



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 10:20 pm BST

PDB ID : 3BG1  
Title : Architecture of a Coat for the Nuclear Pore Membrane  
Authors : Hoelz, A.  
Deposited on : 2007-11-23  
Resolution : 3.00 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

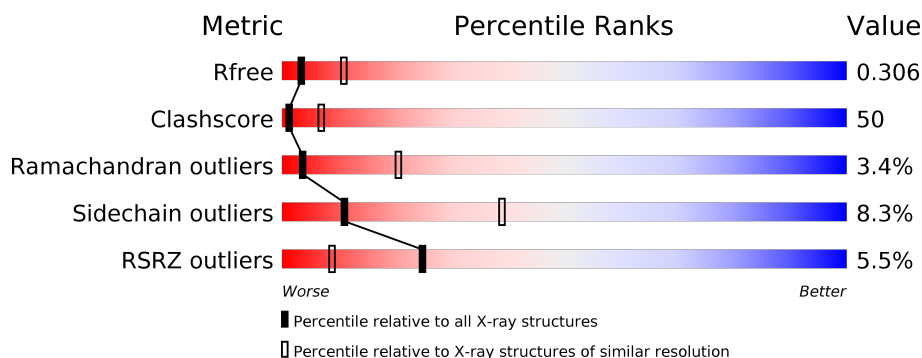
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	316	<div> <div>2%</div> <div>34% 50% 6% 10%</div> </div>
1	D	316	<div> <div>16%</div> <div>34% 49% 7% 10%</div> </div>
1	E	316	<div> <div>5%</div> <div>34% 50% 6% 10%</div> </div>
1	H	316	<div> <div>9%</div> <div>32% 51% 7% 10%</div> </div>
2	B	442	<div> <div>2%</div> <div>31% 56% 8% 5%</div> </div>
2	C	442	<div> <div>3%</div> <div>33% 55% 7% 5%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	442	<div><div></div><div>3%</div><div>33%</div><div>53%</div><div>8%</div><div></div><div></div></div>
2	G	442	<div><div></div><div>3%</div><div>36%</div><div>52%</div><div>7%</div><div>5%</div><div></div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 22614 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 Protein SEC13 homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	S	0	0	0
			2233	1407	389	425	12			
1	D	283	Total	C	N	O	S	0	0	0
			2218	1398	386	422	12			
1	E	285	Total	C	N	O	S	0	0	0
			2233	1407	389	425	12			
1	H	283	Total	C	N	O	S	0	0	0
			2218	1398	386	422	12			

- Molecule 2 is a protein called Nucleoporin NUP145.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	423	Total	C	N	O	S	0	0	0
			3438	2201	570	656	11			
2	C	420	Total	C	N	O	S	0	0	0
			3418	2188	566	653	11			
2	F	423	Total	C	N	O	S	0	0	0
			3438	2201	570	656	11			
2	G	420	Total	C	N	O	S	0	0	0
			3418	2188	566	653	11			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	111	MET	-	EXPRESSION TAG	UNP P49687
B	112	GLY	-	EXPRESSION TAG	UNP P49687
B	113	SER	-	EXPRESSION TAG	UNP P49687
B	114	SER	-	EXPRESSION TAG	UNP P49687
B	115	HIS	-	EXPRESSION TAG	UNP P49687
B	116	HIS	-	EXPRESSION TAG	UNP P49687
B	117	HIS	-	EXPRESSION TAG	UNP P49687
B	118	HIS	-	EXPRESSION TAG	UNP P49687

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Chain	Residue	Modelled	Actual	Comment	Reference
B	119	HIS	-	EXPRESSION TAG	UNP P49687
B	120	HIS	-	EXPRESSION TAG	UNP P49687
B	121	SER	-	EXPRESSION TAG	UNP P49687
B	122	GLY	-	EXPRESSION TAG	UNP P49687
B	123	ASP	-	EXPRESSION TAG	UNP P49687
B	124	PRO	-	EXPRESSION TAG	UNP P49687
C	111	MET	-	EXPRESSION TAG	UNP P49687
C	112	GLY	-	EXPRESSION TAG	UNP P49687
C	113	SER	-	EXPRESSION TAG	UNP P49687
C	114	SER	-	EXPRESSION TAG	UNP P49687
C	115	HIS	-	EXPRESSION TAG	UNP P49687
C	116	HIS	-	EXPRESSION TAG	UNP P49687
C	117	HIS	-	EXPRESSION TAG	UNP P49687
C	118	HIS	-	EXPRESSION TAG	UNP P49687
C	119	HIS	-	EXPRESSION TAG	UNP P49687
C	120	HIS	-	EXPRESSION TAG	UNP P49687
C	121	SER	-	EXPRESSION TAG	UNP P49687
C	122	GLY	-	EXPRESSION TAG	UNP P49687
C	123	ASP	-	EXPRESSION TAG	UNP P49687
C	124	PRO	-	EXPRESSION TAG	UNP P49687
F	111	MET	-	EXPRESSION TAG	UNP P49687
F	112	GLY	-	EXPRESSION TAG	UNP P49687
F	113	SER	-	EXPRESSION TAG	UNP P49687
F	114	SER	-	EXPRESSION TAG	UNP P49687
F	115	HIS	-	EXPRESSION TAG	UNP P49687
F	116	HIS	-	EXPRESSION TAG	UNP P49687
F	117	HIS	-	EXPRESSION TAG	UNP P49687
F	118	HIS	-	EXPRESSION TAG	UNP P49687
F	119	HIS	-	EXPRESSION TAG	UNP P49687
F	120	HIS	-	EXPRESSION TAG	UNP P49687
F	121	SER	-	EXPRESSION TAG	UNP P49687
F	122	GLY	-	EXPRESSION TAG	UNP P49687
F	123	ASP	-	EXPRESSION TAG	UNP P49687
F	124	PRO	-	EXPRESSION TAG	UNP P49687
G	111	MET	-	EXPRESSION TAG	UNP P49687
G	112	GLY	-	EXPRESSION TAG	UNP P49687
G	113	SER	-	EXPRESSION TAG	UNP P49687
G	114	SER	-	EXPRESSION TAG	UNP P49687
G	115	HIS	-	EXPRESSION TAG	UNP P49687
G	116	HIS	-	EXPRESSION TAG	UNP P49687
G	117	HIS	-	EXPRESSION TAG	UNP P49687
G	118	HIS	-	EXPRESSION TAG	UNP P49687

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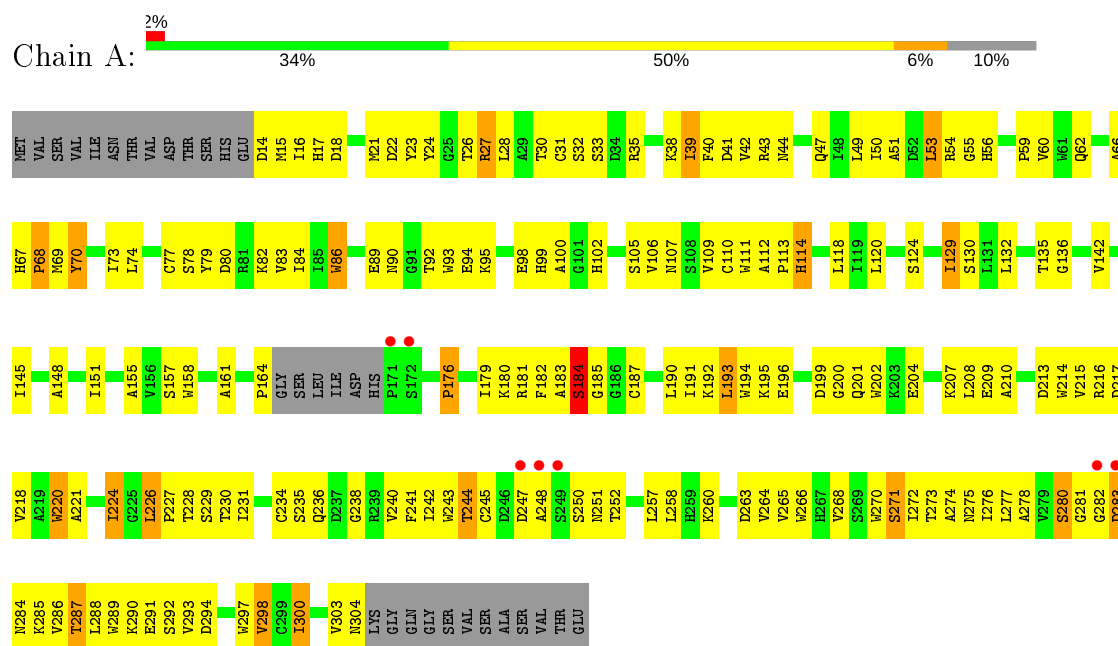
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Chain	Residue	Modelled	Actual	Comment	Reference
G	119	HIS	-	EXPRESSION TAG	UNP P49687
G	120	HIS	-	EXPRESSION TAG	UNP P49687
G	121	SER	-	EXPRESSION TAG	UNP P49687
G	122	GLY	-	EXPRESSION TAG	UNP P49687
G	123	ASP	-	EXPRESSION TAG	UNP P49687
G	124	PRO	-	EXPRESSION TAG	UNP P49687

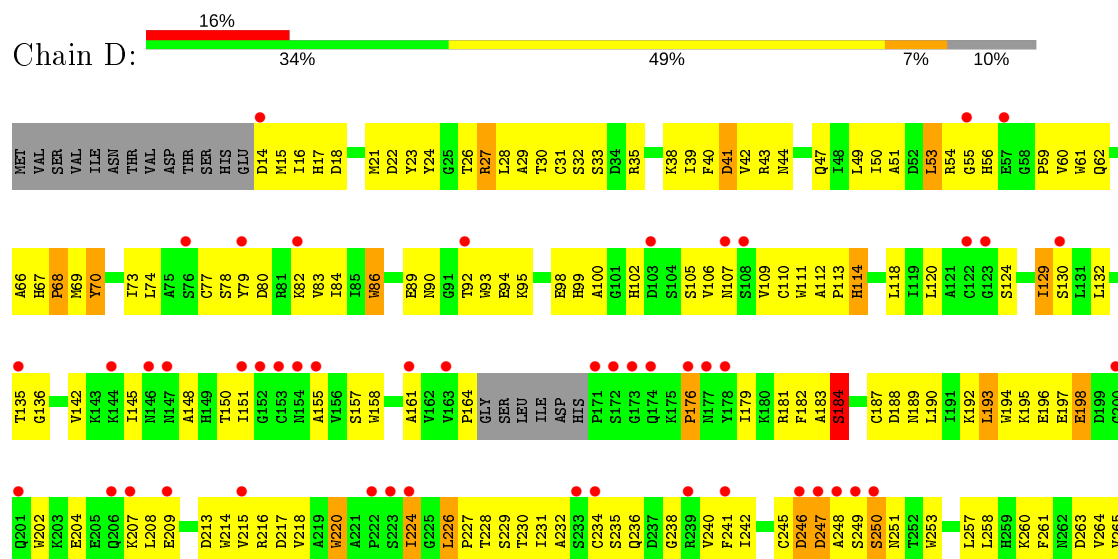
### 3 Residue-property plots

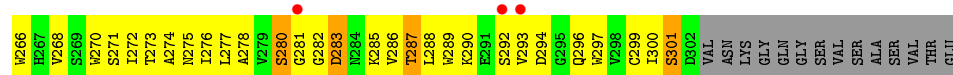
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

#### • Molecule 1: Protein SEC13 homolog

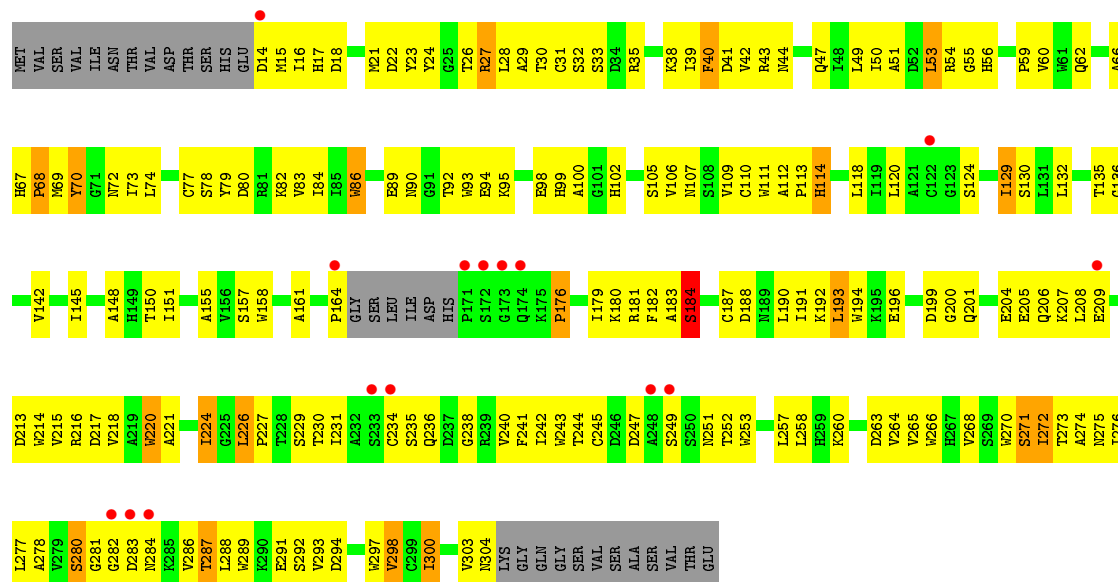


#### • Molecule 1: Protein SEC13 homolog

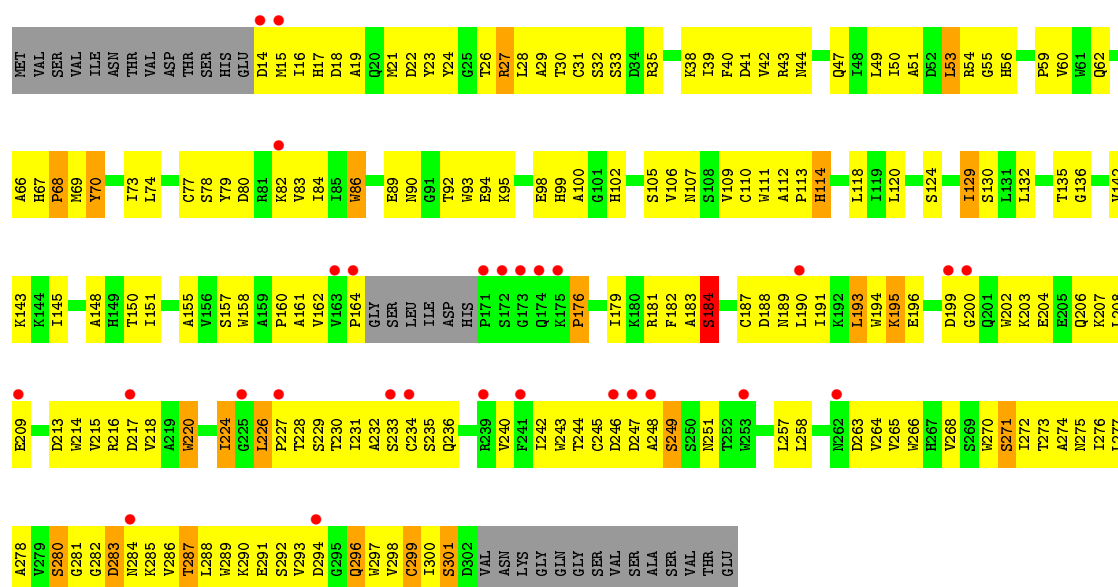




• Molecule 1: Protein SEC13 homolog



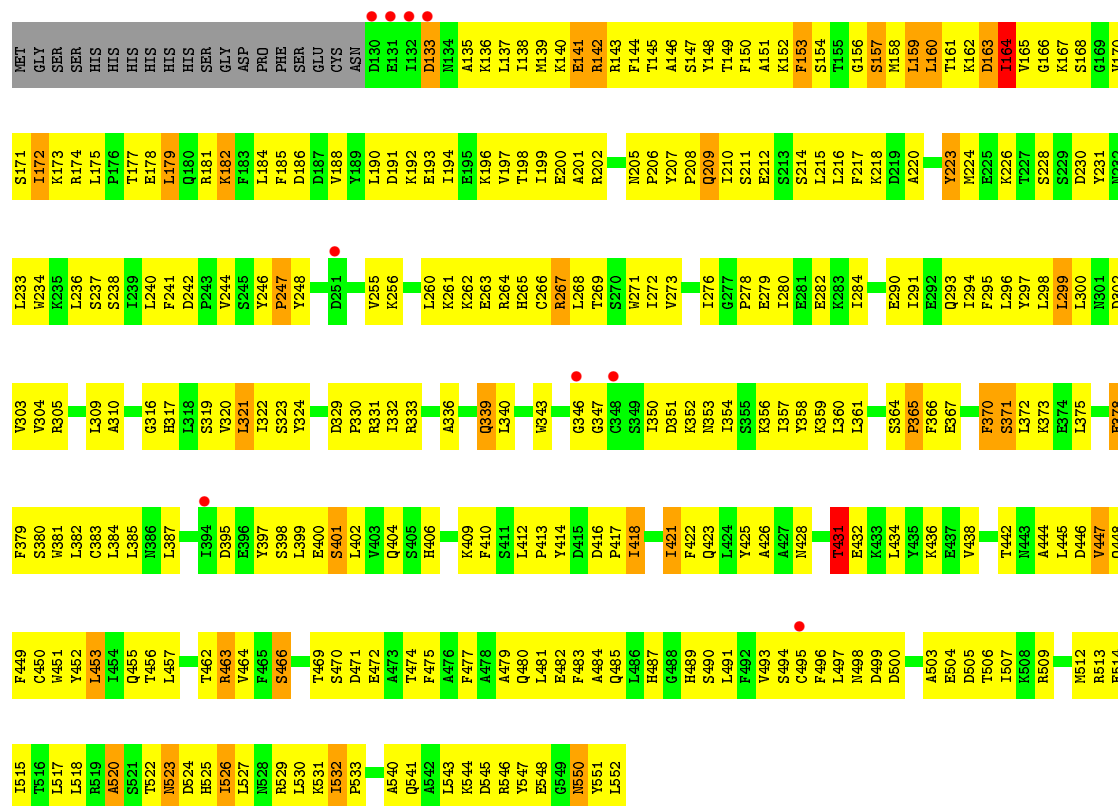
• Molecule 1: Protein SEC13 homolog



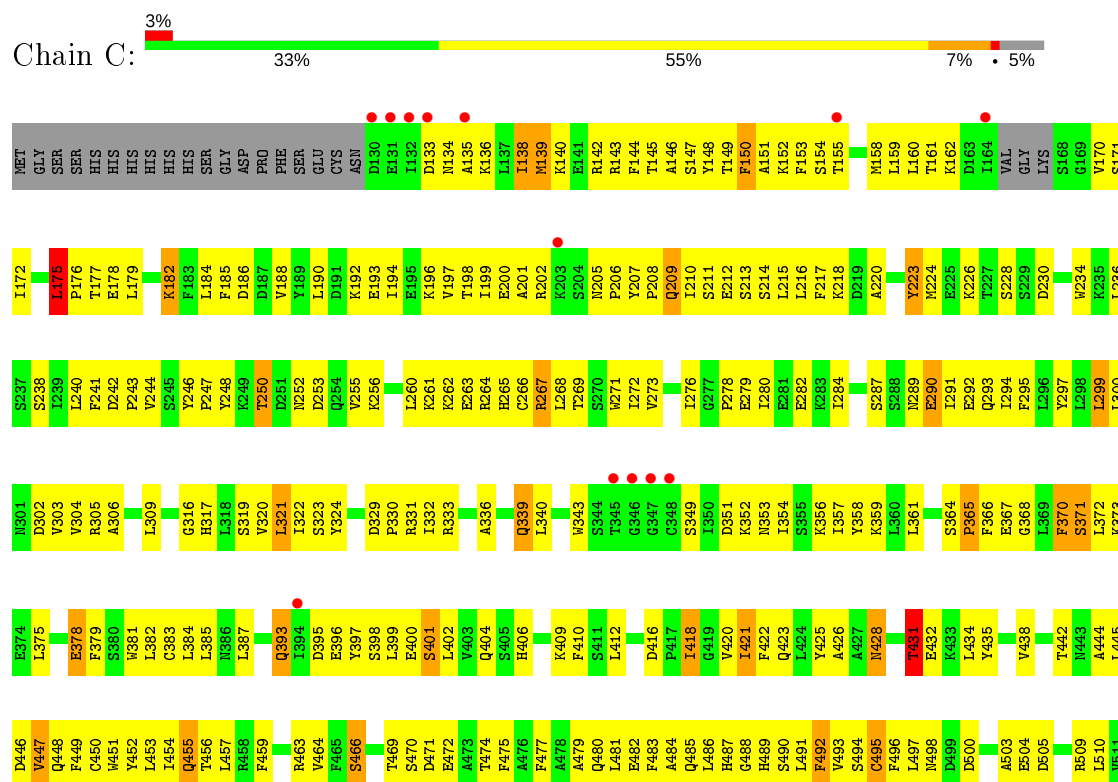
• Molecule 2: Nucleoporin NUP145

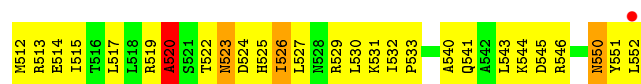




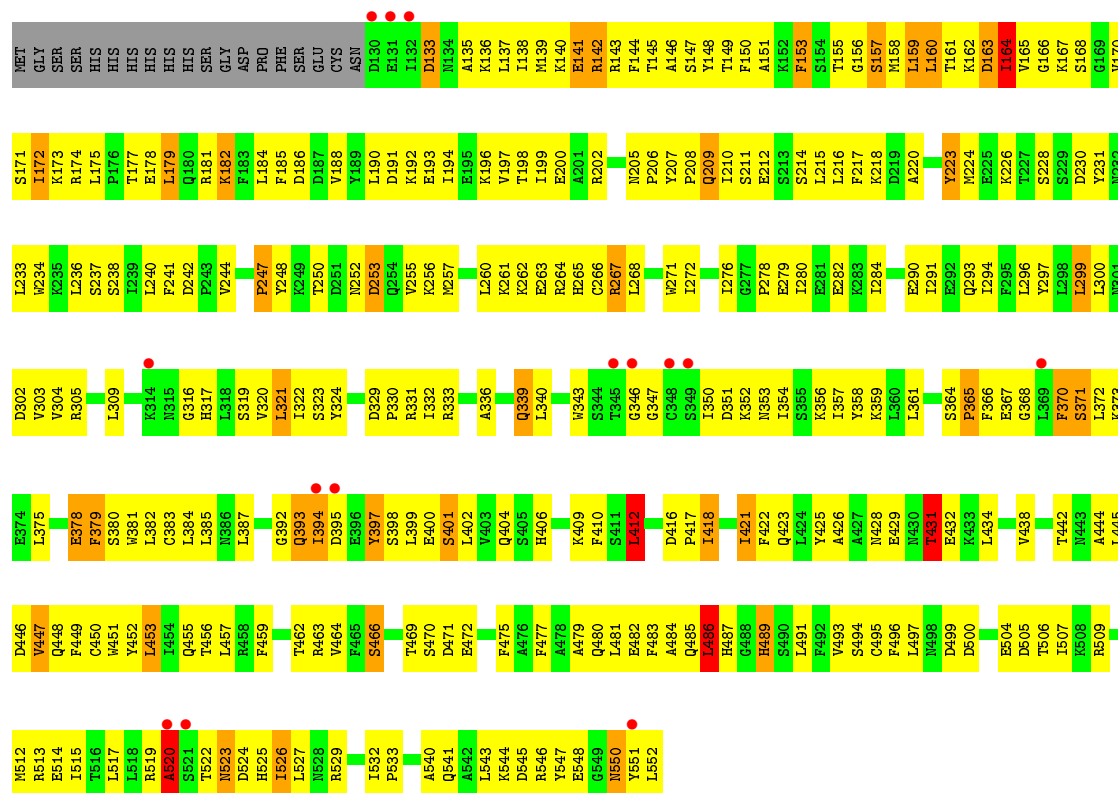


### • Molecule 2: Nucleoporin NUP145

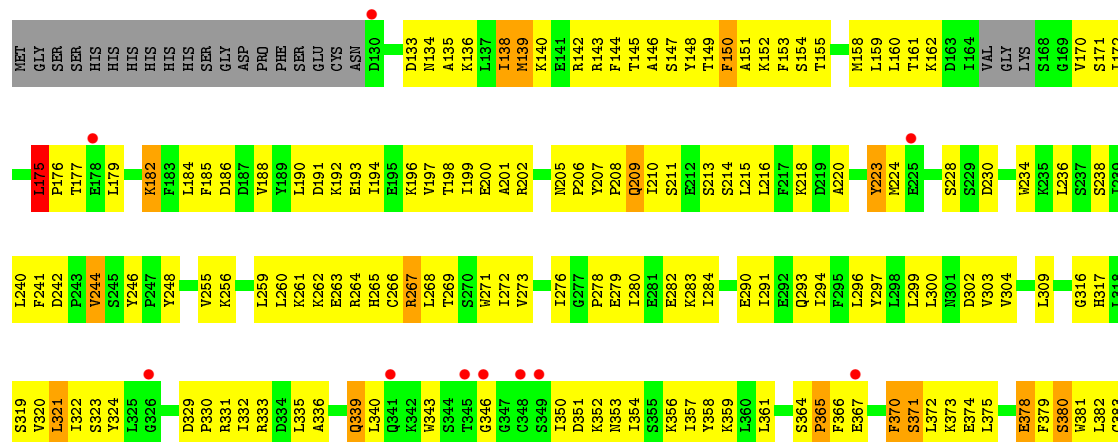


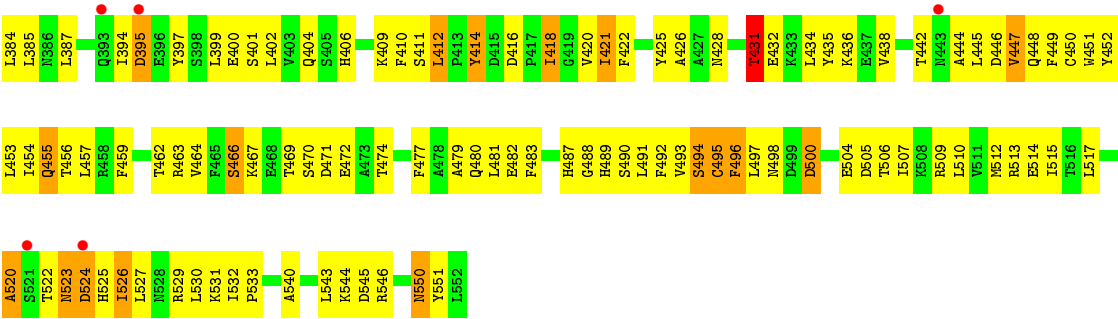


• Molecule 2: Nucleoporin NUP145



• Molecule 2: Nucleoporin NUP145





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	181.37Å 216.79Å 192.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 20.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.3 (20.00-3.00) 84.6 (20.00-3.00)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.38 (at 2.98Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.249 , 0.294 0.262 , 0.306	Depositor DCC
$R_{free}$ test set	5815 reflections (8.15%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	87.9	Xtriage
Anisotropy	0.769	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 78.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	22614	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	149.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.84 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.5507e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.48	0/2297	0.74	1/3131 (0.0%)
1	D	0.45	0/2282	0.76	1/3110 (0.0%)
1	E	0.47	0/2297	0.74	2/3131 (0.1%)
1	H	0.43	0/2282	0.72	1/3110 (0.0%)
2	B	0.52	1/3504 (0.0%)	0.76	1/4728 (0.0%)
2	C	0.49	0/3483	0.76	3/4699 (0.1%)
2	F	0.52	1/3504 (0.0%)	0.77	2/4728 (0.0%)
2	G	0.48	0/3483	0.75	2/4699 (0.0%)
All	All	0.49	2/23132 (0.0%)	0.75	13/31336 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	153	PHE	CE2-CZ	5.19	1.47	1.37
2	B	153	PHE	CE2-CZ	5.05	1.47	1.37

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	175	LEU	CA-CB-CG	5.86	128.77	115.30
2	G	175	LEU	CA-CB-CG	5.85	128.75	115.30
2	C	397	TYR	N-CA-C	5.74	126.49	111.00
1	H	272	ILE	N-CA-C	5.58	126.06	111.00
1	D	272	ILE	N-CA-C	5.51	125.89	111.00
1	E	272	ILE	N-CA-C	5.48	125.80	111.00
1	A	272	ILE	N-CA-C	5.46	125.74	111.00
2	C	520	ALA	N-CA-C	5.23	125.12	111.00
2	B	520	ALA	N-CA-C	5.22	125.09	111.00
2	F	520	ALA	N-CA-C	5.19	125.02	111.00
2	G	520	ALA	N-CA-C	5.19	125.02	111.00
2	F	412	LEU	CA-CB-CG	-5.18	103.38	115.30
1	E	40	PHE	CB-CA-C	-5.06	100.28	110.40

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	2233	0	2109	240	0
1	D	2218	0	2094	244	0
1	E	2233	0	2109	255	0
1	H	2218	0	2094	238	0
2	B	3438	0	3452	370	0
2	C	3418	0	3426	341	0
2	F	3438	0	3452	375	0
2	G	3418	0	3426	334	0
All	All	22614	0	22162	2245	0

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 50.

