2.24	0.53
1:A:198:LEU:HD13	1:A:406:LEU:HG	1.89	0.53
1:E:449:LEU:O	1:E:453:LEU:HB2	2.09	0.53
1:B:98:ARG:NH1	1:B:291:TRP:CZ3	2.77	0.53
1:D:98:ARG:NH1	1:D:291:TRP:CZ3	2.77	0.53
1:A:148:GLU:O	1:A:149:GLY:C	2.48	0.53
1:B:148:GLU:O	1:B:149:GLY:C	2.48	0.53
1:F:244:LEU:HD13	1:F:418:ASN:ND2	2.24	0.53
1:E:244:LEU:HD13	1:E:418:ASN:ND2	2.24	0.53
1:A:419:TYR:OH	1:B:414:GLU:OE1	2.19	0.53
1:E:274:LEU:HD12	1:E:277:GLN:HE21	1.74	0.52
1:A:109:ILE:N	1:A:110:PRO:HD2	2.24	0.52
1:A:110:PRO:O	1:A:449:LEU:HD13	2.09	0.52
1:C:109:ILE:N	1:C:110:PRO:HD2	2.24	0.52
1:F:148:GLU:O	1:F:149:GLY:C	2.48	0.52
1:C:148:GLU:O	1:C:149:GLY:C	2.48	0.52
1:E:198:LEU:HD13	1:E:406:LEU:HG	1.89	0.52
1:F:131:LYS:HZ2	1:F:153:GLN:NE2	2.07	0.52
1:E:28:ARG:NH2	1:F:207:GLN:HE22	2.05	0.52
1:E:28:ARG:NH1	1:F:446:SER:OG	2.42	0.52
1:B:284:HIS:O	1:B:286:GLY:N	2.42	0.52
1:F:288:ILE:HD12	1:F:288:ILE:N	2.24	0.52
1:A:288:ILE:N	1:A:288:ILE:HD12	2.24	0.52
1:E:98:ARG:NH1	1:E:291:TRP:CZ3	2.77	0.52
1:D:148:GLU:O	1:D:149:GLY:C	2.48	0.52
1:D:109:ILE:N	1:D:110:PRO:HD2	2.24	0.52
1:D:284:HIS:O	1:D:286:GLY:N	2.43	0.52
1:D:244:LEU:HD13	1:D:418:ASN:ND2	2.24	0.52
1:D:198:LEU:HD13	1:D:406:LEU:HG	1.89	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:21:LEU:O	1:F:25:LEU:N	2.34	0.52
1:F:110:PRO:O	1:F:449:LEU:HD13	2.09	0.52
1:B:110:PRO:O	1:B:449:LEU:HD13	2.09	0.52
1:D:191:ASN:HB2	1:D:229:TYR:CE2	2.44	0.52
1:E:224:MET:O	1:E:228:MET:HG2	2.08	0.52
1:B:109:ILE:N	1:B:110:PRO:HD2	2.24	0.52
1:D:288:ILE:N	1:D:288:ILE:HD12	2.24	0.52
1:C:98:ARG:NH1	1:C:291:TRP:CZ3	2.77	0.52
1:A:284:HIS:O	1:A:286:GLY:N	2.43	0.52
1:F:90:ALA:O	1:F:94:TYR:HD1	1.93	0.52
1:C:191:ASN:HB2	1:C:229:TYR:CE2	2.44	0.52
1:D:444:LEU:HD13	1:D:444:LEU:O	2.10	0.52
1:B:191:ASN:HB2	1:B:229:TYR:CE2	2.44	0.52
1:B:288:ILE:HD12	1:B:288:ILE:N	2.24	0.52
1:A:44:THR:HG23	1:A:228:MET:HE3	1.92	0.52
1:A:44:THR:HG23	1:A:228:MET:HE2	1.90	0.52
1:B:244:LEU:HD13	1:B:418:ASN:ND2	2.24	0.52
1:C:419:TYR:OH	1:D:414:GLU:OE1	2.19	0.52
1:E:110:PRO:O	1:E:449:LEU:HD13	2.09	0.52
1:C:274:LEU:HD12	1:C:277:GLN:HE21	1.74	0.52
1:F:444:LEU:HD13	1:F:444:LEU:O	2.10	0.52
1:B:444:LEU:O	1:B:444:LEU:HD13	2.10	0.52
1:D:274:LEU:HD12	1:D:277:GLN:HE21	1.75	0.52
1:C:284:HIS:O	1:C:286:GLY:N	2.43	0.52
1:A:98:ARG:NH1	1:A:291:TRP:CZ3	2.77	0.52
1:E:98:ARG:NH2	1:E:102:PRO:HB3	2.21	0.52
1:E:191:ASN:HB2	1:E:229:TYR:CE2	2.44	0.52
1:B:200:ILE:HA	1:B:204:MET:HB2	1.92	0.52
1:A:444:LEU:HD13	1:A:444:LEU:O	2.10	0.52
1:F:98:ARG:NH2	1:F:102:PRO:HB3	2.21	0.52
1:F:284:HIS:O	1:F:286:GLY:N	2.43	0.52
1:E:284:HIS:O	1:E:286:GLY:N	2.43	0.52
1:E:90:ALA:O	1:E:94:TYR:HD1	1.93	0.52
1:D:110:PRO:O	1:D:449:LEU:HD13	2.09	0.52
1:D:109:ILE:HG21	1:D:445:TYR:CD1	2.45	0.52
1:A:90:ALA:O	1:A:94:TYR:HD1	1.93	0.52
1:E:444:LEU:O	1:E:444:LEU:HD13	2.10	0.52
1:A:200:ILE:HA	1:A:204:MET:HB2	1.92	0.52
1:A:274:LEU:HD12	1:A:277:GLN:HE21	1.74	0.52
1:C:444:LEU:HD13	1:C:444:LEU:O	2.10	0.52
1:F:30:LYS:HZ3	1:F:30:LYS:HB3	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:ASN:HB2	1:A:229:TYR:CE2	2.44	0.52
1:D:200:ILE:HA	1:D:204:MET:HB2	1.92	0.51
1:B:109:ILE:HG21	1:B:445:TYR:CD1	2.45	0.51
1:F:98:ARG:NH1	1:F:291:TRP:CZ3	2.77	0.51
1:E:288:ILE:HD12	1:E:288:ILE:N	2.24	0.51
1:A:321:PRO:HA	1:A:365:THR:HG21	1.92	0.51
1:E:321:PRO:HA	1:E:365:THR:HG21	1.92	0.51
1:F:274:LEU:HD12	1:F:277:GLN:HE21	1.74	0.51
1:C:200:ILE:HA	1:C:204:MET:HB2	1.92	0.51
1:B:274:LEU:HD12	1:B:277:GLN:HE21	1.74	0.51
1:E:148:GLU:O	1:E:149:GLY:C	2.48	0.51
1:B:30:LYS:HB3	1:B:30:LYS:HZ3	1.73	0.51
1:E:109:ILE:HG21	1:E:445:TYR:CD1	2.45	0.51
1:C:321:PRO:HA	1:C:365:THR:HG21	1.93	0.51
1:E:430:LEU:CD1	1:F:219:PHE:HB3	2.40	0.51
1:E:200:ILE:HA	1:E:204:MET:HB2	1.92	0.51
1:F:449:LEU:O	1:F:453:LEU:HB2	2.09	0.51
1:C:90:ALA:O	1:C:94:TYR:HD1	1.93	0.51
1:F:200:ILE:HA	1:F:204:MET:HB2	1.92	0.51
1:F:321:PRO:HA	1:F:365:THR:HG21	1.92	0.51
1:F:176:THR:HG22	1:F:177:LEU:N	2.26	0.51
1:D:90:ALA:O	1:D:94:TYR:HD1	1.93	0.51
1:C:419:TYR:CZ	1:D:414:GLU:OE1	2.64	0.51
1:A:176:THR:HG22	1:A:177:LEU:N	2.26	0.51
1:D:356:ILE:HG13	1:D:360:MET:HE1	1.93	0.51
1:F:449:LEU:HA	1:F:452:THR:HG22	1.93	0.51
1:A:109:ILE:HG21	1:A:445:TYR:CD1	2.45	0.51
1:D:321:PRO:HA	1:D:365:THR:HG21	1.92	0.51
1:C:249:LEU:HD11	1:D:230:ARG:HB3	1.93	0.51
1:B:308:VAL:O	1:B:309:ALA:HB3	2.11	0.51
1:C:176:THR:HG22	1:C:177:LEU:N	2.26	0.50
1:B:176:THR:HG22	1:B:177:LEU:N	2.26	0.50
1:F:109:ILE:HG21	1:F:445:TYR:CD1	2.45	0.50
1:E:419:TYR:CZ	1:F:414:GLU:OE1	2.64	0.50
1:A:419:TYR:CZ	1:B:414:GLU:OE1	2.64	0.50
1:B:42:VAL:HG21	1:B:177:LEU:HD13	1.94	0.50
1:A:249:LEU:HD11	1:B:230:ARG:HB3	1.93	0.50
1:B:90:ALA:O	1:B:94:TYR:HD1	1.93	0.50
1:D:308:VAL:O	1:D:309:ALA:HB3	2.11	0.50
1:E:176:THR:HG22	1:E:177:LEU:N	2.26	0.50
1:D:176:THR:HG22	1:D:177:LEU:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:211:THR:C	1:D:212:LEU:HD12	2.32	0.50
1:E:249:LEU:HD11	1:F:230:ARG:HB3	1.94	0.50
1:E:244:LEU:CD1	1:E:418:ASN:HD21	2.25	0.50
1:F:308:VAL:O	1:F:309:ALA:HB3	2.12	0.50
1:E:449:LEU:HA	1:E:452:THR:HG22	1.93	0.50
1:F:318:ASN:O	1:F:319:LEU:HD13	2.12	0.50
1:C:109:ILE:HG21	1:C:445:TYR:CD1	2.45	0.50
1:C:449:LEU:HA	1:C:452:THR:HG22	1.93	0.50
1:A:211:THR:C	1:A:212:LEU:HD12	2.32	0.50
1:D:148:GLU:HG2	1:D:357:PHE:HD2	1.77	0.50
1:D:42:VAL:HG21	1:D:177:LEU:HD13	1.94	0.50
1:B:211:THR:C	1:B:212:LEU:HD12	2.32	0.50
1:D:249:LEU:C	1:D:251:THR:H	2.15	0.50
1:A:249:LEU:C	1:A:251:THR:H	2.15	0.50
1:B:148:GLU:HG2	1:B:357:PHE:HD2	1.77	0.50
1:C:148:GLU:HG2	1:C:357:PHE:HD2	1.77	0.50
1:F:112:ILE:HD12	1:F:156:GLY:HA3	1.94	0.50
1:A:430:LEU:CD1	1:B:219:PHE:HB3	2.40	0.50
1:B:249:LEU:C	1:B:251:THR:H	2.15	0.50
1:E:249:LEU:C	1:E:251:THR:H	2.15	0.50
1:A:148:GLU:HG2	1:A:357:PHE:HD2	1.77	0.50
1:E:318:ASN:O	1:E:319:LEU:HD13	2.12	0.50
1:B:321:PRO:HA	1:B:365:THR:HG21	1.93	0.50
1:C:430:LEU:CD1	1:D:219:PHE:HB3	2.41	0.50
1:E:211:THR:C	1:E:212:LEU:HD12	2.32	0.50
1:D:122:VAL:HB	1:D:160:ARG:HD2	1.94	0.50
1:A:112:ILE:HD12	1:A:156:GLY:HA3	1.94	0.50
1:C:211:THR:C	1:C:212:LEU:HD12	2.32	0.50
1:B:122:VAL:HB	1:B:160:ARG:HD2	1.94	0.50
1:F:249:LEU:C	1:F:251:THR:H	2.15	0.50
1:C:44:THR:HG23	1:C:228:MET:HE2	1.93	0.50
1:A:30:LYS:HB3	1:A:30:LYS:HZ2	1.77	0.50
1:E:112:ILE:HD12	1:E:156:GLY:HA3	1.94	0.50
1:A:449:LEU:HA	1:A:452:THR:HG22	1.93	0.50
1:E:294:MET:O	1:E:297:ALA:HB3	2.12	0.50
1:A:21:LEU:O	1:A:25:LEU:N	2.34	0.50
1:C:269:PHE:O	1:C:273:VAL:HG12	2.12	0.49
1:E:42:VAL:HG21	1:E:177:LEU:HD13	1.94	0.49
1:C:42:VAL:HG21	1:C:177:LEU:HD13	1.94	0.49
1:D:449:LEU:HA	1:D:452:THR:HG22	1.93	0.49
1:C:249:LEU:C	1:C:251:THR:H	2.15	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:356:ILE:HG13	1:B:360:MET:HE1	1.94	0.49
1:C:308:VAL:O	1:C:309:ALA:HB3	2.12	0.49
1:C:112:ILE:HD12	1:C:156:GLY:HA3	1.94	0.49
1:E:269:PHE:O	1:E:273:VAL:HG12	2.12	0.49
1:F:269:PHE:O	1:F:273:VAL:HG12	2.12	0.49
1:F:148:GLU:HG2	1:F:357:PHE:CD2	2.48	0.49
1:A:308:VAL:O	1:A:309:ALA:HB3	2.11	0.49
1:E:459:GLU:O	1:E:459:GLU:HG2	2.12	0.49
1:F:459:GLU:O	1:F:459:GLU:HG2	2.12	0.49
1:A:269:PHE:O	1:A:273:VAL:HG12	2.12	0.49
1:A:430:LEU:CD2	1:B:223:ILE:HD12	2.40	0.49
