



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 18, 2018 – 06:56 pm GMT

PDB ID : 1HQM  
Title : CRYSTAL STRUCTURE OF THERMUS AQUATICUS CORE RNA POLYMERASE-INCLUDES COMPLETE STRUCTURE WITH SIDE-CHAINS (EXCEPT FOR DISORDERED REGIONS)-FURTHER REFINED FROM ORIGINAL DEPOSITION-CONTAINS ADDITIONAL SEQUENCE INFORMATION  
Authors : Minakhin, L.; Bhagat, S.; Brunning, A.; Campbell, E.A.; Darst, S.A.; Ebright, R.H.; Severinov, K.  
Deposited on : 2000-12-18  
Resolution : 3.30 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk30686

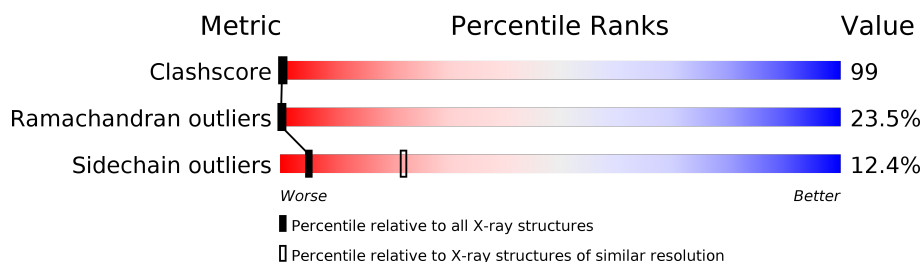
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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))
Clashscore	122078	1021 (3.34-3.26)
Ramachandran outliers	120005	1003 (3.34-3.26)
Sidechain outliers	119972	1002 (3.34-3.26)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	313	
1	B	313	
2	C	1119	
3	D	1265	
4	E	99	

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 21254 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total	C	N	O	S	0	0	0
			1750	1118	302	328	2			
1	B	229	Total	C	N	O	S	0	0	0
			1776	1135	305	334	2			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LYS	deletion	UNP Q9KWU8
A	93	ARG	MET	conflict	UNP Q9KWU8
A	94	TRP	ALA	conflict	UNP Q9KWU8
A	95	ARG	SER	conflict	UNP Q9KWU8
A	111	VAL	GLY	conflict	UNP Q9KWU8
B	?	-	LYS	deletion	UNP Q9KWU8
B	93	ARG	MET	conflict	UNP Q9KWU8
B	94	TRP	ALA	conflict	UNP Q9KWU8
B	95	ARG	SER	conflict	UNP Q9KWU8
B	111	VAL	GLY	conflict	UNP Q9KWU8

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1113	Total	C	N	O	S	12	0	0
			8508	5386	1514	1585	23			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	2	LYS	GLU	conflict	UNP Q9KWU7

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1175	Total	C	N	O	S	17	0	0
			8499	5328	1549	1595	27			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	119	PHE	SER	conflict	UNP Q9KWU6
D	863	THR	VAL	conflict	UNP Q9KWU6
D	866	THR	VAL	conflict	UNP Q9KWU6
D	876	ASN	SER	conflict	UNP Q9KWU6
D	947	ILE	-	insertion	UNP Q9KWU6
D	1010	ASN	LYS	conflict	UNP Q9KWU6
D	1117	LYS	ASN	conflict	UNP Q9KWU6
D	1389	PRO	ARG	conflict	UNP Q9KWU6

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	98	Total	C	N	O	S	0	0	0
			719	453	132	130	4			

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	1	Total	Mg	0	0
			1	1		

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

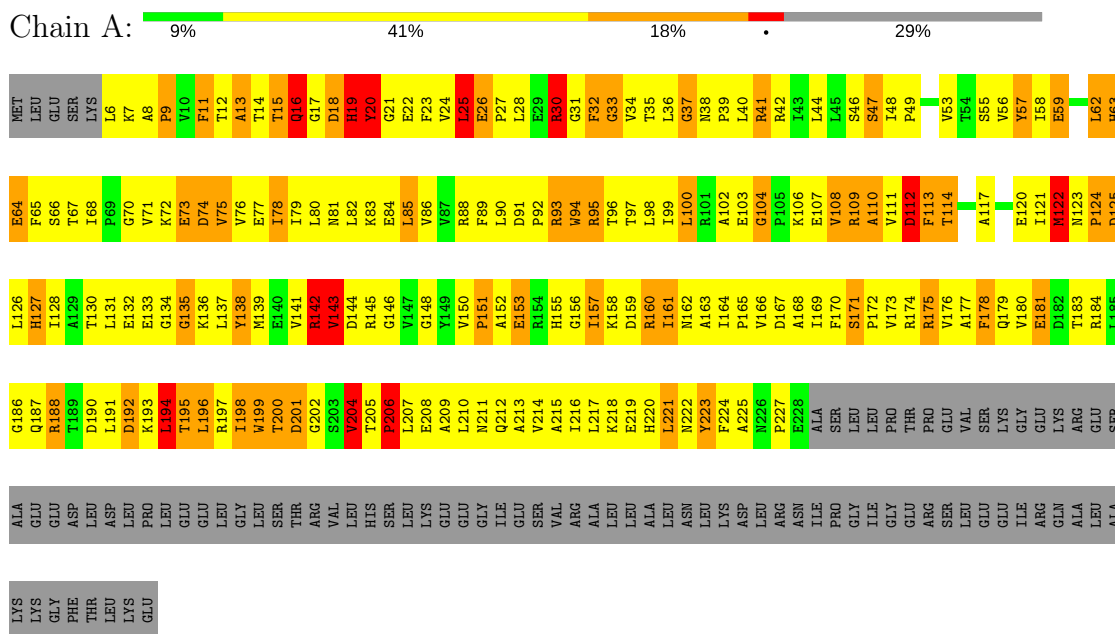
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Zn	0	0
			1	1		

### 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.

Note EDS was not executed.