All (2245) 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:E:278:ALA:HB2	2:F:153:PHE:CE1	1.79	1.18
2:G:481:LEU:HD13	2:G:489:HIS:HB3	1.23	1.17
2:C:479:ALA:CB	1:D:273:THR:HG21	1.76	1.14
1:E:107:ASN:HD21	2:F:142:ARG:NH2	1.47	1.12
1:E:278:ALA:HB2	2:F:153:PHE:HE1	0.98	1.10
2:C:479:ALA:HB1	1:D:273:THR:HG21	1.34	1.09
1:A:278:ALA:HB2	2:B:153:PHE:HE1	1.07	1.08
1:E:69:MET:HE3	1:E:70:TYR:HE1	1.19	1.08
1:A:278:ALA:HB2	2:B:153:PHE:CE1	1.89	1.07
1:A:69:MET:HE3	1:A:70:TYR:HE1	1.19	1.07
1:D:135:THR:HG22	1:D:136:GLY:H	1.17	1.05
1:A:135:THR:HG22	1:A:136:GLY:H	1.17	1.05
2:B:432:GLU:OE2	2:B:466:SER:HB3	1.56	1.05
2:B:350:ILE:HG23	2:B:354:ILE:HD12	1.39	1.04
1:A:41:ASP:HB2	1:A:50:ILE:HD11	1.38	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:479:ALA:CB	1:H:273:THR:HG21	1.87	1.04
2:C:481:LEU:HD13	2:C:489:HIS:HB3	1.39	1.04
2:G:432:GLU:OE2	2:G:466:SER:HB3	1.56	1.03
1:E:135:THR:HG22	1:E:136:GLY:H	1.17	1.03
2:B:404:GLN:HG2	2:B:426:ALA:HB1	1.39	1.03
1:D:69:MET:HE3	1:D:70:TYR:HE1	1.19	1.03
1:H:69:MET:HE3	1:H:70:TYR:HE1	1.19	1.02
1:H:135:THR:HG22	1:H:136:GLY:H	1.17	1.02
2:G:479:ALA:HB1	1:H:273:THR:CG2	1.90	1.01
2:G:155:THR:HG22	2:G:513:ARG:HD2	1.42	1.01
2:F:484:ALA:HB3	2:F:486:LEU:CD1	1.90	1.01
2:C:479:ALA:HB1	1:D:273:THR:CG2	1.90	1.00
1:A:107:ASN:HD21	2:B:142:ARG:NH2	1.57	1.00
2:F:202:ARG:HG3	2:F:500:ASP:OD1	1.61	0.98
1:E:70:TYR:CE2	1:E:118:LEU:HB2	1.98	0.98
2:F:432:GLU:OE2	2:F:466:SER:HB3	1.63	0.98
2:C:442:THR:HG22	2:C:444:ALA:H	1.28	0.98
1:A:70:TYR:CE2	1:A:118:LEU:HB2	1.98	0.98
1:D:70:TYR:CE2	1:D:118:LEU:HB2	1.99	0.98
1:E:102:HIS:ND1	1:E:124:SER:HB3	1.79	0.98
1:H:102:HIS:ND1	1:H:124:SER:HB3	1.79	0.98
1:E:206:GLN:OE1	1:E:251:ASN:HB3	1.62	0.98
1:A:102:HIS:ND1	1:A:124:SER:HB3	1.79	0.97
2:B:276:ILE:HD13	2:B:383:CYS:HA	1.44	0.97
2:C:479:ALA:CB	1:D:273:THR:CG2	2.41	0.97
2:C:162:LYS:HZ3	1:D:15:MET:CE	1.76	0.97
1:H:70:TYR:CE2	1:H:118:LEU:HB2	1.99	0.97
2:F:442:THR:HG22	2:F:444:ALA:H	1.29	0.97
2:G:479:ALA:CB	1:H:273:THR:CG2	2.41	0.96
1:D:102:HIS:ND1	1:D:124:SER:HB3	1.79	0.96
2:B:487:HIS:HD2	2:B:517:LEU:HD23	1.31	0.95
2:G:479:ALA:HB1	1:H:273:THR:HG21	1.46	0.95
2:G:291:ILE:HG22	2:G:353:ASN:HB2	1.47	0.94
2:G:177:THR:HG22	2:G:179:LEU:H	1.29	0.94
2:G:276:ILE:HD13	2:G:383:CYS:HA	1.47	0.94
2:G:442:THR:HG22	2:G:444:ALA:H	1.30	0.94
2:C:291:ILE:HG22	2:C:353:ASN:HB2	1.49	0.93
2:B:149:THR:HG22	2:B:150:PHE:H	1.32	0.93
2:B:201:ALA:H	2:B:531:LYS:HZ2	1.12	0.93
2:C:177:THR:HG22	2:C:179:LEU:H	1.29	0.93
2:F:149:THR:HG22	2:F:150:PHE:H	1.33	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:162:LYS:HZ3	1:D:15:MET:HE2	1.33	0.92
1:E:242:ILE:HD13	1:E:297:TRP:NE1	1.84	0.92
2:G:159:LEU:HD12	2:G:160:LEU:H	1.35	0.91
2:G:462:THR:O	2:G:463:ARG:HD3	1.71	0.91
2:B:522:THR:O	2:B:523:ASN:CG	2.09	0.91
2:C:159:LEU:HD12	2:C:160:LEU:H	1.35	0.91
1:E:107:ASN:ND2	2:F:142:ARG:HH22	1.67	0.91
1:A:28:LEU:HD21	2:B:170:VAL:HG11	1.54	0.90
2:B:184:LEU:HD21	2:B:448:GLN:HE22	1.34	0.90
2:F:207:TYR:CD2	2:F:504:GLU:HA	2.05	0.90
2:G:267:ARG:HG3	2:G:267:ARG:HH11	1.37	0.90
1:H:288:LEU:H	1:H:301:SER:HB3	1.37	0.89
1:E:41:ASP:HB2	1:E:50:ILE:HD11	1.51	0.89
1:A:40:PHE:CZ	2:B:168:SER:HB2	2.07	0.89
1:E:107:ASN:HD21	2:F:142:ARG:HH22	1.10	0.89
2:G:294:ILE:HG12	2:G:309:LEU:HD23	1.54	0.89
2:F:238:SER:HA	2:F:242:ASP:OD2	1.73	0.89
1:A:214:TRP:O	1:A:235:SER:HB2	1.74	0.88
1:D:195:LYS:HG2	1:D:196:GLU:H	1.36	0.88
1:E:214:TRP:O	1:E:235:SER:HB2	1.73	0.88
1:A:107:ASN:HD21	2:B:142:ARG:HH22	1.14	0.88
2:F:484:ALA:HB3	2:F:486:LEU:HD12	1.52	0.88
2:F:522:THR:O	2:F:523:ASN:CG	2.12	0.88
2:F:267:ARG:HG3	2:F:267:ARG:HH11	1.38	0.88
1:H:82:LYS:HG2	1:H:100:ALA:HB2	1.56	0.88
2:B:163:ASP:HB2	2:B:171:SER:OG	1.73	0.88
1:D:82:LYS:HG2	1:D:100:ALA:HB2	1.56	0.88
2:F:404:GLN:HG2	2:F:426:ALA:HB1	1.54	0.88
1:E:135:THR:HG22	1:E:136:GLY:N	1.90	0.87
1:E:69:MET:HE3	1:E:70:TYR:CE1	2.09	0.87
2:F:163:ASP:HB2	2:F:171:SER:OG	1.73	0.87
1:A:82:LYS:HG2	1:A:100:ALA:HB2	1.56	0.87
2:B:442:THR:HG22	2:B:444:ALA:H	1.39	0.87
1:D:214:TRP:O	1:D:235:SER:HB2	1.74	0.87
2:G:551:TYR:HD1	1:H:27:ARG:HE	1.23	0.87
2:B:267:ARG:HH11	2:B:267:ARG:HG3	1.38	0.87
1:D:69:MET:HE3	1:D:70:TYR:CE1	2.10	0.87
1:H:135:THR:HG22	1:H:136:GLY:N	1.90	0.87
1:D:135:THR:HG22	1:D:136:GLY:N	1.90	0.87
1:A:69:MET:HE3	1:A:70:TYR:CE1	2.09	0.87
2:B:202:ARG:HG3	2:B:500:ASP:OD1	1.75	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:249:SER:O	1:D:250:SER:HB2	1.73	0.86
1:E:107:ASN:ND2	2:F:142:ARG:NH2	2.20	0.86
1:A:49:LEU:HD12	1:A:50:ILE:H	1.40	0.86
1:H:151:ILE:HB	1:H:187:CYS:HB2	1.55	0.86
1:A:135:THR:HG22	1:A:136:GLY:N	1.90	0.86
2:B:515:ILE:HD11	2:B:540:ALA:HB3	1.54	0.86
1:H:69:MET:HE3	1:H:70:TYR:CE1	2.10	0.86
2:C:267:ARG:HG3	2:C:267:ARG:HH11	1.37	0.86
2:B:487:HIS:CD2	2:B:517:LEU:HD23	2.08	0.86
1:E:82:LYS:HG2	1:E:100:ALA:HB2	1.56	0.86
1:A:107:ASN:ND2	2:B:142:ARG:HH22	1.73	0.86
2:G:291:ILE:HG22	2:G:353:ASN:CB	2.04	0.86
1:E:49:LEU:HD12	1:E:50:ILE:H	1.40	0.86
1:H:41:ASP:HB2	1:H:50:ILE:HD11	1.58	0.86
1:H:49:LEU:HD12	1:H:50:ILE:H	1.40	0.85
2:B:365:PRO:HB2	2:B:372:LEU:HD12	1.58	0.85
2:F:276:ILE:HD13	2:F:383:CYS:HA	1.56	0.85
1:H:214:TRP:O	1:H:235:SER:HB2	1.74	0.85
1:E:40:PHE:CZ	2:F:168:SER:HB2	2.12	0.85
2:F:365:PRO:HB2	2:F:372:LEU:HD12	1.59	0.85
2:G:218:LYS:HG2	2:G:238:SER:OG	1.76	0.85
2:F:218:LYS:HG2	2:F:238:SER:OG	1.76	0.85
2:C:365:PRO:HB2	2:C:372:LEU:HD12	1.59	0.85
2:B:149:THR:HG22	2:B:150:PHE:N	1.92	0.84
2:C:218:LYS:HG2	2:C:238:SER:OG	1.76	0.84
2:C:280:ILE:HG13	2:C:300:LEU:HD21	1.58	0.84
2:F:481:LEU:HD13	2:F:489:HIS:HB3	1.58	0.84
2:B:184:LEU:HD21	2:B:448:GLN:NE2	1.93	0.84
1:D:155:ALA:HB2	1:D:217:ASP:HA	1.60	0.84
2:B:218:LYS:HG2	2:B:238:SER:OG	1.76	0.84
1:D:49:LEU:HD12	1:D:50:ILE:H	1.41	0.84
2:F:149:THR:HG22	2:F:150:PHE:N	1.92	0.84
2:G:343:TRP:CZ3	2:G:350:ILE:HG13	2.12	0.84
1:A:28:LEU:HD11	2:B:160:LEU:HD13	1.60	0.83
2:C:416:ASP:OD1	2:C:418:ILE:HG13	1.78	0.83
2:B:151:ALA:HB1	2:B:159:LEU:HD11	1.60	0.83
2:B:416:ASP:OD1	2:B:418:ILE:HG13	1.78	0.83
2:C:276:ILE:HD13	2:C:383:CYS:HA	1.59	0.83
2:F:151:ALA:HB1	2:F:159:LEU:HD11	1.60	0.83
2:G:365:PRO:HB2	2:G:372:LEU:HD12	1.58	0.83
2:G:416:ASP:OD1	2:G:418:ILE:HG13	1.78	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:175:LEU:HD13	2:G:176:PRO:HD2	1.60	0.82
2:G:494:SER:O	2:G:497:LEU:HG	1.79	0.82
2:F:416:ASP:OD1	2:F:418:ILE:HG13	1.78	0.82
2:C:175:LEU:HD13	2:C:176:PRO:HD2	1.60	0.82
2:F:484:ALA:HB3	2:F:486:LEU:HD11	1.60	0.82
2:B:350:ILE:CG2	2:B:354:ILE:HD12	2.09	0.82
2:F:216:LEU:HB3	2:F:242:ASP:OD1	1.78	0.82
2:B:218:LYS:HG3	2:B:242:ASP:OD2	1.80	0.82
1:H:155:ALA:HB2	1:H:217:ASP:HA	1.59	0.82
2:F:515:ILE:HD11	2:F:540:ALA:HB3	1.62	0.81
2:C:142:ARG:O	2:C:143:ARG:HB2	1.79	0.81
2:B:497:LEU:HD12	2:B:503:ALA:HA	1.62	0.81
2:C:276:ILE:CD1	2:C:383:CYS:HA	2.10	0.81
2:F:320:VAL:O	2:F:323:SER:HB3	1.81	0.81
2:C:291:ILE:HG22	2:C:353:ASN:CB	2.10	0.80
2:C:145:THR:HG22	2:C:147:SER:H	1.46	0.80
2:C:515:ILE:HD11	2:C:540:ALA:HB3	1.62	0.80
2:G:145:THR:HG22	2:G:147:SER:H	1.46	0.80
2:G:471:ASP:OD1	2:G:497:LEU:HD22	1.82	0.80
2:C:155:THR:HG22	2:C:513:ARG:HD2	1.63	0.80
1:E:245:CYS:HB2	1:E:253:TRP:CE3	2.17	0.80
2:B:320:VAL:O	2:B:323:SER:HB3	1.82	0.80
2:B:159:LEU:HD12	2:B:160:LEU:N	1.97	0.80
2:F:159:LEU:HD12	2:F:160:LEU:N	1.96	0.80
2:G:320:VAL:O	2:G:323:SER:HB3	1.82	0.80
1:H:220:TRP:CE2	1:H:231:ILE:HD11	2.17	0.80
2:F:431:THR:HG22	2:F:432:GLU:N	1.97	0.79
2:B:190:LEU:HD13	2:B:489:HIS:ND1	1.97	0.79
2:B:431:THR:HG22	2:B:432:GLU:N	1.96	0.79
1:E:208:LEU:HB3	1:E:243:TRP:CZ3	2.18	0.79
1:A:220:TRP:CE2	1:A:231:ILE:HD11	2.18	0.79
2:C:149:THR:HG23	2:C:162:LYS:HG2	1.64	0.79
2:G:479:ALA:CA	1:H:273:THR:HG21	2.11	0.79
2:B:207:TYR:CD2	2:B:504:GLU:HA	2.18	0.79
2:C:320:VAL:O	2:C:323:SER:HB3	1.82	0.79
2:C:431:THR:HG22	2:C:432:GLU:N	1.97	0.79
2:G:149:THR:HG23	2:G:162:LYS:HG2	1.64	0.79
2:F:238:SER:O	2:F:242:ASP:HB2	1.81	0.79
1:E:28:LEU:HD21	2:F:170:VAL:HG11	1.65	0.79
2:G:431:THR:HG22	2:G:432:GLU:N	1.97	0.79
1:A:107:ASN:ND2	2:B:142:ARG:NH2	2.30	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:494:SER:O	2:C:497:LEU:HG	1.82	0.79
1:E:220:TRP:CE2	1:E:231:ILE:HD11	2.17	0.79
2:F:445:LEU:HD22	2:F:449:PHE:CD2	2.18	0.78
2:G:142:ARG:O	2:G:143:ARG:HB2	1.79	0.78
2:B:276:ILE:CD1	2:B:383:CYS:HA	2.13	0.78
1:D:220:TRP:CE2	1:D:231:ILE:HD11	2.18	0.78
2:B:172:ILE:HG22	2:B:172:ILE:O	1.83	0.78
1:E:180:LYS:HD2	1:E:196:GLU:OE1	1.82	0.78
2:G:479:ALA:HB1	1:H:273:THR:HG22	1.65	0.78
1:H:244:THR:HG22	1:H:245:CYS:H	1.48	0.78
1:A:41:ASP:HB2	1:A:50:ILE:CD1	2.13	0.78
2:B:398:SER:OG	2:B:401:SER:HB3	1.83	0.78
1:E:273:THR:HG21	2:F:479:ALA:CB	2.14	0.77
2:G:512:MET:SD	2:G:540:ALA:HB2	2.24	0.77
2:F:177:THR:HG21	2:F:179:LEU:HD23	1.67	0.77
2:B:177:THR:HG21	2:B:179:LEU:HD23	1.67	0.77
2:C:442:THR:CG2	2:C:444:ALA:H	1.96	0.77
2:C:432:GLU:OE2	2:C:466:SER:HB3	1.85	0.77
1:E:135:THR:CG2	1:E:136:GLY:H	1.98	0.77
2:F:442:THR:CG2	2:F:444:ALA:H	1.97	0.77
2:C:134:ASN:O	2:C:138:ILE:HB	1.85	0.76
2:C:487:HIS:HD2	2:C:517:LEU:HD23	1.49	0.76
2:F:172:ILE:O	2:F:172:ILE:HG22	1.84	0.76
2:F:250:THR:HG21	2:G:335:LEU:HD13	1.67	0.76
2:G:134:ASN:O	2:G:138:ILE:HB	1.85	0.76
2:C:522:THR:O	2:C:523:ASN:CG	2.23	0.76
2:G:352:LYS:CE	2:G:374:GLU:OE2	2.33	0.76
2:G:291:ILE:CG2	2:G:353:ASN:HB2	2.16	0.76
1:H:226:LEU:HD13	1:H:227:PRO:HD2	1.67	0.76
1:A:220:TRP:CZ3	1:A:229:SER:HB2	2.21	0.76
2:B:210:ILE:HD11	2:B:495:CYS:HB2	1.65	0.76
2:F:343:TRP:CZ3	2:F:350:ILE:HG21	2.21	0.76
2:G:359:LYS:HD2	2:G:365:PRO:HA	1.68	0.76
1:D:220:TRP:CZ3	1:D:229:SER:HB2	2.21	0.76
1:E:220:TRP:CZ3	1:E:229:SER:HB2	2.21	0.76
1:H:220:TRP:CZ3	1:H:229:SER:HB2	2.21	0.76
2:B:177:THR:CG2	2:B:179:LEU:HD23	2.16	0.75
2:F:159:LEU:C	2:F:160:LEU:HD23	2.06	0.75
2:C:284:ILE:HD13	2:C:297:TYR:CE1	2.22	0.75
1:D:226:LEU:HD13	1:D:227:PRO:HD2	1.68	0.75
1:A:102:HIS:HE2	1:A:130:SER:HB3	1.52	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:364:SER:HB3	2:F:394:ILE:HG12	1.69	0.75
1:H:79:TYR:HA	1:H:105:SER:HB2	1.68	0.75
2:B:321:LEU:HB3	2:B:361:LEU:HD11	1.67	0.75
2:B:359:LYS:HD2	2:B:365:PRO:HA	1.68	0.75
2:G:276:ILE:CD1	2:G:383:CYS:HA	2.15	0.75
2:G:216:LEU:HB3	2:G:242:ASP:OD1	1.86	0.75
1:H:102:HIS:HE2	1:H:130:SER:HB3	1.52	0.75
1:A:226:LEU:HD13	1:A:227:PRO:HD2	1.67	0.74
1:D:102:HIS:HE2	1:D:130:SER:HB3	1.52	0.74
2:F:359:LYS:HD2	2:F:365:PRO:HA	1.68	0.74
2:F:484:ALA:CB	2:F:486:LEU:HD11	2.17	0.74
2:C:359:LYS:HD2	2:C:365:PRO:HA	1.68	0.74
1:D:195:LYS:HG2	1:D:196:GLU:N	2.01	0.74
1:E:79:TYR:HA	1:E:105:SER:HB2	1.69	0.74
1:A:242:ILE:HD11	1:A:258:LEU:HD22	1.69	0.74
1:E:226:LEU:HD13	1:E:227:PRO:HD2	1.68	0.74
1:A:135:THR:CG2	1:A:136:GLY:H	1.98	0.74
2:B:159:LEU:C	2:B:160:LEU:HD23	2.07	0.74
2:C:151:ALA:HA	2:C:160:LEU:O	1.87	0.74
2:G:151:ALA:HA	2:G:160:LEU:O	1.87	0.74
2:C:294:ILE:HG12	2:C:309:LEU:HD23	1.67	0.74
1:A:41:ASP:CB	1:A:50:ILE:HD11	2.17	0.74
1:A:79:TYR:HA	1:A:105:SER:HB2	1.68	0.74
1:D:151:ILE:HB	1:D:187:CYS:HB2	1.70	0.74
2:F:177:THR:CG2	2:F:179:LEU:HD23	2.16	0.74
2:G:284:ILE:HD13	2:G:297:TYR:CE1	2.23	0.74
1:D:79:TYR:HA	1:D:105:SER:HB2	1.68	0.74
1:D:135:THR:CG2	1:D:136:GLY:H	1.98	0.74
1:D:29:ALA:HB2	1:D:39:ILE:CD1	2.18	0.74
2:F:179:LEU:O	2:F:179:LEU:HG	1.88	0.74
1:E:107:ASN:OD1	2:F:142:ARG:NH1	2.21	0.74
2:G:280:ILE:HB	2:G:300:LEU:HD21	1.68	0.74
2:B:177:THR:HG22	2:B:179:LEU:HB3	1.70	0.73
1:E:17:HIS:CE1	2:F:148:TYR:CE2	2.76	0.73
1:D:290:LYS:HB3	1:D:300:ILE:HD11	1.70	0.73
2:G:240:LEU:HD21	2:G:268:LEU:CD1	2.17	0.73
1:D:249:SER:O	1:D:250:SER:CB	2.34	0.73
1:E:102:HIS:HE2	1:E:130:SER:HB3	1.52	0.73
2:B:244:VAL:HG23	2:B:264:ARG:HH21	1.54	0.73
2:C:197:VAL:HG12	2:C:198:THR:N	2.04	0.73
2:C:483:PHE:O	2:C:485:GLN:HG2	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:197:VAL:HG12	2:B:198:THR:N	2.03	0.73
2:B:216:LEU:HB3	2:B:242:ASP:OD2	1.88	0.73
2:C:421:ILE:HD11	2:C:449:PHE:HZ	1.54	0.73
2:G:197:VAL:HG12	2:G:198:THR:N	2.03	0.73
2:G:412:LEU:N	2:G:412:LEU:HD12	2.04	0.73
1:H:95:LYS:HE3	1:H:98:GLU:HB2	1.71	0.73
1:D:95:LYS:HE3	1:D:98:GLU:HB2	1.71	0.73
2:F:336:ALA:O	2:F:340:LEU:HD23	1.89	0.73
2:C:199:ILE:CD1	2:C:530:LEU:HA	2.19	0.72
2:F:179:LEU:HD11	2:F:184:LEU:CD1	2.19	0.72
2:G:442:THR:CG2	2:G:444:ALA:H	2.01	0.72
1:H:195:LYS:HE2	1:H:203:LYS:HB2	1.71	0.72
1:E:41:ASP:CB	1:E:50:ILE:HD11	2.18	0.72
2:C:428:ASN:HA	2:C:463:ARG:NH1	2.04	0.72
2:C:471:ASP:OD1	2:C:497:LEU:HA	1.89	0.72
1:D:41:ASP:CB	1:D:50:ILE:HD11	2.19	0.72
1:A:95:LYS:HE3	1:A:98:GLU:HB2	1.71	0.72
2:B:336:ALA:O	2:B:340:LEU:HD23	1.89	0.72
1:E:230:THR:HG22	1:E:231:ILE:H	1.55	0.72
2:F:197:VAL:HG12	2:F:198:THR:N	2.04	0.72
2:C:336:ALA:O	2:C:340:LEU:HD23	1.90	0.72
2:C:421:ILE:HD11	2:C:449:PHE:CZ	2.24	0.72
2:F:177:THR:HG22	2:F:179:LEU:HB3	1.70	0.72
2:G:336:ALA:O	2:G:340:LEU:HD23	1.89	0.72
1:H:69:MET:CE	1:H:114:HIS:HB2	2.20	0.72
2:C:162:LYS:NZ	1:D:15:MET:CE	2.52	0.72
2:F:184:LEU:HD21	2:F:448:GLN:HE22	1.52	0.72
2:B:179:LEU:O	2:B:179:LEU:HG	1.87	0.72
2:G:175:LEU:CD1	2:G:176:PRO:HD2	2.18	0.72
2:C:175:LEU:CD1	2:C:176:PRO:HD2	2.18	0.71
2:G:149:THR:HG22	2:G:150:PHE:H	1.55	0.71
1:D:69:MET:CE	1:D:114:HIS:HB2	2.20	0.71
2:C:223:TYR:CD1	2:C:223:TYR:N	2.58	0.71
2:B:223:TYR:CD1	2:B:223:TYR:N	2.58	0.71
1:D:234:CYS:SG	1:D:268:VAL:HG23	2.30	0.71
2:F:343:TRP:CE3	2:F:350:ILE:HD13	2.25	0.71
1:A:69:MET:CE	1:A:114:HIS:HB2	2.20	0.71
1:A:230:THR:HG22	1:A:231:ILE:H	1.55	0.71
1:E:69:MET:CE	1:E:114:HIS:HB2	2.20	0.71
2:G:148:TYR:HB2	1:H:266:TRP:CG	2.24	0.71
2:G:280:ILE:CB	2:G:300:LEU:HD21	2.19	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:512:MET:SD	2:C:540:ALA:HB2	2.30	0.71
2:C:149:THR:HG22	2:C:150:PHE:H	1.55	0.71
2:C:194:ILE:HG12	2:C:492:PHE:CE2	2.26	0.71
2:F:276:ILE:CD1	2:F:383:CYS:HA	2.21	0.71
1:D:29:ALA:CB	1:D:39:ILE:CD1	2.69	0.71
1:E:95:LYS:HE3	1:E:98:GLU:HB2	1.72	0.71
2:F:247:PRO:HG2	2:F:248:TYR:CE1	2.26	0.71
2:F:385:LEU:HA	2:F:406:HIS:CE1	2.26	0.71
2:F:343:TRP:HZ3	2:F:350:ILE:CG2	2.04	0.70
2:C:216:LEU:HB3	2:C:242:ASP:OD1	1.92	0.70
1:H:230:THR:HG22	1:H:231:ILE:H	1.56	0.70
2:C:149:THR:HG22	2:C:150:PHE:N	2.06	0.70
2:F:223:TYR:CD1	2:F:223:TYR:N	2.58	0.70
1:A:22:ASP:OD1	1:A:23:TYR:N	2.24	0.70
2:F:445:LEU:HD22	2:F:449:PHE:HD2	1.56	0.70
1:H:22:ASP:OD1	1:H:23:TYR:N	2.25	0.70
1:D:230:THR:HG22	1:D:231:ILE:H	1.56	0.70
2:F:480:GLN:HA	2:F:480:GLN:OE1	1.91	0.70
2:F:524:ASP:O	2:F:524:ASP:OD1	2.10	0.70
2:C:480:GLN:HA	2:C:480:GLN:OE1	1.92	0.70
1:E:145:ILE:HD13	1:E:194:TRP:CZ3	2.26	0.70
1:A:107:ASN:OD1	2:B:142:ARG:NH1	2.24	0.70
1:E:22:ASP:OD1	1:E:23:TYR:N	2.24	0.70
1:A:242:ILE:HD12	1:A:297:TRP:CE2	2.27	0.70
2:C:291:ILE:CG2	2:C:353:ASN:HB2	2.21	0.70
2:F:294:ILE:HG12	2:F:309:LEU:HD23	1.72	0.70
2:G:149:THR:HG22	2:G:150:PHE:N	2.06	0.70
2:G:223:TYR:N	2:G:223:TYR:CD1	2.58	0.70
1:D:22:ASP:OD1	1:D:23:TYR:N	2.25	0.70
1:D:190:LEU:CD2	1:D:209:GLU:HB3	2.22	0.69
1:E:179:ILE:HG21	1:E:181:ARG:HE	1.57	0.69
2:F:244:VAL:HG23	2:F:264:ARG:HH21	1.56	0.69
2:F:395:ASP:HB2	2:F:397:TYR:CE2	2.27	0.69
2:F:431:THR:HG22	2:F:432:GLU:H	1.56	0.69
2:G:215:LEU:O	2:G:456:THR:HG23	1.92	0.69
1:D:179:ILE:HG21	1:D:181:ARG:HE	1.57	0.69
1:E:26:THR:HB	2:F:547:TYR:OH	1.92	0.69
1:H:135:THR:CG2	1:H:136:GLY:H	1.98	0.69
2:F:343:TRP:HZ3	2:F:350:ILE:HG21	1.56	0.69
2:C:162:LYS:HZ3	1:D:15:MET:HE1	1.56	0.69
2:C:170:VAL:HG12	2:C:171:SER:N	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:479:ALA:HB2	1:D:273:THR:CG2	2.21	0.69
2:F:475:PHE:HE2	2:F:497:LEU:HD21	1.56	0.69
2:B:480:GLN:HA	2:B:480:GLN:OE1	1.92	0.69
2:C:431:THR:HG22	2:C:432:GLU:H	1.57	0.69
1:D:41:ASP:HB3	1:D:50:ILE:HD11	1.75	0.69
2:G:353:ASN:O	2:G:357:ILE:HG13	1.92	0.69
2:B:385:LEU:HA	2:B:406:HIS:CE1	2.28	0.69
2:G:480:GLN:OE1	2:G:480:GLN:HA	1.92	0.69
2:B:524:ASP:O	2:B:524:ASP:OD1	2.10	0.69
2:C:479:ALA:CA	1:D:273:THR:HG21	2.23	0.69
2:F:353:ASN:O	2:F:357:ILE:HG13	1.93	0.69
1:H:29:ALA:HB2	1:H:39:ILE:CD1	2.23	0.69
1:A:179:ILE:CG2	1:A:181:ARG:HE	2.06	0.69
2:B:404:GLN:CG	2:B:426:ALA:HB1	2.21	0.69
1:H:179:ILE:HG21	1:H:181:ARG:HE	1.57	0.69
2:B:304:VAL:HG21	2:C:302:ASP:HA	1.75	0.68
1:E:29:ALA:HB2	1:E:39:ILE:CD1	2.23	0.68
2:F:224:MET:CE	2:F:230:ASP:HB3	2.24	0.68
2:C:224:MET:CE	2:C:230:ASP:HB3	2.23	0.68
2:G:479:ALA:HA	1:H:273:THR:HG21	1.74	0.68
2:G:291:ILE:HD12	2:G:351:ASP:OD2	1.93	0.68
1:H:53:LEU:N	1:H:53:LEU:HD23	2.09	0.68
1:A:28:LEU:HD11	2:B:160:LEU:CD1	2.23	0.68
2:C:353:ASN:O	2:C:357:ILE:HG13	1.93	0.68
1:E:39:ILE:HD11	1:E:74:LEU:HD22	1.75	0.68
2:F:432:GLU:CD	2:F:466:SER:HB3	2.13	0.68
1:H:288:LEU:N	1:H:301:SER:HB3	2.06	0.68
2:B:353:ASN:O	2:B:357:ILE:HG13	1.92	0.68
2:B:491:LEU:O	2:B:494:SER:HB2	1.93	0.68
2:G:170:VAL:HG12	2:G:171:SER:N	2.08	0.68
2:G:202:ARG:HG2	2:G:209:GLN:OE1	1.94	0.68
2:G:284:ILE:HG12	2:G:296:LEU:HD12	1.76	0.68
1:H:220:TRP:HZ3	1:H:229:SER:HB2	1.58	0.68
2:B:202:ARG:HG2	2:B:209:GLN:OE1	1.94	0.68
2:B:223:TYR:HD1	2:B:223:TYR:H	1.42	0.68
2:C:215:LEU:O	2:C:456:THR:HG23	1.93	0.68
2:G:352:LYS:HG2	2:G:356:LYS:HE3	1.73	0.68
2:G:400:GLU:HG3	2:G:425:TYR:CZ	2.28	0.68
2:G:404:GLN:HG2	2:G:426:ALA:HB1	1.74	0.68
2:G:431:THR:HG22	2:G:432:GLU:H	1.56	0.68
1:E:107:ASN:OD1	2:F:142:ARG:CZ	2.42	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:202:ARG:HG2	2:F:209:GLN:OE1	1.94	0.68
2:C:238:SER:O	2:C:242:ASP:HB2	1.93	0.68
2:C:378:GLU:N	2:C:378:GLU:OE1	2.27	0.68
2:F:280:ILE:HG13	2:F:300:LEU:HD21	1.75	0.68
1:A:53:LEU:HD23	1:A:53:LEU:N	2.09	0.68
2:B:156:GLY:O	2:B:157:SER:HB2	1.94	0.68
2:C:159:LEU:HD12	2:C:160:LEU:N	2.09	0.68
2:F:184:LEU:HD21	2:F:448:GLN:NE2	2.08	0.68
2:B:431:THR:HG22	2:B:432:GLU:H	1.56	0.67
1:H:179:ILE:CG2	1:H:181:ARG:HE	2.06	0.67
1:A:42:VAL:HG12	1:A:42:VAL:O	1.94	0.67
1:E:53:LEU:N	1:E:53:LEU:HD23	2.08	0.67
2:F:378:GLU:N	2:F:378:GLU:OE1	2.27	0.67
2:G:210:ILE:CD1	2:G:495:CYS:HB3	2.24	0.67
2:G:224:MET:CE	2:G:230:ASP:HB3	2.23	0.67
1:A:268:VAL:CG1	1:A:277:LEU:HD11	2.25	0.67
2:C:202:ARG:HG2	2:C:209:GLN:OE1	1.94	0.67
1:E:271:SER:HB2	2:F:153:PHE:CD2	2.29	0.67
2:B:224:MET:CE	2:B:230:ASP:HB3	2.23	0.67
2:C:280:ILE:CG1	2:C:300:LEU:HD21	2.24	0.67
2:C:364:SER:HB2	2:C:367:GLU:HG2	1.76	0.67
1:D:179:ILE:CG2	1:D:181:ARG:HE	2.06	0.67
1:D:288:LEU:H	1:D:301:SER:HB3	1.59	0.67
2:G:352:LYS:HE2	2:G:374:GLU:OE2	1.94	0.67
1:A:179:ILE:HG21	1:A:181:ARG:HE	1.57	0.67
2:B:378:GLU:OE1	2:B:378:GLU:N	2.27	0.67
2:B:487:HIS:CE1	2:B:514:GLU:HG3	2.30	0.67
1:D:53:LEU:HD23	1:D:53:LEU:N	2.08	0.67
1:H:268:VAL:CG1	1:H:277:LEU:HD11	2.25	0.67
1:D:232:ALA:HB2	1:D:270:TRP:CZ2	2.29	0.67
2:G:202:ARG:CZ	2:G:209:GLN:HB3	2.25	0.67
1:H:23:TYR:HD2	1:H:24:TYR:CD1	2.12	0.67
1:E:28:LEU:HD11	2:F:160:LEU:HD13	1.76	0.67
2:F:156:GLY:O	2:F:157:SER:HB2	1.94	0.67
2:F:202:ARG:CZ	2:F:209:GLN:HB3	2.25	0.67
1:E:179:ILE:CG2	1:E:181:ARG:HE	2.06	0.67
2:F:421:ILE:HD11	2:F:449:PHE:HZ	1.59	0.67
2:G:138:ILE:HG22	2:G:139:MET:HG2	1.77	0.67
1:H:230:THR:CG2	1:H:242:ILE:HG23	2.25	0.67
1:A:273:THR:HG21	2:B:479:ALA:CB	2.25	0.66
1:E:23:TYR:HD2	1:E:24:TYR:CD1	2.13	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:167:LYS:O	2:B:167:LYS:HD3	1.95	0.66
2:B:284:ILE:HG12	2:B:296:LEU:HD12	1.76	0.66
2:C:202:ARG:CZ	2:C:209:GLN:HB3	2.25	0.66
2:F:167:LYS:O	2:F:167:LYS:HD3	1.95	0.66
1:A:17:HIS:CE1	2:B:148:TYR:CE2	2.83	0.66
2:C:223:TYR:HD1	2:C:223:TYR:H	1.42	0.66
1:D:268:VAL:CG1	1:D:277:LEU:HD11	2.24	0.66
1:E:208:LEU:HD13	1:E:243:TRP:CE3	2.30	0.66
2:G:240:LEU:HD21	2:G:268:LEU:HD12	1.75	0.66
2:B:364:SER:HB2	2:B:367:GLU:HG2	1.77	0.66
2:B:522:THR:CG2	2:B:526:ILE:HD11	2.25	0.66
2:B:491:LEU:HD21	2:B:532:ILE:HD11	1.78	0.66
1:D:274:ALA:HB1	1:D:290:LYS:HE3	1.78	0.66
1:E:220:TRP:HZ3	1:E:229:SER:HB2	1.58	0.66
1:E:242:ILE:HD13	1:E:297:TRP:CE2	2.30	0.66
2:G:223:TYR:HD1	2:G:223:TYR:H	1.42	0.66
1:H:39:ILE:HD11	1:H:74:LEU:HD22	1.75	0.66
1:A:23:TYR:HD2	1:A:24:TYR:CD1	2.13	0.66
2:C:487:HIS:CD2	2:C:517:LEU:HD23	2.31	0.66
1:D:23:TYR:HD2	1:D:24:TYR:CD1	2.12	0.66
2:F:223:TYR:HD1	2:F:223:TYR:H	1.42	0.66
2:G:479:ALA:CB	1:H:273:THR:HG22	2.24	0.66
1:A:26:THR:HB	2:B:547:TYR:OH	1.96	0.66
2:C:240:LEU:HD21	2:C:268:LEU:CD1	2.26	0.66
2:B:202:ARG:CZ	2:B:209:GLN:HB3	2.25	0.66
2:C:177:THR:HG22	2:C:179:LEU:N	2.08	0.66
2:C:321:LEU:HB3	2:C:361:LEU:HD11	1.76	0.66
1:E:26:THR:HG22	1:E:27:ARG:HD2	1.78	0.66
2:G:364:SER:HB2	2:G:367:GLU:HG2	1.77	0.66
1:A:220:TRP:HZ3	1:A:229:SER:HB2	1.58	0.66
2:B:246:TYR:CD1	2:B:247:PRO:HD2	2.31	0.66
1:D:39:ILE:HD11	1:D:74:LEU:HD22	1.77	0.65
1:E:268:VAL:CG1	1:E:277:LEU:HD11	2.25	0.65
1:E:288:LEU:HB2	1:E:300:ILE:HG13	1.78	0.65
2:F:364:SER:HB2	2:F:367:GLU:HG2	1.77	0.65
2:G:202:ARG:HG3	2:G:500:ASP:OD1	1.97	0.65
2:G:378:GLU:N	2:G:378:GLU:OE1	2.27	0.65
1:A:26:THR:HG22	1:A:27:ARG:HD2	1.78	0.65
2:C:138:ILE:HG22	2:C:139:MET:HG2	1.77	0.65
1:D:220:TRP:HZ3	1:D:229:SER:HB2	1.58	0.65
2:C:223:TYR:HD1	2:C:223:TYR:N	1.94	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:MET:HG3	2:B:162:LYS:NZ	2.12	0.65
1:A:107:ASN:OD1	2:B:142:ARG:CZ	2.45	0.65
2:C:487:HIS:O	2:C:488:GLY:C	2.35	0.65
2:G:421:ILE:HD11	2:G:449:PHE:HZ	1.62	0.65
1:H:244:THR:HG22	1:H:245:CYS:N	2.11	0.65
1:H:26:THR:HG22	1:H:27:ARG:HD2	1.78	0.65
1:H:29:ALA:CB	1:H:39:ILE:CD1	2.75	0.65
2:C:291:ILE:HD12	2:C:351:ASP:OD2	1.96	0.65
2:C:491:LEU:O	2:C:494:SER:HB3	1.97	0.65
2:F:484:ALA:CB	2:F:486:LEU:CD1	2.70	0.65
2:B:280:ILE:CB	2:B:300:LEU:HD21	2.27	0.65
1:D:26:THR:HG22	1:D:27:ARG:HD2	1.78	0.65
2:F:149:THR:CG2	2:F:150:PHE:H	2.06	0.65
2:F:223:TYR:HD1	2:F:223:TYR:N	1.94	0.65
2:G:280:ILE:HG13	2:G:300:LEU:HD21	1.78	0.65
2:G:421:ILE:HD11	2:G:449:PHE:CZ	2.31	0.65
1:E:29:ALA:CB	1:E:39:ILE:CD1	2.75	0.65
2:B:431:THR:CG2	2:B:432:GLU:N	2.60	0.65
2:B:522:THR:O	2:B:523:ASN:ND2	2.29	0.65
2:C:435:TYR:CE2	2:C:454:ILE:HD11	2.32	0.65
1:D:209:GLU:O	1:D:209:GLU:HG3	1.97	0.65
1:E:288:LEU:CB	1:E:300:ILE:HG13	2.27	0.65
2:G:159:LEU:HD12	2:G:160:LEU:N	2.09	0.65
2:G:431:THR:CG2	2:G:432:GLU:N	2.60	0.65
1:A:190:LEU:CD2	1:A:209:GLU:HB3	2.27	0.64
2:B:149:THR:CG2	2:B:150:PHE:H	2.06	0.64
2:C:210:ILE:HG22	2:C:459:PHE:HE2	1.61	0.64
1:H:16:ILE:HD12	1:H:30:THR:HG21	1.79	0.64
1:A:151:ILE:HB	1:A:187:CYS:HB2	1.80	0.64
1:E:16:ILE:HD12	1:E:30:THR:HG21	1.79	0.64
2:F:252:ASN:HB3	2:F:255:VAL:HB	1.79	0.64
1:A:113:PRO:CB	1:A:161:ALA:HB2	2.27	0.64
1:H:209:GLU:O	1:H:209:GLU:HG3	1.97	0.64
2:B:280:ILE:HB	2:B:300:LEU:HD21	1.79	0.64
2:C:479:ALA:HB1	1:D:273:THR:HG22	1.79	0.64
2:G:210:ILE:HD12	2:G:495:CYS:HB3	1.77	0.64
1:A:16:ILE:HD12	1:A:30:THR:HG21	1.79	0.64
1:A:182:PHE:CD1	1:A:182:PHE:O	2.51	0.64
2:B:197:VAL:CG1	2:B:198:THR:N	2.61	0.64
2:C:524:ASP:O	2:C:524:ASP:OD1	2.15	0.64
1:D:29:ALA:HB2	1:D:39:ILE:HD12	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:182:PHE:O	1:E:182:PHE:CD1	2.50	0.64
1:E:278:ALA:CB	2:F:153:PHE:HE1	1.93	0.64
1:A:155:ALA:HB2	1:A:217:ASP:HA	1.79	0.64
2:G:223:TYR:N	2:G:223:TYR:HD1	1.94	0.64
2:G:246:TYR:HE2	2:G:248:TYR:HB2	1.63	0.64
1:D:274:ALA:O	1:D:275:ASN:HB2	1.97	0.64
1:E:15:MET:HG3	2:F:162:LYS:NZ	2.12	0.64
2:F:431:THR:CG2	2:F:432:GLU:N	2.60	0.64
2:B:179:LEU:HD11	2:B:184:LEU:CD1	2.28	0.64
2:B:384:LEU:O	2:B:387:LEU:HB2	1.98	0.64
2:F:197:VAL:CG1	2:F:198:THR:N	2.61	0.64
2:F:284:ILE:HG12	2:F:296:LEU:HD12	1.80	0.64
1:A:274:ALA:HB3	1:A:276:ILE:HG13	1.80	0.64
2:C:170:VAL:HG12	2:C:171:SER:H	1.63	0.64
2:C:384:LEU:O	2:C:387:LEU:HB2	1.98	0.64
2:C:420:VAL:HG11	2:C:445:LEU:HD11	1.80	0.64
2:G:481:LEU:CD1	2:G:489:HIS:HB3	2.15	0.64
2:B:404:GLN:HG2	2:B:426:ALA:CB	2.23	0.63
1:D:182:PHE:CD1	1:D:182:PHE:O	2.51	0.63
2:C:152:LYS:NZ	1:D:62:GLN:HE21	1.96	0.63
1:H:151:ILE:HB	1:H:187:CYS:CB	2.28	0.63
2:C:280:ILE:CB	2:C:300:LEU:HD21	2.29	0.63
2:C:381:TRP:CZ3	2:C:382:LEU:HD13	2.33	0.63
1:A:193:LEU:C	1:A:194:TRP:CD1	2.72	0.63
1:A:209:GLU:O	1:A:209:GLU:HG3	1.97	0.63
2:B:485:GLN:HE21	2:B:517:LEU:HD22	1.63	0.63
2:C:162:LYS:NZ	1:D:15:MET:HE2	2.11	0.63
1:D:193:LEU:C	1:D:194:TRP:CD1	2.72	0.63
1:E:274:ALA:O	1:E:275:ASN:HB2	1.98	0.63
2:F:321:LEU:HB3	2:F:361:LEU:HD11	1.78	0.63
2:C:431:THR:CG2	2:C:432:GLU:N	2.61	0.63
1:E:193:LEU:C	1:E:194:TRP:CD1	2.72	0.63
2:G:384:LEU:O	2:G:387:LEU:HB2	1.98	0.63
2:B:223:TYR:HD1	2:B:223:TYR:N	1.94	0.63
2:G:512:MET:HA	2:G:540:ALA:HB1	1.81	0.63
2:C:197:VAL:CG1	2:C:198:THR:N	2.61	0.63
1:D:79:TYR:CD1	1:D:105:SER:HB3	2.34	0.63
1:E:209:GLU:O	1:E:209:GLU:HG3	1.98	0.63
2:G:197:VAL:CG1	2:G:198:THR:N	2.61	0.63
2:G:201:ALA:HB2	2:G:531:LYS:NZ	2.14	0.63
1:H:274:ALA:HB3	1:H:276:ILE:HG13	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:ALA:O	1:A:275:ASN:HB2	1.98	0.63
2:B:164:ILE:HG23	2:B:164:ILE:O	1.98	0.63
2:B:494:SER:O	2:B:497:LEU:HG	1.99	0.63
1:D:16:ILE:HD12	1:D:30:THR:HG21	1.79	0.63
2:G:155:THR:HG22	2:G:513:ARG:CD	2.25	0.63
1:H:226:LEU:HD13	1:H:227:PRO:CD	2.29	0.63
1:A:79:TYR:CD1	1:A:105:SER:HB3	2.34	0.63
2:C:381:TRP:CE3	2:C:412:LEU:CD2	2.82	0.63
1:H:190:LEU:CD2	1:H:209:GLU:HB3	2.29	0.63