1:F:211:THR:C	1:F:212:LEU:HD12	2.32	0.49
1:E:308:VAL:O	1:E:309:ALA:HB3	2.11	0.49
1:A:315:GLY:H	1:A:318:ASN:ND2	2.10	0.49
1:D:443:PRO:O	1:D:446:SER:N	2.41	0.49
1:E:30:LYS:HG2	1:E:30:LYS:O	2.12	0.49
1:F:358:ALA:O	1:F:361:LEU:HB2	2.13	0.49
1:B:322:ILE:CD1	1:B:322:ILE:N	2.42	0.49
1:A:42:VAL:HG21	1:A:177:LEU:HD13	1.94	0.49
1:B:131:LYS:HZ2	1:B:153:GLN:NE2	2.10	0.49
1:B:449:LEU:HA	1:B:452:THR:HG22	1.93	0.49
1:D:269:PHE:O	1:D:273:VAL:HG12	2.12	0.49
1:F:288:ILE:HD12	1:F:288:ILE:H	1.77	0.49
1:D:288:ILE:HD12	1:D:288:ILE:H	1.77	0.49
1:E:198:LEU:HD13	1:E:406:LEU:CD2	2.43	0.49
1:D:294:MET:O	1:D:297:ALA:HB3	2.12	0.49
1:C:315:GLY:H	1:C:318:ASN:ND2	2.10	0.49
1:B:318:ASN:O	1:B:319:LEU:HD13	2.12	0.49
1:B:288:ILE:HD12	1:B:288:ILE:H	1.77	0.49
1:C:288:ILE:H	1:C:288:ILE:HD12	1.77	0.49
1:D:30:LYS:HZ3	1:D:30:LYS:HB3	1.76	0.49
1:D:198:LEU:HD13	1:D:406:LEU:CD2	2.43	0.49
1:A:294:MET:O	1:A:297:ALA:HB3	2.12	0.49
1:A:459:GLU:HG2	1:A:459:GLU:O	2.12	0.49
1:C:459:GLU:O	1:C:459:GLU:HG2	2.12	0.49
1:A:318:ASN:O	1:A:319:LEU:HD13	2.12	0.49
1:C:122:VAL:HB	1:C:160:ARG:HD2	1.94	0.49
1:F:123:ARG:CZ	1:F:127:VAL:HG21	2.43	0.49
1:B:443:PRO:O	1:B:446:SER:N	2.41	0.49
1:A:288:ILE:H	1:A:288:ILE:HD12	1.77	0.49
1:E:44:THR:HG23	1:E:228:MET:HE3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:148:GLU:HG2	1:F:357:PHE:HD2	1.77	0.49
1:C:148:GLU:HG2	1:C:357:PHE:CD2	2.48	0.49
1:E:148:GLU:HG2	1:E:357:PHE:CD2	2.48	0.49
1:A:30:LYS:HG2	1:A:30:LYS:O	2.12	0.49
1:B:294:MET:O	1:B:297:ALA:HB3	2.12	0.49
1:C:294:MET:O	1:C:297:ALA:HB3	2.12	0.49
1:F:315:GLY:H	1:F:318:ASN:ND2	2.10	0.49
1:A:122:VAL:HB	1:A:160:ARG:HD2	1.94	0.49
1:B:269:PHE:O	1:B:273:VAL:HG12	2.12	0.49
1:A:148:GLU:HG2	1:A:357:PHE:CD2	2.48	0.49
1:F:30:LYS:HG2	1:F:30:LYS:O	2.12	0.49
1:C:198:LEU:HD13	1:C:406:LEU:CD2	2.43	0.49
1:A:198:LEU:HD13	1:A:406:LEU:CD2	2.43	0.49
1:E:209:ARG:HG3	1:E:209:ARG:O	2.13	0.49
1:B:112:ILE:HD12	1:B:156:GLY:HA3	1.94	0.49
1:E:358:ALA:O	1:E:361:LEU:HB2	2.13	0.49
1:C:318:ASN:O	1:C:319:LEU:HD13	2.12	0.49
1:C:430:LEU:CD2	1:D:223:ILE:HD12	2.40	0.49
1:F:42:VAL:HG21	1:F:177:LEU:HD13	1.94	0.49
1:D:112:ILE:HD12	1:D:156:GLY:HA3	1.94	0.49
1:D:318:ASN:O	1:D:319:LEU:HD13	2.12	0.49
1:B:124:TRP:HA	1:B:157:ASN:HD22	1.78	0.49
1:E:216:LYS:O	1:E:220:ILE:HG13	2.13	0.49
1:B:148:GLU:HG2	1:B:357:PHE:CD2	2.48	0.49
1:C:30:LYS:O	1:C:30:LYS:HG2	2.12	0.49
1:D:30:LYS:HG2	1:D:30:LYS:O	2.12	0.49
1:A:358:ALA:O	1:A:361:LEU:HB2	2.13	0.49
1:E:26:LEU:HD21	1:F:450:ALA:CB	2.43	0.49
1:F:216:LYS:O	1:F:220:ILE:HG13	2.13	0.48
1:D:216:LYS:O	1:D:220:ILE:HG13	2.13	0.48
1:F:122:VAL:HB	1:F:160:ARG:HD2	1.94	0.48
1:D:124:TRP:HA	1:D:157:ASN:HD22	1.78	0.48
1:D:148:GLU:HG2	1:D:357:PHE:CD2	2.48	0.48
1:C:30:LYS:HZ2	1:C:30:LYS:HB3	1.78	0.48
1:B:30:LYS:O	1:B:30:LYS:HG2	2.12	0.48
1:B:459:GLU:O	1:B:459:GLU:HG2	2.12	0.48
1:E:124:TRP:HA	1:E:157:ASN:HD22	1.78	0.48
1:E:123:ARG:CZ	1:E:127:VAL:HG21	2.43	0.48
1:D:123:ARG:CZ	1:D:127:VAL:HG21	2.43	0.48
1:F:198:LEU:HD13	1:F:406:LEU:CD2	2.43	0.48
1:D:244:LEU:CD1	1:D:418:ASN:HD21	2.25	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:430:LEU:HD21	1:F:220:ILE:CG1	2.32	0.48
1:A:124:TRP:HA	1:A:157:ASN:HD22	1.78	0.48
1:F:443:PRO:O	1:F:446:SER:N	2.41	0.48
1:E:288:ILE:HD12	1:E:288:ILE:H	1.77	0.48
1:A:223:ILE:HD11	1:B:430:LEU:HD22	1.93	0.48
1:C:223:ILE:HD11	1:D:430:LEU:HD22	1.93	0.48
1:B:198:LEU:HD13	1:B:406:LEU:CD2	2.43	0.48
1:A:26:LEU:HD21	1:B:450:ALA:CB	2.43	0.48
1:F:294:MET:O	1:F:297:ALA:HB3	2.12	0.48
1:C:109:ILE:HD11	1:C:152:VAL:CG2	2.43	0.48
1:B:216:LYS:O	1:B:220:ILE:HG13	2.13	0.48
1:E:122:VAL:HB	1:E:160:ARG:HD2	1.94	0.48
1:C:108:GLY:HA2	1:C:153:GLN:NE2	2.29	0.48
1:C:131:LYS:HZ2	1:C:153:GLN:NE2	2.09	0.48
1:A:108:GLY:HA2	1:A:153:GLN:NE2	2.29	0.48
1:B:128:LEU:HB2	1:B:129:PRO:HD2	1.96	0.48
1:D:44:THR:HG23	1:D:228:MET:HE2	1.94	0.48
1:B:244:LEU:CD1	1:B:418:ASN:HD21	2.25	0.48
1:C:123:ARG:CZ	1:C:127:VAL:HG21	2.43	0.48
1:D:128:LEU:HB2	1:D:129:PRO:HD2	1.96	0.48
1:E:148:GLU:HG2	1:E:357:PHE:HD2	1.77	0.48
1:C:26:LEU:HD21	1:D:450:ALA:CB	2.43	0.48
1:E:433:THR:HG22	1:F:216:LYS:HZ3	1.77	0.48
1:C:157:ASN:C	1:C:159:GLY:H	2.16	0.48
1:F:124:TRP:HA	1:F:157:ASN:HD22	1.78	0.48
1:C:98:ARG:NH2	1:C:102:PRO:HB3	2.21	0.48
1:C:30:LYS:HZ3	1:C:30:LYS:HB3	1.78	0.48
1:A:356:ILE:HG13	1:A:360:MET:HE1	1.95	0.48
1:C:358:ALA:O	1:C:361:LEU:HB2	2.13	0.48
1:D:459:GLU:HG2	1:D:459:GLU:O	2.12	0.48
1:A:267:PRO:O	1:A:270:ASN:HB2	2.14	0.48
1:D:315:GLY:H	1:D:318:ASN:ND2	2.10	0.48
1:C:124:TRP:HA	1:C:157:ASN:HD22	1.78	0.48
1:D:157:ASN:C	1:D:159:GLY:H	2.16	0.48
1:B:123:ARG:CZ	1:B:127:VAL:HG21	2.43	0.48
1:D:91:MET:O	1:D:93:GLY:N	2.47	0.48
1:E:91:MET:O	1:E:93:GLY:N	2.47	0.48
1:D:358:ALA:O	1:D:361:LEU:HB2	2.13	0.48
1:A:312:THR:HG22	1:A:339:ALA:HB1	1.96	0.48
1:B:209:ARG:HG3	1:B:209:ARG:O	2.13	0.48
1:C:128:LEU:HB2	1:C:129:PRO:HD2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:GLY:HA2	1:B:153:GLN:NE2	2.29	0.48
1:F:267:PRO:O	1:F:270:ASN:HB2	2.14	0.48
1:B:91:MET:O	1:B:93:GLY:N	2.47	0.48
1:C:216:LYS:O	1:C:220:ILE:HG13	2.13	0.48
1:E:356:ILE:HG13	1:E:360:MET:HE1	1.96	0.48
1:C:312:THR:HG22	1:C:339:ALA:HB1	1.96	0.48
1:D:209:ARG:HG3	1:D:209:ARG:O	2.13	0.48
1:C:267:PRO:O	1:C:270:ASN:HB2	2.14	0.48
1:C:433:THR:CG2	1:D:216:LYS:HE2	2.44	0.48
1:D:312:THR:HG22	1:D:339:ALA:HB1	1.96	0.48
1:B:312:THR:HG22	1:B:339:ALA:HB1	1.96	0.48
1:D:179:ALA:HB1	1:D:200:ILE:HG21	1.96	0.48
1:E:179:ALA:HB1	1:E:200:ILE:HG21	1.96	0.48
1:B:315:GLY:H	1:B:318:ASN:ND2	2.10	0.48
1:E:430:LEU:CD2	1:F:223:ILE:HD12	2.40	0.48
1:E:131:LYS:HZ2	1:E:153:GLN:NE2	2.10	0.48
1:E:108:GLY:HA2	1:E:153:GLN:NE2	2.29	0.48
1:F:157:ASN:C	1:F:159:GLY:H	2.16	0.48
1:A:123:ARG:CZ	1:A:127:VAL:HG21	2.43	0.48
1:A:128:LEU:HB2	1:A:129:PRO:HD2	1.96	0.48
1:F:91:MET:O	1:F:93:GLY:N	2.47	0.48
1:B:179:ALA:HB1	1:B:200:ILE:HG21	1.96	0.47
1:E:443:PRO:O	1:E:446:SER:N	2.41	0.47
1:A:433:THR:CG2	1:B:216:LYS:HE2	2.44	0.47
1:A:157:ASN:C	1:A:159:GLY:H	2.16	0.47
1:D:209:ARG:O	1:D:210:TYR:C	2.52	0.47
1:D:42:VAL:HG22	1:D:162:VAL:HG21	1.96	0.47
1:B:209:ARG:O	1:B:210:TYR:C	2.52	0.47
1:E:209:ARG:O	1:E:210:TYR:C	2.52	0.47
1:E:267:PRO:O	1:E:270:ASN:HB2	2.14	0.47
1:D:108:GLY:HA2	1:D:153:GLN:NE2	2.29	0.47
1:F:266:GLY:HA3	1:F:400:ALA:HB1	1.97	0.47
1:B:267:PRO:O	1:B:270:ASN:HB2	2.14	0.47
1:B:358:ALA:O	1:B:361:LEU:HB2	2.13	0.47
1:A:216:LYS:O	1:A:220:ILE:HG13	2.13	0.47
1:C:244:LEU:CD1	1:C:418:ASN:HD21	2.25	0.47
1:A:209:ARG:O	1:A:210:TYR:C	2.52	0.47
1:E:315:GLY:H	1:E:318:ASN:ND2	2.10	0.47
1:C:266:GLY:HA3	1:C:400:ALA:HB1	1.97	0.47
1:F:108:GLY:HA2	1:F:153:GLN:NE2	2.29	0.47
1:B:157:ASN:C	1:B:159:GLY:H	2.16	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:VAL:HG22	1:B:162:VAL:HG21	1.97	0.47
1:A:91:MET:O	1:A:93:GLY:N	2.47	0.47
1:A:98:ARG:NH2	1:A:102:PRO:HB3	2.21	0.47
1:C:209:ARG:O	1:C:210:TYR:C	2.52	0.47
1:F:209:ARG:O	1:F:209:ARG:HG3	2.13	0.47
1:E:266:GLY:HA3	1:E:400:ALA:HB1	1.97	0.47
1:E:451:ARG:C	1:E:453:LEU:H	2.18	0.47
1:F:314:GLY:C	1:F:316:GLY:H	2.18	0.47
1:A:266:GLY:HA3	1:A:400:ALA:HB1	1.97	0.47
1:E:314:GLY:C	1:E:316:GLY:H	2.18	0.47
1:E:433:THR:CG2	1:F:216:LYS:HE2	2.44	0.47