- Molecule 1: DNA-directed RNA polymerase subunit alpha

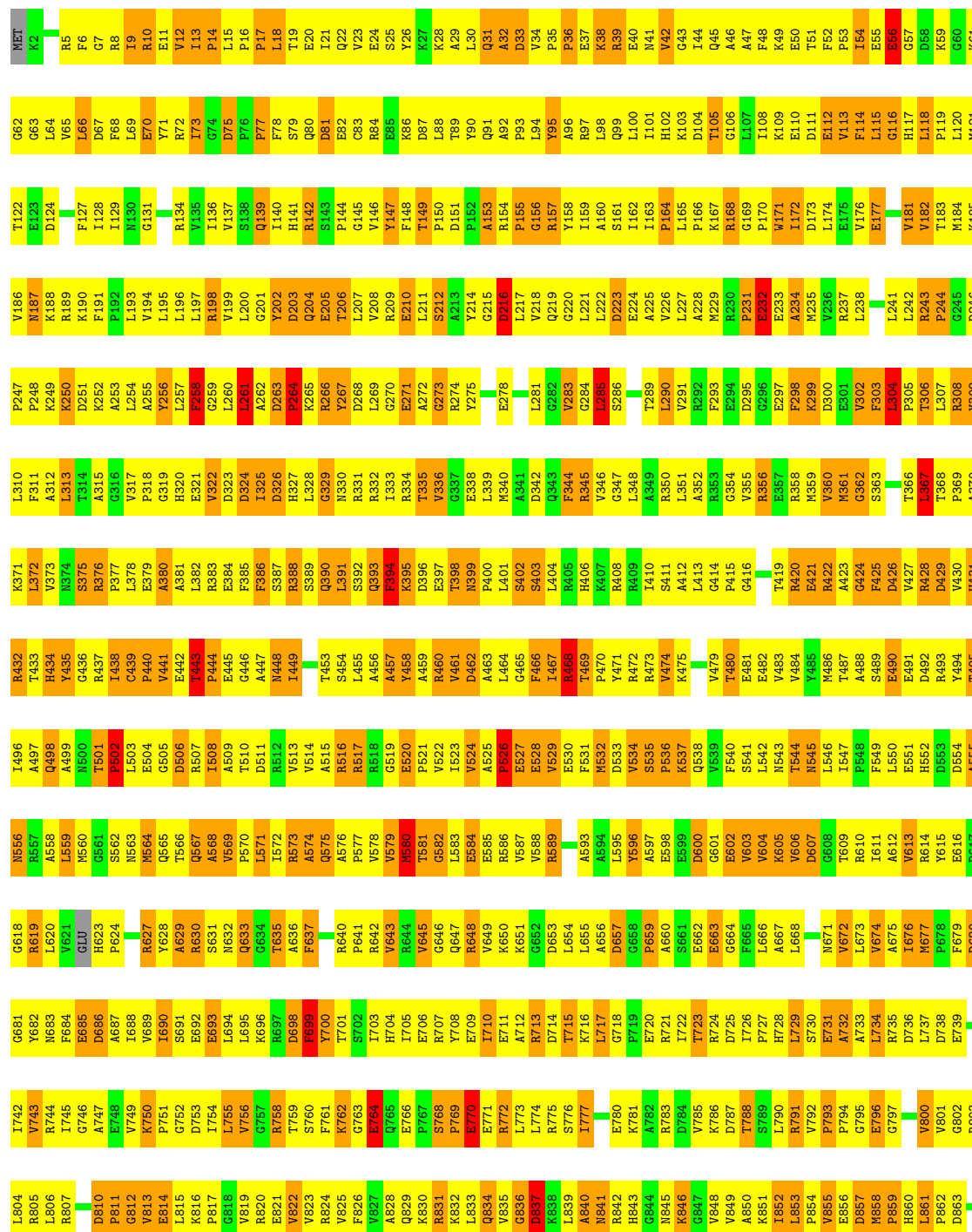


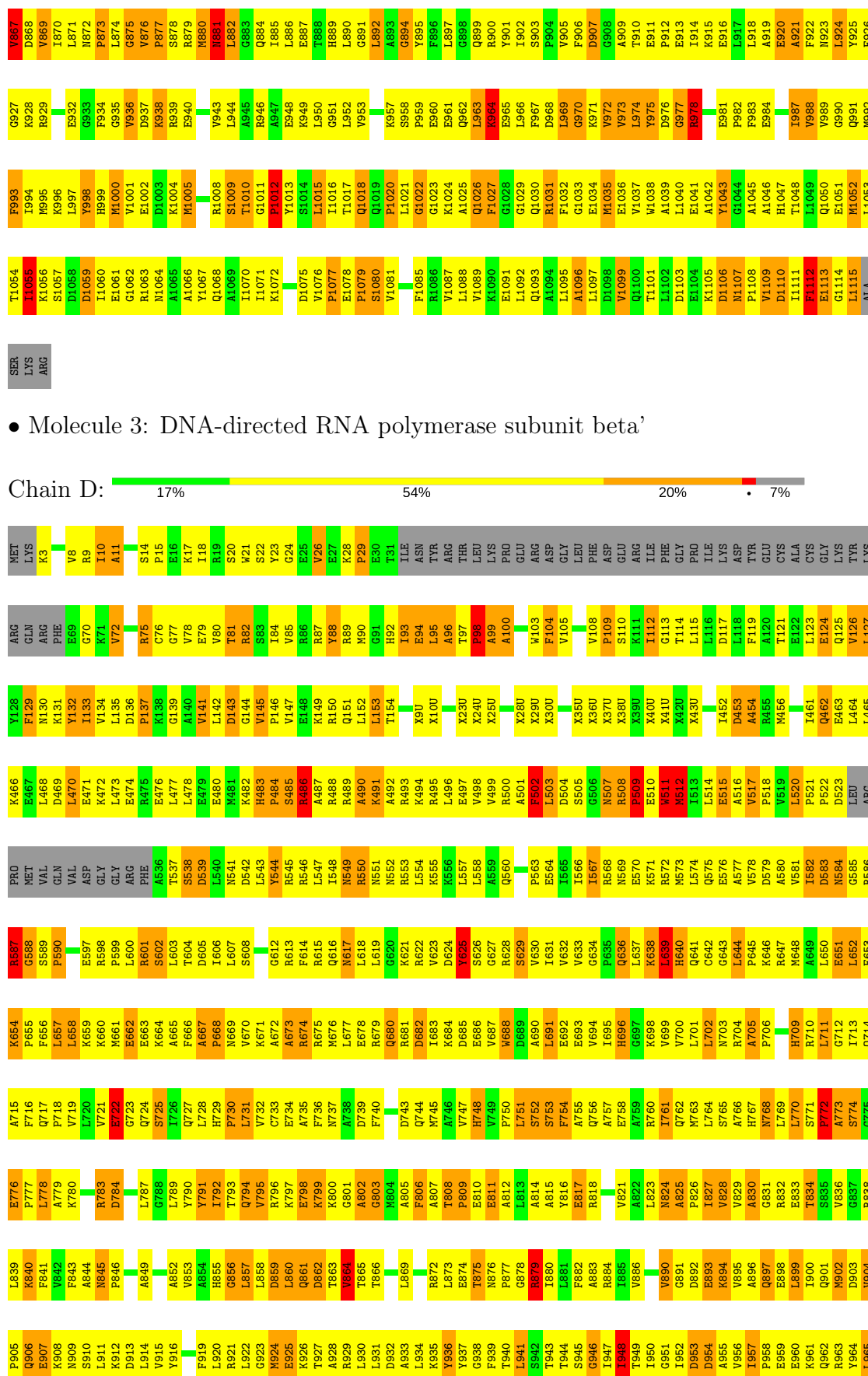
ASP LEU ASP ASP LEU PRO LEU LEU LEU LEU LEU SER THR ARG VAL LEU LEU SER SER LEU LYS GLU GLY ILE LEU SER VAL ARG ALA LEU LEU ALA LEU LEU ASN LYS ASP LEU ARG LEU ASN ILE PRO GLY ILE GLY ILE GLY

PHE THR LEU LYS GLU

# • Molecule 2: DNA-directed RNA polymerase subunit beta

Chain C: 15% 56% 26% ..





• Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain D:





## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	200.76Å 200.76Å 292.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.30	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-3.30)	Depositor
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, $R_{free}$	0.300 , 0.360	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	21254	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

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	0.42	0/1786	0.77	0/2434
1	B	0.39	0/1812	0.74	0/2471
2	C	0.42	0/8672	0.78	5/11752 (0.0%)
3	D	0.42	0/8437	0.78	14/11443 (0.1%)
4	E	0.35	0/730	0.65	0/991
All	All	0.41	0/21437	0.77	19/29091 (0.1%)

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

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

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	834	THR	N-CA-C	-6.40	93.72	111.00
3	D	137	PRO	N-CA-CB	6.22	110.77	103.30
2	C	580	MET	N-CA-C	6.19	127.70	111.00
2	C	836	GLY	N-CA-C	-6.04	97.99	113.10
2	C	329	GLY	N-CA-C	-5.97	98.17	113.10
3	D	1280	GLY	N-CA-C	5.83	127.66	113.10
3	D	639	LEU	N-CA-C	-5.70	95.62	111.00
3	D	1205	CYS	N-CA-C	-5.66	95.72	111.00
2	C	831	ARG	N-CA-C	5.58	126.05	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	29	PRO	N-CA-CB	5.57	109.98	103.30
3	D	512	MET	N-CA-C	-5.51	96.12	111.00
2	C	73	ILE	N-CA-C	-5.42	96.38	111.00
3	D	1066	LEU	CA-CB-CG	5.40	127.73	115.30
3	D	109	PRO	N-CA-CB	5.37	109.74	103.30
3	D	98	PRO	N-CA-CB	5.31	109.67	103.30
3	D	1043	ARG	N-CA-C	-5.29	96.71	111.00
3	D	1066	LEU	N-CA-C	-5.25	96.83	111.00
3	D	146	PRO	N-CA-CB	5.23	109.58	103.30
3	D	1070	GLU	N-CA-C	-5.21	96.94	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	138	TYR	Sidechain
2	C	975	TYR	Sidechain

## 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	1750	0	1759	403	0
1	B	1776	0	1776	323	0
2	C	8508	0	8418	1886	0
3	D	8499	0	7993	1651	0
4	E	719	0	685	125	0
5	D	1	0	0	0	0
6	D	1	0	0	0	0
All	All	21254	0	20631	4161	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 99.