1:H:274:ALA:O	1:H:275:ASN:HB2	1.98	0.63
1:A:224:ILE:C	1:A:226:LEU:H	2.03	0.62
2:C:240:LEU:HD21	2:C:268:LEU:HD12	1.81	0.62
1:D:224:ILE:C	1:D:226:LEU:H	2.03	0.62
1:E:17:HIS:ND1	2:F:148:TYR:HE2	1.96	0.62
2:B:238:SER:O	2:B:242:ASP:HB3	1.99	0.62
2:C:151:ALA:HB2	1:D:286:VAL:HG21	1.81	0.62
2:G:138:ILE:HG22	2:G:139:MET:H	1.64	0.62
1:A:226:LEU:HD13	1:A:227:PRO:CD	2.29	0.62
2:C:267:ARG:CG	2:C:267:ARG:HH11	2.10	0.62
1:E:230:THR:HG22	1:E:231:ILE:N	2.14	0.62
1:E:274:ALA:HB3	1:E:276:ILE:HG13	1.80	0.62
1:H:182:PHE:O	1:H:182:PHE:CD1	2.51	0.62
2:C:136:LYS:O	2:C:140:LYS:HB2	1.99	0.62
1:D:274:ALA:HB3	1:D:276:ILE:HG13	1.80	0.62
1:E:30:THR:HG22	1:E:31:CYS:N	2.14	0.62
2:F:149:THR:CG2	2:F:150:PHE:N	2.63	0.62
2:F:164:ILE:O	2:F:164:ILE:HG23	1.99	0.62
2:F:240:LEU:HD21	2:F:268:LEU:HD12	1.80	0.62
1:H:79:TYR:CD1	1:H:105:SER:HB3	2.34	0.62
1:H:42:VAL:HG12	1:H:42:VAL:O	1.98	0.62
1:D:226:LEU:HD13	1:D:227:PRO:CD	2.29	0.62
1:E:226:LEU:HD13	1:E:227:PRO:CD	2.29	0.62
2:F:177:THR:C	2:F:179:LEU:H	2.03	0.62
2:F:237:SER:OG	2:F:421:ILE:CD1	2.48	0.62
2:G:515:ILE:HD11	2:G:540:ALA:HB3	1.82	0.62
1:H:193:LEU:C	1:H:194:TRP:CD1	2.72	0.62
1:H:30:THR:HG22	1:H:31:CYS:N	2.15	0.62
2:B:177:THR:C	2:B:179:LEU:H	2.02	0.62
2:C:148:TYR:HB2	1:D:266:TRP:CG	2.35	0.62
1:E:79:TYR:CD1	1:E:105:SER:HB3	2.35	0.62
2:F:384:LEU:O	2:F:387:LEU:HB2	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:155:THR:HG22	2:F:513:ARG:CD	2.30	0.62
2:G:432:GLU:CD	2:G:466:SER:HB3	2.18	0.62
1:H:39:ILE:HD11	1:H:74:LEU:CD2	2.29	0.62
2:B:276:ILE:HD13	2:B:383:CYS:CA	2.27	0.62
2:F:522:THR:O	2:F:523:ASN:ND2	2.32	0.62
2:G:136:LYS:O	2:G:140:LYS:HB2	1.99	0.62
2:G:194:ILE:HG12	2:G:492:PHE:CE2	2.35	0.62
1:A:238:GLY:O	1:A:260:LYS:HA	2.00	0.62
1:E:221:ALA:HB2	1:E:270:TRP:CE2	2.34	0.62
2:F:155:THR:HG22	2:F:513:ARG:HD2	1.82	0.62
2:G:162:LYS:NZ	1:H:15:MET:HE2	2.15	0.62
1:H:208:LEU:HB3	1:H:243:TRP:CZ3	2.35	0.62
2:B:240:LEU:HD21	2:B:268:LEU:CD1	2.30	0.61
2:B:267:ARG:CG	2:B:267:ARG:HH11	2.11	0.61
2:B:421:ILE:HD11	2:B:449:PHE:HZ	1.63	0.61
2:C:138:ILE:HG22	2:C:139:MET:H	1.64	0.61
2:F:210:ILE:HD11	2:F:495:CYS:HB2	1.81	0.61
2:G:524:ASP:O	2:G:524:ASP:OD1	2.18	0.61
1:A:30:THR:HG22	1:A:31:CYS:N	2.15	0.61
1:E:190:LEU:HD13	1:E:207:LYS:HD3	1.80	0.61
1:E:27:ARG:HE	2:F:551:TYR:HD1	1.46	0.61
2:G:343:TRP:HZ3	2:G:350:ILE:HG21	1.65	0.61
1:D:30:THR:HG22	1:D:31:CYS:N	2.15	0.61
2:F:280:ILE:CB	2:F:300:LEU:HD21	2.30	0.61
1:A:180:LYS:HD2	1:A:196:GLU:OE1	2.00	0.61
1:D:263:ASP:OD1	1:D:264:VAL:N	2.34	0.61
1:E:70:TYR:CD2	1:E:118:LEU:HB2	2.35	0.61
1:A:271:SER:HB2	2:B:153:PHE:CD2	2.35	0.61
2:C:160:LEU:HA	2:C:171:SER:O	2.00	0.61
2:C:512:MET:HA	2:C:540:ALA:HB1	1.81	0.61
1:D:230:THR:HG22	1:D:231:ILE:N	2.16	0.61
2:G:175:LEU:HG	2:G:483:PHE:CD2	2.35	0.61
1:A:70:TYR:CD2	1:A:118:LEU:HB2	2.35	0.61
1:A:263:ASP:OD1	1:A:264:VAL:N	2.33	0.61
1:D:145:ILE:HD11	1:D:202:TRP:CB	2.30	0.61
1:E:224:ILE:C	1:E:226:LEU:H	2.02	0.61
1:E:263:ASP:OD1	1:E:264:VAL:N	2.33	0.61
2:F:263:GLU:HA	2:G:320:VAL:HG22	1.83	0.61
2:F:512:MET:SD	2:F:540:ALA:HB2	2.41	0.61
2:G:160:LEU:HA	2:G:171:SER:O	2.00	0.61
2:G:479:ALA:HB2	1:H:273:THR:CG2	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:138:ILE:O	2:B:142:ARG:HB2	2.00	0.61
1:D:70:TYR:CD2	1:D:118:LEU:HB2	2.35	0.61
1:D:39:ILE:HD11	1:D:74:LEU:CD2	2.30	0.61
1:E:39:ILE:HD11	1:E:74:LEU:CD2	2.30	0.61
2:F:145:THR:HG22	2:F:147:SER:H	1.66	0.61
2:F:491:LEU:HD21	2:F:532:ILE:CD1	2.30	0.61
1:H:224:ILE:C	1:H:226:LEU:H	2.03	0.61
1:H:263:ASP:OD1	1:H:264:VAL:N	2.33	0.61
1:H:70:TYR:CD2	1:H:118:LEU:HB2	2.36	0.61
2:B:284:ILE:HG12	2:B:296:LEU:CD1	2.30	0.61
1:D:248:ALA:O	1:D:249:SER:OG	2.16	0.61
2:G:238:SER:HA	2:G:242:ASP:OD2	2.01	0.61
2:C:138:ILE:CG2	2:C:139:MET:N	2.64	0.61
2:G:236:LEU:HD22	2:G:418:ILE:HG22	1.83	0.61
1:H:208:LEU:HB3	1:H:243:TRP:CH2	2.36	0.61
1:A:230:THR:HG22	1:A:231:ILE:N	2.15	0.61
1:D:70:TYR:HE2	1:D:118:LEU:HB2	1.64	0.61
1:D:238:GLY:O	1:D:260:LYS:HA	2.01	0.61
2:F:138:ILE:O	2:F:142:ARG:HB2	2.01	0.60
2:F:399:LEU:HD23	2:F:425:TYR:OH	2.01	0.60
2:F:487:HIS:CD2	2:F:517:LEU:HD23	2.36	0.60
2:G:177:THR:HG22	2:G:179:LEU:N	2.08	0.60
2:G:205:ASN:HB2	2:G:206:PRO:HD2	1.83	0.60
2:G:162:LYS:HZ2	1:H:15:MET:HE2	1.66	0.60
1:H:208:LEU:HD13	1:H:243:TRP:CE3	2.36	0.60
2:B:375:LEU:HB2	2:B:384:LEU:HD21	1.82	0.60
2:F:142:ARG:HB3	2:F:144:PHE:CD1	2.36	0.60
2:B:240:LEU:HD21	2:B:268:LEU:HD12	1.82	0.60
1:H:230:THR:HG22	1:H:231:ILE:N	2.15	0.60
2:B:205:ASN:HB2	2:B:206:PRO:HD2	1.84	0.60
2:G:142:ARG:NH2	1:H:107:ASN:OD1	2.35	0.60
2:B:442:THR:HG22	2:B:444:ALA:N	2.15	0.60
2:F:412:LEU:H	2:F:412:LEU:CD1	2.10	0.60
2:G:210:ILE:HG22	2:G:459:PHE:HE2	1.66	0.60
2:B:237:SER:OG	2:B:421:ILE:CD1	2.49	0.60
2:C:224:MET:HE2	2:C:230:ASP:HB3	1.83	0.60
1:E:183:ALA:O	1:E:184:SER:HB3	2.00	0.60
1:H:287:THR:CG2	1:H:299:CYS:SG	2.89	0.60
1:A:70:TYR:HE2	1:A:118:LEU:HB2	1.64	0.60
2:F:224:MET:HE1	2:F:230:ASP:HB3	1.82	0.60
2:F:240:LEU:HD21	2:F:268:LEU:CD1	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:170:VAL:HG12	2:G:171:SER:H	1.64	0.60
2:G:283:LYS:NZ	2:G:378:GLU:HB2	2.16	0.60
2:G:138:ILE:CG2	2:G:139:MET:N	2.64	0.60
2:B:149:THR:CG2	2:B:150:PHE:N	2.63	0.60
2:F:446:ASP:O	2:F:449:PHE:N	2.35	0.60
2:B:294:ILE:HG12	2:B:309:LEU:HD23	1.83	0.60
2:B:446:ASP:O	2:B:449:PHE:N	2.35	0.60
1:E:151:ILE:HB	1:E:187:CYS:HB2	1.83	0.60
2:F:485:GLN:O	2:F:487:HIS:N	2.35	0.60
2:G:451:TRP:CZ2	2:G:493:VAL:HG13	2.36	0.60
1:H:113:PRO:HB2	1:H:161:ALA:HB2	1.84	0.60
2:B:142:ARG:HB3	2:B:144:PHE:CD1	2.37	0.59
2:B:522:THR:HG22	2:B:526:ILE:HD11	1.83	0.59
2:C:205:ASN:HB2	2:C:206:PRO:HD2	1.83	0.59
1:D:195:LYS:CG	1:D:196:GLU:H	2.11	0.59
1:E:190:LEU:CD2	1:E:209:GLU:HB3	2.32	0.59
2:F:205:ASN:HB2	2:F:206:PRO:HD2	1.83	0.59
2:F:532:ILE:HG23	2:F:533:PRO:HD2	1.84	0.59
1:A:221:ALA:HB2	1:A:270:TRP:CE2	2.38	0.59
1:D:145:ILE:HD11	1:D:202:TRP:HB2	1.83	0.59
1:D:183:ALA:O	1:D:184:SER:HB3	2.01	0.59
1:D:213:ASP:HB3	1:D:236:GLN:HB2	1.84	0.59
1:E:238:GLY:O	1:E:260:LYS:HA	2.01	0.59
1:H:287:THR:HA	1:H:301:SER:CB	2.32	0.59
1:A:89:GLU:O	1:A:90:ASN:HB2	2.02	0.59
2:B:162:LYS:O	2:B:162:LYS:HG3	2.02	0.59
2:B:332:ILE:H	2:B:332:ILE:HD12	1.67	0.59
1:D:77:CYS:HB3	1:D:109:VAL:CG2	2.32	0.59
1:E:192:LYS:HD3	1:E:204:GLU:OE1	2.02	0.59
2:F:162:LYS:O	2:F:162:LYS:HG3	2.02	0.59
2:F:198:THR:HG22	2:F:211:SER:HB3	1.84	0.59
2:F:332:ILE:H	2:F:332:ILE:HD12	1.67	0.59
2:B:497:LEU:CD1	2:B:503:ALA:HA	2.31	0.59
2:C:202:ARG:HG3	2:C:500:ASP:OD1	2.02	0.59
1:E:155:ALA:HB2	1:E:217:ASP:HA	1.84	0.59
1:E:258:LEU:HD13	1:E:297:TRP:CB	2.32	0.59
2:B:145:THR:HG22	2:B:147:SER:H	1.66	0.59
2:C:451:TRP:CD1	2:C:474:THR:HA	2.37	0.59
1:H:183:ALA:O	1:H:184:SER:HB3	2.01	0.59
1:E:49:LEU:HD12	1:E:50:ILE:N	2.16	0.59
2:F:423:GLN:HB3	2:F:434:LEU:HD21	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:190:LEU:HD22	1:H:209:GLU:HB3	1.85	0.59
2:B:464:VAL:HG23	2:B:464:VAL:O	2.03	0.59
1:D:29:ALA:HA	1:D:39:ILE:HD13	1.85	0.59
1:E:213:ASP:HB3	1:E:236:GLN:HB2	1.84	0.59
1:A:183:ALA:O	1:A:184:SER:HB3	2.01	0.59
1:A:213:ASP:HB3	1:A:236:GLN:HB2	1.84	0.59
2:C:446:ASP:O	2:C:449:PHE:N	2.36	0.59
2:G:321:LEU:HB3	2:G:361:LEU:HD11	1.84	0.59
1:A:77:CYS:HB3	1:A:109:VAL:CG2	2.33	0.59
2:B:198:THR:HG22	2:B:211:SER:HB3	1.84	0.59
2:C:160:LEU:CD2	2:C:172:ILE:HG12	2.33	0.59
1:D:41:ASP:HB2	1:D:50:ILE:HD11	1.85	0.58
2:F:384:LEU:HD13	2:F:410:PHE:CE1	2.38	0.58
1:H:89:GLU:O	1:H:90:ASN:HB2	2.02	0.58
2:C:332:ILE:H	2:C:332:ILE:HD12	1.67	0.58
1:D:242:ILE:HG12	1:D:297:TRP:CE2	2.38	0.58
2:B:491:LEU:HD21	2:B:532:ILE:CD1	2.33	0.58
2:G:199:ILE:CD1	2:G:530:LEU:HA	2.32	0.58
2:G:464:VAL:HG23	2:G:464:VAL:O	2.04	0.58
2:G:491:LEU:HD13	2:G:510:LEU:HD23	1.85	0.58
1:H:77:CYS:HB3	1:H:109:VAL:CG2	2.33	0.58
2:C:152:LYS:HZ1	1:D:62:GLN:NE2	2.00	0.58
2:C:218:LYS:HG3	2:C:242:ASP:OD2	2.03	0.58
2:F:233:LEU:HD13	2:F:417:PRO:HB2	1.85	0.58
2:G:332:ILE:HD12	2:G:332:ILE:H	1.67	0.58
1:E:89:GLU:O	1:E:90:ASN:HB2	2.02	0.58
2:F:267:ARG:CG	2:F:267:ARG:HH11	2.11	0.58
2:G:160:LEU:CD2	2:G:172:ILE:HG12	2.33	0.58
1:H:213:ASP:HB3	1:H:236:GLN:HB2	1.84	0.58
2:C:351:ASP:HB2	2:C:354:ILE:HG13	1.86	0.58
1:D:89:GLU:O	1:D:90:ASN:HB2	2.02	0.58
1:E:70:TYR:CD1	1:E:70:TYR:N	2.72	0.58
2:F:247:PRO:HG2	2:F:248:TYR:CD1	2.38	0.58
2:G:198:THR:HG22	2:G:211:SER:HB3	1.84	0.58
2:G:238:SER:O	2:G:242:ASP:HB2	2.04	0.58
1:A:208:LEU:HB3	1:A:243:TRP:CZ3	2.39	0.58
2:C:152:LYS:NZ	1:D:62:GLN:NE2	2.51	0.58
1:H:70:TYR:CD1	1:H:70:TYR:N	2.72	0.58
1:A:193:LEU:N	1:A:193:LEU:CD2	2.67	0.58
2:B:210:ILE:CD1	2:B:495:CYS:HB2	2.33	0.58
2:C:262:LYS:O	2:C:265:HIS:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:29:ALA:HB2	1:E:39:ILE:HD12	1.85	0.58
1:E:23:TYR:CD2	1:E:68:PRO:HG3	2.39	0.58
2:F:340:LEU:HD21	2:F:358:TYR:HB3	1.85	0.58
1:H:191:ILE:HG23	1:H:218:VAL:HG21	1.86	0.58
1:A:190:LEU:HD22	1:A:209:GLU:HB3	1.86	0.58
2:B:160:LEU:N	2:B:160:LEU:HD23	2.18	0.58
2:B:210:ILE:CD1	2:B:495:CYS:CB	2.82	0.58
1:E:77:CYS:HB3	1:E:109:VAL:CG2	2.33	0.58
2:F:381:TRP:CG	2:F:382:LEU:N	2.71	0.58
2:F:421:ILE:HD11	2:F:449:PHE:CZ	2.39	0.58
2:G:487:HIS:HD2	2:G:517:LEU:HD23	1.69	0.58
1:H:132:LEU:HD23	1:H:142:VAL:HG13	1.86	0.58
2:C:400:GLU:HG3	2:C:425:TYR:CZ	2.39	0.58
1:D:132:LEU:HD23	1:D:142:VAL:HG13	1.86	0.58
1:E:109:VAL:HG12	1:E:120:LEU:HD11	1.86	0.58
2:G:175:LEU:HG	2:G:483:PHE:HD2	1.69	0.58
1:H:287:THR:HA	1:H:301:SER:HB3	1.86	0.58
1:H:291:GLU:HG3	1:H:291:GLU:O	2.01	0.58
1:A:16:ILE:HG22	1:A:17:HIS:N	2.19	0.57
1:D:16:ILE:HG22	1:D:17:HIS:N	2.19	0.57
1:E:208:LEU:HB3	1:E:243:TRP:CH2	2.38	0.57
2:F:262:LYS:O	2:F:265:HIS:N	2.36	0.57
2:G:351:ASP:HB2	2:G:354:ILE:HG13	1.86	0.57
2:C:492:PHE:CD1	2:C:492:PHE:C	2.77	0.57
1:D:193:LEU:N	1:D:193:LEU:CD2	2.68	0.57
2:G:291:ILE:HG22	2:G:353:ASN:HB3	1.86	0.57
2:G:207:TYR:CD2	2:G:504:GLU:HA	2.39	0.57
2:G:551:TYR:HD1	1:H:27:ARG:NE	1.99	0.57
1:H:23:TYR:CD2	1:H:68:PRO:HG3	2.39	0.57
2:B:532:ILE:HG23	2:B:533:PRO:HD2	1.84	0.57
1:E:286:VAL:O	1:E:303:VAL:HG23	2.05	0.57
2:F:464:VAL:HG23	2:F:464:VAL:O	2.04	0.57
1:A:17:HIS:ND1	2:B:148:TYR:HE2	2.03	0.57
1:A:208:LEU:HB3	1:A:243:TRP:CH2	2.39	0.57
1:D:42:VAL:HG12	1:D:42:VAL:O	2.05	0.57
1:E:16:ILE:HG22	1:E:17:HIS:N	2.18	0.57
2:F:215:LEU:O	2:F:456:THR:HG23	2.04	0.57
2:G:202:ARG:NH2	2:G:209:GLN:HB3	2.20	0.57
2:G:294:ILE:CG1	2:G:309:LEU:HD23	2.31	0.57
1:H:16:ILE:HG22	1:H:17:HIS:N	2.19	0.57
2:B:280:ILE:HG13	2:B:300:LEU:HD21	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:289:ASN:O	2:C:292:GLU:N	2.37	0.57
1:D:23:TYR:CD2	1:D:68:PRO:HG3	2.39	0.57
1:E:109:VAL:CG1	1:E:120:LEU:HD11	2.35	0.57
2:F:177:THR:OG1	2:F:483:PHE:HB2	2.05	0.57
2:F:339:GLN:O	2:F:343:TRP:HD1	1.87	0.57
2:G:210:ILE:HD13	2:G:496:PHE:CD1	2.39	0.57
2:C:149:THR:CG2	2:C:162:LYS:HG2	2.35	0.57
2:F:351:ASP:HB2	2:F:354:ILE:HG13	1.86	0.57
2:G:446:ASP:O	2:G:449:PHE:N	2.36	0.57
1:A:70:TYR:CD1	1:A:70:TYR:N	2.72	0.57
2:B:246:TYR:CG	2:B:247:PRO:HD2	2.40	0.57
2:B:262:LYS:O	2:B:265:HIS:N	2.36	0.57
1:E:132:LEU:HD23	1:E:142:VAL:HG13	1.86	0.57
1:E:193:LEU:N	1:E:193:LEU:CD2	2.67	0.57
2:F:267:ARG:NH1	2:F:267:ARG:HG3	2.15	0.57
1:A:132:LEU:HD23	1:A:142:VAL:HG13	1.86	0.57
2:C:198:THR:HG22	2:C:211:SER:HB3	1.84	0.57
2:C:371:SER:OG	2:C:373:LYS:HG3	2.05	0.57
1:A:258:LEU:HD13	1:A:297:TRP:CB	2.35	0.57
1:E:41:ASP:OD1	1:E:41:ASP:C	2.43	0.57
1:H:292:SER:C	1:H:294:ASP:H	2.08	0.57
1:H:29:ALA:HB2	1:H:39:ILE:HD12	1.85	0.57
1:A:113:PRO:HB2	1:A:161:ALA:HB2	1.86	0.57
2:C:201:ALA:HB2	2:C:531:LYS:HE2	1.87	0.57
2:C:464:VAL:HG23	2:C:464:VAL:O	2.04	0.57
1:D:109:VAL:CG1	1:D:120:LEU:HD11	2.35	0.57
2:G:149:THR:CG2	2:G:150:PHE:H	2.18	0.57
1:A:23:TYR:CD2	1:A:68:PRO:HG3	2.39	0.56
2:B:190:LEU:O	2:B:194:ILE:HG13	2.05	0.56
2:C:149:THR:CG2	2:C:150:PHE:H	2.18	0.56
2:C:190:LEU:O	2:C:194:ILE:HG13	2.05	0.56
2:C:451:TRP:CZ2	2:C:493:VAL:HG13	2.39	0.56
2:F:371:SER:OG	2:F:373:LYS:HG3	2.05	0.56
2:G:371:SER:OG	2:G:373:LYS:HG3	2.05	0.56
1:H:193:LEU:CD2	1:H:193:LEU:N	2.68	0.56
2:B:351:ASP:HB2	2:B:354:ILE:HG13	1.86	0.56
2:C:194:ILE:HG12	2:C:492:PHE:HE2	1.69	0.56
2:F:284:ILE:HD13	2:F:297:TYR:CE1	2.40	0.56
2:G:280:ILE:CG1	2:G:300:LEU:HD21	2.35	0.56
2:G:332:ILE:HD12	2:G:332:ILE:N	2.21	0.56
2:G:532:ILE:HG23	2:G:533:PRO:HD2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:109:VAL:HG12	1:H:120:LEU:HD11	1.88	0.56
1:H:150:THR:HB	1:H:188:ASP:HB3	1.86	0.56
2:B:233:LEU:HD13	2:B:417:PRO:HB2	1.87	0.56
1:D:70:TYR:CD1	1:D:70:TYR:N	2.72	0.56
1:E:151:ILE:O	1:E:151:ILE:HG22	2.06	0.56
1:E:35:ARG:HD3	1:E:56:HIS:O	2.05	0.56
2:F:151:ALA:HB1	2:F:159:LEU:CD1	2.33	0.56
2:G:339:GLN:O	2:G:343:TRP:HD1	1.87	0.56
1:A:35:ARG:HD3	1:A:56:HIS:O	2.05	0.56
2:C:339:GLN:O	2:C:343:TRP:HD1	1.87	0.56
2:C:381:TRP:CE3	2:C:412:LEU:HD21	2.40	0.56
1:D:80:ASP:OD2	1:D:82:LYS:HB2	2.05	0.56
2:F:352:LYS:O	2:F:356:LYS:HG3	2.05	0.56
1:H:234:CYS:SG	1:H:268:VAL:HG23	2.45	0.56
1:A:80:ASP:OD2	1:A:82:LYS:HB2	2.05	0.56
2:C:284:ILE:HD13	2:C:297:TYR:HE1	1.68	0.56
1:D:35:ARG:HD3	1:D:56:HIS:O	2.05	0.56
2:F:280:ILE:HB	2:F:300:LEU:HD21	1.85	0.56
2:F:332:ILE:N	2:F:332:ILE:HD12	2.21	0.56
2:F:392:GLY:C	2:F:394:ILE:H	2.08	0.56
2:G:262:LYS:O	2:G:265:HIS:N	2.37	0.56
1:H:35:ARG:HD3	1:H:56:HIS:O	2.05	0.56
1:H:80:ASP:OD2	1:H:82:LYS:HB2	2.06	0.56
1:D:151:ILE:HG22	1:D:151:ILE:O	2.06	0.56
2:B:321:LEU:HD23	2:B:321:LEU:N	2.20	0.56
2:B:431:THR:OG1	2:B:463:ARG:HG2	2.06	0.56
2:B:177:THR:OG1	2:B:483:PHE:HB3	2.06	0.56
2:C:267:ARG:HG3	2:C:267:ARG:NH1	2.14	0.56
1:D:112:ALA:HB2	1:D:158:TRP:CZ2	2.41	0.56
2:C:162:LYS:NZ	1:D:15:MET:HE1	2.18	0.56
1:H:232:ALA:HB2	1:H:270:TRP:CZ2	2.41	0.56
2:B:339:GLN:O	2:B:343:TRP:HD1	1.87	0.56
2:C:202:ARG:NH2	2:C:209:GLN:HB3	2.20	0.56
2:F:160:LEU:N	2:F:160:LEU:HD23	2.18	0.56
2:F:181:ARG:HD2	2:F:448:GLN:OE1	2.05	0.56
2:G:352:LYS:O	2:G:356:LYS:HG3	2.06	0.56
1:H:109:VAL:CG1	1:H:120:LEU:HD11	2.36	0.56
1:E:80:ASP:OD2	1:E:82:LYS:HB2	2.05	0.56
2:G:162:LYS:NZ	1:H:15:MET:CE	2.68	0.56
2:G:495:CYS:O	2:G:497:LEU:N	2.38	0.56
1:A:304:ASN:OD1	2:B:161:THR:HG21	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:448:GLN:HB2	2:B:477:PHE:CE1	2.41	0.56
2:C:352:LYS:O	2:C:356:LYS:HG3	2.05	0.56
1:E:112:ALA:HB2	1:E:158:TRP:CZ2	2.41	0.56
2:G:224:MET:HE2	2:G:230:ASP:HB3	1.88	0.56
2:G:321:LEU:N	2:G:321:LEU:HD23	2.20	0.56
1:H:70:TYR:HE2	1:H:118:LEU:HB2	1.64	0.56
1:A:190:LEU:HD13	1:A:207:LYS:HD3	1.88	0.56
2:B:179:LEU:HD11	2:B:184:LEU:HD13	1.87	0.56
2:B:197:VAL:CG1	2:B:198:THR:H	2.19	0.56
2:B:371:SER:OG	2:B:373:LYS:HG3	2.05	0.56
1:E:31:CYS:HB2	1:E:60:VAL:HB	1.88	0.56
2:F:156:GLY:O	2:F:157:SER:CB	2.54	0.56
2:F:202:ARG:NH2	2:F:209:GLN:HB3	2.20	0.56
2:G:190:LEU:O	2:G:194:ILE:HG13	2.05	0.56
1:H:290:LYS:HB3	1:H:300:ILE:HD11	1.87	0.56
2:C:321:LEU:N	2:C:321:LEU:HD23	2.20	0.55
2:F:190:LEU:O	2:F:194:ILE:HG13	2.05	0.55
2:G:451:TRP:CD1	2:G:474:THR:HA	2.41	0.55
1:A:112:ALA:HB2	1:A:158:TRP:CZ2	2.41	0.55
2:B:202:ARG:NH2	2:B:209:GLN:HB3	2.20	0.55
2:B:332:ILE:N	2:B:332:ILE:HD12	2.20	0.55
2:B:210:ILE:HD12	2:B:495:CYS:HB3	1.89	0.55
2:F:321:LEU:HD23	2:F:321:LEU:N	2.21	0.55
2:F:343:TRP:HE3	2:F:350:ILE:HD13	1.69	0.55
1:H:151:ILE:O	1:H:151:ILE:HG22	2.06	0.55
1:A:109:VAL:CG1	1:A:120:LEU:HD11	2.35	0.55
1:A:151:ILE:HG22	1:A:151:ILE:O	2.06	0.55
1:A:273:THR:HG21	2:B:479:ALA:HB2	1.87	0.55
1:A:31:CYS:HB2	1:A:60:VAL:HB	1.89	0.55
2:B:352:LYS:O	2:B:356:LYS:HG3	2.05	0.55
1:D:49:LEU:HD12	1:D:50:ILE:N	2.17	0.55
1:E:42:VAL:O	1:E:42:VAL:HG12	2.05	0.55
1:H:112:ALA:HB2	1:H:158:TRP:CZ2	2.41	0.55
1:D:31:CYS:HB2	1:D:60:VAL:HB	1.88	0.55
2:G:224:MET:HE1	2:G:230:ASP:HB3	1.88	0.55
1:A:304:ASN:HA	2:B:173:LYS:NZ	2.22	0.55
2:C:512:MET:HA	2:C:540:ALA:CB	2.37	0.55
1:D:29:ALA:CB	1:D:39:ILE:HD13	2.36	0.55
1:E:289:TRP:HA	1:E:298:VAL:O	2.06	0.55
2:G:149:THR:CG2	2:G:162:LYS:HG2	2.34	0.55
2:G:190:LEU:HB2	2:G:489:HIS:CE1	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:197:VAL:CG1	2:F:198:THR:H	2.19	0.55
2:F:268:LEU:HD21	2:F:272:ILE:HD11	1.88	0.55
2:B:224:MET:HE1	2:B:230:ASP:HB3	1.86	0.55
1:D:109:VAL:HG12	1:D:120:LEU:HD11	1.87	0.55
1:E:113:PRO:CB	1:E:161:ALA:HB2	2.36	0.55
1:E:207:LYS:O	1:E:208:LEU:HD23	2.07	0.55
2:F:491:LEU:HD21	2:F:532:ILE:HD11	1.88	0.55
1:A:109:VAL:HG12	1:A:120:LEU:HD11	1.87	0.55
2:C:154:SER:HB2	1:D:21:MET:HB3	1.88	0.55
2:F:462:THR:O	2:F:463:ARG:HD3	2.07	0.55
2:G:512:MET:SD	2:G:540:ALA:CB	2.95	0.55
2:C:210:ILE:HG22	2:C:459:PHE:CE2	2.41	0.55
2:C:332:ILE:N	2:C:332:ILE:HD12	2.21	0.55
2:G:197:VAL:CG1	2:G:198:THR:H	2.19	0.55
1:H:242:ILE:HD11	1:H:258:LEU:HD22	1.89	0.55
1:A:250:SER:O	1:A:252:THR:N	2.35	0.55
2:B:151:ALA:HB1	2:B:159:LEU:CD1	2.33	0.55
2:B:268:LEU:HD21	2:B:272:ILE:HD11	1.89	0.55
2:C:268:LEU:HD21	2:C:272:ILE:HD11	1.89	0.55
2:C:375:LEU:HB3	2:C:379:PHE:HD2	1.71	0.55
2:C:375:LEU:HB2	2:C:384:LEU:HD21	1.88	0.55
1:D:207:LYS:O	1:D:208:LEU:HD23	2.07	0.55
2:F:381:TRP:CZ2	2:F:382:LEU:HD13	2.42	0.55
2:B:512:MET:SD	2:B:540:ALA:HB2	2.46	0.54
2:C:207:TYR:CD2	2:C:504:GLU:HA	2.43	0.54
1:D:190:LEU:HD13	1:D:207:LYS:HD3	1.89	0.54
1:E:145:ILE:HD13	1:E:194:TRP:CE3	2.43	0.54
2:G:267:ARG:CG	2:G:267:ARG:HH11	2.10	0.54
2:G:268:LEU:HD21	2:G:272:ILE:HD11	1.89	0.54
1:D:79:TYR:HD1	1:D:105:SER:HB3	1.72	0.54
2:G:343:TRP:CZ3	2:G:350:ILE:HG21	2.42	0.54
1:A:265:VAL:HA	1:A:281:GLY:HA3	1.89	0.54
2:B:156:GLY:O	2:B:157:SER:CB	2.55	0.54
1:D:190:LEU:HD22	1:D:209:GLU:HB3	1.90	0.54
1:E:242:ILE:HD13	1:E:297:TRP:CD1	2.43	0.54
1:A:207:LYS:O	1:A:208:LEU:HD23	2.07	0.54
2:B:484:ALA:O	2:B:485:GLN:HB3	2.07	0.54
2:F:280:ILE:CG1	2:F:300:LEU:HD21	2.37	0.54
2:F:491:LEU:O	2:F:494:SER:HB2	2.08	0.54
2:G:242:ASP:O	2:G:264:ARG:NH2	2.40	0.54
2:B:477:PHE:CE2	2:B:493:VAL:HG21	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:194:ILE:HG12	2:C:492:PHE:CD2	2.42	0.54
2:C:451:TRP:HE1	2:C:474:THR:HG23	1.73	0.54
1:D:60:VAL:HG13	1:D:77:CYS:O	2.08	0.54
2:G:210:ILE:HD13	2:G:496:PHE:CG	2.42	0.54
1:H:265:VAL:HA	1:H:281:GLY:HA3	1.89	0.54
1:H:31:CYS:HB2	1:H:60:VAL:HB	1.88	0.54
2:C:138:ILE:HG22	2:C:139:MET:N	2.23	0.54
1:D:41:ASP:OD1	1:D:41:ASP:C	2.46	0.54
1:E:304:ASN:OD1	2:F:161:THR:HG21	2.08	0.54
1:E:60:VAL:HG13	1:E:77:CYS:O	2.08	0.54
2:G:382:LEU:HD12	2:G:385:LEU:HD23	1.90	0.54
1:H:291:GLU:HB3	1:H:297:TRP:CD2	2.42	0.54
2:C:267:ARG:NH1	2:C:267:ARG:CG	2.71	0.54
2:C:482:GLU:CD	2:C:509:ARG:HH22	2.11	0.54
2:F:512:MET:HA	2:F:540:ALA:HB1	1.90	0.54
2:G:170:VAL:H	1:H:47:GLN:HE22	1.55	0.54
2:G:284:ILE:HG12	2:G:296:LEU:CD1	2.37	0.54
2:G:367:GLU:O	2:G:367:GLU:HG3	2.08	0.54
1:A:56:HIS:NE2	1:A:84:ILE:HD12	2.22	0.54
2:B:145:THR:HG22	2:B:146:ALA:N	2.23	0.54
1:D:265:VAL:HA	1:D:281:GLY:HA3	1.89	0.54
1:D:67:HIS:ND1	1:D:69:MET:HB3	2.23	0.54
1:D:82:LYS:HG2	1:D:100:ALA:CB	2.35	0.54
1:E:70:TYR:HE2	1:E:118:LEU:HB2	1.64	0.54
1:E:67:HIS:ND1	1:E:69:MET:HB3	2.23	0.54
2:F:145:THR:HG22	2:F:146:ALA:N	2.23	0.54
2:F:379:PHE:CD1	2:F:379:PHE:N	2.75	0.54
2:F:375:LEU:HB2	2:F:384:LEU:HD21	1.90	0.54
1:H:60:VAL:HG13	1:H:77:CYS:O	2.07	0.54
1:A:67:HIS:ND1	1:A:69:MET:HB3	2.23	0.54
2:B:382:LEU:HD12	2:B:385:LEU:HD23	1.90	0.54
2:F:236:LEU:HD21	2:F:422:PHE:CE1	2.43	0.54
1:H:79:TYR:HD1	1:H:105:SER:HB3	1.72	0.54
1:A:102:HIS:HE2	1:A:130:SER:CB	2.21	0.54
2:B:177:THR:OG1	2:B:483:PHE:CB	2.56	0.54
2:B:201:ALA:H	2:B:531:LYS:NZ	1.96	0.54
2:C:197:VAL:CG1	2:C:198:THR:H	2.19	0.54
2:C:366:PHE:CZ	2:C:384:LEU:HD22	2.42	0.54
2:C:236:LEU:HD21	2:C:422:PHE:CE1	2.42	0.54
2:C:428:ASN:HA	2:C:463:ARG:HH12	1.73	0.54
2:G:244:VAL:HG12	2:G:263:GLU:OE2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:ILE:HG21	1:A:181:ARG:NE	2.23	0.53
1:A:82:LYS:HG2	1:A:100:ALA:CB	2.34	0.53
1:A:60:VAL:HG13	1:A:77:CYS:O	2.07	0.53
2:G:241:PHE:CD2	2:G:457:LEU:HD21	2.43	0.53
1:H:113:PRO:CB	1:H:161:ALA:HB2	2.38	0.53
1:A:49:LEU:HD12	1:A:50:ILE:N	2.16	0.53
2:B:159:LEU:HD12	2:B:160:LEU:H	1.74	0.53
2:C:142:ARG:HG3	1:D:61:TRP:CZ2	2.44	0.53
1:E:205:GLU:HG2	1:E:251:ASN:ND2	2.22	0.53
2:G:487:HIS:HA	2:G:490:SER:HB2	1.91	0.53
2:G:495:CYS:C	2:G:497:LEU:H	2.11	0.53
1:H:207:LYS:O	1:H:208:LEU:HD23	2.07	0.53
1:H:56:HIS:NE2	1:H:84:ILE:HD12	2.23	0.53
1:A:145:ILE:HD13	1:A:194:TRP:CZ3	2.43	0.53
2:F:174:ARG:HG2	2:F:175:LEU:H	1.74	0.53
1:A:291:GLU:N	1:A:297:TRP:CE3	2.77	0.53
2:B:291:ILE:HG22	2:B:353:ASN:HB2	1.90	0.53
1:D:245:CYS:SG	1:D:251:ASN:HB2	2.48	0.53
1:E:273:THR:HG21	2:F:479:ALA:HB2	1.89	0.53
2:F:272:ILE:HG23	2:F:382:LEU:HG	1.90	0.53
1:A:145:ILE:O	1:A:145:ILE:HG22	2.08	0.53
2:B:236:LEU:HD21	2:B:422:PHE:CE1	2.44	0.53
2:C:515:ILE:HD12	2:C:541:GLN:N	2.24	0.53
1:D:242:ILE:HD11	1:D:258:LEU:HB2	1.89	0.53
1:D:38:LYS:HB2	1:D:40:PHE:HE1	1.73	0.53
2:G:138:ILE:HG22	2:G:139:MET:N	2.22	0.53
1:H:78:SER:HB3	1:H:80:ASP:OD1	2.09	0.53
2:B:175:LEU:HD23	2:B:483:PHE:CE2	2.44	0.53
2:C:208:PRO:HG3	2:C:530:LEU:O	2.08	0.53
2:F:382:LEU:HD12	2:F:385:LEU:HD23	1.90	0.53
1:H:82:LYS:HG2	1:H:100:ALA:CB	2.34	0.53
1:D:263:ASP:HB3	1:D:282:GLY:HA2	1.91	0.53
2:B:291:ILE:HG22	2:B:353:ASN:CB	2.39	0.53
2:C:404:GLN:HG2	2:C:426:ALA:HB1	1.90	0.53
1:E:29:ALA:CB	1:E:39:ILE:HD13	2.39	0.53
1:E:56:HIS:NE2	1:E:84:ILE:HD12	2.23	0.53
1:H:145:ILE:HG22	1:H:145:ILE:O	2.08	0.53
1:H:67:HIS:ND1	1:H:69:MET:HB3	2.23	0.53
2:B:210:ILE:HD12	2:B:495:CYS:CB	2.39	0.52
2:B:331:ARG:HB2	2:B:332:ILE:HD12	1.91	0.52
2:C:149:THR:CG2	2:C:150:PHE:N	2.72	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:280:ILE:HB	2:C:300:LEU:HD21	1.91	0.52
2:C:382:LEU:HD12	2:C:385:LEU:HD23	1.90	0.52
2:C:236:LEU:HD22	2:C:418:ILE:HG22	1.89	0.52
1:D:56:HIS:NE2	1:D:84:ILE:HD12	2.24	0.52
1:E:145:ILE:HG22	1:E:145:ILE:O	2.08	0.52
1:E:243:TRP:CD1	1:E:243:TRP:N	2.76	0.52
1:E:276:ILE:CG2	1:E:300:ILE:HD11	2.38	0.52
1:E:38:LYS:HB2	1:E:40:PHE:HE1	1.73	0.52
1:E:67:HIS:O	1:E:69:MET:N	2.42	0.52
2:F:155:THR:O	2:F:513:ARG:NH1	2.39	0.52
1:H:49:LEU:HD12	1:H:50:ILE:N	2.16	0.52
1:A:78:SER:HB3	1:A:80:ASP:OD1	2.09	0.52
2:F:284:ILE:HG12	2:F:296:LEU:CD1	2.38	0.52
2:F:272:ILE:CG2	2:F:382:LEU:HG	2.39	0.52
1:H:102:HIS:HE2	1:H:130:SER:CB	2.21	0.52
1:H:292:SER:C	1:H:294:ASP:N	2.62	0.52
2:B:224:MET:HE2	2:B:230:ASP:HB3	1.90	0.52
2:B:359:LYS:HZ1	2:B:370:PHE:H	1.57	0.52
1:D:197:GLU:O	1:D:198:GLU:HB2	2.08	0.52
1:E:79:TYR:HD1	1:E:105:SER:HB3	1.73	0.52
1:E:263:ASP:HB3	1:E:282:GLY:HA2	1.91	0.52
2:F:302:ASP:HA	2:G:304:VAL:HG21	1.92	0.52
2:G:162:LYS:HZ3	1:H:15:MET:CE	2.22	0.52
2:C:367:GLU:O	2:C:367:GLU:HG3	2.08	0.52
1:D:290:LYS:CB	1:D:300:ILE:HD11	2.36	0.52
1:E:265:VAL:HA	1:E:281:GLY:HA3	1.90	0.52
1:A:39:ILE:HD11	1:A:74:LEU:HD22	1.90	0.52
1:A:79:TYR:HD1	1:A:105:SER:HB3	1.72	0.52
2:C:170:VAL:H	1:D:47:GLN:HE22	1.58	0.52
1:D:67:HIS:O	1:D:69:MET:N	2.43	0.52
1:E:264:VAL:HG12	1:E:265:VAL:N	2.25	0.52
2:F:302:ASP:OD1	2:F:305:ARG:HB2	2.10	0.52
1:H:38:LYS:HB2	1:H:40:PHE:HE1	1.73	0.52
1:H:29:ALA:HA	1:H:39:ILE:HD13	1.91	0.52
1:A:234:CYS:HB2	1:A:265:VAL:HB	1.91	0.52
2:B:174:ARG:HG2	2:B:175:LEU:H	1.74	0.52
1:E:292:SER:C	1:E:294:ASP:H	2.13	0.52
2:F:367:GLU:HG3	2:F:367:GLU:O	2.08	0.52
1:H:263:ASP:HB3	1:H:282:GLY:HA2	1.91	0.52
1:A:220:TRP:CH2	1:A:229:SER:HB2	2.45	0.52
2:B:181:ARG:HD2	2:B:448:GLN:OE1	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:145:ILE:O	1:D:145:ILE:HG22	2.09	0.52
2:F:175:LEU:HD23	2:F:483:PHE:CE2	2.44	0.52
1:H:258:LEU:CD1	1:H:297:TRP:HB2	2.40	0.52
1:H:29:ALA:CB	1:H:39:ILE:HD13	2.39	0.52
1:A:28:LEU:HD13	2:B:172:ILE:HD11	1.92	0.52
2:B:471:ASP:OD1	2:B:497:LEU:HA	2.10	0.52
2:C:375:LEU:HB3	2:C:379:PHE:CD2	2.44	0.52
1:E:220:TRP:CH2	1:E:229:SER:HB2	2.45	0.52
1:E:78:SER:HB3	1:E:80:ASP:OD1	2.09	0.52
2:F:304:VAL:HG21	2:G:302:ASP:HA	1.92	0.52
1:H:109:VAL:HG12	1:H:110:CYS:N	2.25	0.52
2:B:367:GLU:HG3	2:B:367:GLU:O	2.08	0.52
1:E:273:THR:CG2	2:F:479:ALA:CB	2.85	0.52
1:E:273:THR:CG2	2:F:479:ALA:HB2	2.40	0.52
2:G:372:LEU:O	2:G:375:LEU:HG	2.10	0.52
1:A:67:HIS:O	1:A:69:MET:N	2.43	0.52
2:B:372:LEU:O	2:B:375:LEU:HG	2.10	0.52
2:B:421:ILE:HD11	2:B:449:PHE:CZ	2.44	0.52
1:D:220:TRP:CH2	1:D:229:SER:HB2	2.45	0.52
1:D:292:SER:C	1:D:294:ASP:H	2.13	0.52
1:E:29:ALA:HA	1:E:39:ILE:HD13	1.91	0.52
2:F:372:LEU:O	2:F:375:LEU:HG	2.10	0.52
2:F:412:LEU:HD12	2:F:412:LEU:H	1.75	0.52
2:F:236:LEU:HD23	2:F:421:ILE:HG21	1.92	0.52
2:G:148:TYR:HB2	1:H:266:TRP:CD2	2.44	0.52
2:G:175:LEU:HD12	2:G:176:PRO:N	2.24	0.52
2:G:412:LEU:N	2:G:412:LEU:CD1	2.71	0.52
2:G:420:VAL:HG11	2:G:445:LEU:HD11	1.92	0.52
1:H:67:HIS:O	1:H:69:MET:N	2.43	0.52
2:C:175:LEU:HD12	2:C:176:PRO:N	2.24	0.51
2:C:242:ASP:O	2:C:264:ARG:NH2	2.42	0.51
1:D:151:ILE:HB	1:D:187:CYS:CB	2.38	0.51
1:D:78:SER:HB3	1:D:80:ASP:OD1	2.09	0.51
1:E:28:LEU:HD13	2:F:172:ILE:HD11	1.92	0.51
2:G:138:ILE:HD11	1:H:79:TYR:CD2	2.45	0.51
2:C:340:LEU:HD21	2:C:358:TYR:HB3	1.92	0.51
1:H:23:TYR:CD2	1:H:24:TYR:CD1	2.97	0.51
1:A:263:ASP:HB3	1:A:282:GLY:HA2	1.91	0.51
1:A:264:VAL:HG12	1:A:265:VAL:N	2.25	0.51
2:C:522:THR:HG21	2:C:526:ILE:CD1	2.41	0.51