1:F:109:ILE:HD11	1:F:152:VAL:CG2	2.43	0.47
1:D:267:PRO:O	1:D:270:ASN:HB2	2.14	0.47
1:C:91:MET:O	1:C:93:GLY:N	2.47	0.47
1:B:314:GLY:C	1:B:316:GLY:H	2.18	0.47
1:B:44:THR:HG23	1:B:228:MET:HE2	1.96	0.47
1:A:244:LEU:CD1	1:A:418:ASN:HD21	2.25	0.47
1:D:132:PHE:C	1:D:132:PHE:CD2	2.88	0.47
1:C:209:ARG:O	1:C:209:ARG:HG3	2.13	0.47
1:C:74:ASN:ND2	1:C:77:LEU:HB3	2.29	0.47
1:F:74:ASN:ND2	1:F:77:LEU:HB3	2.29	0.47
1:C:287:ASN:HB3	1:C:290:LYS:HB2	1.97	0.47
1:F:287:ASN:HB3	1:F:290:LYS:HB2	1.97	0.47
1:E:183:ALA:HB2	1:E:200:ILE:CG1	2.39	0.47
1:C:314:GLY:C	1:C:316:GLY:H	2.18	0.47
1:A:451:ARG:C	1:A:453:LEU:H	2.18	0.47
1:C:451:ARG:C	1:C:453:LEU:H	2.18	0.47
1:C:433:THR:HG21	1:D:216:LYS:HE2	1.97	0.47
1:F:128:LEU:HB2	1:F:129:PRO:HD2	1.96	0.47
1:B:451:ARG:C	1:B:453:LEU:H	2.18	0.47
1:D:314:GLY:C	1:D:316:GLY:H	2.18	0.47
1:E:223:ILE:HD11	1:F:430:LEU:HD22	1.93	0.47
1:B:132:PHE:CD2	1:B:132:PHE:C	2.88	0.47
1:E:287:ASN:HB3	1:E:290:LYS:HB2	1.97	0.47
1:A:314:GLY:C	1:A:316:GLY:H	2.18	0.47
1:A:179:ALA:HB1	1:A:200:ILE:HG21	1.96	0.47
1:E:157:ASN:C	1:E:159:GLY:H	2.16	0.47
1:E:249:LEU:HD11	1:F:230:ARG:CB	2.45	0.47
1:B:74:ASN:ND2	1:B:77:LEU:HB3	2.29	0.47
1:A:287:ASN:HB3	1:A:290:LYS:HB2	1.97	0.47
1:B:287:ASN:HB3	1:B:290:LYS:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:THR:HG21	1:B:216:LYS:HE2	1.97	0.47
1:E:42:VAL:HG22	1:E:162:VAL:HG21	1.97	0.47
1:B:266:GLY:HA3	1:B:400:ALA:HB1	1.97	0.47
1:D:451:ARG:C	1:D:453:LEU:H	2.18	0.47
1:F:312:THR:HG22	1:F:339:ALA:HB1	1.96	0.47
1:E:312:THR:HG22	1:E:339:ALA:HB1	1.96	0.47
1:A:209:ARG:O	1:A:209:ARG:HG3	2.13	0.47
1:F:209:ARG:O	1:F:210:TYR:C	2.52	0.47
1:E:74:ASN:ND2	1:E:77:LEU:HB3	2.29	0.47
1:A:74:ASN:ND2	1:A:77:LEU:HB3	2.29	0.47
1:C:179:ALA:HB1	1:C:200:ILE:HG21	1.96	0.46
1:E:216:LYS:HD3	1:F:434:LEU:CD2	2.45	0.46
1:A:30:LYS:HB3	1:A:30:LYS:HZ3	1.80	0.46
1:E:30:LYS:HZ3	1:E:30:LYS:HB3	1.79	0.46
1:A:12:GLN:O	1:A:16:LEU:HB2	2.16	0.46
1:C:12:GLN:O	1:C:16:LEU:HB2	2.16	0.46
1:E:203:GLU:O	1:E:204:MET:C	2.54	0.46
1:A:203:GLU:O	1:A:204:MET:C	2.54	0.46
1:A:430:LEU:HD21	1:B:220:ILE:CG1	2.32	0.46
1:E:108:GLY:HA3	1:E:153:GLN:HE21	1.81	0.46
1:C:42:VAL:HG22	1:C:162:VAL:HG21	1.97	0.46
1:C:356:ILE:HG13	1:C:360:MET:HE1	1.96	0.46
1:F:179:ALA:HB1	1:F:200:ILE:HG21	1.96	0.46
1:E:109:ILE:HD11	1:E:152:VAL:CG2	2.43	0.46
1:C:274:LEU:O	1:C:277:GLN:HG2	2.15	0.46
1:E:101:ALA:C	1:E:103:GLU:H	2.19	0.46
1:F:12:GLN:O	1:F:16:LEU:HB2	2.16	0.46
1:A:274:LEU:O	1:A:277:GLN:HG2	2.15	0.46
1:E:128:LEU:HB2	1:E:129:PRO:HD2	1.96	0.46
1:B:101:ALA:C	1:B:103:GLU:H	2.19	0.46
1:F:451:ARG:C	1:F:453:LEU:H	2.18	0.46
1:F:244:LEU:CD1	1:F:418:ASN:HD21	2.25	0.46
1:C:132:PHE:CD2	1:C:132:PHE:C	2.88	0.46
1:F:356:ILE:HG13	1:F:360:MET:HE1	1.97	0.46
1:D:74:ASN:ND2	1:D:77:LEU:HB3	2.29	0.46
1:E:358:ALA:HB3	1:E:359:PRO:CD	2.46	0.46
1:D:287:ASN:HB3	1:D:290:LYS:HB2	1.97	0.46
1:C:203:GLU:O	1:C:204:MET:C	2.54	0.46
1:D:274:LEU:O	1:D:277:GLN:HG2	2.15	0.46
1:D:266:GLY:HA3	1:D:400:ALA:HB1	1.97	0.46
1:C:216:LYS:HD3	1:D:434:LEU:CD2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:ASN:ND2	1:B:77:LEU:CB	2.79	0.46
1:D:74:ASN:ND2	1:D:77:LEU:CB	2.79	0.46
1:A:74:ASN:ND2	1:A:77:LEU:CB	2.79	0.46
1:F:101:ALA:C	1:F:103:GLU:H	2.19	0.46
1:E:255:TYR:CG	1:E:424:PRO:HB3	2.51	0.46
1:A:132:PHE:C	1:A:132:PHE:CD2	2.88	0.46
1:E:74:ASN:ND2	1:E:77:LEU:CB	2.79	0.46
1:B:12:GLN:O	1:B:16:LEU:HB2	2.16	0.46
1:C:108:GLY:HA3	1:C:153:GLN:HE21	1.81	0.46
1:D:101:ALA:C	1:D:103:GLU:H	2.19	0.46
1:A:101:ALA:C	1:A:103:GLU:H	2.19	0.46
1:A:249:LEU:HD11	1:B:230:ARG:CB	2.45	0.46
1:E:30:LYS:HZ2	1:E:30:LYS:HB3	1.78	0.46
1:F:132:PHE:C	1:F:132:PHE:CD2	2.88	0.46
1:C:74:ASN:ND2	1:C:77:LEU:CB	2.79	0.46
1:E:12:GLN:O	1:E:16:LEU:HB2	2.16	0.46
1:E:22:ILE:HD13	1:F:454:ALA:HB2	1.98	0.46
1:A:42:VAL:HG22	1:A:162:VAL:HG21	1.97	0.46
1:F:274:LEU:O	1:F:277:GLN:HG2	2.15	0.46
1:C:249:LEU:HD11	1:D:230:ARG:CB	2.45	0.46
1:C:255:TYR:CG	1:C:424:PRO:HB3	2.51	0.46
1:D:94:TYR:CZ	1:D:352:ALA:HB2	2.51	0.46
1:A:244:LEU:H	1:A:418:ASN:ND2	2.14	0.46
1:F:358:ALA:HB3	1:F:359:PRO:CD	2.46	0.46
1:A:109:ILE:HD11	1:A:152:VAL:CG2	2.43	0.46
1:C:430:LEU:HD21	1:D:220:ILE:CG1	2.32	0.46
1:B:274:LEU:O	1:B:277:GLN:HG2	2.15	0.46
1:F:255:TYR:CG	1:F:424:PRO:HB3	2.51	0.46
1:A:255:TYR:CG	1:A:424:PRO:HB3	2.51	0.46
1:A:216:LYS:HD3	1:B:434:LEU:CD2	2.45	0.46
1:B:94:TYR:CZ	1:B:352:ALA:HB2	2.51	0.46
1:E:94:TYR:CZ	1:E:352:ALA:HB2	2.51	0.46
1:C:391:ILE:N	1:C:391:ILE:HD12	2.31	0.46
1:F:203:GLU:O	1:F:204:MET:C	2.54	0.46
1:B:203:GLU:O	1:B:204:MET:C	2.54	0.46
1:E:127:VAL:HB	1:E:157:ASN:HD21	1.81	0.46
1:A:108:GLY:HA3	1:A:153:GLN:HE21	1.81	0.46
1:B:358:ALA:HB3	1:B:359:PRO:CD	2.46	0.46
1:F:74:ASN:ND2	1:F:77:LEU:CB	2.79	0.46
1:D:12:GLN:O	1:D:16:LEU:HB2	2.16	0.46
1:F:283:VAL:O	1:F:283:VAL:HG12	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:433:THR:HG21	1:F:216:LYS:HE2	1.97	0.45
1:C:101:ALA:C	1:C:103:GLU:H	2.19	0.45
1:C:284:HIS:CE1	1:C:291:TRP:CD2	3.04	0.45
1:C:244:LEU:H	1:C:418:ASN:ND2	2.14	0.45
1:D:358:ALA:HB3	1:D:359:PRO:CD	2.46	0.45
1:D:283:VAL:O	1:D:283:VAL:HG12	2.16	0.45
1:F:391:ILE:HD12	1:F:391:ILE:N	2.31	0.45
1:C:434:LEU:C	1:C:436:ALA:N	2.70	0.45
1:A:434:LEU:C	1:A:436:ALA:N	2.70	0.45
1:C:128:LEU:CB	1:C:129:PRO:CD	2.95	0.45
1:F:108:GLY:HA3	1:F:153:GLN:HE21	1.81	0.45
1:F:42:VAL:HG22	1:F:162:VAL:HG21	1.97	0.45
1:D:244:LEU:H	1:D:418:ASN:ND2	2.14	0.45
1:D:276:MET:HG2	1:D:280:LEU:HD23	1.98	0.45
1:E:132:PHE:C	1:E:132:PHE:CD2	2.88	0.45
1:E:283:VAL:HG12	1:E:283:VAL:O	2.16	0.45
1:A:391:ILE:N	1:A:391:ILE:HD12	2.31	0.45
1:D:128:LEU:CB	1:D:129:PRO:CD	2.95	0.45
1:D:255:TYR:CG	1:D:424:PRO:HB3	2.51	0.45
1:B:255:TYR:CG	1:B:424:PRO:HB3	2.51	0.45
1:D:284:HIS:CE1	1:D:291:TRP:CD2	3.04	0.45
1:E:276:MET:HG2	1:E:280:LEU:HD23	1.98	0.45
1:A:316:GLY:HA2	1:A:340:ARG:NH2	2.32	0.45
1:A:127:VAL:HB	1:A:157:ASN:HD21	1.81	0.45
1:A:284:HIS:CE1	1:A:291:TRP:CD2	3.04	0.45
1:E:286:GLY:O	1:E:288:ILE:HD12	2.17	0.45
1:C:94:TYR:CZ	1:C:352:ALA:HB2	2.51	0.45
1:F:94:TYR:CZ	1:F:352:ALA:HB2	2.51	0.45
1:B:276:MET:HG2	1:B:280:LEU:HD23	1.98	0.45
1:C:372:GLY:O	1:C:373:MET:C	2.55	0.45
1:E:372:GLY:O	1:E:373:MET:C	2.55	0.45
1:E:391:ILE:N	1:E:391:ILE:HD12	2.31	0.45
1:C:316:GLY:HA2	1:C:340:ARG:NH2	2.32	0.45
1:E:316:GLY:HA2	1:E:340:ARG:NH2	2.32	0.45
1:C:430:LEU:HD11	1:D:219:PHE:HB3	1.99	0.45
1:A:430:LEU:HD11	1:B:219:PHE:HB3	1.99	0.45
1:A:128:LEU:CB	1:A:129:PRO:CD	2.95	0.45
1:F:286:GLY:O	1:F:288:ILE:HD12	2.17	0.45
1:B:434:LEU:C	1:B:436:ALA:N	2.70	0.45
1:A:94:TYR:CZ	1:A:352:ALA:HB2	2.51	0.45
1:A:244:LEU:CD1	1:A:244:LEU:N	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:372:GLY:O	1:F:373:MET:C	2.55	0.45
1:D:391:ILE:N	1:D:391:ILE:HD12	2.31	0.45
1:B:283:VAL:HG12	1:B:283:VAL:O	2.16	0.45
1:B:186:LEU:HD22	1:B:199:PHE:CD2	2.52	0.45
1:E:274:LEU:O	1:E:277:GLN:HG2	2.15	0.45
1:E:444:LEU:O	1:E:448:ILE:HG13	2.17	0.45
1:C:321:PRO:C	1:C:322:ILE:HD12	2.36	0.45
1:E:128:LEU:CB	1:E:129:PRO:CD	2.95	0.45
1:D:127:VAL:HB	1:D:157:ASN:HD21	1.81	0.45
1:A:372:GLY:O	1:A:373:MET:C	2.55	0.45
1:F:316:GLY:HA2	1:F:340:ARG:NH2	2.32	0.45