All (4161) 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)
3:D:1020:PRO:HB2	3:D:1023:VAL:HB	1.20	1.18
2:C:508:ILE:H	2:C:508:ILE:HD13	1.10	1.15
2:C:438:ILE:HG21	2:C:470:PRO:HB3	1.22	1.15
2:C:605:LYS:HG2	2:C:606:VAL:H	1.05	1.14
2:C:262:ALA:HB1	2:C:266:ARG:HD2	1.23	1.14
1:A:41:ARG:HB3	1:A:41:ARG:HH11	1.03	1.12
3:D:483:HIS:H	3:D:484:PRO:HD2	1.10	1.12
3:D:129:PHE:HA	3:D:454:ALA:HB1	1.19	1.12
3:D:1148:ARG:HB3	3:D:1189:VAL:HG21	1.32	1.11
3:D:860:LEU:HA	3:D:877:PRO:HG2	1.16	1.11
3:D:772:PRO:HG3	3:D:778:LEU:HB2	1.24	1.10
2:C:438:ILE:HD13	2:C:470:PRO:HD3	1.32	1.10
3:D:890:VAL:HG11	3:D:922:LEU:HD13	1.23	1.10
2:C:256:TYR:HA	2:C:260:LEU:HD13	1.28	1.10
3:D:879:ARG:HG3	3:D:904:VAL:HG22	1.26	1.09
2:C:12:VAL:HG12	2:C:13:ILE:H	0.97	1.08
1:B:26:GLU:HB3	1:B:27:PRO:HD3	1.25	1.08
3:D:1080:LYS:HG3	3:D:1081:GLY:H	0.99	1.07
3:D:1035:GLN:HA	3:D:1035:GLN:HE21	1.16	1.07
2:C:580:MET:HB2	2:C:584:GLU:HG3	1.34	1.07
1:A:157:ILE:HD11	1:A:160:ARG:HE	1.19	1.06
3:D:1025:ALA:HA	3:D:1029:ALA:HB3	1.32	1.06
2:C:892:LEU:HD23	2:C:892:LEU:H	1.17	1.06
2:C:253:ALA:HA	2:C:256:TYR:HB2	1.27	1.05
1:A:62:LEU:HD12	1:A:62:LEU:H	1.19	1.05
1:A:26:GLU:HB3	1:A:27:PRO:CD	1.85	1.05
3:D:862:ASP:HA	3:D:876:ASN:HB3	1.38	1.05
2:C:630:ARG:HB3	2:C:705:ILE:HD11	1.35	1.04
2:C:159:ILE:HD11	2:C:310:LEU:HD22	1.39	1.04
3:D:521:PRO:HG2	3:D:522:PRO:HD3	1.35	1.04
2:C:195:LEU:HB2	2:C:227:LEU:HD13	1.38	1.04
2:C:969:LEU:HD13	3:D:952:ILE:HB	1.33	1.04
2:C:110:GLU:HG2	2:C:369:PRO:HG2	1.38	1.03
2:C:813:VAL:HG12	2:C:814:GLU:H	1.24	1.03
1:B:26:GLU:HB3	1:B:27:PRO:CD	1.85	1.03
2:C:551:GLU:HG3	2:C:906:PHE:HD2	1.21	1.03
2:C:110:GLU:CG	2:C:369:PRO:HG2	1.89	1.03
2:C:605:LYS:HG3	2:C:612:ALA:H	1.20	1.02
2:C:605:LYS:HA	2:C:612:ALA:HB3	1.07	1.02
3:D:1460:LEU:HB3	3:D:1466:ASN:HD21	1.19	1.01
3:D:1281:VAL:HG13	3:D:1316:ASP:HA	1.42	1.01
3:D:1016:TYR:HA	3:D:1019:ASN:HD22	1.24	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1016:TYR:HB3	3:D:1020:PRO:HD3	1.41	1.01
1:A:41:ARG:HB3	1:A:41:ARG:NH1	1.76	1.01
2:C:15:LEU:HD21	2:C:461:VAL:HG21	1.43	1.00
3:D:1281:VAL:HG12	3:D:1282:VAL:HG23	1.41	1.00
2:C:376:ARG:H	2:C:377:PRO:HD2	1.26	1.00
3:D:1253:ILE:HD12	3:D:1270:LYS:HB2	1.41	1.00
2:C:502:PRO:HB2	2:C:507:ARG:CZ	1.91	1.00
2:C:257:LEU:HD13	2:C:264:PRO:HG3	1.42	1.00
2:C:701:THR:HG22	2:C:832:LYS:HA	1.44	1.00
2:C:99:GLN:HB3	2:C:109:LYS:HG2	1.41	1.00
2:C:17:PRO:HG2	2:C:19:THR:H	1.23	1.00
3:D:772:PRO:CG	3:D:778:LEU:HB2	1.91	0.99
1:A:157:ILE:HG23	1:A:158:LYS:H	1.27	0.99
2:C:597:ALA:HA	2:C:614:ARG:NH1	1.77	0.99
3:D:1080:LYS:HG3	3:D:1081:GLY:N	1.78	0.98
2:C:1060:ILE:HG22	2:C:1064:ASN:HD21	1.27	0.98
3:D:795:VAL:HG23	3:D:904:VAL:HG11	1.42	0.98
2:C:613:VAL:HG11	2:C:619:ARG:HD2	1.43	0.98
2:C:889:HIS:CE1	3:D:951:GLY:H	1.81	0.98
2:C:159:ILE:HG12	2:C:310:LEU:HD13	1.42	0.97
2:C:654:LEU:HD11	2:C:657:ASP:HA	1.45	0.97
2:C:211:LEU:HD22	2:C:304:LEU:HD12	1.45	0.97
3:D:901:GLN:HB2	3:D:905:PRO:HG3	1.44	0.97
2:C:631:SER:HB2	2:C:635:THR:H	1.30	0.96
2:C:672:VAL:HG22	2:C:868:ASP:OD2	1.64	0.96
2:C:841:ASN:HD21	2:C:845:ASN:H	1.12	0.96
3:D:1267:ARG:O	3:D:1269:PRO:HD3	1.63	0.96
2:C:438:ILE:CG2	2:C:470:PRO:HB3	1.95	0.96
1:B:149:TYR:HE1	1:B:169:ILE:HG22	1.30	0.96
2:C:796:GLU:HG3	3:D:681:ARG:HH12	1.28	0.96
2:C:13:ILE:HG22	2:C:14:PRO:HD2	1.46	0.96
3:D:948:ILE:HD13	3:D:948:ILE:H	1.29	0.96
2:C:208:VAL:HG11	2:C:218:VAL:HG11	1.45	0.95
2:C:579:VAL:HG21	2:C:887:GLU:HG3	1.47	0.95
2:C:918:LEU:HD22	2:C:968:ASP:HA	1.48	0.95
3:D:1232:GLU:HB3	3:D:1233:PRO:HD3	1.46	0.95
3:D:1096:THR:O	3:D:1100:VAL:HG23	1.66	0.95
1:A:16:GLN:HE21	1:A:17:GLY:H	1.06	0.95
2:C:1045:ALA:HB1	2:C:1048:THR:HB	1.46	0.95
2:C:845:ASN:HD22	2:C:884:GLN:HE22	0.96	0.95
2:C:162:ILE:HA	2:C:171:TRP:HZ3	1.28	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:879:ARG:NH1	3:D:904:VAL:HA	1.81	0.95
2:C:101:ILE:HG22	2:C:102:HIS:H	1.31	0.94
3:D:1365:HIS:CG	3:D:1366:ASP:H	1.84	0.94
2:C:12:VAL:HG12	2:C:13:ILE:N	1.80	0.94
1:B:85:LEU:HA	1:B:123:ASN:HD21	1.33	0.94
2:C:140:ILE:HG22	2:C:333:ILE:HG12	1.49	0.94
2:C:161:SER:HB2	2:C:172:ILE:HG22	1.49	0.94
2:C:181:VAL:HG12	2:C:182:VAL:HG23	1.50	0.94
2:C:710:ILE:HD13	2:C:823:VAL:HB	1.48	0.94
2:C:168:ARG:HH21	2:C:266:ARG:HD3	1.33	0.94
2:C:676:ILE:CG2	2:C:873:PRO:HB3	1.97	0.93
3:D:879:ARG:HH11	3:D:904:VAL:HA	1.29	0.93
2:C:137:VAL:HG21	2:C:393:GLN:OE1	1.69	0.93
3:D:1263:LEU:HD23	3:D:1353:ILE:HG12	1.50	0.93
3:D:1126:MET:HG2	3:D:1127:ASP:H	1.32	0.93
2:C:401:LEU:HD21	2:C:543:ASN:HB2	1.49	0.93
2:C:551:GLU:HG3	2:C:906:PHE:CD2	2.04	0.93
2:C:845:ASN:HD22	2:C:884:GLN:NE2	1.66	0.93
2:C:77:PRO:HD3	2:C:93:PRO:HD3	1.47	0.93
1:B:86:VAL:HG23	1:B:123:ASN:CG	1.88	0.92
2:C:860:HIS:HD2	2:C:977:GLY:HA3	1.33	0.92