1:D:110:CYS:O	1:D:120:LEU:HD12	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:210:ILE:HG22	2:G:459:PHE:CE2	2.45	0.51
2:G:487:HIS:O	2:G:488:GLY:C	2.47	0.51
1:H:268:VAL:HG13	1:H:277:LEU:HD11	1.93	0.51
1:D:290:LYS:HB2	1:D:300:ILE:HD12	1.93	0.51
1:E:110:CYS:O	1:E:120:LEU:HD12	2.10	0.51
1:H:264:VAL:HG12	1:H:265:VAL:N	2.25	0.51
1:A:258:LEU:CD1	1:A:297:TRP:CB	2.89	0.51
1:D:102:HIS:HE2	1:D:130:SER:CB	2.22	0.51
1:D:109:VAL:HG12	1:D:110:CYS:N	2.25	0.51
2:C:551:TYR:HD1	1:D:27:ARG:HE	1.57	0.51
1:E:234:CYS:HB2	1:E:265:VAL:HB	1.93	0.51
2:F:548:GLU:O	2:F:552:LEU:HG	2.10	0.51
2:G:385:LEU:HD21	2:G:422:PHE:CE2	2.45	0.51
1:H:157:SER:HB2	1:H:218:VAL:O	2.11	0.51
2:B:400:GLU:HG3	2:B:425:TYR:CZ	2.46	0.51
2:C:449:PHE:O	2:C:450:CYS:C	2.49	0.51
2:F:210:ILE:CD1	2:F:495:CYS:HB2	2.40	0.51
2:G:175:LEU:CD1	2:G:176:PRO:CD	2.88	0.51
2:G:236:LEU:HD21	2:G:422:PHE:CE1	2.46	0.51
2:F:320:VAL:HG22	2:G:263:GLU:HA	1.92	0.51
2:G:366:PHE:CZ	2:G:387:LEU:HD12	2.46	0.51
1:A:292:SER:C	1:A:294:ASP:H	2.13	0.51
2:B:475:PHE:CE2	2:B:497:LEU:HD21	2.46	0.51
2:C:170:VAL:CG1	2:C:171:SER:N	2.74	0.51
2:C:475:PHE:HE2	2:C:497:LEU:HD11	1.74	0.51
1:E:41:ASP:HB2	1:E:50:ILE:CD1	2.33	0.51
2:C:175:LEU:CD1	2:C:176:PRO:CD	2.88	0.51
1:D:179:ILE:HG21	1:D:181:ARG:NE	2.23	0.51
1:D:23:TYR:CD2	1:D:24:TYR:CD1	2.98	0.51
1:E:109:VAL:HG12	1:E:110:CYS:N	2.26	0.51
1:E:17:HIS:ND1	2:F:148:TYR:CE2	2.76	0.51
2:F:331:ARG:HB2	2:F:332:ILE:HD12	1.91	0.51
1:H:220:TRP:CH2	1:H:229:SER:HB2	2.45	0.51
2:C:216:LEU:HD13	2:C:243:PRO:HD2	1.93	0.51
2:C:385:LEU:HA	2:C:406:HIS:CE1	2.46	0.51
2:F:179:LEU:HD11	2:F:184:LEU:HD13	1.91	0.51
2:F:196:LYS:HD2	2:F:214:SER:O	2.11	0.51
2:G:331:ARG:HB2	2:G:332:ILE:HD12	1.92	0.51
2:G:462:THR:O	2:G:463:ARG:CD	2.53	0.51
1:H:179:ILE:HG21	1:H:181:ARG:NE	2.23	0.51
1:A:109:VAL:HG12	1:A:110:CYS:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:LYS:HB2	1:A:40:PHE:HE1	1.74	0.51
1:A:98:GLU:HG2	1:A:99:HIS:N	2.26	0.51
2:C:366:PHE:CE2	2:C:384:LEU:HD22	2.46	0.51
2:C:479:ALA:CB	1:D:273:THR:HG22	2.35	0.51
2:C:210:ILE:HD13	2:C:496:PHE:CG	2.46	0.51
2:C:199:ILE:HD12	2:C:530:LEU:HA	1.92	0.51
1:D:111:TRP:CD2	1:D:120:LEU:HD13	2.47	0.51
2:F:398:SER:OG	2:F:401:SER:HB3	2.11	0.51
2:G:267:ARG:CG	2:G:267:ARG:NH1	2.71	0.51
1:A:110:CYS:O	1:A:120:LEU:HD12	2.10	0.50
1:A:185:GLY:HA3	1:A:215:VAL:HG11	1.91	0.50
1:A:268:VAL:HG13	1:A:277:LEU:HD11	1.93	0.50
1:A:28:LEU:CD2	2:B:170:VAL:HG11	2.35	0.50
2:B:196:LYS:HD2	2:B:214:SER:O	2.11	0.50
2:C:457:LEU:HD13	2:C:463:ARG:HG3	1.93	0.50
1:D:264:VAL:HG12	1:D:265:VAL:N	2.25	0.50
2:F:434:LEU:O	2:F:438:VAL:HG23	2.11	0.50
2:F:482:GLU:CD	2:F:509:ARG:HH22	2.14	0.50
2:G:170:VAL:CG1	2:G:171:SER:N	2.74	0.50
2:G:191:ASP:OD1	2:G:529:ARG:NH1	2.44	0.50
1:A:230:THR:CG2	1:A:242:ILE:HG22	2.42	0.50
2:B:208:PRO:HB3	2:B:531:LYS:HB3	1.93	0.50
2:C:153:PHE:CE2	1:D:278:ALA:HB2	2.46	0.50
2:C:431:THR:HG21	2:C:463:ARG:HB3	1.93	0.50
2:C:471:ASP:OD2	2:C:498:ASN:ND2	2.44	0.50
1:E:111:TRP:CD2	1:E:120:LEU:HD13	2.46	0.50
1:E:92:THR:HG22	1:E:94:GLU:HG3	1.93	0.50
2:F:347:GLY:O	2:F:350:ILE:HD12	2.12	0.50
1:H:16:ILE:HD12	1:H:30:THR:CG2	2.41	0.50
1:A:111:TRP:CD2	1:A:120:LEU:HD13	2.46	0.50
2:C:276:ILE:HD13	2:C:383:CYS:CA	2.38	0.50
2:C:372:LEU:O	2:C:375:LEU:HG	2.10	0.50
1:E:98:GLU:HG2	1:E:99:HIS:N	2.26	0.50
2:F:486:LEU:H	2:F:486:LEU:HD12	1.76	0.50
2:G:184:LEU:HD21	2:G:448:GLN:HE22	1.76	0.50
1:A:40:PHE:CZ	2:B:168:SER:CB	2.89	0.50
2:B:174:ARG:HG2	2:B:175:LEU:N	2.27	0.50
2:B:236:LEU:HD23	2:B:421:ILE:HG21	1.93	0.50
2:B:241:PHE:O	2:B:242:ASP:C	2.49	0.50
2:B:215:LEU:O	2:B:456:THR:HG23	2.11	0.50
2:B:477:PHE:HD2	2:B:493:VAL:HG11	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:142:ARG:NH2	1:D:107:ASN:OD1	2.44	0.50
2:G:196:LYS:HD2	2:G:214:SER:O	2.12	0.50
2:G:359:LYS:HZ1	2:G:370:PHE:H	1.58	0.50
1:H:98:GLU:HG2	1:H:99:HIS:N	2.27	0.50
2:B:255:VAL:HG12	2:B:256:LYS:N	2.27	0.50
2:C:331:ARG:HB2	2:C:332:ILE:HD12	1.91	0.50
1:E:102:HIS:HE2	1:E:130:SER:CB	2.21	0.50
2:F:159:LEU:HD12	2:F:160:LEU:H	1.74	0.50
2:G:409:LYS:C	2:G:410:PHE:CD2	2.85	0.50
2:G:474:THR:CG2	2:G:493:VAL:HG12	2.42	0.50
2:G:474:THR:HG23	2:G:493:VAL:HG12	1.93	0.50
1:H:111:TRP:CD2	1:H:120:LEU:HD13	2.46	0.50
1:A:16:ILE:HD12	1:A:30:THR:CG2	2.41	0.50
1:A:43:ARG:O	1:A:44:ASN:HB2	2.11	0.50
2:C:448:GLN:HB2	2:C:477:PHE:CE1	2.46	0.50
1:D:245:CYS:HB2	1:D:253:TRP:CE3	2.46	0.50
1:E:179:ILE:HG21	1:E:181:ARG:NE	2.23	0.50
2:F:451:TRP:HZ2	2:F:496:PHE:CD1	2.30	0.50
1:H:110:CYS:O	1:H:120:LEU:HD12	2.11	0.50
1:H:43:ARG:O	1:H:44:ASN:HB2	2.11	0.50
1:H:92:THR:HG22	1:H:94:GLU:HG3	1.93	0.50
1:A:49:LEU:CD1	1:A:50:ILE:H	2.20	0.50
2:B:215:LEU:HD22	2:B:452:TYR:OH	2.11	0.50
2:C:434:LEU:O	2:C:438:VAL:HG23	2.12	0.50
1:E:258:LEU:HD13	1:E:297:TRP:HB2	1.92	0.50
1:E:43:ARG:O	1:E:44:ASN:HB2	2.11	0.50
2:B:449:PHE:O	2:B:450:CYS:C	2.49	0.50
1:E:205:GLU:HG2	1:E:251:ASN:HD21	1.77	0.50
2:F:332:ILE:H	2:F:332:ILE:CD1	2.25	0.50
1:H:230:THR:HG21	1:H:242:ILE:HG23	1.92	0.50
2:B:434:LEU:O	2:B:438:VAL:HG23	2.11	0.50
2:C:409:LYS:C	2:C:410:PHE:CD2	2.85	0.50
2:C:184:LEU:O	2:C:486:LEU:HD13	2.12	0.50
1:D:98:GLU:HG2	1:D:99:HIS:N	2.26	0.50
1:E:23:TYR:CD2	1:E:24:TYR:CD1	2.98	0.50
2:F:255:VAL:HG12	2:F:256:LYS:N	2.27	0.50
2:G:175:LEU:HD12	2:G:176:PRO:CD	2.42	0.50
2:G:255:VAL:HG12	2:G:256:LYS:N	2.27	0.50
2:G:380:SER:OG	2:G:382:LEU:N	2.45	0.50
2:G:436:LYS:HE3	2:G:469:THR:OG1	2.12	0.50
2:B:267:ARG:CG	2:B:267:ARG:NH1	2.71	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:196:LYS:HD2	2:C:214:SER:O	2.12	0.49
2:C:477:PHE:CD2	2:C:493:VAL:HG21	2.47	0.49
2:C:479:ALA:HA	1:D:273:THR:HG21	1.94	0.49
2:F:224:MET:HE2	2:F:230:ASP:HB3	1.94	0.49
2:F:372:LEU:HD22	2:F:375:LEU:HD11	1.94	0.49
1:A:27:ARG:HE	2:B:551:TYR:HD1	1.60	0.49
1:A:30:THR:CG2	1:A:31:CYS:N	2.75	0.49
1:D:92:THR:HG22	1:D:94:GLU:HG3	1.93	0.49
1:E:16:ILE:HD12	1:E:30:THR:CG2	2.41	0.49
1:E:268:VAL:HG13	1:E:277:LEU:HD11	1.93	0.49
2:F:174:ARG:HG2	2:F:175:LEU:N	2.27	0.49
2:F:385:LEU:CA	2:F:406:HIS:CE1	2.95	0.49
2:F:449:PHE:O	2:F:450:CYS:C	2.49	0.49
2:B:244:VAL:HG23	2:B:264:ARG:NH2	2.24	0.49
2:B:409:LYS:C	2:B:410:PHE:CD2	2.86	0.49
2:C:255:VAL:HG12	2:C:256:LYS:N	2.27	0.49
2:C:332:ILE:CD1	2:C:332:ILE:H	2.25	0.49
1:D:241:PHE:CD2	1:D:257:LEU:HA	2.48	0.49
2:G:290:GLU:O	2:G:293:GLN:HB2	2.12	0.49
2:G:449:PHE:O	2:G:450:CYS:C	2.49	0.49
1:A:111:TRP:CE2	1:A:120:LEU:HD13	2.48	0.49
2:B:525:HIS:O	2:B:527:LEU:N	2.45	0.49
2:C:175:LEU:HD12	2:C:176:PRO:CD	2.42	0.49
1:E:242:ILE:HD11	1:E:258:LEU:HD22	1.94	0.49
2:F:409:LYS:C	2:F:410:PHE:CD2	2.86	0.49
2:F:404:GLN:CG	2:F:426:ALA:HB1	2.34	0.49
1:H:287:THR:HG22	1:H:299:CYS:SG	2.52	0.49
2:B:332:ILE:H	2:B:332:ILE:CD1	2.25	0.49
2:B:340:LEU:HD21	2:B:358:TYR:HB3	1.94	0.49
2:C:372:LEU:HD22	2:C:375:LEU:HD11	1.94	0.49
1:D:240:VAL:O	1:D:258:LEU:HB3	2.11	0.49
1:D:43:ARG:O	1:D:44:ASN:HB2	2.11	0.49
1:E:190:LEU:HD22	1:E:209:GLU:HB3	1.94	0.49
1:E:82:LYS:HG2	1:E:100:ALA:CB	2.34	0.49
2:F:217:PHE:HE2	2:F:449:PHE:CE1	2.31	0.49
2:F:475:PHE:CE2	2:F:497:LEU:HD21	2.44	0.49
2:G:170:VAL:CG1	2:G:171:SER:H	2.25	0.49
2:G:356:LYS:O	2:G:359:LYS:HB3	2.12	0.49
1:A:192:LYS:HD3	1:A:204:GLU:OE1	2.13	0.49
1:A:92:THR:HG22	1:A:94:GLU:HG3	1.93	0.49
2:B:290:GLU:O	2:B:293:GLN:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:548:GLU:O	2:B:552:LEU:HG	2.13	0.49
2:C:170:VAL:CG1	2:C:171:SER:H	2.25	0.49
2:C:252:ASN:OD1	2:C:253:ASP:N	2.46	0.49
1:D:157:SER:HB2	1:D:218:VAL:O	2.13	0.49
2:F:145:THR:C	2:F:147:SER:H	2.15	0.49
2:F:191:ASP:OD1	2:F:529:ARG:NH1	2.45	0.49
2:F:210:ILE:HG22	2:F:459:PHE:HE2	1.78	0.49
2:G:409:LYS:C	2:G:410:PHE:HD2	2.16	0.49
1:H:106:VAL:HA	1:H:124:SER:HA	1.94	0.49
2:B:515:ILE:HD12	2:B:541:GLN:N	2.26	0.49
2:C:280:ILE:HG13	2:C:300:LEU:CD2	2.37	0.49
2:C:356:LYS:O	2:C:359:LYS:HB3	2.13	0.49
1:D:242:ILE:HG12	1:D:297:TRP:NE1	2.28	0.49
1:D:16:ILE:HD12	1:D:30:THR:CG2	2.41	0.49
2:F:290:GLU:O	2:F:293:GLN:HB2	2.13	0.49
2:F:525:HIS:O	2:F:527:LEU:N	2.46	0.49
1:H:112:ALA:HA	1:H:158:TRP:CD2	2.48	0.49
2:G:152:LYS:NZ	1:H:62:GLN:HE21	2.11	0.49
1:A:157:SER:HB2	1:A:218:VAL:O	2.12	0.49
1:A:56:HIS:CE1	1:A:84:ILE:HD12	2.48	0.49
2:B:170:VAL:O	2:B:170:VAL:HG12	2.12	0.49
2:B:280:ILE:HD11	2:B:383:CYS:SG	2.53	0.49
2:C:224:MET:HE1	2:C:230:ASP:HB3	1.93	0.49
1:D:49:LEU:CD1	1:D:50:ILE:H	2.21	0.49
1:D:70:TYR:HD1	1:D:70:TYR:N	2.11	0.49
2:F:182:LYS:O	2:F:185:PHE:HD1	1.96	0.49
2:F:356:LYS:O	2:F:359:LYS:HB3	2.13	0.49
1:H:111:TRP:CE2	1:H:120:LEU:HD13	2.48	0.49
1:A:70:TYR:HD1	1:A:70:TYR:N	2.10	0.49
2:B:145:THR:C	2:B:147:SER:H	2.15	0.49
1:D:268:VAL:HG13	1:D:277:LEU:HD11	1.92	0.49
1:E:291:GLU:N	1:E:297:TRP:CE3	2.80	0.49
2:F:135:ALA:O	2:F:139:MET:HB3	2.12	0.49
2:G:267:ARG:HG3	2:G:267:ARG:NH1	2.14	0.49
2:B:140:LYS:C	2:B:142:ARG:H	2.16	0.49
2:B:236:LEU:HD22	2:B:418:ILE:HG22	1.95	0.49
2:C:145:THR:HG22	2:C:146:ALA:N	2.28	0.49
2:C:246:TYR:CD1	2:C:247:PRO:HD2	2.48	0.49
2:C:290:GLU:O	2:C:293:GLN:HB2	2.13	0.49
2:C:385:LEU:HD21	2:C:422:PHE:CE2	2.48	0.49
2:C:491:LEU:HD13	2:C:510:LEU:HD23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:164:PRO:CD	1:D:176:PRO:HB2	2.43	0.49
2:G:372:LEU:HD22	2:G:375:LEU:HD11	1.95	0.49
2:G:208:PRO:HG3	2:G:530:LEU:O	2.12	0.49
2:C:199:ILE:HG22	2:C:200:GLU:N	2.27	0.48
1:E:208:LEU:HD22	1:E:243:TRP:CZ3	2.48	0.48
1:E:28:LEU:HD11	2:F:160:LEU:CD1	2.40	0.48
2:G:145:THR:HG22	2:G:146:ALA:N	2.28	0.48
2:G:434:LEU:O	2:G:438:VAL:HG23	2.12	0.48
1:H:244:THR:CG2	1:H:245:CYS:H	2.23	0.48
1:H:49:LEU:CD1	1:H:50:ILE:H	2.20	0.48
1:H:70:TYR:HD1	1:H:70:TYR:N	2.11	0.48
2:B:135:ALA:O	2:B:139:MET:HB3	2.13	0.48
2:B:238:SER:O	2:B:242:ASP:CB	2.60	0.48
2:B:409:LYS:C	2:B:410:PHE:HD2	2.16	0.48
2:B:436:LYS:HE3	2:B:469:THR:OG1	2.13	0.48
2:C:182:LYS:O	2:C:185:PHE:HD1	1.96	0.48
1:E:113:PRO:HB2	1:E:161:ALA:HB2	1.95	0.48
2:F:207:TYR:CZ	2:F:504:GLU:HG3	2.49	0.48
1:H:30:THR:CG2	1:H:31:CYS:N	2.75	0.48
2:C:398:SER:HB3	2:C:401:SER:HB3	1.96	0.48
2:C:492:PHE:HD1	2:C:492:PHE:C	2.16	0.48
1:D:112:ALA:HA	1:D:158:TRP:CD2	2.48	0.48
1:D:182:PHE:HE2	1:D:202:TRP:CD1	2.31	0.48
1:D:30:THR:CG2	1:D:31:CYS:N	2.75	0.48
1:D:74:LEU:O	1:D:86:TRP:HD1	1.96	0.48
1:E:240:VAL:HB	1:E:258:LEU:HB3	1.96	0.48
1:E:30:THR:CG2	1:E:31:CYS:N	2.75	0.48
2:F:487:HIS:HD2	2:F:517:LEU:HD23	1.77	0.48
1:A:164:PRO:CD	1:A:176:PRO:HB2	2.44	0.48
1:A:288:LEU:HB2	1:A:300:ILE:HG13	1.95	0.48
2:B:372:LEU:HD22	2:B:375:LEU:HD11	1.95	0.48
2:B:485:GLN:HG3	2:B:485:GLN:O	2.13	0.48
2:C:423:GLN:HB3	2:C:434:LEU:HD21	1.94	0.48
2:C:525:HIS:O	2:C:527:LEU:N	2.46	0.48
1:E:112:ALA:HA	1:E:158:TRP:CD2	2.48	0.48
2:F:142:ARG:HG3	2:F:142:ARG:HH11	1.79	0.48
2:F:215:LEU:HD13	2:F:452:TYR:HE1	1.78	0.48
2:F:515:ILE:HD12	2:F:541:GLN:N	2.28	0.48
2:G:332:ILE:CD1	2:G:332:ILE:H	2.25	0.48
1:H:220:TRP:NE1	1:H:231:ILE:HD11	2.28	0.48
1:A:220:TRP:NE1	1:A:231:ILE:HD11	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:294:ILE:HD11	2:B:310:ALA:HA	1.95	0.48
2:B:356:LYS:O	2:B:359:LYS:HB3	2.13	0.48
1:E:47:GLN:OE1	2:F:167:LYS:N	2.46	0.48
2:F:237:SER:OG	2:F:421:ILE:HD13	2.13	0.48
2:G:332:ILE:O	2:G:333:ARG:C	2.52	0.48
1:A:73:ILE:HG22	1:A:74:LEU:N	2.28	0.48
1:A:74:LEU:O	1:A:86:TRP:HD1	1.97	0.48
2:C:409:LYS:C	2:C:410:PHE:HD2	2.16	0.48
2:C:409:LYS:O	2:C:410:PHE:HD2	1.97	0.48
1:D:106:VAL:HA	1:D:124:SER:HA	1.94	0.48
1:D:111:TRP:CE2	1:D:120:LEU:HD13	2.48	0.48
1:D:242:ILE:HG12	1:D:297:TRP:CZ2	2.48	0.48
1:E:40:PHE:CZ	2:F:168:SER:CB	2.93	0.48
2:F:267:ARG:NH1	2:F:267:ARG:CG	2.71	0.48
2:F:409:LYS:C	2:F:410:PHE:HD2	2.16	0.48
2:F:241:PHE:CD2	2:F:457:LEU:HD21	2.48	0.48
2:F:207:TYR:CE2	2:F:504:GLU:HA	2.45	0.48
2:G:394:ILE:O	2:G:397:TYR:CE1	2.66	0.48
1:A:112:ALA:HA	1:A:158:TRP:CD2	2.48	0.48
1:A:23:TYR:CD2	1:A:24:TYR:CD1	2.98	0.48
2:B:485:GLN:HE21	2:B:517:LEU:CD2	2.26	0.48
2:C:524:ASP:O	2:C:524:ASP:CG	2.51	0.48
1:D:274:ALA:O	1:D:275:ASN:CB	2.61	0.48
2:F:170:VAL:HG12	2:F:170:VAL:O	2.13	0.48
2:F:525:HIS:CD2	2:F:529:ARG:HG3	2.49	0.48
2:G:210:ILE:HD11	2:G:495:CYS:HB3	1.93	0.48
1:A:112:ALA:HB2	1:A:158:TRP:CH2	2.49	0.48
2:B:182:LYS:O	2:B:185:PHE:HD1	1.96	0.48
2:C:525:HIS:CD2	2:C:529:ARG:HG3	2.49	0.48
1:E:70:TYR:N	1:E:70:TYR:HD1	2.10	0.48
2:G:492:PHE:O	2:G:495:CYS:HB2	2.14	0.48
1:H:112:ALA:HB2	1:H:158:TRP:CH2	2.49	0.48
1:H:16:ILE:HA	1:H:32:SER:HB3	1.96	0.48
1:A:284:ASN:HA	2:B:149:THR:OG1	2.12	0.48
2:B:199:ILE:HG22	2:B:200:GLU:N	2.27	0.48
2:B:471:ASP:OD2	2:B:498:ASN:ND2	2.37	0.48
2:C:135:ALA:O	2:C:139:MET:HG3	2.14	0.48
2:C:297:TYR:CE2	2:C:305:ARG:HB3	2.48	0.48
1:D:112:ALA:HB2	1:D:158:TRP:CH2	2.49	0.48
1:D:213:ASP:OD1	1:D:214:TRP:N	2.38	0.48
1:E:106:VAL:HA	1:E:124:SER:HA	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:111:TRP:CE2	1:E:120:LEU:HD13	2.48	0.48
1:E:215:VAL:HA	1:E:235:SER:HB3	1.96	0.48
2:F:364:SER:CB	2:F:394:ILE:HG12	2.42	0.48
2:F:448:GLN:HB2	2:F:477:PHE:CE1	2.48	0.48
2:F:485:GLN:O	2:F:487:HIS:CG	2.67	0.48
2:G:199:ILE:HG22	2:G:200:GLU:N	2.27	0.48
1:A:106:VAL:HA	1:A:124:SER:HA	1.95	0.48
2:B:299:LEU:HD13	2:B:379:PHE:HE2	1.79	0.48
2:B:332:ILE:O	2:B:333:ARG:C	2.52	0.48
2:B:409:LYS:O	2:B:410:PHE:HD2	1.97	0.48
2:C:291:ILE:HG22	2:C:353:ASN:HB3	1.95	0.48
2:C:451:TRP:CE2	2:C:493:VAL:HG13	2.49	0.48
1:D:16:ILE:HA	1:D:32:SER:HB3	1.96	0.48
1:E:164:PRO:CD	1:E:176:PRO:HB2	2.44	0.48
2:G:276:ILE:HG22	2:G:276:ILE:O	2.14	0.48
2:G:284:ILE:HD13	2:G:297:TYR:HE1	1.78	0.48
2:G:210:ILE:CD1	2:G:496:PHE:CD1	2.97	0.48
1:A:18:ASP:OD2	2:B:152:LYS:NZ	2.43	0.47
1:A:258:LEU:CD1	1:A:297:TRP:HB2	2.43	0.47
1:A:234:CYS:SG	1:A:268:VAL:HG23	2.54	0.47
2:B:142:ARG:HH11	2:B:142:ARG:HG3	1.79	0.47
1:A:17:HIS:ND1	2:B:148:TYR:CE2	2.82	0.47
2:B:217:PHE:HZ	2:B:453:LEU:HD23	1.77	0.47
2:B:487:HIS:CD2	2:B:517:LEU:CD2	2.91	0.47
2:B:532:ILE:CG2	2:B:533:PRO:HD2	2.44	0.47
2:C:495:CYS:C	2:C:497:LEU:H	2.17	0.47
2:F:199:ILE:HG22	2:F:200:GLU:N	2.27	0.47
2:F:215:LEU:HD22	2:F:452:TYR:OH	2.14	0.47
2:G:283:LYS:HZ3	2:G:378:GLU:HB2	1.77	0.47
2:G:409:LYS:O	2:G:410:PHE:HD2	1.97	0.47
1:E:112:ALA:HB2	1:E:158:TRP:CH2	2.49	0.47
1:E:276:ILE:HG21	1:E:300:ILE:HD11	1.96	0.47
2:F:409:LYS:O	2:F:410:PHE:HD2	1.97	0.47
2:F:190:LEU:HD13	2:F:489:HIS:ND1	2.29	0.47
2:B:174:ARG:NH2	2:B:485:GLN:OE1	2.47	0.47
2:C:299:LEU:HD22	2:C:383:CYS:SG	2.54	0.47
2:C:471:ASP:OD1	2:C:497:LEU:CA	2.59	0.47
2:C:190:LEU:HB2	2:C:489:HIS:CE1	2.48	0.47
1:D:56:HIS:CE1	1:D:84:ILE:HD12	2.49	0.47
2:F:471:ASP:OD1	2:F:497:LEU:HA	2.14	0.47
2:F:543:LEU:O	2:F:546:ARG:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:284:ILE:HD13	2:G:297:TYR:CD1	2.48	0.47
2:G:215:LEU:HD22	2:G:452:TYR:OH	2.15	0.47
2:G:525:HIS:O	2:G:527:LEU:N	2.47	0.47
1:H:189:ASN:OD1	1:H:213:ASP:C	2.52	0.47
1:H:274:ALA:O	1:H:275:ASN:CB	2.62	0.47
2:C:370:PHE:O	2:C:371:SER:O	2.33	0.47
1:D:220:TRP:NE1	1:D:231:ILE:HD11	2.29	0.47
1:D:251:ASN:ND2	1:D:253:TRP:HE1	2.13	0.47
1:E:74:LEU:O	1:E:86:TRP:HD1	1.96	0.47
2:F:370:PHE:O	2:F:371:SER:O	2.32	0.47
2:G:525:HIS:CD2	2:G:529:ARG:HG3	2.49	0.47
1:H:215:VAL:HA	1:H:235:SER:HB3	1.96	0.47
1:H:56:HIS:CE1	1:H:84:ILE:HD12	2.49	0.47
2:B:149:THR:O	2:B:150:PHE:HB3	2.15	0.47
2:B:215:LEU:HD13	2:B:452:TYR:HE1	1.78	0.47
2:B:525:HIS:CD2	2:B:529:ARG:HG3	2.49	0.47
2:C:217:PHE:HE2	2:C:449:PHE:CE1	2.32	0.47
2:C:276:ILE:O	2:C:276:ILE:HG22	2.14	0.47
2:C:332:ILE:O	2:C:333:ARG:C	2.52	0.47
2:C:522:THR:O	2:C:523:ASN:OD1	2.31	0.47
1:E:182:PHE:O	1:E:182:PHE:CG	2.68	0.47
2:F:332:ILE:O	2:F:333:ARG:C	2.52	0.47
2:F:359:LYS:HZ1	2:F:370:PHE:H	1.62	0.47
2:G:135:ALA:O	2:G:139:MET:HG3	2.14	0.47
2:G:370:PHE:O	2:G:371:SER:O	2.33	0.47
1:H:129:ILE:HG22	1:H:129:ILE:O	2.15	0.47
1:H:74:LEU:O	1:H:86:TRP:HD1	1.97	0.47
2:B:145:THR:HG22	2:B:147:SER:N	2.29	0.47
2:B:237:SER:OG	2:B:421:ILE:HD13	2.15	0.47
2:B:425:TYR:O	2:B:463:ARG:NH2	2.47	0.47
2:C:497:LEU:HD12	2:C:503:ALA:HA	1.97	0.47
2:C:152:LYS:HZ2	1:D:62:GLN:HE21	1.62	0.47
2:F:140:LYS:C	2:F:142:ARG:H	2.16	0.47
1:H:79:TYR:HD1	1:H:105:SER:CB	2.28	0.47
1:H:73:ILE:HG22	1:H:74:LEU:N	2.30	0.47
1:A:16:ILE:HA	1:A:32:SER:HB3	1.96	0.47
1:A:27:ARG:HH12	1:A:93:TRP:HZ2	1.62	0.47
2:B:164:ILE:CG2	2:B:164:ILE:O	2.63	0.47
2:B:515:ILE:HD11	2:B:540:ALA:CB	2.35	0.47
2:B:323:SER:OG	2:C:262:LYS:HE2	2.14	0.47
2:C:276:ILE:HG21	2:C:383:CYS:SG	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:79:TYR:HD1	1:D:105:SER:CB	2.28	0.47
1:E:291:GLU:HA	1:E:297:TRP:HA	1.96	0.47
1:E:27:ARG:HH12	1:E:93:TRP:HZ2	1.62	0.47
2:G:172:ILE:CD1	1:H:42:VAL:HG21	2.44	0.47
2:G:182:LYS:O	2:G:185:PHE:HD1	1.96	0.47
2:G:474:THR:HG23	2:G:493:VAL:CG1	2.45	0.47
1:H:280:SER:HA	1:H:286:VAL:HG22	1.96	0.47
1:A:240:VAL:HB	1:A:258:LEU:HB3	1.97	0.47
2:B:280:ILE:CG1	2:B:300:LEU:HD21	2.45	0.47
1:E:220:TRP:NE1	1:E:231:ILE:HD11	2.28	0.47
1:E:56:HIS:CE1	1:E:84:ILE:HD12	2.49	0.47
2:F:217:PHE:HA	2:F:452:TYR:HE2	1.78	0.47
2:G:271:TRP:HE3	2:G:272:ILE:HG12	1.80	0.47
1:A:241:PHE:HD2	1:A:257:LEU:HA	1.80	0.47
2:C:199:ILE:HD13	2:C:530:LEU:HA	1.95	0.47
1:E:16:ILE:HA	1:E:32:SER:HB3	1.96	0.47
2:F:177:THR:CG2	2:F:179:LEU:HB3	2.43	0.47
1:H:145:ILE:HD11	1:H:202:TRP:HB2	1.97	0.47
2:G:162:LYS:HZ3	1:H:15:MET:HE1	1.78	0.47
1:H:27:ARG:HH12	1:H:93:TRP:HZ2	1.63	0.47
1:A:244:THR:HG22	1:A:245:CYS:N	2.30	0.47
2:C:209:GLN:HG2	2:C:497:LEU:O	2.15	0.47
1:D:73:ILE:HG22	1:D:74:LEU:N	2.30	0.47
2:F:291:ILE:HG22	2:F:353:ASN:HB2	1.97	0.47
2:F:207:TYR:CE1	2:F:504:GLU:HG3	2.50	0.47
2:G:543:LEU:O	2:G:546:ARG:HB3	2.15	0.47
1:H:53:LEU:H	1:H:53:LEU:HD23	1.80	0.47
1:A:79:TYR:HD1	1:A:105:SER:CB	2.28	0.46
2:B:370:PHE:O	2:B:371:SER:O	2.33	0.46
1:D:292:SER:C	1:D:294:ASP:N	2.69	0.46
2:F:299:LEU:HD22	2:F:383:CYS:SG	2.55	0.46
2:F:515:ILE:HD11	2:F:540:ALA:CB	2.40	0.46
1:E:43:ARG:NH2	2:F:551:TYR:CE2	2.83	0.46
2:G:394:ILE:O	2:G:395:ASP:HB2	2.15	0.46
1:H:164:PRO:CD	1:H:176:PRO:HB2	2.43	0.46
2:B:276:ILE:HG22	2:B:276:ILE:O	2.15	0.46
2:B:423:GLN:HB3	2:B:434:LEU:HD21	1.97	0.46
1:D:290:LYS:CB	1:D:300:ILE:CD1	2.93	0.46
1:E:273:THR:HG21	2:F:479:ALA:HB1	1.94	0.46
1:E:276:ILE:HG23	1:E:289:TRP:O	2.15	0.46
1:E:242:ILE:CD1	1:E:297:TRP:CD1	2.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:343:TRP:CE3	2:F:350:ILE:HG21	2.51	0.46
2:G:194:ILE:HG12	2:G:492:PHE:CD2	2.50	0.46
2:G:445:LEU:HD23	2:G:445:LEU:HA	1.74	0.46
2:B:142:ARG:HA	2:B:142:ARG:HD3	1.52	0.46
2:B:543:LEU:O	2:B:546:ARG:HB3	2.15	0.46
2:C:543:LEU:O	2:C:546:ARG:HB3	2.15	0.46
1:E:49:LEU:CD1	1:E:50:ILE:H	2.20	0.46
2:F:149:THR:O	2:F:150:PHE:HB3	2.14	0.46
1:H:214:TRP:O	1:H:235:SER:CB	2.56	0.46
1:A:215:VAL:HA	1:A:235:SER:HB3	1.96	0.46
2:B:241:PHE:CD2	2:B:457:LEU:HD21	2.51	0.46
2:F:153:PHE:HE2	2:F:175:LEU:HD22	1.81	0.46
2:F:255:VAL:HG11	2:G:335:LEU:HD22	1.97	0.46
2:G:153:PHE:CE2	1:H:278:ALA:HB2	2.51	0.46
1:A:50:ILE:HG22	1:A:50:ILE:O	2.16	0.46
2:B:177:THR:CG2	2:B:179:LEU:HB3	2.43	0.46
1:D:27:ARG:HH12	1:D:93:TRP:HZ2	1.62	0.46
1:E:234:CYS:SG	1:E:268:VAL:HG23	2.56	0.46
2:F:202:ARG:HA	2:F:202:ARG:HD3	1.55	0.46
2:G:161:THR:O	2:G:170:VAL:HG13	2.15	0.46
1:H:16:ILE:HG22	1:H:17:HIS:H	1.80	0.46
1:H:224:ILE:HG13	1:H:226:LEU:HB2	1.98	0.46
2:B:136:LYS:O	2:B:140:LYS:HB2	2.15	0.46
2:B:163:ASP:O	2:B:164:ILE:HB	2.16	0.46
2:C:161:THR:O	2:C:170:VAL:HG13	2.15	0.46
1:D:16:ILE:HG22	1:D:17:HIS:H	1.81	0.46
1:D:190:LEU:HD21	1:D:209:GLU:HB3	1.97	0.46
1:D:215:VAL:HA	1:D:235:SER:HB3	1.96	0.46
1:D:280:SER:HA	1:D:286:VAL:HG22	1.96	0.46
1:E:280:SER:HA	1:E:286:VAL:HG22	1.96	0.46
1:E:289:TRP:CE3	1:E:298:VAL:C	2.89	0.46
1:E:53:LEU:N	1:E:53:LEU:CD2	2.77	0.46
2:F:165:VAL:O	2:F:165:VAL:HG12	2.14	0.46
2:F:276:ILE:O	2:F:276:ILE:HG22	2.15	0.46
2:G:303:VAL:HG13	2:G:322:ILE:CG2	2.46	0.46
2:G:151:ALA:HB2	1:H:286:VAL:HG21	1.97	0.46
1:H:296:GLN:O	1:H:296:GLN:NE2	2.48	0.46
1:A:16:ILE:HG22	1:A:17:HIS:H	1.80	0.46
1:A:280:SER:HA	1:A:286:VAL:HG22	1.96	0.46
2:B:271:TRP:HE3	2:B:272:ILE:HG12	1.80	0.46
2:B:272:ILE:HG23	2:B:382:LEU:HG	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:272:ILE:HD11	2:F:155:THR:HA	1.97	0.46
2:F:343:TRP:CZ3	2:F:350:ILE:CG2	2.88	0.46
2:F:429:GLU:O	2:F:464:VAL:HG21	2.16	0.46
1:H:143:LYS:HD2	1:H:200:GLY:O	2.15	0.46
1:H:296:GLN:HE21	1:H:298:VAL:HG23	1.80	0.46
2:B:284:ILE:HD13	2:B:297:TYR:CE1	2.51	0.46
1:D:145:ILE:HG22	1:D:148:ALA:HB2	1.98	0.46
1:E:292:SER:C	1:E:294:ASP:N	2.69	0.46
2:F:136:LYS:O	2:F:140:LYS:HB2	2.15	0.46
1:E:304:ASN:HA	2:F:173:LYS:NZ	2.30	0.46
2:F:177:THR:HG22	2:F:179:LEU:HD23	1.97	0.46
2:G:471:ASP:OD1	2:G:497:LEU:CD2	2.58	0.46
1:H:216:ARG:HD3	1:H:216:ARG:HA	1.67	0.46
1:A:292:SER:C	1:A:294:ASP:N	2.69	0.46
1:E:50:ILE:HG22	1:E:50:ILE:O	2.16	0.46
2:F:137:LEU:O	2:F:141:GLU:HB3	2.16	0.46
2:F:271:TRP:HE3	2:F:272:ILE:HG12	1.81	0.46
1:H:145:ILE:HG22	1:H:148:ALA:HB2	1.98	0.46
1:A:53:LEU:N	1:A:53:LEU:CD2	2.78	0.46
2:B:256:LYS:O	2:B:260:LEU:HG	2.16	0.46
1:D:129:ILE:O	1:D:129:ILE:HG22	2.15	0.46
1:D:50:ILE:O	1:D:50:ILE:HG22	2.16	0.46
1:D:53:LEU:CD2	1:D:53:LEU:N	2.77	0.46
1:D:77:CYS:HB3	1:D:109:VAL:HG23	1.98	0.46
1:E:192:LYS:HE2	1:E:207:LYS:HE2	1.98	0.46
1:E:73:ILE:HG22	1:E:74:LEU:N	2.30	0.46
2:F:217:PHE:HZ	2:F:453:LEU:HD23	1.80	0.46
2:F:532:ILE:HG23	2:F:533:PRO:CD	2.45	0.46
1:A:182:PHE:O	1:A:182:PHE:CG	2.68	0.45
1:A:224:ILE:HG13	1:A:226:LEU:HB2	1.98	0.45
1:A:77:CYS:HB3	1:A:109:VAL:HG23	1.98	0.45
2:B:137:LEU:O	2:B:141:GLU:N	2.32	0.45
1:A:15:MET:HG3	2:B:162:LYS:HZ2	1.81	0.45
2:B:295:PHE:CE1	2:B:360:LEU:HD11	2.52	0.45
2:C:213:SER:HB3	2:C:459:PHE:CD2	2.52	0.45
2:F:244:VAL:HG11	2:F:263:GLU:HB3	1.98	0.45
2:F:550:ASN:OD1	2:F:550:ASN:N	2.50	0.45
1:H:50:ILE:O	1:H:50:ILE:HG22	2.16	0.45
2:B:165:VAL:O	2:B:165:VAL:HG12	2.15	0.45
2:C:271:TRP:HE3	2:C:272:ILE:HG12	1.80	0.45
2:C:303:VAL:HG13	2:C:322:ILE:CG2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:182:PHE:CG	1:D:182:PHE:O	2.69	0.45
1:E:191:ILE:HB	1:E:208:LEU:HB2	1.98	0.45
1:E:53:LEU:HD12	1:E:86:TRP:CD2	2.52	0.45
2:F:303:VAL:HG13	2:F:322:ILE:CG2	2.47	0.45
2:F:475:PHE:CE2	2:F:497:LEU:HD11	2.50	0.45
2:G:350:ILE:HG22	2:G:351:ASP:N	2.30	0.45
2:G:394:ILE:O	2:G:397:TYR:CD1	2.70	0.45
2:G:550:ASN:N	2:G:550:ASN:OD1	2.49	0.45
1:A:129:ILE:O	1:A:129:ILE:HG22	2.14	0.45
1:A:28:LEU:HD13	2:B:172:ILE:CD1	2.46	0.45
2:B:487:HIS:HE1	2:B:513:ARG:HH21	1.65	0.45
2:C:359:LYS:HZ1	2:C:370:PHE:H	1.65	0.45
1:E:79:TYR:HD1	1:E:105:SER:CB	2.29	0.45
1:E:145:ILE:HG22	1:E:148:ALA:HB2	1.98	0.45
1:E:150:THR:HB	1:E:188:ASP:HB3	1.99	0.45
1:E:294:ASP:O	1:E:294:ASP:OD1	2.34	0.45
2:G:375:LEU:HB2	2:G:384:LEU:HD21	1.98	0.45
2:B:137:LEU:O	2:B:141:GLU:HB3	2.15	0.45
1:D:242:ILE:CD1	1:D:258:LEU:HB2	2.46	0.45
1:H:248:ALA:O	1:H:249:SER:HB3	2.16	0.45
1:H:276:ILE:HG23	1:H:289:TRP:O	2.16	0.45
1:A:276:ILE:HG23	1:A:289:TRP:O	2.16	0.45
1:A:53:LEU:HD12	1:A:86:TRP:CD2	2.52	0.45
2:B:153:PHE:HE2	2:B:175:LEU:HD22	1.81	0.45
2:B:409:LYS:H	2:B:409:LYS:HG2	1.56	0.45
2:B:484:ALA:O	2:B:485:GLN:CB	2.65	0.45
2:B:482:GLU:CD	2:B:509:ARG:HH22	2.20	0.45
2:B:512:MET:HA	2:B:540:ALA:HB1	1.98	0.45
1:D:189:ASN:HA	1:D:215:VAL:HG23	1.98	0.45
1:D:232:ALA:HB2	1:D:270:TRP:HZ2	1.77	0.45
1:E:266:TRP:HD1	1:E:281:GLY:HA2	1.81	0.45
2:F:164:ILE:O	2:F:164:ILE:CG2	2.63	0.45
2:G:155:THR:CG2	2:G:513:ARG:HD2	2.30	0.45
1:H:145:ILE:HD11	1:H:202:TRP:CB	2.47	0.45
1:H:266:TRP:HD1	1:H:281:GLY:HA2	1.82	0.45
1:A:193:LEU:N	1:A:193:LEU:HD23	2.32	0.45
2:B:199:ILE:HG21	2:B:208:PRO:HB2	1.99	0.45
2:C:519:ARG:HB3	2:C:520:ALA:H	1.48	0.45
1:D:214:TRP:O	1:D:235:SER:CB	2.56	0.45
1:E:77:CYS:SG	1:E:106:VAL:O	2.67	0.45
1:E:129:ILE:HG22	1:E:129:ILE:O	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:224:ILE:HG13	1:E:226:LEU:HB2	1.98	0.45
1:E:258:LEU:CD1	1:E:297:TRP:CB	2.94	0.45
1:E:70:TYR:CD2	1:E:118:LEU:HD13	2.52	0.45
2:G:256:LYS:O	2:G:260:LEU:HG	2.16	0.45
2:G:209:GLN:HG3	2:G:495:CYS:O	2.17	0.45
1:A:213:ASP:OD1	1:A:214:TRP:N	2.38	0.45
1:A:216:ARG:HA	1:A:216:ARG:HD3	1.66	0.45
2:B:299:LEU:HD13	2:B:379:PHE:CE2	2.52	0.45
2:C:522:THR:CG2	2:C:526:ILE:HG13	2.47	0.45
1:D:150:THR:HB	1:D:188:ASP:HB3	1.98	0.45
1:D:294:ASP:O	1:D:294:ASP:OD1	2.34	0.45
2:F:163:ASP:O	2:F:164:ILE:HB	2.16	0.45
2:F:513:ARG:HE	2:F:514:GLU:HG2	1.82	0.45
2:G:201:ALA:HB2	2:G:531:LYS:HZ2	1.80	0.45
2:G:266:CYS:O	2:G:267:ARG:C	2.55	0.45
2:G:385:LEU:HA	2:G:406:HIS:CE1	2.52	0.45
2:B:177:THR:O	2:B:179:LEU:N	2.49	0.45
2:B:272:ILE:CG2	2:B:382:LEU:HG	2.47	0.45
2:B:469:THR:O	2:B:472:GLU:HB3	2.17	0.45
2:B:513:ARG:HE	2:B:514:GLU:HG2	1.81	0.45
2:C:215:LEU:HD22	2:C:452:TYR:OH	2.17	0.45
2:C:256:LYS:O	2:C:260:LEU:HG	2.17	0.45
2:C:469:THR:O	2:C:472:GLU:HB3	2.17	0.45
2:C:486:LEU:HA	2:C:486:LEU:HD23	1.83	0.45
1:D:290:LYS:HB2	1:D:300:ILE:CD1	2.46	0.45
1:E:213:ASP:OD1	1:E:214:TRP:N	2.38	0.45
1:E:284:ASN:HA	2:F:149:THR:OG1	2.16	0.45
2:F:469:THR:O	2:F:472:GLU:HB3	2.17	0.45
2:G:373:LYS:HE2	2:G:410:PHE:HE2	1.81	0.45
2:C:184:LEU:HD21	2:C:448:GLN:HE22	1.81	0.45
2:C:475:PHE:HE2	2:C:497:LEU:CD1	2.30	0.45
1:E:193:LEU:N	1:E:193:LEU:HD23	2.32	0.45