1:B:127:VAL:HB	1:B:157:ASN:HD21	1.81	0.45
1:F:444:LEU:O	1:F:448:ILE:HG13	2.17	0.45
1:F:284:HIS:CE1	1:F:291:TRP:CD2	3.04	0.45
1:B:244:LEU:H	1:B:418:ASN:ND2	2.14	0.45
1:C:244:LEU:CD1	1:C:244:LEU:N	2.79	0.45
1:F:244:LEU:H	1:F:418:ASN:ND2	2.14	0.45
1:E:244:LEU:H	1:E:418:ASN:ND2	2.14	0.45
1:A:358:ALA:HB3	1:A:359:PRO:CD	2.46	0.45
1:F:258:LEU:HD13	1:F:371:PHE:CB	2.47	0.45
1:D:186:LEU:HD22	1:D:199:PHE:CD2	2.52	0.45
1:E:186:LEU:HD22	1:E:199:PHE:CD2	2.52	0.45
1:D:203:GLU:O	1:D:204:MET:C	2.54	0.45
1:B:108:GLY:HA3	1:B:153:GLN:HE21	1.81	0.45
1:F:423:LEU:HA	1:F:423:LEU:HD12	1.81	0.45
1:A:251:THR:HG22	1:A:255:TYR:CE1	2.47	0.45
1:B:284:HIS:CE1	1:B:291:TRP:CD2	3.04	0.45
1:D:286:GLY:O	1:D:288:ILE:HD12	2.17	0.45
1:D:434:LEU:C	1:D:436:ALA:N	2.70	0.45
1:A:22:ILE:HD13	1:B:454:ALA:HB2	1.98	0.45
1:B:391:ILE:HD12	1:B:391:ILE:N	2.31	0.45
1:C:127:VAL:HB	1:C:157:ASN:HD21	1.81	0.45
1:B:42:VAL:O	1:B:46:VAL:HG23	2.17	0.45
1:B:286:GLY:O	1:B:288:ILE:HD12	2.17	0.45
1:B:434:LEU:C	1:B:436:ALA:H	2.21	0.45
1:D:434:LEU:C	1:D:436:ALA:H	2.20	0.45
1:A:258:LEU:HD13	1:A:371:PHE:CB	2.47	0.45
1:D:258:LEU:HD13	1:D:371:PHE:CB	2.47	0.45
1:B:258:LEU:HD13	1:B:371:PHE:CB	2.47	0.45
1:F:186:LEU:HD22	1:F:199:PHE:CD2	2.52	0.45
1:B:51:VAL:HG21	1:B:232:PHE:CG	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:51:VAL:HG21	1:D:232:PHE:CG	2.52	0.45
1:F:320:ILE:C	1:F:322:ILE:H	2.21	0.45
1:F:127:VAL:HB	1:F:157:ASN:HD21	1.81	0.45
1:D:108:GLY:HA3	1:D:153:GLN:HE21	1.81	0.45
1:E:91:MET:C	1:E:93:GLY:N	2.70	0.45
1:A:75:TYR:N	1:A:76:PRO:CD	2.80	0.45
1:F:30:LYS:CG	1:F:30:LYS:O	2.65	0.45
1:F:276:MET:HG2	1:F:280:LEU:HD23	1.98	0.45
1:E:258:LEU:HD13	1:E:371:PHE:CB	2.47	0.45
1:C:22:ILE:HD13	1:D:454:ALA:HB2	1.98	0.45
1:D:243:LYS:HD2	1:D:243:LYS:O	2.17	0.45
1:F:128:LEU:CB	1:F:129:PRO:CD	2.95	0.44
1:D:122:VAL:HB	1:D:160:ARG:HD3	1.99	0.44
1:D:42:VAL:O	1:D:46:VAL:HG23	2.17	0.44
1:A:153:GLN:C	1:A:155:GLY:N	2.69	0.44
1:B:128:LEU:CB	1:B:129:PRO:CD	2.95	0.44
1:E:284:HIS:CE1	1:E:291:TRP:CD2	3.04	0.44
1:D:244:LEU:N	1:D:244:LEU:CD1	2.79	0.44
1:D:30:LYS:HB3	1:D:30:LYS:HZ2	1.81	0.44
1:C:358:ALA:HB3	1:C:359:PRO:CD	2.46	0.44
1:B:243:LYS:O	1:B:243:LYS:HD2	2.17	0.44
1:A:283:VAL:O	1:A:283:VAL:HG12	2.16	0.44
1:F:252:LEU:HD22	1:F:427:ILE:HD12	1.99	0.44
1:A:444:LEU:O	1:A:448:ILE:HG13	2.17	0.44
1:E:104:ALA:HB2	1:E:127:VAL:HG13	1.99	0.44
1:F:122:VAL:HB	1:F:160:ARG:HD3	1.98	0.44
1:C:258:LEU:HD13	1:C:371:PHE:CB	2.47	0.44
1:A:51:VAL:HG21	1:A:232:PHE:CG	2.52	0.44
1:F:243:LYS:O	1:F:243:LYS:HD2	2.17	0.44
1:E:267:PRO:HG2	1:E:268:ILE:H	1.82	0.44
1:A:321:PRO:C	1:A:322:ILE:HD12	2.36	0.44
1:E:340:ARG:HB3	1:E:340:ARG:HH11	1.82	0.44
1:C:444:LEU:O	1:C:448:ILE:HG13	2.17	0.44
1:F:251:THR:HG22	1:F:255:TYR:CE1	2.47	0.44
1:B:316:GLY:HA2	1:B:340:ARG:NH2	2.32	0.44
1:C:286:GLY:O	1:C:288:ILE:HD12	2.17	0.44
1:A:30:LYS:O	1:A:30:LYS:CG	2.65	0.44
1:E:51:VAL:HG21	1:E:232:PHE:CG	2.52	0.44
1:E:243:LYS:HD2	1:E:243:LYS:O	2.17	0.44
1:F:340:ARG:HH11	1:F:340:ARG:HB3	1.83	0.44
1:B:444:LEU:O	1:B:448:ILE:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:444:LEU:O	1:D:448:ILE:HG13	2.17	0.44
1:D:316:GLY:HA2	1:D:340:ARG:NH2	2.32	0.44
1:E:406:LEU:HD21	1:F:198:LEU:HD21	2.00	0.44
1:E:75:TYR:N	1:E:76:PRO:CD	2.80	0.44
1:C:186:LEU:HD22	1:C:199:PHE:CD2	2.52	0.44
1:A:186:LEU:HD22	1:A:199:PHE:CD2	2.52	0.44
1:C:252:LEU:HD22	1:C:427:ILE:HD12	1.99	0.44
1:C:51:VAL:HG21	1:C:232:PHE:CG	2.52	0.44
1:E:122:VAL:HB	1:E:160:ARG:HD3	1.99	0.44
1:C:153:GLN:C	1:C:155:GLY:N	2.69	0.44
1:F:42:VAL:O	1:F:46:VAL:HG23	2.17	0.44
1:D:340:ARG:HB3	1:D:340:ARG:HH11	1.83	0.44
1:F:434:LEU:C	1:F:436:ALA:H	2.21	0.44
1:C:75:TYR:N	1:C:76:PRO:CD	2.80	0.44
1:A:276:MET:HG2	1:A:280:LEU:HD23	1.98	0.44
1:E:252:LEU:HD22	1:E:427:ILE:HD12	1.99	0.44
1:E:207:GLN:HE22	1:F:28:ARG:NH2	2.15	0.44
1:E:434:LEU:C	1:E:436:ALA:N	2.70	0.44
1:E:124:TRP:HB2	1:E:128:LEU:HG	2.00	0.44
1:F:104:ALA:HB2	1:F:127:VAL:HG13	1.99	0.44
1:A:124:TRP:HB2	1:A:128:LEU:HG	2.00	0.44
1:A:122:VAL:HB	1:A:160:ARG:HD3	1.99	0.44
1:B:340:ARG:HH11	1:B:340:ARG:HB3	1.83	0.44
1:A:286:GLY:O	1:A:288:ILE:HD12	2.17	0.44
1:C:198:LEU:HD21	1:D:406:LEU:HD21	2.00	0.44
1:A:198:LEU:HD21	1:B:406:LEU:HD21	2.00	0.44
1:C:283:VAL:O	1:C:283:VAL:HG12	2.16	0.44
1:F:321:PRO:C	1:F:322:ILE:HD12	2.36	0.44
1:A:340:ARG:HH11	1:A:340:ARG:HB3	1.83	0.44
1:E:434:LEU:CD2	1:F:216:LYS:HD3	2.46	0.44
1:C:124:TRP:HB2	1:C:128:LEU:HG	2.00	0.44
1:A:42:VAL:O	1:A:46:VAL:HG23	2.17	0.44
1:B:153:GLN:C	1:B:155:GLY:N	2.69	0.44
1:B:122:VAL:HB	1:B:160:ARG:HD3	1.99	0.44
1:D:288:ILE:CG2	1:D:288:ILE:O	2.66	0.44
1:B:244:LEU:CD1	1:B:244:LEU:N	2.79	0.44
1:A:278:ASP:C	1:A:280:LEU:N	2.71	0.44
1:C:243:LYS:O	1:C:243:LYS:HD2	2.17	0.44
1:C:340:ARG:HH11	1:C:340:ARG:HB3	1.83	0.44
1:E:434:LEU:C	1:E:436:ALA:H	2.21	0.44
1:E:430:LEU:HD11	1:F:219:PHE:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:VAL:O	1:C:46:VAL:HG23	2.17	0.44
1:D:153:GLN:C	1:D:155:GLY:N	2.69	0.44
1:B:108:GLY:CA	1:B:153:GLN:NE2	2.81	0.44
1:B:267:PRO:HG2	1:B:268:ILE:H	1.82	0.44
1:D:109:ILE:HD11	1:D:152:VAL:CG2	2.43	0.44
1:F:91:MET:C	1:F:93:GLY:N	2.70	0.44
1:B:91:MET:C	1:B:93:GLY:N	2.70	0.44
1:C:251:THR:HG22	1:C:255:TYR:CE1	2.47	0.44
1:E:288:ILE:CG2	1:E:288:ILE:O	2.66	0.44
1:F:44:THR:HG23	1:F:228:MET:HE3	1.99	0.44
1:E:198:LEU:HD21	1:F:406:LEU:HD21	2.00	0.44
1:C:30:LYS:O	1:C:30:LYS:CG	2.65	0.44
1:B:252:LEU:HD22	1:B:427:ILE:HD12	1.99	0.44
1:A:243:LYS:O	1:A:243:LYS:HD2	2.17	0.44
1:F:379:PHE:CD1	1:F:379:PHE:N	2.86	0.44
1:E:42:VAL:O	1:E:46:VAL:HG23	2.17	0.44
1:C:122:VAL:HB	1:C:160:ARG:HD3	1.99	0.44
1:D:91:MET:C	1:D:93:GLY:N	2.70	0.44
1:F:90:ALA:HB3	1:F:296:GLY:HA2	2.00	0.44
1:E:30:LYS:CG	1:E:30:LYS:O	2.65	0.44
1:C:276:MET:HG2	1:C:280:LEU:HD23	1.98	0.44
1:E:278:ASP:C	1:E:280:LEU:N	2.71	0.44
1:A:252:LEU:HD22	1:A:427:ILE:HD12	1.99	0.44
1:F:122:VAL:HA	1:F:123:ARG:NH1	2.34	0.43
1:F:124:TRP:HB2	1:F:128:LEU:HG	2.00	0.43
1:D:122:VAL:HA	1:D:123:ARG:NH1	2.33	0.43
1:E:98:ARG:NH2	1:E:102:PRO:CB	2.79	0.43
1:F:434:LEU:C	1:F:436:ALA:N	2.70	0.43
1:E:90:ALA:HB3	1:E:296:GLY:HA2	2.00	0.43
1:E:132:PHE:C	1:E:132:PHE:HD2	2.22	0.43
1:B:21:LEU:O	1:B:24:GLN:N	2.52	0.43
1:B:320:ILE:C	1:B:322:ILE:H	2.21	0.43
1:C:207:GLN:HE22	1:D:28:ARG:NH2	2.15	0.43
1:C:434:LEU:C	1:C:436:ALA:H	2.21	0.43
1:E:108:GLY:CA	1:E:153:GLN:NE2	2.81	0.43
1:E:153:GLN:O	1:E:154:ILE:C	2.57	0.43
1:C:104:ALA:HB2	1:C:127:VAL:HG13	1.99	0.43
1:D:108:GLY:CA	1:D:153:GLN:NE2	2.81	0.43
1:A:104:ALA:HB2	1:A:127:VAL:HG13	1.99	0.43
1:B:122:VAL:HA	1:B:123:ARG:NH1	2.34	0.43
1:F:267:PRO:HG2	1:F:268:ILE:H	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:ILE:O	1:B:288:ILE:CG2	2.66	0.43
1:A:450:ALA:CB	1:B:26:LEU:CD2	2.94	0.43
1:C:278:ASP:C	1:C:280:LEU:N	2.71	0.43
1:D:252:LEU:HD22	1:D:427:ILE:HD12	1.99	0.43
1:A:434:LEU:C	1:A:436:ALA:H	2.21	0.43
1:A:122:VAL:HA	1:A:123:ARG:NH1	2.34	0.43
1:F:288:ILE:CG2	1:F:288:ILE:O	2.66	0.43
1:C:288:ILE:CG2	1:C:288:ILE:O	2.66	0.43
1:D:21:LEU:O	1:D:24:GLN:N	2.52	0.43
1:F:21:LEU:O	1:F:24:GLN:N	2.51	0.43
1:B:379:PHE:N	1:B:379:PHE:CD1	2.86	0.43
1:D:183:ALA:HB2	1:D:200:ILE:CG1	2.39	0.43