3:D:1038:GLN:HG3	3:D:1043:ARG:HD3	1.52	0.92
1:A:75:VAL:HA	1:A:78:ILE:HD12	1.50	0.92
2:C:768:SER:HB2	2:C:769:PRO:HD2	1.52	0.92
3:D:631:ILE:HD13	3:D:745:MET:HE2	1.51	0.92
3:D:1157:LEU:HD12	3:D:1178:ALA:HA	1.50	0.92
3:D:966:GLU:HA	3:D:969:ASP:HB2	1.51	0.91
2:C:861:LEU:HG	2:C:862:PRO:HD2	1.49	0.91
3:D:1282:VAL:HG13	3:D:1315:LYS:HA	1.51	0.91
2:C:742:ILE:HG23	2:C:756:VAL:HG22	1.52	0.91
3:D:477:LEU:HA	3:D:480:GLU:HB3	1.51	0.91
3:D:699:VAL:H	3:D:756:GLN:NE2	1.69	0.91
3:D:721:VAL:HG12	3:D:722:GLU:H	1.33	0.91
1:A:194:LEU:HD23	1:A:195:THR:H	1.33	0.91
3:D:1278:ILE:HG22	3:D:1280:GLY:H	1.34	0.91
3:D:129:PHE:CA	3:D:454:ALA:HB1	2.00	0.91
3:D:92:HIS:HA	3:D:517:VAL:HG12	1.49	0.91
3:D:483:HIS:HA	3:D:489:ARG:HG3	1.51	0.91
3:D:1458:ASP:OD1	3:D:1460:LEU:HD23	1.70	0.91
3:D:1148:ARG:HB3	3:D:1189:VAL:CG2	2.00	0.90
2:C:1103:ASP:HB2	2:C:1108:PRO:HB2	1.49	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1276:SER:H	3:D:1323:GLY:HA2	1.37	0.90
2:C:22:GLN:HE21	2:C:336:VAL:HG21	1.36	0.90
2:C:195:LEU:HD13	2:C:227:LEU:HD22	1.52	0.90
3:D:1004:VAL:O	3:D:1008:VAL:HG12	1.71	0.90
3:D:1274:VAL:N	3:D:1325:PRO:HG3	1.87	0.90
1:B:142:ARG:HG2	1:B:143:VAL:H	1.35	0.89
3:D:772:PRO:HG3	3:D:778:LEU:CB	2.02	0.89
3:D:836:VAL:O	3:D:865:THR:HG23	1.71	0.89
2:C:889:HIS:HE1	3:D:951:GLY:H	1.20	0.89
3:D:654:LYS:HB3	3:D:655:PRO:HD3	1.53	0.89
1:A:79:ILE:HD11	1:A:164:ILE:CD1	2.02	0.89
2:C:605:LYS:HG2	2:C:607:ASP:H	1.35	0.89
2:C:882:LEU:N	2:C:882:LEU:HD23	1.88	0.89
1:B:213:ALA:HA	1:B:216:ILE:HD12	1.54	0.89
2:C:762:LYS:HD2	2:C:786:LYS:HD2	1.51	0.89
3:D:483:HIS:N	3:D:484:PRO:HD2	1.87	0.89
2:C:31:GLN:HE21	2:C:39:ARG:HD2	1.38	0.89
3:D:127:LEU:HA	3:D:456:MET:HB2	1.54	0.89
1:A:179:GLN:HG3	2:C:934:PHE:CD2	2.08	0.89
2:C:1076:VAL:HG11	3:D:753:SER:HB2	1.53	0.89
3:D:1031:GLY:O	3:D:1032:ASN:HB3	1.72	0.89
3:D:1324:GLN:H	3:D:1325:PRO:HD2	1.35	0.89
2:C:12:VAL:CG1	2:C:13:ILE:H	1.81	0.89
2:C:897:LEU:HB2	2:C:921:ALA:HB2	1.55	0.89
1:A:164:ILE:HG13	1:A:164:ILE:O	1.73	0.88
2:C:162:ILE:HA	2:C:171:TRP:CZ3	2.08	0.88
2:C:969:LEU:HD11	3:D:953:ASP:H	1.38	0.88
2:C:577:PRO:HG2	2:C:580:MET:HB3	1.56	0.88
2:C:613:VAL:HA	2:C:620:LEU:O	1.73	0.88
2:C:428:ARG:HA	2:C:431:HIS:CD2	2.08	0.88
3:D:1035:GLN:HA	3:D:1035:GLN:NE2	1.89	0.88
3:D:860:LEU:C	3:D:862:ASP:H	1.67	0.88
3:D:1102:VAL:HG21	3:D:1425:VAL:HG13	1.55	0.88
3:D:1460:LEU:HB3	3:D:1466:ASN:ND2	1.89	0.88
3:D:675:ARG:HA	3:D:678:GLU:HB3	1.55	0.88
3:D:824:ASN:O	3:D:830:ALA:HB1	1.74	0.88
2:C:730:SER:O	2:C:732:ALA:N	2.06	0.88
3:D:787:LEU:HD21	3:D:947:ILE:HD11	1.54	0.88
2:C:845:ASN:ND2	2:C:884:GLN:HE22	1.70	0.87
2:C:605:LYS:HG2	2:C:606:VAL:N	1.89	0.87
1:A:41:ARG:HG2	1:A:176:VAL:HG12	1.55	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:605:LYS:HA	2:C:612:ALA:CB	2.01	0.87
2:C:801:VAL:HG21	2:C:828:ALA:HB2	1.55	0.87
2:C:257:LEU:HD22	2:C:264:PRO:HD3	1.57	0.87
2:C:333:ILE:CD1	2:C:468:ARG:HE	1.87	0.87
2:C:816:LYS:HD2	2:C:817:PRO:HD2	1.56	0.87
3:D:1060:SER:HB3	3:D:1066:LEU:HD22	1.54	0.87
3:D:811:GLU:HA	3:D:814:ALA:HB3	1.54	0.87
2:C:491:GLU:HA	2:C:531:PHE:HA	1.56	0.87
2:C:836:GLY:HA3	2:C:1001:VAL:HG21	1.57	0.87
1:B:173:VAL:HA	1:B:200:THR:HG22	1.55	0.87
2:C:508:ILE:CD1	2:C:508:ILE:H	1.88	0.86
2:C:642:ARG:NH1	2:C:663:GLU:HB3	1.89	0.86
2:C:875:GLY:HA2	2:C:879:ARG:HG3	1.57	0.86
1:A:90:LEU:HD11	1:A:120:GLU:HG3	1.54	0.86
2:C:729:LEU:HD21	2:C:754:ILE:HG13	1.57	0.86
1:A:199:TRP:HD1	1:A:200:THR:H	1.23	0.86
2:C:5:ARG:HH22	2:C:10:ARG:NH1	1.73	0.86
2:C:15:LEU:HD21	2:C:461:VAL:CG2	2.04	0.86
2:C:159:ILE:CG1	2:C:310:LEU:HD13	2.04	0.86
1:A:26:GLU:HB3	1:A:27:PRO:HD3	1.55	0.86
2:C:671:ASN:HA	2:C:993:PHE:HA	1.56	0.86
3:D:1124:PHE:CE2	3:D:1185:ARG:HG2	2.10	0.86
3:D:684:LYS:HD3	3:D:685:ASP:H	1.40	0.86
2:C:304:LEU:H	2:C:305:PRO:CD	1.89	0.86
2:C:266:ARG:HG2	2:C:268:ASP:H	1.38	0.86
3:D:558:LEU:HG	3:D:567:ILE:HD11	1.57	0.86
2:C:735:ARG:HA	2:C:737:LEU:O	1.76	0.86
2:C:263:ASP:HB3	2:C:264:PRO:HD3	1.56	0.85
2:C:726:ILE:HD12	2:C:726:ILE:H	1.38	0.85
3:D:890:VAL:CG1	3:D:922:LEU:HD13	2.06	0.85
2:C:605:LYS:NZ	2:C:611:ILE:HG13	1.90	0.85
2:C:253:ALA:CA	2:C:256:TYR:HB2	2.06	0.85
3:D:1193:LEU:HG	3:D:1370:GLU:HB3	1.58	0.85
3:D:691:LEU:HA	3:D:694:VAL:HB	1.59	0.85
3:D:1365:HIS:ND1	3:D:1366:ASP:N	2.24	0.85
2:C:398:THR:O	2:C:635:THR:HG21	1.77	0.85
2:C:841:ASN:ND2	2:C:845:ASN:H	1.73	0.85
2:C:551:GLU:HA	2:C:906:PHE:HE2	1.41	0.85
2:C:915:LYS:HD2	2:C:968:ASP:HB3	1.56	0.85
1:A:161:ILE:HG12	1:A:162:ASN:OD1	1.75	0.85
1:B:78:ILE:HG13	1:B:129:ALA:HB2	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:183:THR:HG21	2:C:190:LYS:HG3	1.55	0.85
3:D:1016:TYR:HB3	3:D:1019:ASN:HB2	1.59	0.84
3:D:899:LEU:HD11	3:D:921:ARG:HD2	1.59	0.84