1:E:199:ASP:OD1	1:E:200:GLY:N	2.50	0.45
1:E:258:LEU:CD1	1:E:297:TRP:HB2	2.47	0.45
1:E:41:ASP:OD1	1:E:42:VAL:N	2.49	0.45
2:G:202:ARG:HD3	2:G:202:ARG:HA	1.55	0.45
1:A:199:ASP:OD1	1:A:200:GLY:N	2.50	0.45
1:A:208:LEU:HD13	1:A:243:TRP:CE3	2.52	0.45
2:B:350:ILE:CG2	2:B:351:ASP:N	2.80	0.45
2:C:139:MET:HE2	2:C:144:PHE:HB2	1.98	0.45
2:C:155:THR:HG22	2:C:513:ARG:CD	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:145:THR:HG22	2:F:147:SER:N	2.30	0.45
2:F:256:LYS:O	2:F:260:LEU:HG	2.16	0.45
2:G:469:THR:O	2:G:472:GLU:HB3	2.18	0.45
2:G:513:ARG:HE	2:G:514:GLU:HG2	1.81	0.45
1:H:182:PHE:O	1:H:182:PHE:CG	2.69	0.45
1:H:232:ALA:HB2	1:H:270:TRP:HZ2	1.79	0.45
1:A:145:ILE:HD13	1:A:194:TRP:CE3	2.53	0.44
2:B:487:HIS:CE1	2:B:513:ARG:HH21	2.35	0.44
1:D:38:LYS:HB2	1:D:40:PHE:CE1	2.52	0.44
1:D:95:LYS:O	1:D:95:LYS:HG2	2.18	0.44
1:E:157:SER:HB2	1:E:218:VAL:O	2.17	0.44
2:F:250:THR:O	2:F:256:LYS:HE3	2.17	0.44
2:G:149:THR:CG2	2:G:150:PHE:N	2.72	0.44
2:G:276:ILE:HD13	2:G:383:CYS:CA	2.34	0.44
2:G:366:PHE:HZ	2:G:387:LEU:HD12	1.82	0.44
1:A:191:ILE:HB	1:A:208:LEU:HB2	1.99	0.44
1:A:210:ALA:HB3	1:A:243:TRP:CZ2	2.52	0.44
1:A:258:LEU:HD13	1:A:297:TRP:HB2	1.99	0.44
1:A:294:ASP:O	1:A:294:ASP:OD1	2.34	0.44
2:B:133:ASP:N	2:B:133:ASP:OD1	2.50	0.44
1:A:21:MET:HB3	2:B:154:SER:OG	2.17	0.44
2:B:215:LEU:HD23	2:B:215:LEU:HA	1.83	0.44
2:B:321:LEU:HB3	2:B:361:LEU:CD1	2.42	0.44
2:B:491:LEU:HD23	2:B:530:LEU:HD12	1.99	0.44
2:C:193:GLU:O	2:C:196:LYS:HB2	2.18	0.44
2:C:295:PHE:CE2	2:C:356:LYS:HD3	2.53	0.44
2:C:481:LEU:O	2:C:484:ALA:HB3	2.18	0.44
2:C:474:THR:CG2	2:C:493:VAL:HG12	2.47	0.44
2:C:513:ARG:HE	2:C:514:GLU:HG2	1.82	0.44
1:D:266:TRP:HD1	1:D:281:GLY:HA2	1.82	0.44
1:D:53:LEU:HD12	1:D:86:TRP:CD2	2.51	0.44
2:F:210:ILE:HG22	2:F:459:PHE:CE2	2.53	0.44
2:F:218:LYS:HG2	2:F:238:SER:HG	1.79	0.44
1:A:70:TYR:CD2	1:A:118:LEU:HD13	2.53	0.44
1:A:145:ILE:HG22	1:A:148:ALA:HB2	1.98	0.44
1:A:300:ILE:HG12	1:A:300:ILE:H	1.59	0.44
1:A:43:ARG:O	1:A:44:ASN:CB	2.66	0.44
1:A:280:SER:HB2	2:B:150:PHE:HA	1.99	0.44
2:B:210:ILE:H	2:B:210:ILE:HD12	1.82	0.44
2:C:208:PRO:HD3	2:C:533:PRO:HD3	1.98	0.44
1:D:77:CYS:HB3	1:D:109:VAL:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:16:ILE:HG22	1:E:17:HIS:H	1.80	0.44
1:E:43:ARG:O	1:E:44:ASN:CB	2.66	0.44
1:E:95:LYS:HG2	1:E:95:LYS:O	2.17	0.44
2:F:133:ASP:OD1	2:F:133:ASP:N	2.50	0.44
2:F:193:GLU:O	2:F:196:LYS:HB2	2.17	0.44
1:H:77:CYS:HB3	1:H:109:VAL:HG23	1.98	0.44
1:H:95:LYS:O	1:H:95:LYS:HG2	2.17	0.44
1:D:224:ILE:HG13	1:D:226:LEU:HB2	1.98	0.44
2:G:551:TYR:CE2	1:H:43:ARG:NH2	2.85	0.44
1:H:199:ASP:O	1:H:199:ASP:OD1	2.36	0.44
1:H:53:LEU:HD12	1:H:86:TRP:CD2	2.52	0.44
1:A:266:TRP:HD1	1:A:281:GLY:HA2	1.82	0.44
2:B:135:ALA:O	2:B:139:MET:CB	2.65	0.44
2:C:284:ILE:O	2:C:287:SER:HB3	2.17	0.44
2:C:396:GLU:OE1	2:C:396:GLU:HA	2.16	0.44
2:C:435:TYR:CD2	2:C:454:ILE:HD11	2.53	0.44
2:C:550:ASN:N	2:C:550:ASN:OD1	2.49	0.44
1:D:193:LEU:N	1:D:193:LEU:HD23	2.33	0.44
1:D:53:LEU:HD23	1:D:53:LEU:H	1.80	0.44
1:D:78:SER:OG	1:D:79:TYR:N	2.51	0.44
1:E:264:VAL:CG1	1:E:265:VAL:N	2.81	0.44
1:E:287:THR:O	1:E:288:LEU:HD23	2.17	0.44
2:F:145:THR:C	2:F:147:SER:N	2.70	0.44
2:F:210:ILE:HD12	2:F:210:ILE:H	1.82	0.44
1:A:40:PHE:CD1	1:A:40:PHE:N	2.84	0.44
1:A:95:LYS:HG2	1:A:95:LYS:O	2.17	0.44
2:B:193:GLU:O	2:B:196:LYS:HB2	2.17	0.44
2:B:495:CYS:C	2:B:497:LEU:H	2.20	0.44
2:C:178:GLU:HG2	2:C:480:GLN:NE2	2.32	0.44
1:D:29:ALA:CA	1:D:39:ILE:HD13	2.46	0.44
1:E:245:CYS:HB2	1:E:253:TRP:CZ3	2.51	0.44
2:F:199:ILE:HG21	2:F:208:PRO:HB2	1.99	0.44
2:B:210:ILE:HD12	2:B:495:CYS:C	2.38	0.44
2:B:266:CYS:O	2:B:267:ARG:C	2.56	0.44
2:C:216:LEU:HB3	2:C:242:ASP:CG	2.37	0.44
2:C:246:TYR:CE2	2:C:250:THR:OG1	2.67	0.44
2:C:185:PHE:HA	2:C:486:LEU:HD11	2.00	0.44
1:D:276:ILE:HG23	1:D:289:TRP:O	2.17	0.44
1:E:78:SER:OG	1:E:79:TYR:N	2.51	0.44
2:F:137:LEU:O	2:F:141:GLU:N	2.33	0.44
2:F:238:SER:CA	2:F:242:ASP:OD2	2.54	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:323:SER:OG	2:G:262:LYS:HE2	2.18	0.44
1:H:77:CYS:HB3	1:H:109:VAL:HG21	2.00	0.44
1:A:38:LYS:HB2	1:A:40:PHE:CE1	2.52	0.44
2:B:185:PHE:CD1	2:B:185:PHE:N	2.86	0.44
2:B:276:ILE:HG21	2:B:383:CYS:SG	2.58	0.44
2:B:412:LEU:HB3	2:B:413:PRO:HD2	1.99	0.44
2:C:272:ILE:HG23	2:C:382:LEU:HG	2.00	0.44
2:C:448:GLN:HB2	2:C:477:PHE:HE1	1.81	0.44
1:E:280:SER:HB2	2:F:150:PHE:HA	1.98	0.44
2:F:177:THR:CG2	2:F:179:LEU:CD2	2.93	0.44
2:F:266:CYS:O	2:F:267:ARG:C	2.55	0.44
2:F:519:ARG:HB3	2:F:520:ALA:H	1.48	0.44
2:G:199:ILE:HG21	2:G:208:PRO:HB2	1.99	0.44
2:G:278:PRO:HG2	2:G:279:GLU:H	1.83	0.44
2:G:446:ASP:O	2:G:447:VAL:C	2.56	0.44
1:A:77:CYS:HB3	1:A:109:VAL:HG21	2.00	0.44
2:B:303:VAL:HG13	2:B:322:ILE:CG2	2.46	0.44
2:B:451:TRP:CD1	2:B:474:THR:HA	2.53	0.44
2:B:485:GLN:NE2	2:B:517:LEU:HD22	2.31	0.44
2:C:210:ILE:HD13	2:C:496:PHE:HA	2.00	0.44
2:C:266:CYS:O	2:C:267:ARG:C	2.56	0.44
2:C:297:TYR:HB3	2:C:306:ALA:HB2	2.00	0.44
1:D:70:TYR:CD2	1:D:118:LEU:HD13	2.53	0.44
1:D:216:ARG:HA	1:D:216:ARG:HD3	1.67	0.44
2:C:172:ILE:CD1	1:D:42:VAL:HG21	2.47	0.44
1:E:183:ALA:O	1:E:184:SER:CB	2.66	0.44
1:E:303:VAL:O	1:E:304:ASN:HB2	2.17	0.44
2:F:142:ARG:HA	2:F:142:ARG:HD3	1.51	0.44
2:G:139:MET:HE2	2:G:144:PHE:HB2	2.00	0.44
2:G:152:LYS:HZ1	1:H:62:GLN:NE2	2.16	0.44
1:A:89:GLU:O	1:A:90:ASN:CB	2.66	0.43
2:B:297:TYR:CE2	2:B:305:ARG:HB3	2.53	0.43
2:C:188:VAL:O	2:C:192:LYS:HB2	2.18	0.43
2:C:199:ILE:HG21	2:C:208:PRO:HB2	1.99	0.43
2:C:317:HIS:O	2:C:320:VAL:HB	2.18	0.43
1:D:66:ALA:HB3	1:D:73:ILE:HB	2.00	0.43
1:E:245:CYS:HB2	1:E:253:TRP:CD2	2.53	0.43
2:F:177:THR:O	2:F:179:LEU:N	2.50	0.43
2:F:218:LYS:CG	2:F:238:SER:OG	2.59	0.43
2:G:153:PHE:HE1	2:G:175:LEU:HD22	1.82	0.43
2:G:404:GLN:CG	2:G:426:ALA:HB1	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:152:LYS:NZ	1:H:62:GLN:NE2	2.66	0.43
1:A:303:VAL:O	1:A:304:ASN:HB2	2.17	0.43
2:B:145:THR:C	2:B:147:SER:N	2.71	0.43
2:B:199:ILE:CD1	2:B:530:LEU:HA	2.48	0.43
2:B:299:LEU:HD22	2:B:383:CYS:SG	2.58	0.43
2:B:330:PRO:O	2:B:331:ARG:C	2.57	0.43
2:B:481:LEU:HB2	2:B:490:SER:HB2	1.99	0.43
2:B:522:THR:HG21	2:B:526:ILE:HD11	1.98	0.43
2:B:550:ASN:N	2:B:550:ASN:OD1	2.50	0.43
2:C:153:PHE:HE1	2:C:175:LEU:HD22	1.82	0.43
1:D:204:GLU:HG3	1:D:204:GLU:O	2.18	0.43
1:E:288:LEU:HB3	1:E:300:ILE:HG13	2.00	0.43
1:E:77:CYS:HB3	1:E:109:VAL:HG23	1.98	0.43
1:E:79:TYR:CE2	2:F:138:ILE:CD1	3.01	0.43
2:F:188:VAL:O	2:F:192:LYS:HB2	2.19	0.43
2:F:380:SER:O	2:F:383:CYS:N	2.45	0.43
2:F:522:THR:CG2	2:F:526:ILE:CD1	2.96	0.43
2:G:188:VAL:O	2:G:192:LYS:HB2	2.18	0.43
2:G:317:HIS:O	2:G:320:VAL:HB	2.19	0.43
1:H:160:PRO:O	1:H:162:VAL:HG23	2.18	0.43
1:A:204:GLU:HG3	1:A:204:GLU:O	2.18	0.43
1:A:78:SER:OG	1:A:79:TYR:N	2.51	0.43
2:B:487:HIS:HD2	2:B:517:LEU:CD2	2.15	0.43
2:C:359:LYS:NZ	2:C:370:PHE:H	2.16	0.43
2:C:194:ILE:CG1	2:C:492:PHE:CE2	2.99	0.43
2:C:544:LYS:O	2:C:545:ASP:C	2.56	0.43
1:E:33:SER:HA	1:E:59:PRO:HB3	2.00	0.43
2:F:135:ALA:O	2:F:139:MET:CB	2.65	0.43
2:F:253:ASP:O	2:F:257:MET:HB2	2.18	0.43
2:F:317:HIS:O	2:F:320:VAL:HB	2.19	0.43
2:G:330:PRO:O	2:G:331:ARG:C	2.57	0.43
1:H:193:LEU:HD21	1:H:208:LEU:CD1	2.48	0.43
1:H:70:TYR:CD2	1:H:118:LEU:HD13	2.53	0.43
2:B:188:VAL:O	2:B:192:LYS:HB2	2.18	0.43
2:B:217:PHE:HA	2:B:452:TYR:HE2	1.82	0.43
2:C:410:PHE:N	2:C:410:PHE:CD2	2.84	0.43
1:D:234:CYS:HB2	1:D:265:VAL:CG1	2.47	0.43
2:F:410:PHE:N	2:F:410:PHE:CD2	2.84	0.43
2:G:193:GLU:O	2:G:196:LYS:HB2	2.18	0.43
2:G:262:LYS:O	2:G:263:GLU:C	2.56	0.43
1:H:193:LEU:HD23	1:H:193:LEU:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:213:ASP:OD1	1:H:214:TRP:N	2.38	0.43
1:H:78:SER:OG	1:H:79:TYR:N	2.51	0.43
1:H:89:GLU:O	1:H:90:ASN:CB	2.66	0.43
1:A:287:THR:O	1:A:288:LEU:HD23	2.19	0.43
1:A:33:SER:HA	1:A:59:PRO:HB3	2.01	0.43
2:B:262:LYS:O	2:B:263:GLU:C	2.56	0.43
2:C:246:TYR:HA	2:C:247:PRO:HD2	1.80	0.43
2:C:359:LYS:HZ1	2:C:368:GLY:HA3	1.83	0.43
1:D:77:CYS:SG	1:D:106:VAL:O	2.66	0.43
1:E:79:TYR:CD2	2:F:138:ILE:HD13	2.53	0.43
2:F:244:VAL:HG23	2:F:264:ARG:NH2	2.27	0.43
2:F:544:LYS:O	2:F:545:ASP:C	2.56	0.43
1:H:40:PHE:N	1:H:40:PHE:CD1	2.85	0.43
1:A:53:LEU:HD23	1:A:53:LEU:H	1.81	0.43
2:B:278:PRO:HG2	2:B:279:GLU:H	1.84	0.43
2:B:359:LYS:NZ	2:B:370:PHE:H	2.17	0.43
2:B:410:PHE:N	2:B:410:PHE:CD2	2.84	0.43
2:B:522:THR:O	2:B:522:THR:HG22	2.18	0.43
2:B:544:LYS:O	2:B:545:ASP:C	2.56	0.43
2:C:185:PHE:N	2:C:185:PHE:CD1	2.87	0.43
2:C:220:ALA:HB3	2:C:234:TRP:CE3	2.54	0.43
2:C:484:ALA:O	2:C:485:GLN:HB2	2.19	0.43
2:F:379:PHE:HD1	2:F:379:PHE:N	2.17	0.43
2:F:446:ASP:O	2:F:447:VAL:C	2.56	0.43
2:B:177:THR:C	2:B:179:LEU:N	2.71	0.43
2:B:294:ILE:HD13	2:B:310:ALA:HB2	1.99	0.43
2:B:446:ASP:O	2:B:447:VAL:C	2.56	0.43
2:C:289:ASN:O	2:C:290:GLU:C	2.56	0.43
2:C:339:GLN:O	2:C:343:TRP:CD1	2.71	0.43
2:C:399:LEU:O	2:C:402:LEU:HB3	2.19	0.43
1:D:264:VAL:CG1	1:D:265:VAL:N	2.82	0.43
1:D:287:THR:O	1:D:288:LEU:HD23	2.19	0.43
1:D:43:ARG:O	1:D:44:ASN:CB	2.66	0.43
1:E:216:ARG:HA	1:E:216:ARG:HD3	1.67	0.43
1:E:66:ALA:HB3	1:E:73:ILE:HB	2.01	0.43
1:E:77:CYS:HB3	1:E:109:VAL:HG21	2.00	0.43
2:F:262:LYS:O	2:F:263:GLU:C	2.56	0.43
2:F:359:LYS:NZ	2:F:370:PHE:H	2.16	0.43
2:G:220:ALA:HB3	2:G:234:TRP:CE3	2.54	0.43
2:G:272:ILE:HG23	2:G:382:LEU:HG	1.99	0.43
2:F:262:LYS:HE2	2:G:323:SER:OG	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:404:GLN:HG2	2:G:426:ALA:C	2.39	0.43
1:H:43:ARG:O	1:H:44:ASN:CB	2.66	0.43
2:B:267:ARG:HG3	2:B:267:ARG:NH1	2.15	0.43
2:C:194:ILE:CG1	2:C:492:PHE:HE2	2.29	0.43
2:C:446:ASP:O	2:C:447:VAL:C	2.57	0.43
1:E:89:GLU:O	1:E:90:ASN:CB	2.66	0.43
2:F:381:TRP:CD1	2:F:382:LEU:N	2.86	0.43
2:G:201:ALA:HB2	2:G:531:LYS:HZ3	1.80	0.43
2:G:410:PHE:N	2:G:410:PHE:CD2	2.84	0.43
1:H:287:THR:HG21	1:H:299:CYS:SG	2.58	0.43
1:A:264:VAL:CG1	1:A:265:VAL:N	2.81	0.43
1:A:266:TRP:CZ3	2:B:144:PHE:HD2	2.37	0.43
2:B:339:GLN:O	2:B:343:TRP:CD1	2.71	0.43
2:C:218:LYS:HG2	2:C:238:SER:HG	1.81	0.43
2:F:215:LEU:HA	2:F:215:LEU:HD23	1.84	0.43
2:F:278:PRO:HG2	2:F:279:GLU:H	1.83	0.43
2:G:399:LEU:O	2:G:402:LEU:HB3	2.19	0.43
2:G:431:THR:HG21	2:G:463:ARG:HB3	2.00	0.43
1:H:164:PRO:HD2	1:H:176:PRO:HB2	2.01	0.43
1:H:292:SER:OG	1:H:294:ASP:HB2	2.19	0.43
1:H:33:SER:HA	1:H:59:PRO:HB3	2.01	0.43
1:A:224:ILE:C	1:A:226:LEU:N	2.72	0.43
2:B:317:HIS:O	2:B:320:VAL:HB	2.19	0.43
2:B:487:HIS:HB3	2:B:518:LEU:HD21	2.01	0.43
2:C:330:PRO:O	2:C:331:ARG:C	2.57	0.43
1:D:183:ALA:O	1:D:184:SER:CB	2.67	0.43
1:E:164:PRO:HD2	1:E:176:PRO:HB2	2.01	0.43
2:F:494:SER:O	2:F:497:LEU:HB2	2.18	0.43
2:G:544:LYS:O	2:G:545:ASP:C	2.56	0.43
2:B:399:LEU:O	2:B:402:LEU:HB3	2.19	0.42
2:B:493:VAL:O	2:B:493:VAL:HG12	2.19	0.42
2:C:210:ILE:H	2:C:210:ILE:HD12	1.83	0.42
1:E:38:LYS:HB2	1:E:40:PHE:CE1	2.53	0.42
2:F:400:GLU:HG3	2:F:425:TYR:CZ	2.54	0.42
2:G:244:VAL:CG1	2:G:263:GLU:OE2	2.66	0.42
1:H:204:GLU:HG3	1:H:204:GLU:O	2.18	0.42
1:H:49:LEU:HD11	1:H:51:ALA:O	2.19	0.42
1:H:66:ALA:HB3	1:H:73:ILE:HB	2.01	0.42
1:A:21:MET:HA	1:A:28:LEU:HD12	2.01	0.42
1:A:47:GLN:OE1	2:B:166:GLY:CA	2.67	0.42
2:C:393:GLN:HA	2:C:393:GLN:OE1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:89:GLU:O	1:D:90:ASN:CB	2.66	0.42
1:E:274:ALA:O	1:E:275:ASN:CB	2.62	0.42
1:E:293:VAL:O	1:E:293:VAL:HG12	2.20	0.42
2:F:199:ILE:CG2	2:F:200:GLU:N	2.83	0.42
2:F:202:ARG:HG2	2:F:209:GLN:HB2	2.02	0.42
2:F:384:LEU:O	2:F:387:LEU:N	2.51	0.42
2:G:218:LYS:CG	2:G:238:SER:OG	2.59	0.42
2:G:409:LYS:HG2	2:G:409:LYS:H	1.56	0.42
2:G:506:THR:HG22	2:G:507:ILE:N	2.35	0.42
2:G:524:ASP:O	2:G:524:ASP:CG	2.55	0.42
1:H:38:LYS:HB2	1:H:40:PHE:CE1	2.53	0.42
1:A:274:ALA:HB1	1:A:290:LYS:HE3	2.01	0.42
2:B:431:THR:HG21	2:B:463:ARG:HG2	2.01	0.42
2:B:432:GLU:CD	2:B:466:SER:H	2.23	0.42
2:C:145:THR:HG21	2:C:147:SER:OG	2.19	0.42
2:C:218:LYS:CG	2:C:238:SER:OG	2.59	0.42
2:C:278:PRO:HG2	2:C:279:GLU:H	1.83	0.42
2:C:208:PRO:HD3	2:C:531:LYS:O	2.19	0.42
1:D:240:VAL:HB	1:D:258:LEU:HB3	2.00	0.42
1:E:257:LEU:HD12	1:E:258:LEU:N	2.34	0.42
2:G:210:ILE:H	2:G:210:ILE:HD12	1.83	0.42
2:G:384:LEU:O	2:G:387:LEU:N	2.52	0.42
1:A:274:ALA:O	1:A:275:ASN:CB	2.62	0.42
2:B:506:THR:HG22	2:B:507:ILE:N	2.34	0.42
2:B:524:ASP:O	2:B:524:ASP:CG	2.58	0.42
2:C:199:ILE:CG2	2:C:200:GLU:N	2.82	0.42
2:C:271:TRP:CE3	2:C:272:ILE:HG12	2.54	0.42
2:C:321:LEU:O	2:C:324:TYR:N	2.53	0.42
2:F:162:LYS:O	2:F:162:LYS:CG	2.67	0.42
2:F:207:TYR:HA	2:F:208:PRO:HD2	1.81	0.42
2:F:271:TRP:CE3	2:F:272:ILE:HG12	2.55	0.42
2:G:448:GLN:HB2	2:G:477:PHE:CE1	2.55	0.42
2:G:455:GLN:CG	2:G:496:PHE:CD2	3.03	0.42
1:A:288:LEU:CB	1:A:300:ILE:HG13	2.50	0.42
1:A:77:CYS:HA	1:A:83:VAL:HG22	2.01	0.42
1:D:164:PRO:HD2	1:D:176:PRO:HB2	2.01	0.42
1:D:257:LEU:HD12	1:D:258:LEU:N	2.35	0.42
2:B:414:TYR:CD1	2:F:143:ARG:HD3	2.54	0.42
2:F:143:ARG:HH11	2:F:143:ARG:HG3	1.84	0.42
2:F:399:LEU:O	2:F:402:LEU:HB3	2.19	0.42
2:F:495:CYS:C	2:F:497:LEU:H	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:359:LYS:NZ	2:G:370:PHE:H	2.16	0.42
2:G:236:LEU:HD23	2:G:421:ILE:HG21	2.01	0.42
2:G:525:HIS:O	2:G:526:ILE:C	2.57	0.42
1:H:77:CYS:HA	1:H:83:VAL:HG22	2.00	0.42
1:A:102:HIS:NE2	1:A:130:SER:HB3	2.29	0.42
1:A:257:LEU:HD12	1:A:258:LEU:N	2.35	0.42
1:A:291:GLU:N	1:A:297:TRP:CZ3	2.87	0.42
1:A:289:TRP:HA	1:A:298:VAL:O	2.19	0.42
2:B:320:VAL:HG22	2:C:263:GLU:HA	2.01	0.42
2:B:525:HIS:ND1	2:B:525:HIS:N	2.67	0.42
2:C:343:TRP:CZ3	2:C:349:SER:CB	3.03	0.42
2:C:455:GLN:HE21	2:C:496:PHE:HD2	1.66	0.42
1:D:224:ILE:C	1:D:226:LEU:N	2.72	0.42
1:D:241:PHE:HD2	1:D:257:LEU:HA	1.84	0.42
1:D:33:SER:HA	1:D:59:PRO:HB3	2.01	0.42
2:F:177:THR:C	2:F:179:LEU:N	2.72	0.42
2:F:185:PHE:N	2:F:185:PHE:CD1	2.86	0.42
2:G:185:PHE:CD1	2:G:185:PHE:N	2.87	0.42
2:G:321:LEU:O	2:G:324:TYR:N	2.52	0.42
2:G:487:HIS:CD2	2:G:517:LEU:HD23	2.52	0.42
1:A:195:LYS:O	1:A:202:TRP:HA	2.20	0.42
2:B:162:LYS:O	2:B:162:LYS:CG	2.67	0.42
2:B:384:LEU:O	2:B:387:LEU:N	2.51	0.42
2:B:263:GLU:HA	2:C:320:VAL:HG22	2.01	0.42
1:D:293:VAL:HG12	1:D:293:VAL:O	2.19	0.42
1:D:40:PHE:CD1	1:D:40:PHE:N	2.88	0.42
1:E:204:GLU:O	1:E:204:GLU:HG3	2.18	0.42
2:F:385:LEU:N	2:F:406:HIS:CE1	2.87	0.42
2:G:145:THR:HG21	2:G:147:SER:OG	2.19	0.42
2:G:154:SER:OG	2:G:158:MET:HB2	2.20	0.42
2:G:246:TYR:CE1	2:G:259:LEU:HD13	2.55	0.42
2:G:481:LEU:HD13	2:G:489:HIS:CB	2.17	0.42
1:A:164:PRO:HD2	1:A:176:PRO:HB2	2.01	0.42
1:A:214:TRP:O	1:A:235:SER:CB	2.56	0.42
1:A:258:LEU:HD13	1:A:297:TRP:CG	2.53	0.42
1:A:66:ALA:HB3	1:A:73:ILE:HB	2.01	0.42
2:B:199:ILE:CG2	2:B:200:GLU:N	2.82	0.42
2:C:432:GLU:CD	2:C:466:SER:HB3	2.38	0.42
1:E:271:SER:HB2	2:F:153:PHE:CE2	2.55	0.42
2:F:148:TYR:CE1	2:F:149:THR:O	2.73	0.42
2:F:506:THR:HG22	2:F:507:ILE:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:ASP:C	1:A:285:LYS:H	2.23	0.42
2:B:271:TRP:CE3	2:B:272:ILE:HG12	2.54	0.42
2:B:298:LEU:HD23	2:B:298:LEU:HA	1.85	0.42
2:B:321:LEU:O	2:B:324:TYR:N	2.53	0.42
1:D:145:ILE:HD11	1:D:202:TRP:HB3	2.01	0.42
1:D:49:LEU:HD11	1:D:51:ALA:O	2.20	0.42
1:E:72:ASN:HD22	1:E:72:ASN:HA	1.71	0.42
1:E:40:PHE:CE2	2:F:168:SER:HB2	2.52	0.42
2:F:220:ALA:HB3	2:F:234:TRP:CE3	2.54	0.42
2:G:271:TRP:CE3	2:G:272:ILE:HG12	2.54	0.42
2:G:215:LEU:HD13	2:G:452:TYR:HE1	1.85	0.42
1:H:206:GLN:OE1	1:H:251:ASN:O	2.38	0.42
2:B:143:ARG:HG3	2:B:143:ARG:HH11	1.84	0.42
2:B:302:ASP:HA	2:C:304:VAL:HG21	2.01	0.42
2:B:462:THR:O	2:B:463:ARG:HD2	2.19	0.42
2:C:262:LYS:O	2:C:263:GLU:C	2.56	0.42
1:D:192:LYS:HD3	1:D:204:GLU:OE1	2.19	0.42
1:D:245:CYS:SG	1:D:246:ASP:N	2.92	0.42
2:F:522:THR:HG21	2:F:526:ILE:CD1	2.50	0.42
2:F:263:GLU:HB2	2:G:320:VAL:HG21	2.02	0.42
2:G:343:TRP:HZ3	2:G:350:ILE:CG2	2.30	0.42
2:G:375:LEU:HB3	2:G:379:PHE:CD1	2.54	0.42
2:G:435:TYR:CE2	2:G:454:ILE:HD11	2.55	0.42
1:H:258:LEU:HD13	1:H:297:TRP:CB	2.50	0.42
1:A:247:ASP:OD1	1:A:248:ALA:N	2.53	0.41
1:A:49:LEU:HD11	1:A:51:ALA:O	2.19	0.41
2:B:140:LYS:C	2:B:142:ARG:N	2.73	0.41
2:B:148:TYR:CE1	2:B:149:THR:O	2.73	0.41
2:B:329:ASP:HB3	2:B:332:ILE:HD13	2.02	0.41
2:B:432:GLU:OE1	2:B:466:SER:N	2.49	0.41
2:C:236:LEU:HD23	2:C:421:ILE:HG21	2.02	0.41
1:D:77:CYS:HA	1:D:83:VAL:HG22	2.01	0.41
1:E:214:TRP:O	1:E:235:SER:CB	2.56	0.41
1:E:230:THR:O	1:E:231:ILE:HG13	2.20	0.41
1:E:49:LEU:HD11	1:E:51:ALA:O	2.19	0.41
2:G:329:ASP:HB3	2:G:332:ILE:HD13	2.02	0.41
2:G:494:SER:OG	2:G:506:THR:HG21	2.20	0.41
1:H:257:LEU:HD12	1:H:258:LEU:N	2.35	0.41
1:H:258:LEU:HD13	1:H:297:TRP:CG	2.55	0.41
1:H:287:THR:O	1:H:288:LEU:HD23	2.19	0.41
1:A:194:TRP:CD1	1:A:194:TRP:N	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:THR:O	1:A:231:ILE:HG13	2.20	0.41
1:A:293:VAL:O	1:A:293:VAL:HG12	2.20	0.41
1:D:197:GLU:O	1:D:198:GLU:CB	2.68	0.41
1:D:234:CYS:HB3	1:D:268:VAL:HG21	2.02	0.41
1:E:14:ASP:CG	1:E:15:MET:H	2.24	0.41
1:E:247:ASP:C	1:E:249:SER:H	2.23	0.41
1:E:47:GLN:OE1	2:F:166:GLY:CA	2.68	0.41
2:F:321:LEU:O	2:F:324:TYR:N	2.53	0.41
2:F:359:LYS:HZ1	2:F:368:GLY:HA3	1.85	0.41
2:F:451:TRP:CE2	2:F:493:VAL:HG13	2.55	0.41
2:F:525:HIS:ND1	2:F:525:HIS:N	2.67	0.41
2:G:199:ILE:CG2	2:G:200:GLU:N	2.83	0.41
2:G:482:GLU:CD	2:G:509:ARG:HH22	2.24	0.41
2:G:546:ARG:HH11	2:G:546:ARG:HG3	1.86	0.41
1:A:77:CYS:SG	1:A:106:VAL:O	2.67	0.41
1:A:183:ALA:O	1:A:184:SER:CB	2.67	0.41
1:A:241:PHE:CD2	1:A:257:LEU:HA	2.54	0.41
2:B:202:ARG:HG2	2:B:209:GLN:HB2	2.02	0.41
2:B:381:TRP:HA	2:B:384:LEU:HD12	2.01	0.41
2:B:451:TRP:HZ2	2:B:496:PHE:CD1	2.38	0.41
2:C:148:TYR:HB2	1:D:266:TRP:CD2	2.55	0.41
2:C:246:TYR:CD2	2:C:248:TYR:O	2.73	0.41
2:F:432:GLU:OE1	2:F:466:SER:HB3	2.20	0.41
1:H:224:ILE:C	1:H:226:LEU:N	2.72	0.41
1:H:264:VAL:CG1	1:H:265:VAL:N	2.82	0.41
1:H:283:ASP:C	1:H:285:LYS:H	2.23	0.41
1:H:258:LEU:HD13	1:H:297:TRP:HB2	2.02	0.41
2:B:220:ALA:HB3	2:B:234:TRP:CE3	2.54	0.41
2:C:480:GLN:CA	2:C:480:GLN:OE1	2.66	0.41
1:D:194:TRP:N	1:D:194:TRP:CD1	2.88	0.41
1:E:77:CYS:HA	1:E:83:VAL:HG22	2.01	0.41
2:G:143:ARG:HB2	1:H:216:ARG:NH2	2.35	0.41
2:G:269:THR:O	2:G:273:VAL:HG23	2.20	0.41
2:G:340:LEU:HD21	2:G:358:TYR:HB3	2.02	0.41
2:G:375:LEU:HB3	2:G:379:PHE:HD1	1.85	0.41
1:A:266:TRP:CZ3	2:B:144:PHE:CD2	3.08	0.41
2:C:289:ASN:O	2:C:291:ILE:N	2.53	0.41
2:C:546:ARG:HH11	2:C:546:ARG:HG3	1.86	0.41
2:F:140:LYS:C	2:F:142:ARG:N	2.73	0.41
2:F:522:THR:HG21	2:F:526:ILE:HD12	2.03	0.41
2:F:546:ARG:HG3	2:F:546:ARG:HH11	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:343:TRP:HZ3	2:G:350:ILE:CB	2.34	0.41
2:G:291:ILE:CD1	2:G:351:ASP:OD2	2.65	0.41
1:A:271:SER:HB2	2:B:153:PHE:CE2	2.56	0.41
2:B:247:PRO:HG2	2:B:248:TYR:H	1.85	0.41
2:B:366:PHE:O	2:B:373:LYS:HG3	2.21	0.41
2:B:445:LEU:HA	2:B:445:LEU:HD23	1.89	0.41
2:B:217:PHE:HE2	2:B:449:PHE:CE1	2.38	0.41
2:C:481:LEU:HA	2:C:484:ALA:HB3	2.02	0.41
2:C:525:HIS:O	2:C:526:ILE:C	2.58	0.41
1:D:283:ASP:C	1:D:285:LYS:H	2.23	0.41
1:E:241:PHE:C	1:E:242:ILE:HG13	2.40	0.41
2:F:329:ASP:HB3	2:F:332:ILE:HD13	2.03	0.41
2:G:512:MET:HA	2:G:540:ALA:CB	2.50	0.41
1:H:196:GLU:HB3	1:H:202:TRP:CE2	2.55	0.41
1:A:18:ASP:OD2	1:A:62:GLN:HG2	2.21	0.41
2:B:230:ASP:O	2:B:231:TYR:C	2.59	0.41
2:B:269:THR:O	2:B:273:VAL:HG23	2.21	0.41
2:C:154:SER:OG	2:C:158:MET:HB2	2.20	0.41
2:C:244:VAL:HG12	2:C:260:LEU:HD22	2.03	0.41
2:C:474:THR:HG23	2:C:493:VAL:CG1	2.51	0.41
2:C:551:TYR:HD2	2:C:552:LEU:HD23	1.85	0.41
1:D:14:ASP:CG	1:D:15:MET:H	2.24	0.41
1:E:21:MET:HA	1:E:28:LEU:HD12	2.01	0.41
2:G:366:PHE:O	2:G:373:LYS:HG3	2.21	0.41
2:B:139:MET:O	2:B:144:PHE:HB2	2.21	0.41
2:B:145:THR:CG2	2:B:146:ALA:N	2.84	0.41
2:B:399:LEU:HD23	2:B:425:TYR:OH	2.20	0.41
2:C:343:TRP:CE3	2:C:349:SER:HB3	2.56	0.41
2:C:208:PRO:CB	2:C:530:LEU:O	2.69	0.41
1:D:21:MET:HA	1:D:28:LEU:HD12	2.01	0.41
1:E:107:ASN:CG	2:F:142:ARG:NH2	2.73	0.41
2:F:252:ASN:O	2:F:255:VAL:N	2.49	0.41
2:F:291:ILE:HG22	2:F:353:ASN:CB	2.50	0.41
2:F:316:GLY:O	2:F:319:SER:N	2.54	0.41
2:G:213:SER:HB3	2:G:459:PHE:CD2	2.56	0.41
1:H:240:VAL:HB	1:H:258:LEU:HB3	2.03	0.41
1:A:241:PHE:HE2	1:A:257:LEU:HB2	1.84	0.41
2:B:316:GLY:O	2:B:319:SER:N	2.54	0.41
2:B:370:PHE:HA	2:B:370:PHE:HD2	1.75	0.41
2:B:532:ILE:HG23	2:B:533:PRO:CD	2.51	0.41
2:C:153:PHE:HA	2:C:158:MET:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:269:THR:O	2:C:273:VAL:HG23	2.20	0.41
2:C:316:GLY:O	2:C:319:SER:N	2.54	0.41
2:C:152:LYS:NZ	1:D:18:ASP:OD2	2.50	0.41
1:D:18:ASP:OD2	1:D:62:GLN:HG2	2.21	0.41
2:F:230:ASP:O	2:F:231:TYR:C	2.59	0.41
2:F:381:TRP:HA	2:F:384:LEU:HD12	2.02	0.41
2:F:236:LEU:HD22	2:F:418:ILE:HG22	2.02	0.41
2:G:411:SER:C	2:G:412:LEU:HD12	2.41	0.41
1:H:191:ILE:HD13	1:H:233:SER:HB3	2.03	0.41
2:G:153:PHE:CE2	1:H:271:SER:HB3	2.56	0.41
1:A:14:ASP:CG	1:A:15:MET:H	2.24	0.41
1:A:226:LEU:HD12	1:A:228:THR:H	1.86	0.41
2:B:380:SER:O	2:B:383:CYS:N	2.50	0.41
2:B:442:THR:CG2	2:B:444:ALA:CB	2.99	0.41
2:C:186:ASP:OD1	2:C:186:ASP:C	2.60	0.41
2:C:366:PHE:O	2:C:373:LYS:HG3	2.21	0.41
1:E:18:ASP:OD2	1:E:62:GLN:HG2	2.21	0.41
1:E:40:PHE:CD1	1:E:40:PHE:N	2.89	0.41
2:F:139:MET:O	2:F:144:PHE:HB2	2.20	0.41
2:F:155:THR:HG22	2:F:513:ARG:HD3	2.03	0.41
2:F:186:ASP:OD1	2:F:186:ASP:C	2.59	0.41
2:F:330:PRO:O	2:F:331:ARG:C	2.57	0.41
2:F:209:GLN:HG2	2:F:497:LEU:O	2.21	0.41
2:G:352:LYS:HE2	2:G:356:LYS:HE3	2.03	0.41
1:H:293:VAL:O	1:H:293:VAL:HG12	2.21	0.41
2:C:244:VAL:CG1	2:C:260:LEU:HD22	2.51	0.41
1:D:132:LEU:CD2	1:D:142:VAL:HG13	2.51	0.41
1:E:53:LEU:H	1:E:53:LEU:HD23	1.80	0.41
2:F:445:LEU:CD2	2:F:449:PHE:CD2	2.98	0.41
2:G:381:TRP:CH2	2:G:382:LEU:HD13	2.56	0.41
2:G:414:TYR:CD2	2:G:414:TYR:C	2.94	0.41
1:H:18:ASP:OD2	1:H:62:GLN:HG2	2.20	0.41
2:B:186:ASP:OD1	2:B:186:ASP:C	2.59	0.40
2:B:191:ASP:OD1	2:B:529:ARG:NH1	2.54	0.40
2:B:202:ARG:HG2	2:B:209:GLN:CD	2.42	0.40
2:C:202:ARG:HG2	2:C:209:GLN:HB2	2.02	0.40
2:C:343:TRP:HZ3	2:C:349:SER:CB	2.33	0.40
1:D:102:HIS:NE2	1:D:130:SER:HB3	2.29	0.40
1:E:15:MET:HG3	2:F:162:LYS:HZ2	1.83	0.40
1:E:303:VAL:HG12	1:E:304:ASN:N	2.37	0.40
2:F:432:GLU:OE1	2:F:466:SER:N	2.48	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:186:ASP:C	2:G:186:ASP:OD1	2.59	0.40
2:G:467:LYS:HA	2:G:498:ASN:ND2	2.36	0.40
1:H:135:THR:CG2	1:H:136:GLY:N	2.62	0.40
1:A:132:LEU:CD2	1:A:142:VAL:HG13	2.51	0.40
2:B:177:THR:HG22	2:B:179:LEU:HD23	1.98	0.40
2:C:329:ASP:HB3	2:C:332:ILE:HD13	2.03	0.40
2:C:489:HIS:O	2:C:490:SER:C	2.60	0.40
2:C:530:LEU:HB2	2:C:532:ILE:HG12	2.03	0.40
1:D:226:LEU:HD12	1:D:228:THR:H	1.87	0.40
1:D:230:THR:O	1:D:231:ILE:HG13	2.20	0.40
1:D:240:VAL:O	1:D:258:LEU:CB	2.69	0.40
2:F:366:PHE:O	2:F:373:LYS:HG3	2.21	0.40
2:F:210:ILE:HD13	2:F:496:PHE:CG	2.56	0.40
2:G:153:PHE:HA	2:G:158:MET:O	2.21	0.40
1:H:14:ASP:CG	1:H:15:MET:H	2.24	0.40
1:H:194:TRP:N	1:H:194:TRP:CD1	2.88	0.40
1:H:21:MET:HA	1:H:28:LEU:HD12	2.02	0.40
2:B:199:ILE:CG2	2:B:208:PRO:HB2	2.52	0.40
2:B:371:SER:HG	2:B:373:LYS:H	1.66	0.40
2:B:217:PHE:CZ	2:B:453:LEU:HD23	2.56	0.40
1:D:69:MET:HE1	1:D:114:HIS:HB2	2.01	0.40
2:G:261:LYS:HG3	2:G:262:LYS:N	2.36	0.40
2:G:316:GLY:O	2:G:319:SER:N	2.54	0.40
2:G:451:TRP:CE2	2:G:493:VAL:HG13	2.56	0.40
2:G:522:THR:O	2:G:523:ASN:CG	2.59	0.40
1:H:230:THR:O	1:H:231:ILE:HG13	2.20	0.40
1:A:69:MET:HE1	1:A:114:HIS:HB2	2.01	0.40
1:A:113:PRO:HB3	1:A:161:ALA:HB2	2.00	0.40
2:B:161:THR:O	2:B:171:SER:N	2.55	0.40
2:B:381:TRP:CD2	2:B:412:LEU:HD22	2.56	0.40
2:B:480:GLN:OE1	2:B:483:PHE:HD1	2.05	0.40
2:C:177:THR:CG2	2:C:179:LEU:H	2.16	0.40
2:C:198:THR:HB	2:C:212:GLU:HB2	2.03	0.40
2:C:241:PHE:CD2	2:C:457:LEU:HD21	2.57	0.40
2:C:261:LYS:HG3	2:C:262:LYS:N	2.36	0.40
2:C:442:THR:CG2	2:C:444:ALA:CB	2.99	0.40
1:D:113:PRO:HB2	1:D:161:ALA:HB2	2.03	0.40
1:E:194:TRP:N	1:E:194:TRP:CD1	2.89	0.40
1:E:221:ALA:HA	1:E:270:TRP:CD1	2.56	0.40
2:F:145:THR:CG2	2:F:146:ALA:N	2.84	0.40
2:F:198:THR:HB	2:F:212:GLU:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:261:LYS:HG3	2:F:262:LYS:N	2.36	0.40
2:F:276:ILE:HD13	2:F:383:CYS:CA	2.39	0.40
2:G:177:THR:C	2:G:179:LEU:H	2.25	0.40
2:G:272:ILE:HG13	2:G:272:ILE:H	1.67	0.40
1:H:18:ASP:OD1	1:H:19:ALA:N	2.55	0.40
1:H:226:LEU:HD12	1:H:228:THR:H	1.87	0.40
1:A:283:ASP:O	1:A:284:ASN:HB2	2.22	0.40
2:B:177:THR:HG21	2:B:484:ALA:HB2	2.03	0.40
2:B:198:THR:HB	2:B:212:GLU:HB2	2.04	0.40
2:B:261:LYS:HG3	2:B:262:LYS:N	2.36	0.40
2:C:202:ARG:HD3	2:C:202:ARG:HA	1.55	0.40
2:F:174:ARG:NH2	2:F:485:GLN:OE1	2.46	0.40
2:G:202:ARG:HG2	2:G:209:GLN:HB2	2.02	0.40
2:G:175:LEU:CD2	2:G:483:PHE:HE2	2.34	0.40
1:H:102:HIS:NE2	1:H:130:SER:HB3	2.29	0.40
1:H:283:ASP:O	1:H:284:ASN:HB2	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	281/316 (89%)	231 (82%)	42 (15%)	8 (3%)	5	25
1	D	279/316 (88%)	226 (81%)	43 (15%)	10 (4%)	3	19
1	E	281/316 (89%)	231 (82%)	43 (15%)	7 (2%)	5	28
1	H	279/316 (88%)	228 (82%)	43 (15%)	8 (3%)	4	24
2	B	421/442 (95%)	336 (80%)	68 (16%)	17 (4%)	3	17
2	C	416/442 (94%)	330 (79%)	73 (18%)	13 (3%)	4	23
2	F	421/442 (95%)	337 (80%)	65 (15%)	19 (4%)	2	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	G	416/442 (94%)	330 (79%)	73 (18%)	13 (3%)	4	23
All	All	2794/3032 (92%)	2249 (80%)	450 (16%)	95 (3%)	3	20