1:A:320:ILE:C	1:A:322:ILE:H	2.21	0.43
1:C:434:LEU:CD2	1:D:216:LYS:HD3	2.46	0.43
1:C:131:LYS:NZ	1:C:153:GLN:HE21	2.16	0.43
1:D:100:TYR:O	1:D:126:ARG:HD3	2.18	0.43
1:B:100:TYR:O	1:B:126:ARG:HD3	2.18	0.43
1:E:28:ARG:NE	1:F:443:PRO:HG2	2.33	0.43
1:B:30:LYS:CG	1:B:30:LYS:O	2.65	0.43
1:B:372:GLY:O	1:B:373:MET:C	2.55	0.43
1:F:132:PHE:HD2	1:F:132:PHE:C	2.22	0.43
1:F:51:VAL:HG21	1:F:232:PHE:CG	2.52	0.43
1:A:207:GLN:HE22	1:B:28:ARG:NH2	2.15	0.43
1:E:122:VAL:HA	1:E:123:ARG:NH1	2.34	0.43
1:C:122:VAL:HA	1:C:123:ARG:NH1	2.34	0.43
1:C:124:TRP:CG	1:C:125:TRP:N	2.86	0.43
1:C:108:GLY:CA	1:C:153:GLN:NE2	2.81	0.43
1:F:100:TYR:O	1:F:126:ARG:HD3	2.18	0.43
1:B:109:ILE:HD11	1:B:152:VAL:CG2	2.43	0.43
1:D:267:PRO:HG2	1:D:268:ILE:H	1.82	0.43
1:F:191:ASN:OD1	1:F:230:ARG:NH1	2.52	0.43
1:A:288:ILE:O	1:A:288:ILE:CG2	2.66	0.43
1:F:199:PHE:CD1	1:F:407:THR:HG21	2.54	0.43
1:A:265:PHE:CE2	1:A:269:PHE:HB2	2.54	0.43
1:D:315:GLY:N	1:D:318:ASN:ND2	2.67	0.43
1:D:321:PRO:HD2	1:D:322:ILE:CD1	2.49	0.43
1:D:320:ILE:C	1:D:322:ILE:H	2.21	0.43
1:B:315:GLY:N	1:B:318:ASN:ND2	2.67	0.43
1:C:267:PRO:HG2	1:C:268:ILE:H	1.82	0.43
1:E:124:TRP:CG	1:E:125:TRP:N	2.86	0.43
1:F:124:TRP:CG	1:F:125:TRP:N	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:104:ALA:HB2	1:D:127:VAL:HG13	1.99	0.43
1:A:124:TRP:CG	1:A:125:TRP:N	2.86	0.43
1:B:104:ALA:HB2	1:B:127:VAL:HG13	1.99	0.43
1:B:266:GLY:N	1:B:267:PRO:HD2	2.33	0.43
1:F:98:ARG:NH2	1:F:102:PRO:CB	2.80	0.43
1:C:90:ALA:HB3	1:C:296:GLY:HA2	2.00	0.43
1:A:90:ALA:HB3	1:A:296:GLY:HA2	2.00	0.43
1:E:116:LEU:HB3	1:E:206:PRO:HD3	2.01	0.43
1:B:116:LEU:HB3	1:B:206:PRO:HD3	2.01	0.43
1:D:116:LEU:HB3	1:D:206:PRO:HD3	2.01	0.43
1:E:244:LEU:H	1:E:418:ASN:HD21	1.67	0.43
1:D:372:GLY:O	1:D:373:MET:C	2.55	0.43
1:B:199:PHE:CD1	1:B:407:THR:HG21	2.54	0.43
1:C:199:PHE:CD1	1:C:407:THR:HG21	2.54	0.43
1:D:379:PHE:CD1	1:D:379:PHE:N	2.86	0.43
1:E:69:VAL:HG12	1:E:69:VAL:O	2.19	0.43
1:F:183:ALA:HB2	1:F:200:ILE:CG1	2.39	0.43
1:A:321:PRO:HD2	1:A:322:ILE:CD1	2.49	0.43
1:E:315:GLY:N	1:E:318:ASN:ND2	2.67	0.43
1:E:320:ILE:C	1:E:322:ILE:H	2.21	0.43
1:C:265:PHE:CE2	1:C:269:PHE:HB2	2.54	0.43
1:C:100:TYR:O	1:C:126:ARG:HD3	2.18	0.43
1:A:131:LYS:NZ	1:A:153:GLN:HE21	2.16	0.43
1:F:266:GLY:N	1:F:267:PRO:HD2	2.34	0.43
1:E:148:GLU:CD	1:E:357:PHE:HB3	2.39	0.43
1:F:30:LYS:HZ2	1:F:30:LYS:HB3	1.83	0.43
1:C:209:ARG:HG2	1:C:209:ARG:HH11	1.84	0.43
1:E:191:ASN:OD1	1:E:230:ARG:NH1	2.52	0.43
1:D:199:PHE:CD1	1:D:407:THR:HG21	2.54	0.43
1:E:379:PHE:N	1:E:379:PHE:CD1	2.86	0.43
1:E:266:GLY:N	1:E:267:PRO:HD2	2.33	0.43
1:A:267:PRO:HG2	1:A:268:ILE:H	1.82	0.43
1:A:274:LEU:HD12	1:A:277:GLN:NE2	2.34	0.43
1:C:266:GLY:N	1:C:267:PRO:HD2	2.34	0.43
1:F:131:LYS:NZ	1:F:153:GLN:HE21	2.16	0.43
1:F:153:GLN:C	1:F:155:GLY:N	2.69	0.43
1:C:28:ARG:NE	1:D:443:PRO:HG2	2.33	0.43
1:F:288:ILE:CD1	1:F:288:ILE:H	2.32	0.43
1:A:288:ILE:CD1	1:A:288:ILE:H	2.32	0.43
1:D:30:LYS:CG	1:D:30:LYS:O	2.65	0.43
1:A:132:PHE:C	1:A:132:PHE:HD2	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:ARG:HG2	1:A:209:ARG:HH11	1.84	0.43
1:E:273:VAL:HG13	1:E:274:LEU:N	2.34	0.43
1:C:320:ILE:C	1:C:322:ILE:H	2.21	0.43
1:A:321:PRO:CA	1:A:322:ILE:HD12	2.49	0.43
1:A:266:GLY:N	1:A:267:PRO:HD2	2.34	0.43
1:C:274:LEU:HD12	1:C:277:GLN:NE2	2.34	0.43
1:A:100:TYR:O	1:A:126:ARG:HD3	2.18	0.43
1:A:108:GLY:CA	1:A:153:GLN:NE2	2.81	0.43
1:F:270:ASN:HA	1:F:273:VAL:HG12	2.01	0.43
1:B:273:VAL:HG13	1:B:274:LEU:N	2.34	0.43
1:B:191:ASN:OD1	1:B:230:ARG:NH1	2.52	0.43
1:C:288:ILE:H	1:C:288:ILE:CD1	2.32	0.43
1:B:244:LEU:H	1:B:418:ASN:HD21	1.67	0.43
1:A:406:LEU:HD21	1:B:198:LEU:HD21	2.00	0.43
1:C:191:ASN:OD1	1:C:230:ARG:NH1	2.52	0.43
1:E:199:PHE:CD1	1:E:407:THR:HG21	2.54	0.43
1:F:321:PRO:HD2	1:F:322:ILE:CD1	2.49	0.43
1:B:321:PRO:HD2	1:B:322:ILE:CD1	2.49	0.43
1:F:215:ILE:HG22	1:F:216:LYS:N	2.34	0.43
1:E:153:GLN:C	1:E:155:GLY:N	2.69	0.43
1:B:124:TRP:CG	1:B:125:TRP:N	2.86	0.43
1:B:265:PHE:CE2	1:B:269:PHE:HB2	2.54	0.43
1:D:423:LEU:HD12	1:D:423:LEU:HA	1.81	0.43
1:D:191:ASN:OD1	1:D:230:ARG:NH1	2.52	0.43
1:B:57:VAL:HG22	1:B:136:LEU:HD12	2.01	0.43
1:D:132:PHE:C	1:D:132:PHE:HD2	2.21	0.43
1:D:57:VAL:HG22	1:D:136:LEU:HD12	2.01	0.43
1:E:21:LEU:O	1:E:24:GLN:N	2.52	0.43
1:E:202:GLU:HG2	1:E:202:GLU:O	2.19	0.43
1:A:379:PHE:CD1	1:A:379:PHE:N	2.86	0.43
1:C:321:PRO:CA	1:C:322:ILE:HD12	2.49	0.42
1:B:321:PRO:C	1:B:322:ILE:HD12	2.36	0.42
1:E:100:TYR:O	1:E:126:ARG:HD3	2.18	0.42
1:D:124:TRP:CG	1:D:125:TRP:N	2.86	0.42
1:B:131:LYS:NZ	1:B:153:GLN:HE21	2.16	0.42
1:F:273:VAL:HG13	1:F:274:LEU:N	2.34	0.42
1:A:28:ARG:NE	1:B:443:PRO:HG2	2.33	0.42
1:D:265:PHE:CE2	1:D:269:PHE:HB2	2.54	0.42
1:B:288:ILE:H	1:B:288:ILE:CD1	2.32	0.42
1:A:116:LEU:HB3	1:A:206:PRO:HD3	2.01	0.42
1:C:406:LEU:HD21	1:D:198:LEU:HD21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:LEU:HD13	1:B:410:ILE:CD1	2.47	0.42
1:A:191:ASN:OD1	1:A:230:ARG:NH1	2.52	0.42
1:B:150:PRO:CD	1:B:354:GLY:HA2	2.49	0.42
1:C:69:VAL:HG12	1:C:69:VAL:O	2.19	0.42
1:A:69:VAL:HG12	1:A:69:VAL:O	2.19	0.42
1:A:434:LEU:CD2	1:B:216:LYS:HD3	2.46	0.42
1:E:46:VAL:HG11	1:E:181:GLY:O	2.19	0.42
1:F:108:GLY:CA	1:F:153:GLN:NE2	2.81	0.42
1:D:124:TRP:HB2	1:D:128:LEU:HG	2.00	0.42
1:D:266:GLY:N	1:D:267:PRO:HD2	2.34	0.42
1:D:273:VAL:HG13	1:D:274:LEU:N	2.34	0.42
1:D:288:ILE:CD1	1:D:288:ILE:H	2.32	0.42
1:E:215:ILE:HG22	1:E:216:LYS:N	2.34	0.42
1:F:135:GLY:C	1:F:137:GLY:N	2.73	0.42
1:B:209:ARG:HH11	1:B:209:ARG:HG2	1.84	0.42
1:F:209:ARG:HG2	1:F:209:ARG:HH11	1.84	0.42
1:C:379:PHE:CD1	1:C:379:PHE:N	2.86	0.42
1:B:202:GLU:HG2	1:B:202:GLU:O	2.19	0.42
1:F:69:VAL:HG12	1:F:69:VAL:O	2.19	0.42
1:C:321:PRO:HD2	1:C:322:ILE:CD1	2.49	0.42
1:D:324:THR:O	1:D:326:GLY:N	2.53	0.42
1:C:273:VAL:HG13	1:C:274:LEU:N	2.34	0.42
1:E:176:THR:HA	1:E:213:ILE:HG23	2.01	0.42
1:F:176:THR:HA	1:F:213:ILE:HG23	2.01	0.42
1:F:148:GLU:CD	1:F:357:PHE:HB3	2.39	0.42
1:C:21:LEU:O	1:C:24:GLN:N	2.52	0.42
1:C:132:PHE:HD2	1:C:132:PHE:C	2.21	0.42
1:A:21:LEU:O	1:A:24:GLN:N	2.52	0.42
1:F:252:LEU:HD13	1:F:427:ILE:HD11	2.01	0.42
1:A:199:PHE:CD1	1:A:407:THR:HG21	2.54	0.42
1:E:414:GLU:OE1	1:F:419:TYR:CE1	2.73	0.42
1:D:150:PRO:CD	1:D:354:GLY:HA2	2.49	0.42
1:E:150:PRO:CD	1:E:354:GLY:HA2	2.49	0.42
1:B:183:ALA:HB2	1:B:200:ILE:CG1	2.39	0.42
1:E:274:LEU:HD12	1:E:277:GLN:NE2	2.34	0.42
1:A:270:ASN:HA	1:A:273:VAL:HG12	2.01	0.42
1:E:321:PRO:CA	1:E:322:ILE:HD12	2.49	0.42
1:B:324:THR:O	1:B:326:GLY:N	2.53	0.42
1:F:157:ASN:O	1:F:159:GLY:N	2.52	0.42
1:D:153:GLN:O	1:D:154:ILE:C	2.57	0.42
1:D:176:THR:HA	1:D:213:ILE:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:GLN:O	1:B:154:ILE:C	2.57	0.42
1:F:116:LEU:HB3	1:F:206:PRO:HD3	2.01	0.42
1:A:148:GLU:CD	1:A:357:PHE:HB3	2.39	0.42
1:F:244:LEU:H	1:F:418:ASN:HD21	1.67	0.42
1:C:194:LEU:HD13	1:D:410:ILE:CD1	2.47	0.42
1:B:132:PHE:HD2	1:B:132:PHE:C	2.22	0.42
1:E:312:THR:CG2	1:E:339:ALA:HB1	2.50	0.42
1:A:252:LEU:HD13	1:A:427:ILE:HD11	2.01	0.42
1:D:252:LEU:HD13	1:D:427:ILE:HD11	2.01	0.42
1:C:150:PRO:CD	1:C:354:GLY:HA2	2.49	0.42
1:F:315:GLY:N	1:F:318:ASN:ND2	2.67	0.42
1:C:324:THR:O	1:C:326:GLY:N	2.53	0.42