1:A:41:ARG:HH11	1:A:41:ARG:CB	1.88	0.84
1:B:105:PRO:HB3	1:B:133:GLU:H	1.40	0.84
2:C:100:LEU:HD21	2:C:368:THR:HA	1.58	0.84
3:D:1267:ARG:O	3:D:1269:PRO:CD	2.26	0.84
2:C:946:ARG:NE	3:D:861:GLN:HE22	1.74	0.84
2:C:446:GLY:HA2	2:C:449:ILE:HD11	1.58	0.84
2:C:836:GLY:HA3	2:C:1001:VAL:CG2	2.07	0.84
4:E:40:LEU:HD21	4:E:67:GLU:HA	1.59	0.84
3:D:827:ILE:O	3:D:828:VAL:HG23	1.76	0.84
2:C:142:ARG:HE	2:C:324:ASP:HA	1.41	0.84
2:C:564:MET:SD	2:C:840:ALA:HB1	2.17	0.84
2:C:613:VAL:HG13	2:C:620:LEU:H	1.42	0.84
2:C:328:LEU:O	2:C:467:ILE:HG21	1.77	0.84
3:D:1048:LYS:HG2	3:D:1054:PHE:CE1	2.13	0.84
1:B:102:ALA:HB1	1:B:131:LEU:HD11	1.59	0.83
2:C:260:LEU:O	2:C:261:LEU:HD23	1.77	0.83
2:C:397:GLU:H	2:C:633:GLN:NE2	1.76	0.83
3:D:1087:LEU:HD12	3:D:1090:ALA:HB3	1.58	0.83
3:D:783:ARG:O	3:D:784:ASP:HB2	1.77	0.83
2:C:758:ARG:O	2:C:788:THR:HG23	1.78	0.83
1:A:179:GLN:HE21	2:C:934:PHE:HB3	1.42	0.83
3:D:483:HIS:H	3:D:484:PRO:CD	1.85	0.83
3:D:1271:ALA:HB3	3:D:1329:GLY:HA3	1.59	0.83
1:B:77:GLU:O	1:B:81:ASN:HB2	1.77	0.83
1:B:91:ASP:H	1:B:92:PRO:CD	1.91	0.83
2:C:253:ALA:HA	2:C:256:TYR:CB	2.07	0.83
2:C:267:TYR:HD1	2:C:273:GLY:HA3	1.43	0.83
3:D:1148:ARG:CB	3:D:1189:VAL:HG21	2.09	0.83
1:B:150:VAL:HG11	1:B:154:ARG:HG2	1.59	0.83
2:C:533:ASP:HB3	2:C:538:GLN:NE2	1.93	0.83
1:B:90:LEU:HD11	1:B:118:ASP:HA	1.61	0.83
2:C:97:ARG:HG2	2:C:112:GLU:H	1.42	0.83
2:C:632:ASN:HB2	2:C:633:GLN:NE2	1.94	0.83
2:C:1052:MET:O	2:C:1053:LEU:HD13	1.79	0.83
3:D:1016:TYR:HA	3:D:1019:ASN:ND2	1.94	0.83
3:D:721:VAL:HG12	3:D:722:GLU:N	1.92	0.83
2:C:920:GLU:HG2	2:C:921:ALA:H	1.43	0.83
2:C:15:LEU:HD12	2:C:16:PRO:HD2	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:ARG:HB2	1:A:122:MET:SD	2.19	0.82
2:C:605:LYS:CA	2:C:612:ALA:HB3	2.01	0.82
3:D:89:ARG:O	3:D:520:LEU:HD11	1.76	0.82
2:C:861:LEU:CG	2:C:862:PRO:HD2	2.09	0.82
3:D:1275:ILE:HA	3:D:1323:GLY:N	1.95	0.82
3:D:1324:GLN:H	3:D:1325:PRO:CD	1.92	0.82
2:C:749:VAL:HG11	2:C:792:VAL:HG21	1.58	0.82
2:C:102:HIS:HD2	2:C:106:GLY:HA3	1.42	0.82
2:C:860:HIS:CD2	2:C:977:GLY:HA3	2.15	0.82
2:C:940:GLU:HA	2:C:973:VAL:HG21	1.61	0.82
3:D:1311:ARG:HA	3:D:1324:GLN:O	1.80	0.82
3:D:709:HIS:ND1	3:D:1232:GLU:HG3	1.95	0.82
2:C:801:VAL:CG2	2:C:828:ALA:HB2	2.09	0.82
3:D:728:LEU:HD22	3:D:745:MET:CE	2.09	0.82
3:D:1277:GLU:HG3	3:D:1304:TYR:OH	1.79	0.82
3:D:790:TYR:CE2	3:D:906:GLN:HB3	2.14	0.82
2:C:750:LYS:HB2	2:C:751:PRO:HD2	1.61	0.81
2:C:642:ARG:HH11	2:C:654:LEU:HD23	1.45	0.81
3:D:638:LYS:HA	3:D:729:HIS:CG	2.15	0.81
2:C:1013:TYR:HE2	2:C:1018:GLN:HE22	1.28	0.81
2:C:34:VAL:HG11	2:C:39:ARG:HG2	1.63	0.81
2:C:80:GLN:O	2:C:81:ASP:HB2	1.79	0.81
3:D:1237:LEU:HD11	3:D:1357:TYR:CE2	2.16	0.81
3:D:465:LEU:HD23	3:D:509:PRO:HB3	1.61	0.81
3:D:1085:THR:C	3:D:1087:LEU:H	1.82	0.81
1:A:71:VAL:HG13	1:A:131:LEU:HB3	1.61	0.81
2:C:146:VAL:HG22	2:C:161:SER:HA	1.61	0.81
2:C:376:ARG:N	2:C:377:PRO:HD2	1.95	0.81
3:D:1142:GLU:HA	3:D:1172:VAL:HG11	1.63	0.81
3:D:521:PRO:CG	3:D:522:PRO:HD3	2.09	0.81
2:C:1055:ILE:H	2:C:1055:ILE:HD12	1.46	0.81
2:C:216:ASP:O	2:C:218:VAL:HG23	1.81	0.81
2:C:495:THR:HG22	2:C:496:ILE:H	1.45	0.81
2:C:969:LEU:CD1	3:D:952:ILE:HB	2.11	0.81
2:C:1008:ARG:NH1	2:C:1020:PRO:HB3	1.95	0.81
2:C:892:LEU:H	2:C:892:LEU:CD2	1.93	0.81
2:C:892:LEU:HD23	2:C:892:LEU:N	1.94	0.81
3:D:1068:VAL:HG12	3:D:1070:GLU:HB2	1.63	0.81
2:C:574:ALA:O	2:C:667:ALA:HB1	1.82	0.80
2:C:331:ARG:O	2:C:467:ILE:HG12	1.82	0.80
2:C:177:GLU:HG2	2:C:181:VAL:H	1.47	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1275:ILE:HG22	3:D:1322:ALA:HA	1.63	0.80
1:B:56:VAL:O	1:B:164:ILE:HG12	1.82	0.80
3:D:1043:ARG:HH21	3:D:1066:LEU:HD21	1.45	0.80
3:D:750:PRO:HG2	3:D:756:GLN:OE1	1.81	0.80
1:B:150:VAL:HB	1:B:168:ALA:HB3	1.61	0.80
2:C:439:CYS:HB2	2:C:468:ARG:NH1	1.96	0.80
2:C:569:VAL:HG13	2:C:569:VAL:O	1.80	0.80
3:D:1263:LEU:HD23	3:D:1353:ILE:CG1	2.11	0.80
2:C:363:SER:O	2:C:367:LEU:HB2	1.80	0.80
2:C:872:ASN:HD21	2:C:874:LEU:HB3	1.47	0.80
3:D:1221:ALA:HB2	3:D:1475:ALA:HB1	1.63	0.80
2:C:602:GLU:H	2:C:647:GLN:HA	1.46	0.80
3:D:969:ASP:O	3:D:972:LEU:HB2	1.81	0.80
2:C:172:ILE:HD11	2:C:184:MET:SD	2.21	0.80
2:C:21:ILE:HG23	2:C:460:ARG:NH2	1.96	0.80
2:C:613:VAL:HG12	2:C:615:TYR:H	1.46	0.80
3:D:1155:GLU:HB3	3:D:1160:ARG:HA	1.64	0.80
3:D:1275:ILE:HA	3:D:1323:GLY:H	1.46	0.80
3:D:1451:ALA:HA	3:D:1456:LYS:HG3	1.62	0.80
3:D:569:ASN:O	3:D:572:ARG:HG2	1.81	0.80
3:D:864:VAL:HG12	3:D:874:GLU:O	1.82	0.80
2:C:523:ILE:C	2:C:525:ALA:H	1.85	0.79
2:C:1038:TRP:CD1	3:D:1100:VAL:HG11	2.17	0.79
3:D:518:PRO:HA	3:D:544:TYR:CZ	2.16	0.79
2:C:77:PRO:HD3	2:C:93:PRO:CD	2.11	0.79
3:D:662:GLU:HG3	3:D:670:VAL:HG23	1.64	0.79
3:D:688:TRP:HA	3:D:688:TRP:CE3	2.16	0.79
3:D:840:LYS:CB	3:D:846:PRO:HA	2.13	0.79