All (95) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	251	ASN
2	B	164	ILE
2	B	371	SER
2	B	428	ASN
2	B	520	ALA
2	B	523	ASN
2	C	371	SER
2	C	395	ASP
2	C	428	ASN
2	C	520	ALA
2	C	523	ASN
2	F	164	ILE
2	F	371	SER
2	F	428	ASN
2	F	520	ALA
2	F	523	ASN
2	G	371	SER
2	G	428	ASN
2	G	496	PHE
2	G	520	ALA
2	G	523	ASN
1	H	249	SER
1	A	114	HIS
2	B	178	GLU
2	B	247	PRO
2	B	346	GLY
2	B	499	ASP
2	B	526	ILE
2	C	526	ILE
1	D	114	HIS
1	D	250	SER
1	E	114	HIS
2	F	178	GLU
2	F	346	GLY
2	F	394	ILE
2	F	499	ASP

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Mol	Chain	Res	Type
2	F	526	ILE
2	G	500	ASP
2	G	526	ILE
1	H	114	HIS
1	A	184	SER
2	B	157	SER
2	B	447	VAL
2	C	393	GLN
2	C	447	VAL
1	D	184	SER
1	E	184	SER
2	F	157	SER
2	F	447	VAL
2	F	486	LEU
2	G	395	ASP
2	G	447	VAL
1	H	184	SER
1	A	55	GLY
2	B	182	LYS
2	B	431	THR
2	C	182	LYS
2	C	431	THR
1	D	55	GLY
1	D	198	GLU
1	E	55	GLY
2	F	182	LYS
2	F	431	THR
2	G	182	LYS
2	G	431	THR
1	H	55	GLY
1	A	68	PRO
2	C	250	THR
1	D	68	PRO
1	D	247	ASP
1	E	68	PRO
2	F	247	PRO
2	F	393	GLN
2	G	524	ASP
1	H	68	PRO
2	B	226	LYS
2	C	226	LYS
2	C	290	GLU