1:F:46:VAL:HG11	1:F:181:GLY:O	2.19	0.42
1:E:288:ILE:CD1	1:E:288:ILE:H	2.32	0.42
1:D:90:ALA:HB3	1:D:296:GLY:HA2	2.00	0.42
1:A:135:GLY:C	1:A:137:GLY:N	2.73	0.42
1:B:90:ALA:HB3	1:B:296:GLY:HA2	2.00	0.42
1:D:148:GLU:CD	1:D:357:PHE:HB3	2.39	0.42
1:D:244:LEU:H	1:D:418:ASN:HD21	1.67	0.42
1:B:30:LYS:HB3	1:B:30:LYS:HZ2	1.84	0.42
1:A:57:VAL:HG22	1:A:136:LEU:HD12	2.01	0.42
1:B:252:LEU:HD13	1:B:427:ILE:HD11	2.01	0.42
1:C:414:GLU:OE1	1:D:419:TYR:CE1	2.73	0.42
1:F:202:GLU:HG2	1:F:202:GLU:O	2.19	0.42
1:E:321:PRO:HD2	1:E:322:ILE:CD1	2.49	0.42
1:B:321:PRO:CA	1:B:322:ILE:HD12	2.49	0.42
1:C:153:GLN:O	1:C:154:ILE:C	2.57	0.42
1:C:176:THR:HA	1:C:213:ILE:HG23	2.01	0.42
1:F:265:PHE:CE2	1:F:269:PHE:HB2	2.54	0.42
1:C:91:MET:C	1:C:93:GLY:N	2.70	0.42
1:A:91:MET:C	1:A:93:GLY:N	2.70	0.42
1:F:421:LEU:O	1:F:424:PRO:HD2	2.20	0.42
1:C:215:ILE:HG22	1:C:216:LYS:N	2.34	0.42
1:C:116:LEU:HB3	1:C:206:PRO:HD3	2.01	0.42
1:D:312:THR:CG2	1:D:339:ALA:HB1	2.50	0.42
1:D:209:ARG:HG2	1:D:209:ARG:HH11	1.84	0.42
1:A:150:PRO:CD	1:A:354:GLY:HA2	2.49	0.42
1:C:315:GLY:N	1:C:318:ASN:ND2	2.67	0.42
1:A:324:THR:O	1:A:326:GLY:N	2.53	0.42
1:E:157:ASN:O	1:E:159:GLY:N	2.52	0.42
1:F:153:GLN:O	1:F:154:ILE:C	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:ASN:O	1:A:159:GLY:N	2.52	0.42
1:B:212:LEU:CD1	1:B:212:LEU:N	2.81	0.42
1:E:251:THR:HG22	1:E:255:TYR:CE1	2.47	0.42
1:C:223:ILE:HD12	1:D:430:LEU:CD2	2.45	0.42
1:B:312:THR:CG2	1:B:339:ALA:HB1	2.50	0.42
1:C:252:LEU:HD13	1:C:427:ILE:HD11	2.01	0.42
1:A:414:GLU:OE1	1:B:419:TYR:CE1	2.73	0.42
1:D:202:GLU:HG2	1:D:202:GLU:O	2.19	0.42
1:A:202:GLU:O	1:A:202:GLU:HG2	2.19	0.42
1:F:150:PRO:CD	1:F:354:GLY:HA2	2.49	0.42
1:E:265:PHE:CE2	1:E:269:PHE:HB2	2.54	0.42
1:F:324:THR:O	1:F:326:GLY:N	2.52	0.42
1:A:273:VAL:HG13	1:A:274:LEU:N	2.34	0.42
1:E:324:THR:O	1:E:326:GLY:N	2.53	0.42
1:C:270:ASN:HA	1:C:273:VAL:HG12	2.01	0.42
1:C:157:ASN:O	1:C:159:GLY:N	2.52	0.42
1:B:124:TRP:HB2	1:B:128:LEU:HG	2.00	0.42
1:B:46:VAL:HG11	1:B:181:GLY:O	2.19	0.42
1:C:148:GLU:CD	1:C:357:PHE:HB3	2.39	0.42
1:C:244:LEU:H	1:C:418:ASN:HD21	1.67	0.42
1:F:75:TYR:N	1:F:76:PRO:CD	2.79	0.42
1:F:244:LEU:N	1:F:244:LEU:CD1	2.79	0.42
1:F:100:TYR:CD1	1:F:100:TYR:N	2.88	0.42
1:A:153:GLN:O	1:A:154:ILE:C	2.57	0.42
1:B:100:TYR:N	1:B:100:TYR:CD1	2.88	0.42
1:D:270:ASN:HA	1:D:273:VAL:HG12	2.01	0.42
1:E:421:LEU:O	1:E:424:PRO:HD2	2.20	0.42
1:C:135:GLY:C	1:C:137:GLY:N	2.73	0.42
1:A:190:PHE:HE1	1:A:357:PHE:CE2	2.38	0.42
1:A:244:LEU:H	1:A:418:ASN:HD21	1.67	0.42
1:C:57:VAL:HG22	1:C:136:LEU:HD12	2.01	0.42
1:A:312:THR:CG2	1:A:339:ALA:HB1	2.50	0.42
1:A:201:ILE:HA	1:A:205:ARG:HG2	2.01	0.42
1:A:315:GLY:N	1:A:318:ASN:ND2	2.67	0.42
1:E:100:TYR:CD1	1:E:100:TYR:N	2.88	0.42
1:D:100:TYR:N	1:D:100:TYR:CD1	2.88	0.42
1:A:131:LYS:HZ2	1:A:153:GLN:NE2	2.16	0.42
1:A:176:THR:HA	1:A:213:ILE:HG23	2.01	0.42
1:B:176:THR:HA	1:B:213:ILE:HG23	2.01	0.42
1:F:190:PHE:HE1	1:F:357:PHE:CE2	2.38	0.42
1:D:190:PHE:HE1	1:D:357:PHE:CE2	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:53:PHE:CZ	1:D:139:LEU:HD12	2.55	0.42
1:F:201:ILE:HA	1:F:205:ARG:HG2	2.01	0.42
1:A:53:PHE:CZ	1:A:139:LEU:HD12	2.55	0.42
1:C:202:GLU:HG2	1:C:202:GLU:O	2.19	0.42
1:D:321:PRO:CA	1:D:322:ILE:HD12	2.49	0.41
1:A:223:ILE:HD12	1:B:430:LEU:CD2	2.45	0.41
1:C:190:PHE:HE1	1:C:357:PHE:CE2	2.38	0.41
1:E:57:VAL:HG22	1:E:136:LEU:HD12	2.01	0.41
1:B:143:MET:HE2	1:B:347:CYS:HB3	2.02	0.41
1:F:197:ILE:HG12	1:F:222:VAL:HG21	2.02	0.41
1:F:53:PHE:CZ	1:F:139:LEU:HD12	2.55	0.41
1:C:197:ILE:HG12	1:C:222:VAL:HG21	2.02	0.41
1:B:201:ILE:HA	1:B:205:ARG:HG2	2.01	0.41
1:D:321:PRO:C	1:D:322:ILE:HD12	2.36	0.41
1:E:321:PRO:C	1:E:322:ILE:HD12	2.36	0.41
1:B:215:ILE:HG22	1:B:216:LYS:N	2.34	0.41
1:D:131:LYS:NZ	1:D:153:GLN:HE21	2.16	0.41
1:D:46:VAL:HG11	1:D:181:GLY:O	2.19	0.41
1:A:421:LEU:O	1:A:424:PRO:HD2	2.20	0.41
1:E:135:GLY:C	1:E:137:GLY:N	2.73	0.41
1:B:190:PHE:HE1	1:B:357:PHE:CE2	2.38	0.41
1:F:278:ASP:O	1:F:280:LEU:N	2.53	0.41
1:F:57:VAL:HG22	1:F:136:LEU:HD12	2.01	0.41
1:C:197:ILE:CG1	1:C:222:VAL:HG21	2.51	0.41
1:B:53:PHE:CZ	1:B:139:LEU:HD12	2.55	0.41
1:C:53:PHE:CZ	1:C:139:LEU:HD12	2.55	0.41
1:B:69:VAL:HG12	1:B:69:VAL:O	2.19	0.41
1:C:46:VAL:HG11	1:C:181:GLY:O	2.19	0.41
1:F:103:GLU:HG3	1:F:123:ARG:HE	1.85	0.41
1:A:46:VAL:HG11	1:A:181:GLY:O	2.19	0.41
1:B:157:ASN:O	1:B:159:GLY:N	2.52	0.41
1:B:270:ASN:HA	1:B:273:VAL:HG12	2.01	0.41
1:B:274:LEU:HD12	1:B:277:GLN:NE2	2.34	0.41
1:B:421:LEU:O	1:B:424:PRO:HD2	2.20	0.41
1:E:223:ILE:HD12	1:F:430:LEU:CD2	2.45	0.41
1:B:148:GLU:CD	1:B:357:PHE:HB3	2.39	0.41
1:E:194:LEU:HD13	1:F:410:ILE:CD1	2.47	0.41
1:C:312:THR:CG2	1:C:339:ALA:HB1	2.50	0.41
1:E:209:ARG:HG2	1:E:209:ARG:HH11	1.84	0.41
1:E:252:LEU:HD13	1:E:427:ILE:HD11	2.01	0.41
1:E:201:ILE:HA	1:E:205:ARG:HG2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:247:ALA:HA	1:C:248:PRO:HD2	1.93	0.41
1:E:143:MET:HE2	1:E:347:CYS:HB3	2.03	0.41
1:A:197:ILE:CG1	1:A:222:VAL:HG21	2.51	0.41
1:C:201:ILE:HA	1:C:205:ARG:HG2	2.01	0.41
1:A:320:ILE:C	1:A:322:ILE:N	2.74	0.41
1:E:320:ILE:C	1:E:322:ILE:N	2.74	0.41
1:E:430:LEU:HD13	1:F:219:PHE:HD2	1.85	0.41
1:E:103:GLU:HG3	1:E:123:ARG:HE	1.84	0.41
1:B:103:GLU:HG3	1:B:123:ARG:HE	1.84	0.41
1:C:421:LEU:O	1:C:424:PRO:HD2	2.20	0.41
1:C:278:ASP:O	1:C:280:LEU:N	2.53	0.41
1:B:197:ILE:CG1	1:B:222:VAL:HG21	2.51	0.41
1:D:69:VAL:HG12	1:D:69:VAL:O	2.19	0.41
1:C:320:ILE:C	1:C:322:ILE:N	2.74	0.41
1:D:103:GLU:HG3	1:D:123:ARG:HE	1.84	0.41
1:B:124:TRP:O	1:B:126:ARG:N	2.53	0.41
1:D:274:LEU:HD12	1:D:277:GLN:NE2	2.34	0.41
1:A:215:ILE:HG22	1:A:216:LYS:N	2.34	0.41
1:F:190:PHE:CD1	1:F:411:LEU:HD11	2.56	0.41
1:B:190:PHE:CD1	1:B:411:LEU:HD11	2.56	0.41
1:E:197:ILE:CG1	1:E:222:VAL:HG21	2.51	0.41
1:E:53:PHE:CZ	1:E:139:LEU:HD12	2.55	0.41
1:D:215:ILE:HG22	1:D:216:LYS:N	2.34	0.41
1:E:124:TRP:O	1:E:126:ARG:N	2.53	0.41
1:F:124:TRP:CD1	1:F:161:MET:HG3	2.56	0.41
1:D:212:LEU:N	1:D:212:LEU:CD1	2.81	0.41
1:C:411:LEU:O	1:C:415:MET:HG2	2.21	0.41
1:D:190:PHE:CD1	1:D:411:LEU:HD11	2.56	0.41
1:E:190:PHE:CD1	1:E:411:LEU:HD11	2.56	0.41
1:A:197:ILE:HG12	1:A:222:VAL:HG21	2.02	0.41
1:E:197:ILE:HG12	1:E:222:VAL:HG21	2.02	0.41
1:D:143:MET:HE2	1:D:347:CYS:HB3	2.03	0.41
1:C:124:TRP:O	1:C:126:ARG:N	2.53	0.41
1:D:124:TRP:CD1	1:D:125:TRP:N	2.89	0.41
1:F:274:LEU:HD12	1:F:277:GLN:NE2	2.34	0.41
1:E:190:PHE:HE1	1:E:357:PHE:CE2	2.38	0.41
1:D:197:ILE:CG1	1:D:222:VAL:HG21	2.51	0.41
1:D:200:ILE:CG2	1:D:200:ILE:O	2.68	0.41
1:F:321:PRO:CA	1:F:322:ILE:HD12	2.49	0.41
1:A:443:PRO:O	1:A:446:SER:N	2.41	0.41
1:F:124:TRP:O	1:F:126:ARG:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:157:ASN:O	1:D:159:GLY:N	2.52	0.41
1:A:103:GLU:HG3	1:A:123:ARG:HE	1.84	0.41
1:D:251:THR:HG22	1:D:255:TYR:CE1	2.46	0.41
1:D:421:LEU:O	1:D:424:PRO:HD2	2.20	0.41
1:F:284:HIS:CE1	1:F:291:TRP:CE3	3.09	0.41
1:A:411:LEU:O	1:A:415:MET:HG2	2.21	0.41
1:A:356:ILE:HA	1:A:359:PRO:CG	2.51	0.41
1:C:356:ILE:HA	1:C:359:PRO:CG	2.51	0.41
1:F:197:ILE:CG1	1:F:222:VAL:HG21	2.51	0.41
1:D:201:ILE:HA	1:D:205:ARG:HG2	2.01	0.41
1:B:200:ILE:CG2	1:B:200:ILE:O	2.68	0.41