2:C:673:LEU:O	2:C:868:ASP:HB2	1.81	0.79
3:D:507:ASN:O	3:D:508:ARG:HG2	1.82	0.79
3:D:770:LEU:CD1	3:D:770:LEU:H	1.95	0.79
2:C:57:GLY:H	2:C:356:ARG:NH1	1.79	0.79
2:C:134:ARG:HA	2:C:394:PHE:O	1.82	0.79
3:D:858:LEU:HD11	3:D:865:THR:HG21	1.64	0.79
2:C:399:ASN:ND2	2:C:401:LEU:H	1.81	0.79
3:D:1404:LEU:O	3:D:1408:LEU:HB2	1.83	0.79
3:D:1482:VAL:O	3:D:1483:ARG:HG3	1.83	0.79
1:B:25:LEU:HD11	1:B:28:LEU:HD12	1.65	0.79
2:C:200:LEU:HD13	2:C:290:LEU:HD13	1.65	0.79
3:D:772:PRO:HD2	3:D:776:GLU:O	1.83	0.79
3:D:1102:VAL:CG2	3:D:1425:VAL:HG13	2.13	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:508:ARG:O	3:D:510:GLU:HG3	1.84	0.78
2:C:1012:PRO:HB3	2:C:1023:GLY:HA3	1.64	0.78
2:C:469:THR:HG22	2:C:484:VAL:HG23	1.63	0.78
3:D:1049:PRO:HD3	3:D:1076:HIS:ND1	1.98	0.78
1:B:33:GLY:HA2	1:B:194:LEU:HD23	1.64	0.78
2:C:1055:ILE:HG22	2:C:1066:ALA:HB2	1.65	0.78
3:D:1330:ALA:HB3	3:D:1333:PRO:HG3	1.63	0.78
3:D:1157:LEU:O	3:D:1157:LEU:HD23	1.82	0.78
3:D:669:ASN:O	3:D:672:ALA:HB3	1.83	0.78
3:D:860:LEU:HA	3:D:877:PRO:CG	2.08	0.78
2:C:493:ARG:HH12	3:D:1070:GLU:HA	1.49	0.78
1:B:95:ARG:O	1:B:95:ARG:HD2	1.83	0.78
2:C:491:GLU:O	2:C:509:ALA:HB1	1.84	0.78
3:D:776:GLU:HB3	3:D:912:LYS:HE3	1.66	0.78
3:D:1104:HIS:C	3:D:1106:ILE:H	1.86	0.78
3:D:1145:LEU:HB2	3:D:1172:VAL:HG13	1.66	0.78
1:A:41:ARG:HE	2:C:860:HIS:CE1	2.02	0.78
2:C:139:GLN:OE1	2:C:414:GLY:HA3	1.84	0.78
2:C:475:LYS:CB	2:C:527:GLU:H	1.96	0.78
2:C:571:LEU:N	2:C:571:LEU:HD12	1.99	0.78
3:D:705:ALA:HB3	3:D:706:PRO:HD2	1.66	0.78
1:A:25:LEU:HD12	1:A:28:LEU:HD21	1.65	0.77
2:C:274:ARG:HG3	2:C:275:TYR:HD1	1.49	0.77
2:C:565:GLN:HE21	2:C:668:LEU:HD12	1.49	0.77
2:C:722:ILE:HD13	2:C:823:VAL:HG23	1.66	0.77
2:C:950:LEU:HB3	3:D:1019:ASN:OD1	1.85	0.77
3:D:1354:GLN:HE21	3:D:1369:ILE:CD1	1.97	0.77
2:C:460:ARG:HD2	2:C:464:LEU:CD2	2.14	0.77
2:C:66:LEU:HD23	2:C:355:VAL:HG21	1.66	0.77
3:D:709:HIS:CE1	3:D:1232:GLU:HG3	2.20	0.77
2:C:676:ILE:HG23	2:C:873:PRO:HB3	1.65	0.77
3:D:659:LYS:HD3	3:D:659:LYS:O	1.83	0.77
3:D:890:VAL:HG11	3:D:922:LEU:CD1	2.10	0.77
2:C:796:GLU:HG3	3:D:681:ARG:NH1	1.98	0.77
2:C:355:VAL:O	2:C:359:MET:HG2	1.84	0.77
2:C:101:ILE:HG22	2:C:102:HIS:N	1.98	0.77
3:D:630:VAL:O	3:D:725:SER:HA	1.83	0.77
2:C:997:LEU:O	2:C:999:HIS:N	2.17	0.77
3:D:1077:GLY:O	3:D:1080:LYS:HG2	1.85	0.77
3:D:997:TRP:HA	3:D:1000:THR:HG22	1.67	0.77
1:B:147:VAL:HG23	1:B:148:GLY:H	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:613:VAL:HG12	2:C:615:TYR:N	1.99	0.77
2:C:974:LEU:HD23	2:C:987:ILE:HB	1.67	0.77
3:D:795:VAL:HA	3:D:862:ASP:CB	2.14	0.77
2:C:559:LEU:HD12	2:C:559:LEU:C	2.05	0.77
2:C:769:PRO:O	2:C:771:GLU:N	2.18	0.77
1:B:91:ASP:H	1:B:92:PRO:HD2	1.48	0.76
2:C:358:ARG:HB2	2:C:372:LEU:HD23	1.67	0.76
3:D:1381:GLU:CD	3:D:1392:GLU:HG3	2.06	0.76
2:C:525:ALA:HB1	2:C:526:PRO:HD2	1.65	0.76
3:D:75:ARG:O	3:D:77:GLY:N	2.18	0.76
1:A:141:VAL:HG22	1:A:142:ARG:O	1.85	0.76
1:A:142:ARG:O	1:A:143:VAL:HG13	1.86	0.76
2:C:743:VAL:HG11	2:C:800:VAL:HG21	1.68	0.76
3:D:1281:VAL:HG12	3:D:1282:VAL:CG2	2.15	0.76
2:C:567:GLN:O	2:C:997:LEU:HA	1.85	0.76
1:A:159:ASP:O	1:A:161:ILE:HG22	1.85	0.76
1:A:161:ILE:HG23	1:A:162:ASN:N	2.00	0.76
2:C:807:ARG:O	2:C:810:ASP:HB2	1.84	0.76
1:B:85:LEU:HA	1:B:123:ASN:ND2	2.00	0.76
2:C:1034:GLU:CD	3:D:1097:ARG:HH12	1.89	0.76
2:C:915:LYS:O	2:C:919:ALA:N	2.14	0.76
1:B:97:THR:HG22	1:B:98:LEU:H	1.50	0.76
2:C:283:VAL:HG12	2:C:284:GLY:H	1.50	0.76
2:C:595:LEU:HG	2:C:655:LEU:HD22	1.68	0.76
2:C:597:ALA:HA	2:C:614:ARG:HH12	1.51	0.76
3:D:1097:ARG:HH11	3:D:1097:ARG:HG3	1.49	0.76
3:D:731:LEU:HD13	3:D:931:LEU:HD12	1.67	0.76
3:D:1332:ASP:O	3:D:1334:HIS:N	2.15	0.76
3:D:1332:ASP:C	3:D:1334:HIS:H	1.90	0.76
3:D:1102:VAL:HG21	3:D:1425:VAL:HG22	1.67	0.76
2:C:256:TYR:C	2:C:260:LEU:HB3	2.06	0.76
3:D:1020:PRO:HB2	3:D:1023:VAL:CB	2.10	0.76
3:D:10:ILE:HG12	3:D:11:ALA:H	1.49	0.76
3:D:805:ALA:HB3	3:D:827:ILE:HA	1.68	0.76
1:A:205:THR:HG23	1:A:206:PRO:HD2	1.65	0.75
2:C:161:SER:CB	2:C:172:ILE:HG22	2.15	0.75
2:C:291:VAL:HB	2:C:299:LYS:HG3	1.67	0.75
2:C:344:PHE:C	2:C:346:VAL:H	1.89	0.75
2:C:376:ARG:H	2:C:377:PRO:CD	2.00	0.75
2:C:758:ARG:HH11	2:C:758:ARG:HG3	1.51	0.75
3:D:797:LYS:O	3:D:799:LYS:N	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:905:PRO:O	3:D:906:GLN:HB2	1.84	0.75
3:D:909:ASN:O	3:D:912:LYS:HB3	1.87	0.75
1:A:30:ARG:HD3	1:A:30:ARG:H	1.52	0.75
2:C:911:GLU:O	2:C:915:LYS:HG2	1.86	0.75
2:C:525:ALA:O	2:C:527:GLU:N	2.19	0.75
2:C:474:VAL:HG13	2:C:530:GLU:HA	1.67	0.75
2:C:755:LEU:HB3	2:C:790:LEU:HD23	1.67	0.75
2:C:869:VAL:HG21	2:C:871:LEU:HD13	1.66	0.75
2:C:943:VAL:HG21	2:C:973:VAL:HG13	1.65	0.75
3:D:1266:ALA:O	3:D:1267:ARG:HG3	1.85	0.75
1:B:44:LEU:O	1:B:173:VAL:HG21	1.87	0.75