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Mol	Chain	Res	Type
2	F	226	LYS
2	G	346	GLY
2	B	172	ILE
2	F	172	ILE
1	A	129	ILE
1	A	176	PRO
2	B	347	GLY
1	D	129	ILE
1	D	176	PRO
1	E	129	ILE
1	E	176	PRO
1	H	129	ILE
1	H	176	PRO
1	D	224	ILE
1	A	224	ILE
1	E	224	ILE
1	H	224	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	240/267 (90%)	222 (92%)	18 (8%)	13	43
1	D	238/267 (89%)	218 (92%)	20 (8%)	11	38
1	E	240/267 (90%)	222 (92%)	18 (8%)	13	43
1	H	238/267 (89%)	219 (92%)	19 (8%)	12	40
2	B	386/403 (96%)	352 (91%)	34 (9%)	10	36
2	C	384/403 (95%)	356 (93%)	28 (7%)	14	44
2	F	386/403 (96%)	349 (90%)	37 (10%)	8	32
2	G	384/403 (95%)	352 (92%)	32 (8%)	11	39
All	All	2496/2680 (93%)	2290 (92%)	206 (8%)	11	39

All (206) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	27	ARG
1	A	39	ILE
1	A	53	LEU
1	A	54	ARG
1	A	70	TYR
1	A	86	TRP
1	A	184	SER
1	A	193	LEU
1	A	201	GLN
1	A	220	TRP
1	A	226	LEU
1	A	244	THR
1	A	271	SER
1	A	280	SER
1	A	283	ASP
1	A	287	THR
1	A	298	VAL
1	A	300	ILE
2	B	133	ASP
2	B	141	GLU
2	B	142	ARG
2	B	158	MET
2	B	159	LEU
2	B	160	LEU
2	B	163	ASP
2	B	164	ILE
2	B	179	LEU
2	B	209	GLN
2	B	223	TYR
2	B	228	SER
2	B	267	ARG
2	B	282	GLU
2	B	299	LEU
2	B	321	LEU
2	B	339	GLN
2	B	365	PRO
2	B	370	PHE
2	B	378	GLU
2	B	395	ASP
2	B	397	TYR
2	B	401	SER
2	B	418	ILE
2	B	421	ILE