1:E:179:ALA:HB1	1:E:200:ILE:CG2	2.51	0.41
1:F:320:ILE:C	1:F:322:ILE:N	2.74	0.41
1:C:317:PHE:CA	1:C:321:PRO:HD2	2.50	0.41
1:A:317:PHE:CA	1:A:321:PRO:HD2	2.50	0.41
1:A:179:ALA:HB1	1:A:200:ILE:CG2	2.51	0.41
1:E:316:GLY:O	1:E:318:ASN:N	2.54	0.41
1:C:179:ALA:HB1	1:C:200:ILE:CG2	2.51	0.41
1:C:103:GLU:HG3	1:C:123:ARG:HE	1.84	0.41
1:D:124:TRP:O	1:D:126:ARG:N	2.53	0.41
1:A:124:TRP:O	1:A:126:ARG:N	2.53	0.41
1:B:124:TRP:CD1	1:B:125:TRP:N	2.89	0.41
1:B:124:TRP:CD1	1:B:161:MET:HG3	2.56	0.41
1:E:423:LEU:HD12	1:E:423:LEU:HA	1.81	0.41
1:C:98:ARG:NH2	1:C:102:PRO:CB	2.79	0.41
1:B:411:LEU:O	1:B:415:MET:HG2	2.21	0.41
1:C:190:PHE:CD1	1:C:411:LEU:HD11	2.56	0.41
1:F:278:ASP:C	1:F:280:LEU:N	2.71	0.41
1:A:278:ASP:O	1:A:280:LEU:N	2.53	0.41
1:E:278:ASP:O	1:E:280:LEU:N	2.53	0.41
1:D:278:ASP:C	1:D:280:LEU:N	2.71	0.41
1:D:278:ASP:O	1:D:280:LEU:N	2.53	0.41
1:F:312:THR:CG2	1:F:339:ALA:HB1	2.50	0.41
1:A:247:ALA:HA	1:A:248:PRO:HD2	1.93	0.41
1:D:256:LEU:O	1:D:257:ILE:C	2.59	0.41
1:A:443:PRO:HG2	1:B:28:ARG:NE	2.36	0.41
1:C:200:ILE:CG2	1:C:200:ILE:O	2.68	0.41
1:C:443:PRO:HG2	1:D:28:ARG:NE	2.36	0.41
1:B:29:ASP:OD1	1:B:216:LYS:NZ	2.51	0.41
1:C:123:ARG:CD	1:C:123:ARG:N	2.81	0.41
1:D:341:VAL:O	1:D:345:LEU:HG	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:423:LEU:HA	1:B:423:LEU:HD12	1.81	0.41
1:F:284:HIS:C	1:F:286:GLY:H	2.25	0.41
1:E:284:HIS:C	1:E:286:GLY:H	2.25	0.41
1:D:95:PHE:O	1:D:96:LEU:C	2.60	0.41
1:B:95:PHE:O	1:B:96:LEU:C	2.60	0.41
1:B:278:ASP:C	1:B:280:LEU:N	2.71	0.41
1:C:201:ILE:HD13	1:C:201:ILE:HG21	1.87	0.41
1:E:443:PRO:HG2	1:F:28:ARG:NE	2.36	0.40
1:F:317:PHE:C	1:F:317:PHE:CD1	2.95	0.40
1:A:317:PHE:CD1	1:A:317:PHE:C	2.95	0.40
1:F:124:TRP:CD1	1:F:125:TRP:N	2.89	0.40
1:A:124:TRP:CD1	1:A:125:TRP:N	2.89	0.40
1:F:341:VAL:O	1:F:345:LEU:HG	2.21	0.40
1:A:423:LEU:HD12	1:A:423:LEU:HA	1.81	0.40
1:C:284:HIS:CE1	1:C:291:TRP:CE3	3.09	0.40
1:A:190:PHE:CD1	1:A:411:LEU:HD11	2.56	0.40
1:D:356:ILE:HA	1:D:359:PRO:CG	2.51	0.40
1:B:256:LEU:O	1:B:257:ILE:C	2.59	0.40
1:A:316:GLY:C	1:A:318:ASN:H	2.25	0.40
1:E:124:TRP:CD1	1:E:125:TRP:N	2.89	0.40
1:E:131:LYS:NZ	1:E:153:GLN:HE21	2.16	0.40
1:C:100:TYR:CD1	1:C:100:TYR:N	2.88	0.40
1:C:124:TRP:CD1	1:C:125:TRP:N	2.89	0.40
1:D:124:TRP:CD1	1:D:161:MET:HG3	2.56	0.40
1:D:211:THR:CG2	1:D:212:LEU:H	2.26	0.40
1:A:100:TYR:N	1:A:100:TYR:CD1	2.88	0.40
1:D:273:VAL:CA	1:D:345:LEU:HD22	2.49	0.40
1:D:411:LEU:O	1:D:415:MET:HG2	2.21	0.40
1:E:411:LEU:O	1:E:415:MET:HG2	2.21	0.40
1:B:278:ASP:O	1:B:280:LEU:N	2.53	0.40
1:A:201:ILE:HD13	1:A:201:ILE:HG21	1.87	0.40
1:B:197:ILE:HG12	1:B:222:VAL:HG21	2.02	0.40
1:D:197:ILE:HG12	1:D:222:VAL:HG21	2.02	0.40
1:C:316:GLY:C	1:C:318:ASN:H	2.25	0.40
1:A:200:ILE:CG2	1:A:200:ILE:O	2.68	0.40
1:E:316:GLY:C	1:E:318:ASN:H	2.25	0.40
1:B:317:PHE:C	1:B:317:PHE:CD1	2.95	0.40
1:E:426:ILE:HG22	1:F:223:ILE:CD1	2.51	0.40
1:D:123:ARG:CD	1:D:123:ARG:N	2.81	0.40
1:A:98:ARG:NH2	1:A:102:PRO:CB	2.80	0.40
1:F:356:ILE:HA	1:F:359:PRO:CG	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:356:ILE:HA	1:B:359:PRO:CG	2.51	0.40
1:A:143:MET:HE2	1:A:347:CYS:HB3	2.03	0.40
1:B:341:VAL:O	1:B:345:LEU:HG	2.22	0.40
1:B:251:THR:HG22	1:B:255:TYR:CE1	2.47	0.40
1:A:420:GLN:HG2	1:A:420:GLN:H	1.64	0.40
1:A:284:HIS:C	1:A:286:GLY:H	2.25	0.40
1:E:284:HIS:CE1	1:E:291:TRP:CE3	3.09	0.40
1:C:450:ALA:CB	1:D:26:LEU:CD2	2.94	0.40
1:B:361:LEU:HD23	1:B:361:LEU:HA	1.95	0.40
1:F:316:GLY:O	1:F:318:ASN:N	2.54	0.40
1:C:317:PHE:C	1:C:317:PHE:CD1	2.95	0.40
1:A:183:ALA:HB2	1:A:200:ILE:CG1	2.39	0.40
1:C:430:LEU:HD13	1:D:219:PHE:HD2	1.85	0.40
1:D:223:ILE:HG22	1:D:227:ILE:HD11	2.04	0.40
1:B:75:TYR:N	1:B:76:PRO:CD	2.80	0.40

All (53) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:ARG:CA	1:E:12:GLN:NE2[4_455]	0.70	1.50
1:B:16:LEU:CG	1:E:19:ARG:CZ[4_455]	0.73	1.47
1:B:19:ARG:NH1	1:E:16:LEU:CB[4_455]	0.88	1.32
1:B:12:GLN:CD	1:E:15:ARG:CB[4_455]	0.91	1.29
1:B:19:ARG:NH1	1:E:16:LEU:CG[4_455]	0.96	1.24
1:B:16:LEU:CD2	1:E:19:ARG:NH2[4_455]	1.03	1.17
1:B:19:ARG:CD	1:E:16:LEU:CD1[4_455]	1.05	1.15
1:B:12:GLN:NE2	1:E:15:ARG:CB[4_455]	1.07	1.13
1:B:167:ARG:NH1	1:D:12:GLN:OE1[2_554]	1.15	1.05
1:B:15:ARG:CB	1:E:12:GLN:NE2[4_455]	1.18	1.02
1:B:19:ARG:CZ	1:E:16:LEU:CG[4_455]	1.18	1.02
1:B:12:GLN:OE1	1:E:15:ARG:CB[4_455]	1.26	0.94
1:B:19:ARG:CZ	1:E:16:LEU:CB[4_455]	1.28	0.92
1:B:19:ARG:NE	1:E:16:LEU:CD2[4_455]	1.31	0.89
1:B:19:ARG:CZ	1:E:16:LEU:CD2[4_455]	1.34	0.86
1:B:16:LEU:CD2	1:E:19:ARG:CZ[4_455]	1.35	0.85
1:B:12:GLN:N	1:E:15:ARG:NH2[4_455]	1.35	0.85
1:B:16:LEU:CG	1:E:19:ARG:NH2[4_455]	1.38	0.82
1:B:15:ARG:C	1:E:12:GLN:NE2[4_455]	1.39	0.81
1:B:15:ARG:O	1:E:12:GLN:OE1[4_455]	1.40	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:LEU:CG	1:E:19:ARG:NH1[4_455]	1.52	0.68
1:B:15:ARG:CB	1:E:12:GLN:CD[4_455]	1.57	0.63
1:B:12:GLN:NE2	1:E:15:ARG:CG[4_455]	1.57	0.63
1:C:12:GLN:OE1	1:E:167:ARG:NH2[3_645]	1.58	0.62
1:B:16:LEU:CD1	1:E:19:ARG:NE[4_455]	1.59	0.61
1:B:19:ARG:NE	1:E:16:LEU:CG[4_455]	1.61	0.59
1:B:16:LEU:CD2	1:E:19:ARG:NE[4_455]	1.64	0.56
1:B:16:LEU:CG	1:E:19:ARG:NE[4_455]	1.66	0.54
1:B:167:ARG:CZ	1:D:12:GLN:OE1[2_554]	1.66	0.54
1:B:15:ARG:O	1:E:12:GLN:CD[4_455]	1.70	0.50
1:B:12:GLN:NE2	1:E:15:ARG:CA[4_455]	1.74	0.46
1:B:15:ARG:C	1:E:12:GLN:CD[4_455]	1.80	0.40
1:B:19:ARG:NH1	1:E:16:LEU:CA[4_455]	1.81	0.39
1:B:19:ARG:NE	1:E:16:LEU:CD1[4_455]	1.85	0.35
1:B:16:LEU:CD1	1:E:19:ARG:CZ[4_455]	1.85	0.35
1:B:167:ARG:NH1	1:D:12:GLN:CD[2_554]	1.87	0.33
1:B:23:ARG:NH1	1:E:23:ARG:CD[4_455]	1.89	0.31
1:B:12:GLN:NE2	1:E:15:ARG:N[4_455]	1.91	0.29
1:B:12:GLN:CD	1:E:15:ARG:CG[4_455]	1.93	0.27
1:B:16:LEU:CD1	1:E:19:ARG:CD[4_455]	1.93	0.27
1:B:16:LEU:CB	1:E:19:ARG:NH2[4_455]	1.93	0.27
1:B:15:ARG:N	1:E:12:GLN:NE2[4_455]	1.96	0.24
1:B:19:ARG:NH2	1:E:16:LEU:CB[4_455]	1.97	0.23
1:B:19:ARG:CD	1:E:16:LEU:CG[4_455]	1.98	0.22
1:B:15:ARG:CA	1:E:12:GLN:CD[4_455]	2.00	0.20
1:B:167:ARG:NH2	1:D:12:GLN:OE1[2_554]	2.03	0.17
1:B:19:ARG:NH2	1:E:16:LEU:CD2[4_455]	2.06	0.14
1:B:15:ARG:O	1:E:12:GLN:NE2[4_455]	2.09	0.11
1:B:12:GLN:N	1:E:15:ARG:CZ[4_455]	2.14	0.06
1:B:16:LEU:O	1:E:19:ARG:NH1[4_455]	2.17	0.03
1:B:12:GLN:CG	1:E:15:ARG:NE[4_455]	2.18	0.02
1:B:19:ARG:NH1	1:E:16:LEU:CD2[4_455]	2.18	0.02
1:B:16:LEU:CB	1:E:19:ARG:CZ[4_455]	2.19	0.01

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	448/473 (95%)	340 (76%)	75 (17%)	33 (7%)	1	16
1	B	448/473 (95%)	340 (76%)	75 (17%)	33 (7%)	1	16
1	C	448/473 (95%)	340 (76%)	75 (17%)	33 (7%)	1	16
1	D	448/473 (95%)	340 (76%)	76 (17%)	32 (7%)	1	17
1	E	448/473 (95%)	340 (76%)	76 (17%)	32 (7%)	1	17
1	F	448/473 (95%)	340 (76%)	75 (17%)	33 (7%)	1	16
All	All	2688/2838 (95%)	2040 (76%)	452 (17%)	196 (7%)	1	16

All (196) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	319	LEU
1	B	319	LEU
1	C	319	LEU
1	D	319	LEU
1	E	319	LEU
1	F	319	LEU
1	A	33	LEU
1	A	167	ARG
1	A	204	MET
1	A	285	GLY
1	A	318	ASN
1	B	33	LEU
1	B	167	ARG
1	B	204	MET
1	B	285	GLY
1	B	318	ASN
1	C	33	LEU
1	C	167	ARG
1	C	204	MET
1	C	285	GLY
1	C	318	ASN
1	D	33	LEU
1	D	167	ARG
1	D	204	MET
1	D	285	GLY
1	D	318	ASN