2:C:168:ARG:NH2	2:C:266:ARG:HD3	2.00	0.75
2:C:262:ALA:CB	2:C:266:ARG:HD2	2.12	0.75
2:C:836:GLY:C	2:C:837:ASP:OD2	2.25	0.75
3:D:659:LYS:NZ	3:D:663:GLU:HB2	2.01	0.75
2:C:996:LYS:HE2	2:C:1000:MET:HE3	1.69	0.75
2:C:115:LEU:HD12	2:C:116:GLY:H	1.51	0.75
2:C:810:ASP:OD1	2:C:811:PRO:HD2	1.86	0.75
3:D:1015:ASN:O	3:D:1016:TYR:CG	2.39	0.75
3:D:1063:ARG:HH11	3:D:1063:ARG:HG3	1.50	0.75
1:B:212:GLN:O	1:B:216:ILE:HG13	1.86	0.75
2:C:920:GLU:O	2:C:922:PHE:N	2.19	0.75
3:D:1149:VAL:HG23	3:D:1166:TYR:CD2	2.21	0.75
3:D:860:LEU:O	3:D:862:ASP:N	2.20	0.75
3:D:969:ASP:HA	3:D:972:LEU:HD12	1.67	0.75
2:C:1009:SER:O	2:C:1010:THR:HG23	1.86	0.75
2:C:519:GLY:C	2:C:521:PRO:HD3	2.07	0.75
3:D:1108:VAL:O	3:D:1218:ILE:HD13	1.87	0.75
3:D:699:VAL:H	3:D:756:GLN:HE21	1.33	0.75
3:D:972:LEU:O	3:D:975:ILE:HG22	1.85	0.75
2:C:48:PHE:CE2	2:C:71:TYR:HB3	2.22	0.74
3:D:1274:VAL:H	3:D:1325:PRO:HG3	1.52	0.74
3:D:728:LEU:HD22	3:D:745:MET:HE1	1.68	0.74
2:C:804:LEU:HD12	2:C:805:ARG:H	1.51	0.74
3:D:860:LEU:C	3:D:862:ASP:N	2.37	0.74
1:B:89:PHE:HD1	1:B:94:TRP:HB3	1.52	0.74
2:C:614:ARG:CZ	2:C:623:HIS:HE1	2.00	0.74
2:C:755:LEU:HD23	2:C:792:VAL:HG23	1.70	0.74
2:C:438:ILE:CD1	2:C:470:PRO:HD3	2.15	0.74
3:D:643:GLY:HA3	3:D:727:GLN:H	1.52	0.74
1:A:86:VAL:HG13	1:A:122:MET:HB2	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:208:VAL:HG11	2:C:218:VAL:CG1	2.18	0.74
2:C:910:THR:HG22	2:C:912:PRO:HD2	1.70	0.74
2:C:862:PRO:HA	2:C:975:TYR:CE1	2.23	0.74
3:D:518:PRO:HA	3:D:544:TYR:CE1	2.22	0.74
1:A:16:GLN:NE2	1:A:17:GLY:H	1.82	0.74
2:C:184:MET:HB3	2:C:191:PHE:CZ	2.22	0.74
2:C:395:LYS:HG2	2:C:397:GLU:HG3	1.67	0.74
2:C:31:GLN:NE2	2:C:39:ARG:HD2	2.02	0.74
3:D:639:LEU:HD23	3:D:729:HIS:CD2	2.23	0.74
1:A:220:HIS:HA	1:A:223:TYR:CD2	2.23	0.74
3:D:1069:LEU:C	3:D:1071:TYR:H	1.89	0.74
2:C:438:ILE:HG21	2:C:470:PRO:CB	2.12	0.74
2:C:401:LEU:HD21	2:C:543:ASN:CB	2.17	0.74
1:B:105:PRO:HA	1:B:132:GLU:HA	1.70	0.74
2:C:468:ARG:CD	2:C:468:ARG:H	2.01	0.74
2:C:467:ILE:O	2:C:469:THR:HG23	1.87	0.74
3:D:1364:LEU:O	3:D:1365:HIS:O	2.06	0.74
2:C:243:ARG:HG3	2:C:244:PRO:HA	1.70	0.74
2:C:437:ARG:O	2:C:438:ILE:HG23	1.87	0.74
3:D:606:ILE:HD12	3:D:606:ILE:N	2.03	0.74
3:D:731:LEU:CD1	3:D:931:LEU:HD12	2.17	0.74
1:B:86:VAL:HG23	1:B:123:ASN:ND2	2.02	0.73
2:C:1030:GLN:OE1	3:D:628:ARG:HG3	1.87	0.73
2:C:266:ARG:HG2	2:C:268:ASP:N	2.02	0.73
3:D:566:ILE:O	3:D:566:ILE:HG22	1.88	0.73
3:D:586:ARG:O	3:D:587:ARG:HD3	1.88	0.73
2:C:151:ASP:HA	2:C:158:TYR:HD2	1.54	0.73
2:C:461:VAL:HB	2:C:471:TYR:OH	1.89	0.73
3:D:721:VAL:CG1	3:D:722:GLU:H	2.00	0.73
2:C:142:ARG:HG3	2:C:147:TYR:OH	1.87	0.73
2:C:755:LEU:HD23	2:C:792:VAL:CG2	2.18	0.73
3:D:1278:ILE:HG22	3:D:1279:ASP:N	2.03	0.73
1:A:166:VAL:HG12	1:A:167:ASP:N	2.03	0.73
2:C:581:THR:O	2:C:584:GLU:HG2	1.87	0.73
2:C:32:ALA:HB2	2:C:73:ILE:HD13	1.69	0.73
1:B:35:THR:O	1:B:35:THR:HG22	1.87	0.73
3:D:1047:GLN:HA	3:D:1053:THR:HA	1.70	0.73
3:D:675:ARG:HA	3:D:678:GLU:CB	2.18	0.73
2:C:750:LYS:HE3	3:D:680:GLN:HE22	1.54	0.73
1:A:30:ARG:HD2	1:A:191:LEU:N	2.04	0.73
1:B:85:LEU:CA	1:B:123:ASN:HD21	2.01	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:283:VAL:HG12	2:C:284:GLY:N	2.03	0.73
2:C:333:ILE:HD11	2:C:468:ARG:HE	1.53	0.73
3:D:1148:ARG:HH12	3:D:1191:SER:HB2	1.54	0.73
1:B:62:LEU:HD22	1:B:162:ASN:OD1	1.89	0.73
2:C:66:LEU:HA	2:C:100:LEU:HA	1.69	0.73
2:C:722:ILE:HD12	2:C:821:GLU:CD	2.08	0.73
2:C:55:GLU:O	2:C:56:GLU:HB3	1.89	0.73
2:C:775:ARG:HA	2:C:780:GLU:CB	2.18	0.73
2:C:263:ASP:CB	2:C:264:PRO:HD3	2.19	0.73
3:D:590:PRO:C	3:D:600:LEU:HD21	2.09	0.72
3:D:925:GLU:N	3:D:925:GLU:OE1	2.22	0.72
4:E:91:ARG:HB3	4:E:92:LEU:HD12	1.71	0.72
2:C:355:VAL:HG23	2:C:372:LEU:HD22	1.71	0.72
3:D:1012:PHE:HB2	3:D:1020:PRO:HG2	1.71	0.72
3:D:1364:LEU:HD23	3:D:1365:HIS:H	1.53	0.72
1:A:161:ILE:HG12	1:A:162:ASN:CG	2.10	0.72
2:C:17:PRO:HD2	2:C:20:GLU:HB2	1.69	0.72
3:D:1008:VAL:HG21	3:D:1040:CYS:HB2	1.70	0.72
3:D:1135:LEU:H	3:D:1135:LEU:HD23	1.53	0.72
3:D:546:ARG:O	3:D:550:ARG:HB2	1.89	0.72
3:D:87:ARG:HA	3:D:522:PRO:HG2	1.70	0.72
1:A:79:ILE:HD11	1:A:164:ILE:HD12	1.70	0.72
1:B:54:THR:HG21	1:B:144:ASP:HB2	1.72	0.72
3:D:1436:LEU:HB2	3:D:1458:ASP:OD2	1.88	0.72
2:C:9:ILE:HG22	2:C:10:ARG:N	2.05	0.72
2:C:399:ASN:C	2:C:399:ASN:HD22	1.93	0.72
2:C:424:GLY:O	2:C:427:VAL:HG23	1.89	0.72
2:C:508:ILE:N	2:C:508:ILE:HD13	1.95	0.72
3:D:547:LEU:HD13	3:D:577:ALA:O	1.89	0.72
1:A:66:SER:HB2	1:A:75:VAL:HG21	1.72	0.72
1:A:224:PHE:HE1	1:B:36:LEU:HD11	1.54	0.72
2:C:140:ILE:CG2	2:C:333:ILE:HG12	2.19	0.72
2:C:16:PRO:HA	2:C:586:ARG:HH22	1.53	0.72
2:C:881:ASN:HD22	2:C:881:ASN:N	1.87	0.72
3:D:975:ILE:HA	3:D:978:ALA:HB3	1.70	0.72
1:B:58:ILE:HG23	1:B:139:MET:HG2	1.69	0.72