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Mol	Chain	Res	Type
2	B	431	THR
2	B	453	LEU
2	B	455	GLN
2	B	463	ARG
2	B	466	SER
2	B	470	SER
2	B	505	ASP
2	B	532	ILE
2	B	550	ASN
2	C	133	ASP
2	C	138	ILE
2	C	139	MET
2	C	150	PHE
2	C	175	LEU
2	C	209	GLN
2	C	223	TYR
2	C	228	SER
2	C	267	ARG
2	C	282	GLU
2	C	299	LEU
2	C	321	LEU
2	C	339	GLN
2	C	365	PRO
2	C	370	PHE
2	C	378	GLU
2	C	401	SER
2	C	418	ILE
2	C	421	ILE
2	C	431	THR
2	C	453	LEU
2	C	455	GLN
2	C	466	SER
2	C	470	SER
2	C	492	PHE
2	C	495	CYS
2	C	505	ASP
2	C	550	ASN
1	D	27	ARG
1	D	41	ASP
1	D	53	LEU
1	D	54	ARG
1	D	70	TYR

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Mol	Chain	Res	Type
1	D	86	TRP
1	D	184	SER
1	D	193	LEU
1	D	220	TRP
1	D	226	LEU
1	D	246	ASP
1	D	247	ASP
1	D	261	PHE
1	D	271	SER
1	D	280	SER
1	D	283	ASP
1	D	287	THR
1	D	296	GLN
1	D	299	CYS
1	D	301	SER
1	E	27	ARG
1	E	53	LEU
1	E	54	ARG
1	E	70	TYR
1	E	86	TRP
1	E	184	SER
1	E	193	LEU
1	E	201	GLN
1	E	220	TRP
1	E	226	LEU
1	E	244	THR
1	E	252	THR
1	E	271	SER
1	E	280	SER
1	E	283	ASP
1	E	287	THR
1	E	298	VAL
1	E	300	ILE
2	F	133	ASP
2	F	141	GLU
2	F	142	ARG
2	F	158	MET
2	F	159	LEU
2	F	160	LEU
2	F	163	ASP
2	F	164	ILE
2	F	179	LEU

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Mol	Chain	Res	Type
2	F	209	GLN
2	F	223	TYR
2	F	228	SER
2	F	253	ASP
2	F	267	ARG
2	F	282	GLU
2	F	299	LEU
2	F	321	LEU
2	F	339	GLN
2	F	365	PRO
2	F	370	PHE
2	F	378	GLU
2	F	379	PHE
2	F	393	GLN
2	F	397	TYR
2	F	401	SER
2	F	412	LEU
2	F	418	ILE
2	F	421	ILE
2	F	431	THR
2	F	453	LEU
2	F	455	GLN
2	F	466	SER
2	F	470	SER
2	F	486	LEU
2	F	489	HIS
2	F	505	ASP
2	F	550	ASN
2	G	133	ASP
2	G	138	ILE
2	G	139	MET
2	G	150	PHE
2	G	175	LEU
2	G	209	GLN
2	G	223	TYR
2	G	228	SER
2	G	244	VAL
2	G	267	ARG
2	G	282	GLU
2	G	299	LEU
2	G	321	LEU
2	G	339	GLN

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Mol	Chain	Res	Type
2	G	365	PRO
2	G	370	PHE
2	G	378	GLU
2	G	380	SER
2	G	401	SER
2	G	412	LEU
2	G	414	TYR
2	G	418	ILE
2	G	421	ILE
2	G	431	THR
2	G	453	LEU
2	G	455	GLN
2	G	466	SER
2	G	470	SER
2	G	494	SER
2	G	495	CYS
2	G	505	ASP
2	G	550	ASN
1	H	27	ARG
1	H	53	LEU
1	H	54	ARG
1	H	70	TYR
1	H	86	TRP
1	H	184	SER
1	H	193	LEU
1	H	195	LYS
1	H	220	TRP
1	H	226	LEU
1	H	246	ASP
1	H	247	ASP
1	H	271	SER
1	H	280	SER
1	H	283	ASP
1	H	287	THR
1	H	296	GLN
1	H	299	CYS
1	H	301	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	HIS

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Mol	Chain	Res	Type
1	A	275	ASN
1	A	296	GLN
2	B	232	ASN
2	B	341	GLN
2	B	353	ASN
2	B	448	GLN
2	B	455	GLN
2	B	487	HIS
2	C	232	ASN
2	C	275	GLN
2	C	328	ASN
2	C	341	GLN
2	C	455	GLN
2	C	487	HIS
1	D	47	GLN
1	D	62	GLN
1	D	72	ASN
1	D	114	HIS
1	E	17	HIS
1	E	107	ASN
1	E	114	HIS
1	E	251	ASN
1	E	267	HIS
1	E	275	ASN
2	F	232	ASN
2	F	275	GLN
2	F	341	GLN
2	F	455	GLN
2	G	232	ASN
2	G	275	GLN
2	G	341	GLN
2	G	353	ASN
2	G	455	GLN
2	G	487	HIS
2	G	498	ASN
1	H	47	GLN
1	H	114	HIS
1	H	206	GLN
1	H	296	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	285/316 (90%)	-0.03	7 (2%) 57 29	79, 129, 189, 200	0
1	D	283/316 (89%)	0.86	52 (18%) 1 0	119, 185, 200, 200	0
1	E	285/316 (90%)	0.02	15 (5%) 26 10	70, 128, 189, 200	0
1	H	283/316 (89%)	0.48	28 (9%) 7 2	108, 174, 200, 200	0
2	B	423/442 (95%)	-0.22	9 (2%) 63 34	70, 134, 189, 200	0
2	C	420/442 (95%)	-0.18	14 (3%) 46 20	99, 150, 195, 200	0
2	F	423/442 (95%)	-0.21	14 (3%) 46 20	70, 142, 193, 200	0
2	G	420/442 (95%)	-0.22	15 (3%) 42 17	92, 151, 197, 200	0
All	All	2822/3032 (93%)	0.01	154 (5%) 25 9	70, 149, 200, 200	0

All (154) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	248	ALA	10.8
1	H	247	ASP	8.4
1	E	282	GLY	6.0
1	D	155	ALA	5.9
1	D	122	CYS	5.8
1	H	14	ASP	5.2
1	D	233	SER	5.2
1	A	171	PRO	5.0
1	H	234	CYS	4.9
1	A	282	GLY	4.8
1	D	57	GLU	4.8
1	H	171	PRO	4.7
2	F	394	ILE	4.7
1	D	249	SER	4.7
1	D	152	GLY	4.7
2	C	552	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
1	D	123	GLY	4.5
1	E	14	ASP	4.5
1	E	171	PRO	4.4
1	D	174	GLN	4.3
2	C	346	GLY	4.3
1	D	209	GLU	4.3
2	F	349	SER	4.2
1	A	283	ASP	4.1
2	F	395	ASP	4.1
1	E	233	SER	4.0
2	C	130	ASP	3.9
2	B	132	ILE	3.9
1	D	207	LYS	3.9
2	F	551	TYR	3.7
1	D	173	GLY	3.7
1	D	178	TYR	3.6
1	H	284	ASN	3.6
1	D	146	ASN	3.6
1	E	283	ASP	3.6
1	H	174	GLN	3.6
1	D	172	SER	3.5
1	H	209	GLU	3.5
1	D	79	TYR	3.5
2	B	348	CYS	3.5
1	D	201	GLN	3.5
1	D	151	ILE	3.5
1	D	293	VAL	3.4
1	D	239	ARG	3.4
1	H	173	GLY	3.4
1	A	249	SER	3.4
2	C	131	GLU	3.4
1	E	248	ALA	3.3
2	C	203	LYS	3.2
1	E	234	CYS	3.2
2	B	495	CYS	3.2
2	B	133	ASP	3.2
1	D	250	SER	3.2
1	D	177	ASN	3.2
1	D	206	GLN	3.2
2	F	131	GLU	3.1
1	A	172	SER	3.1
1	H	239	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	249	SER	3.1
2	G	367	GLU	3.1
2	G	395	ASP	3.0
2	B	131	GLU	2.9
2	G	345	THR	2.9
1	E	173	GLY	2.9
1	D	154	ASN	2.9
2	G	393	GLN	2.9
2	G	346	GLY	2.9
2	F	520	ALA	2.9
1	D	144	LYS	2.9
1	H	199	ASP	2.8
1	D	222	PRO	2.8
2	G	225	GLU	2.8
1	E	172	SER	2.8
1	D	200	GLY	2.8
2	G	341	GLN	2.8
1	D	108	SER	2.8
1	H	227	PRO	2.8
1	H	163	VAL	2.8
2	G	130	ASP	2.7
2	B	130	ASP	2.7
1	D	223	SER	2.7
2	B	251	ASP	2.7
2	F	132	ILE	2.7
1	D	241	PHE	2.7
1	D	224	ILE	2.6
2	C	394	ILE	2.6
1	H	225	GLY	2.6
2	C	345	THR	2.6
1	H	172	SER	2.6
2	G	521	SER	2.6
1	D	248	ALA	2.6
2	G	349	SER	2.6
2	F	130	ASP	2.6
2	F	314	LYS	2.6
2	F	369	LEU	2.6
1	D	176	PRO	2.5
2	C	348	CYS	2.5
1	H	241	PHE	2.5
2	B	394	ILE	2.5
1	D	171	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	174	GLN	2.5
1	D	147	ASN	2.5
1	D	14	ASP	2.5
2	G	443	ASN	2.5
1	D	161	ALA	2.5
1	H	262	ASN	2.4
2	C	135	ALA	2.4
1	D	292	SER	2.4
1	D	107	ASN	2.4
1	D	76	SER	2.4
1	H	233	SER	2.4
1	D	103	ASP	2.4
1	H	200	GLY	2.4
2	F	521	SER	2.4
1	D	163	VAL	2.4
1	H	175	LYS	2.4
1	E	209	GLU	2.4
1	D	55	GLY	2.4
1	D	281	GLY	2.4
2	C	132	ILE	2.4
2	C	164	ILE	2.3
2	G	348	CYS	2.3
1	H	253	TRP	2.3
2	G	326	GLY	2.3
1	H	294	ASP	2.3
1	H	246	ASP	2.3
2	F	348	CYS	2.3
1	D	153	CYS	2.3
1	D	130	SER	2.3
1	H	217	ASP	2.2
1	A	248	ALA	2.2
1	D	234	CYS	2.2
2	G	178	GLU	2.2
1	A	247	ASP	2.2
2	C	133	ASP	2.2
2	F	346	GLY	2.2
1	D	247	ASP	2.2
1	H	15	MET	2.2
1	E	284	ASN	2.2
1	E	164	PRO	2.1
1	H	190	LEU	2.1
2	F	345	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	246	ASP	2.1
2	G	524	ASP	2.1
2	C	347	GLY	2.1
1	H	82	LYS	2.1
2	B	346	GLY	2.1
1	D	82	LYS	2.1
1	D	135	THR	2.0
1	H	164	PRO	2.0
1	D	215	VAL	2.0
1	E	122	CYS	2.0
2	C	155	THR	2.0
1	D	92	THR	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.