1	E	33	LEU

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Mol	Chain	Res	Type
1	E	167	ARG
1	E	204	MET
1	E	285	GLY
1	E	318	ASN
1	F	33	LEU
1	F	167	ARG
1	F	204	MET
1	F	285	GLY
1	F	318	ASN
1	A	92	PHE
1	A	107	SER
1	A	125	TRP
1	A	172	GLU
1	A	210	TYR
1	A	250	ASN
1	A	279	LEU
1	A	325	ALA
1	A	444	LEU
1	B	92	PHE
1	B	107	SER
1	B	125	TRP
1	B	172	GLU
1	B	210	TYR
1	B	250	ASN
1	B	279	LEU
1	B	325	ALA
1	B	444	LEU
1	C	92	PHE
1	C	107	SER
1	C	125	TRP
1	C	172	GLU
1	C	210	TYR
1	C	250	ASN
1	C	279	LEU
1	C	325	ALA
1	C	444	LEU
1	D	92	PHE
1	D	107	SER
1	D	125	TRP
1	D	172	GLU
1	D	210	TYR
1	D	250	ASN

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Mol	Chain	Res	Type
1	D	279	LEU
1	D	325	ALA
1	D	444	LEU
1	E	92	PHE
1	E	107	SER
1	E	125	TRP
1	E	172	GLU
1	E	210	TYR
1	E	250	ASN
1	E	279	LEU
1	E	325	ALA
1	E	444	LEU
1	F	92	PHE
1	F	107	SER
1	F	125	TRP
1	F	172	GLU
1	F	210	TYR
1	F	250	ASN
1	F	279	LEU
1	F	325	ALA
1	F	444	LEU
1	A	91	MET
1	A	121	PRO
1	A	177	LEU
1	A	242	GLY
1	A	283	VAL
1	A	342	ILE
1	A	343	THR
1	A	452	THR
1	B	91	MET
1	B	121	PRO
1	B	177	LEU
1	B	242	GLY
1	B	283	VAL
1	B	342	ILE
1	B	343	THR
1	B	452	THR
1	C	91	MET
1	C	121	PRO
1	C	177	LEU
1	C	242	GLY
1	C	283	VAL

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Mol	Chain	Res	Type
1	C	342	ILE
1	C	343	THR
1	C	452	THR
1	D	91	MET
1	D	121	PRO
1	D	177	LEU
1	D	242	GLY
1	D	283	VAL
1	D	342	ILE
1	D	343	THR
1	D	452	THR
1	E	91	MET
1	E	121	PRO
1	E	177	LEU
1	E	242	GLY
1	E	283	VAL
1	E	342	ILE
1	E	343	THR
1	E	452	THR
1	F	91	MET
1	F	121	PRO
1	F	177	LEU
1	F	242	GLY
1	F	283	VAL
1	F	342	ILE
1	F	343	THR
1	F	452	THR
1	A	102	PRO
1	A	317	PHE
1	A	326	GLY
1	B	102	PRO
1	B	317	PHE
1	B	326	GLY
1	C	102	PRO
1	C	317	PHE
1	C	326	GLY
1	D	102	PRO
1	D	317	PHE
1	D	326	GLY
1	E	102	PRO
1	E	317	PHE
1	E	326	GLY

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Mol	Chain	Res	Type
1	F	102	PRO
1	F	317	PHE
1	F	326	GLY
1	A	26	LEU
1	A	443	PRO
1	B	26	LEU
1	B	443	PRO
1	C	26	LEU
1	C	443	PRO
1	D	26	LEU
1	D	443	PRO
1	E	26	LEU
1	E	443	PRO
1	F	26	LEU
1	F	443	PRO
1	A	149	GLY
1	A	288	ILE
1	B	149	GLY
1	B	288	ILE
1	C	149	GLY
1	C	288	ILE
1	D	149	GLY
1	D	288	ILE
1	E	149	GLY
1	E	288	ILE
1	F	149	GLY
1	F	288	ILE
1	A	321	PRO
1	A	440	GLY
1	B	321	PRO
1	B	440	GLY
1	C	321	PRO
1	C	440	GLY
1	D	321	PRO
1	D	440	GLY
1	E	321	PRO
1	E	440	GLY
1	F	321	PRO
1	F	440	GLY
1	A	200	ILE
1	B	200	ILE
1	C	200	ILE

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Mol	Chain	Res	Type
1	F	200	ILE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	339/358 (95%)	323 (95%)	16 (5%)	32	72
1	B	339/358 (95%)	323 (95%)	16 (5%)	32	72
1	C	339/358 (95%)	323 (95%)	16 (5%)	32	72
1	D	339/358 (95%)	323 (95%)	16 (5%)	32	72
1	E	339/358 (95%)	323 (95%)	16 (5%)	32	72
1	F	339/358 (95%)	323 (95%)	16 (5%)	32	72
All	All	2034/2148 (95%)	1938 (95%)	96 (5%)	32	72

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	LYS
1	A	62	ASN
1	A	83	PHE
1	A	120	ARG
1	A	123	ARG
1	A	132	PHE
1	A	164	ASP
1	A	177	LEU
1	A	212	LEU
1	A	243	LYS
1	A	284	HIS
1	A	317	PHE
1	A	322	ILE
1	A	397	LEU
1	A	416	THR
1	A	451	ARG
1	B	30	LYS

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Mol	Chain	Res	Type
1	B	62	ASN
1	B	83	PHE
1	B	120	ARG
1	B	123	ARG
1	B	132	PHE
1	B	164	ASP
1	B	177	LEU
1	B	212	LEU
1	B	243	LYS
1	B	284	HIS
1	B	317	PHE
1	B	322	ILE
1	B	397	LEU
1	B	416	THR
1	B	451	ARG
1	C	30	LYS
1	C	62	ASN
1	C	83	PHE
1	C	120	ARG
1	C	123	ARG
1	C	132	PHE
1	C	164	ASP
1	C	177	LEU
1	C	212	LEU
1	C	243	LYS
1	C	284	HIS
1	C	317	PHE
1	C	322	ILE
1	C	397	LEU
1	C	416	THR
1	C	451	ARG
1	D	30	LYS
1	D	62	ASN
1	D	83	PHE
1	D	120	ARG
1	D	123	ARG
1	D	132	PHE
1	D	164	ASP
1	D	177	LEU
1	D	212	LEU
1	D	243	LYS
1	D	284	HIS

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Mol	Chain	Res	Type
1	D	317	PHE
1	D	322	ILE
1	D	397	LEU
1	D	416	THR
1	D	451	ARG
1	E	30	LYS
1	E	62	ASN
1	E	83	PHE
1	E	120	ARG
1	E	123	ARG
1	E	132	PHE
1	E	164	ASP
1	E	177	LEU
1	E	212	LEU
1	E	243	LYS
1	E	284	HIS
1	E	317	PHE
1	E	322	ILE
1	E	397	LEU
1	E	416	THR
1	E	451	ARG
1	F	30	LYS
1	F	62	ASN
1	F	83	PHE
1	F	120	ARG
1	F	123	ARG
1	F	132	PHE
1	F	164	ASP
1	F	177	LEU
1	F	212	LEU
1	F	243	LYS
1	F	284	HIS
1	F	317	PHE
1	F	322	ILE
1	F	397	LEU
1	F	416	THR
1	F	451	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	ASN

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Mol	Chain	Res	Type
1	A	74	ASN
1	A	153	GLN
1	A	157	ASN
1	A	207	GLN
1	A	270	ASN
1	A	277	GLN
1	A	318	ASN
1	A	327	ASN
1	A	418	ASN
1	A	420	GLN
1	A	437	GLN
1	B	62	ASN
1	B	74	ASN
1	B	153	GLN
1	B	157	ASN
1	B	207	GLN
1	B	270	ASN
1	B	277	GLN
1	B	318	ASN
1	B	327	ASN
1	B	418	ASN
1	B	420	GLN
1	B	437	GLN
1	C	62	ASN
1	C	74	ASN
1	C	153	GLN
1	C	157	ASN
1	C	207	GLN
1	C	270	ASN
1	C	277	GLN
1	C	318	ASN
1	C	327	ASN
1	C	418	ASN
1	C	420	GLN
1	C	437	GLN
1	D	62	ASN
1	D	74	ASN
1	D	153	GLN
1	D	157	ASN
1	D	207	GLN
1	D	270	ASN
1	D	277	GLN

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Mol	Chain	Res	Type
1	D	318	ASN
1	D	327	ASN
1	D	418	ASN
1	D	420	GLN
1	D	437	GLN
1	E	62	ASN
1	E	74	ASN
1	E	153	GLN
1	E	157	ASN
1	E	207	GLN
1	E	270	ASN
1	E	277	GLN
1	E	318	ASN
1	E	327	ASN
1	E	418	ASN
1	E	420	GLN
1	E	437	GLN
1	F	62	ASN
1	F	74	ASN
1	F	153	GLN
1	F	157	ASN
1	F	207	GLN
1	F	270	ASN
1	F	277	GLN
1	F	318	ASN
1	F	327	ASN
1	F	418	ASN
1	F	420	GLN
1	F	437	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	450/473 (95%)	-0.35	9 (2%) 68 59	51, 100, 147, 151	0
1	B	450/473 (95%)	-0.33	11 (2%) 62 52	51, 100, 147, 151	0
1	C	450/473 (95%)	-0.31	9 (2%) 68 59	51, 100, 147, 151	0
1	D	450/473 (95%)	-0.29	17 (3%) 44 36	51, 100, 147, 151	0
1	E	450/473 (95%)	-0.28	15 (3%) 50 41	51, 100, 147, 151	0
1	F	450/473 (95%)	-0.28	9 (2%) 68 59	51, 100, 147, 151	0
All	All	2700/2838 (95%)	-0.31	70 (2%) 59 49	51, 100, 147, 151	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	12	GLN	8.2
1	E	12	GLN	7.7
1	B	12	GLN	5.9
1	F	12	GLN	5.3
1	D	169	LYS	4.7
1	C	12	GLN	4.4
1	D	15	ARG	4.3
1	E	235	GLU	4.0
1	E	460	GLN	3.6
1	B	234	HIS	3.5
1	E	282	ARG	3.5
1	C	13	ALA	3.5
1	D	235	GLU	3.4
1	E	15	ARG	3.3
1	E	283	VAL	3.2
1	D	14	ALA	3.1
1	D	243	LYS	3.1
1	D	167	ARG	3.1
1	F	171	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	290	LYS	3.0
1	A	283	VAL	3.0
1	A	234	HIS	3.0
1	E	459	GLU	2.9
1	B	383	HIS	2.9
1	D	171	ASP	2.8
1	A	307	PHE	2.8
1	C	171	ASP	2.8
1	E	234	HIS	2.8
1	B	282	ARG	2.7
1	C	27	GLU	2.7
1	D	286	GLY	2.7
1	A	70	HIS	2.7
1	E	24	GLN	2.7
1	A	460	GLN	2.7
1	C	76	PRO	2.7
1	F	76	PRO	2.6
1	C	234	HIS	2.6
1	F	70	HIS	2.6
1	D	70	HIS	2.6
1	B	235	GLU	2.5
1	B	243	LYS	2.5
1	D	13	ALA	2.5
1	E	13	ALA	2.4
1	D	290	LYS	2.4
1	D	283	VAL	2.4
1	D	12	GLN	2.4
1	D	234	HIS	2.4
1	D	27	GLU	2.3
1	F	26	LEU	2.3
1	F	460	GLN	2.3
1	E	169	LYS	2.3
1	F	29	ASP	2.3
1	B	169	LYS	2.3
1	B	283	VAL	2.3
1	B	15	ARG	2.2
1	B	233	ASN	2.2
1	B	250	ASN	2.2
1	E	279	LEU	2.2
1	F	169	LYS	2.2
1	A	19	ARG	2.2
1	C	75	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	99	LYS	2.2
1	A	308	VAL	2.2
1	F	167	ARG	2.1
1	E	212	LEU	2.1
1	E	70	HIS	2.1
1	D	285	GLY	2.1
1	D	74	ASN	2.0
1	C	169	LYS	2.0
1	E	125	TRP	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.