2:C:129:ILE:HD13	2:C:386:PHE:HB3	1.70	0.72
3:D:1079:ARG:O	3:D:1082:GLY:N	2.21	0.72
2:C:1032:PHE:HB2	3:D:623:VAL:HG23	1.71	0.72
3:D:518:PRO:HB3	3:D:544:TYR:CG	2.24	0.72
4:E:19:LEU:HD11	4:E:23:VAL:HG23	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:ARG:HA	1:A:192:ASP:OD1	1.89	0.72
2:C:399:ASN:ND2	2:C:399:ASN:C	2.43	0.72
3:D:1060:SER:CB	3:D:1066:LEU:HD22	2.19	0.72
3:D:1339:ALA:O	3:D:1340:LYS:HB2	1.89	0.72
3:D:1408:LEU:C	3:D:1410:ALA:H	1.92	0.72
1:B:194:LEU:CD1	1:B:196:LEU:HD13	2.20	0.71
2:C:290:LEU:HD21	2:C:298:PHE:HD2	1.55	0.71
2:C:310:LEU:O	2:C:313:LEU:HD23	1.89	0.71
2:C:115:LEU:HG	2:C:378:LEU:HD22	1.71	0.71
2:C:580:MET:HB2	2:C:584:GLU:CG	2.16	0.71
2:C:703:ILE:HD11	2:C:830:LYS:HE2	1.71	0.71
3:D:1009:PHE:HE1	3:D:1036:ILE:HG13	1.54	0.71
3:D:1104:HIS:HE1	3:D:1463:LEU:H	1.35	0.71
3:D:709:HIS:HA	3:D:1228:GLU:HB3	1.71	0.71
2:C:732:ALA:O	2:C:736:ASP:HB2	1.90	0.71
2:C:804:LEU:HD12	2:C:805:ARG:N	2.05	0.71
2:C:256:TYR:O	2:C:260:LEU:HB3	1.90	0.71
2:C:536:PRO:O	2:C:538:GLN:N	2.23	0.71
3:D:590:PRO:O	3:D:600:LEU:HD11	1.90	0.71
4:E:4:PRO:HB2	4:E:66:LYS:HE2	1.70	0.71
1:B:90:LEU:CD1	1:B:118:ASP:HA	2.19	0.71
2:C:31:GLN:NE2	2:C:39:ARG:HB3	2.05	0.71
4:E:8:LYS:HE2	4:E:69:LEU:HD11	1.71	0.71
1:B:100:LEU:HD22	1:B:139:MET:CE	2.21	0.71
2:C:1051:GLU:HA	2:C:1055:ILE:CD1	2.21	0.71
2:C:492:ASP:O	2:C:532:MET:HA	1.90	0.71
3:D:1209:ASP:O	3:D:1210:LEU:HB3	1.89	0.71
3:D:856:GLY:O	3:D:857:LEU:HD13	1.89	0.71
2:C:511:ASP:OD1	2:C:516:ARG:HB2	1.89	0.71
2:C:588:VAL:O	2:C:589:ARG:HG2	1.91	0.71
2:C:963:LEU:O	2:C:966:LEU:N	2.23	0.71
3:D:1044:GLY:CA	3:D:1058:VAL:H	2.02	0.71
3:D:1075:SER:O	3:D:1078:ALA:HB3	1.91	0.71
3:D:1286:GLU:HG3	3:D:1291:LEU:HD11	1.70	0.71
3:D:772:PRO:HD3	3:D:778:LEU:H	1.54	0.71
2:C:100:LEU:HG	2:C:369:PRO:HD3	1.70	0.71
2:C:198:ARG:HG2	2:C:228:ALA:HA	1.71	0.71
2:C:711:GLU:HG2	2:C:822:VAL:HG22	1.71	0.71
2:C:889:HIS:C	2:C:891:GLY:H	1.92	0.71
2:C:929:ARG:HH11	2:C:936:VAL:H	1.35	0.71
1:A:222:ASN:O	1:A:224:PHE:N	2.24	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:231:PRO:O	2:C:233:GLU:N	2.24	0.71
2:C:420:ARG:HD3	2:C:420:ARG:H	1.56	0.71
1:A:72:LYS:HA	2:C:607:ASP:HB3	1.73	0.71
2:C:603:VAL:HG21	2:C:646:GLY:N	2.05	0.71
3:D:1000:THR:O	3:D:1004:VAL:HG23	1.90	0.71
3:D:1080:LYS:CG	3:D:1081:GLY:H	1.89	0.71
3:D:767:HIS:CE1	4:E:6:ILE:HG13	2.25	0.71
3:D:911:LEU:O	3:D:915:VAL:HG23	1.90	0.71
3:D:969:ASP:O	3:D:972:LEU:N	2.22	0.71
2:C:165:LEU:HD22	2:C:334:ARG:HD3	1.73	0.71
3:D:1018:PHE:HA	3:D:1024:MET:SD	2.30	0.71
2:C:987:ILE:HA	3:D:948:ILE:CG2	2.20	0.71
1:B:77:GLU:HA	1:B:77:GLU:OE1	1.89	0.71
2:C:162:ILE:HG13	2:C:171:TRP:CH2	2.25	0.71
2:C:630:ARG:CB	2:C:705:ILE:HD11	2.19	0.71
2:C:726:ILE:HD12	2:C:726:ILE:N	2.06	0.71
1:A:110:ALA:O	1:A:113:PHE:HB2	1.91	0.70
2:C:1051:GLU:HG3	2:C:1055:ILE:HD13	1.73	0.70
3:D:1063:ARG:C	3:D:1063:ARG:HD3	2.11	0.70
3:D:1110:GLU:O	3:D:1218:ILE:HD11	1.90	0.70
3:D:1365:HIS:CG	3:D:1366:ASP:N	2.55	0.70
3:D:1382:VAL:HG12	3:D:1383:THR:H	1.56	0.70
3:D:770:LEU:H	3:D:770:LEU:HD12	1.55	0.70
4:E:28:GLN:HG2	4:E:28:GLN:O	1.91	0.70
2:C:399:ASN:ND2	2:C:401:LEU:N	2.39	0.70
3:D:1286:GLU:HG3	3:D:1291:LEU:CD1	2.21	0.70
3:D:688:TRP:O	3:D:690:ALA:N	2.23	0.70
2:C:110:GLU:HG3	2:C:369:PRO:O	1.90	0.70
3:D:1482:VAL:HG12	4:E:21:VAL:HG21	1.72	0.70
2:C:1013:TYR:HE2	2:C:1018:GLN:NE2	1.88	0.70
2:C:20:GLU:CD	2:C:461:VAL:HG22	2.12	0.70
2:C:290:LEU:HD21	2:C:298:PHE:CD2	2.27	0.70
2:C:358:ARG:HB2	2:C:372:LEU:CD2	2.20	0.70
2:C:640:ARG:HH11	2:C:640:ARG:HG3	1.56	0.70
2:C:659:PRO:HG2	2:C:660:ALA:H	1.56	0.70
3:D:806:PHE:H	3:D:827:ILE:HA	1.56	0.70
1:B:100:LEU:HD11	1:B:112:ASP:HB2	1.72	0.70
2:C:467:ILE:HG22	2:C:484:VAL:HG21	1.74	0.70
3:D:684:LYS:HD3	3:D:685:ASP:N	2.06	0.70
2:C:567:GLN:HB2	2:C:997:LEU:HD22	1.74	0.70
2:C:546:LEU:HD22	2:C:584:GLU:OE2	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:8:ARG:HB3	2:C:9:ILE:HD12	1.73	0.70
1:A:161:ILE:HG23	1:A:162:ASN:H	1.55	0.70
2:C:614:ARG:CZ	2:C:623:HIS:CE1	2.75	0.70
2:C:743:VAL:HG23	2:C:755:LEU:O	1.92	0.70
2:C:78:PHE:CZ	2:C:812:GLY:HA3	2.26	0.70
3:D:500:ARG:O	3:D:504:ASP:HB2	1.92	0.70
3:D:793:THR:HB	3:D:879:ARG:NH1	2.05	0.70
1:A:211:ASN:O	1:A:214:VAL:HG22	1.91	0.70
2:C:831:ARG:HH12	2:C:1002:GLU:HB2	1.56	0.70
2:C:976:ASP:O	2:C:978:ARG:N	2.24	0.70
2:C:988:VAL:HG12	3:D:948:ILE:HG13	1.72	0.70
3:D:543:LEU:HD13	3:D:581:VAL:HA	1.74	0.70
2:C:1067:TYR:CE1	2:C:1071:ILE:HD11	2.27	0.70
2:C:946:ARG:NE	3:D:861:GLN:NE2	2.39	0.70
2:C:94:LEU:O	2:C:115:LEU:HB3	1.91	0.70
3:D:990:TYR:OH	3:D:1053:THR:HG23	1.91	0.70
1:B:14:THR:OG1	1:B:22:GLU:HB2	1.91	0.70
2:C:13:ILE:N	2:C:13:ILE:HD12	2.07	0.70
2:C:325:ILE:O	2:C:327:HIS:N	2.25	0.70
2:C:15:LEU:CD2	2:C:461:VAL:HG21	2.22	0.70
2:C:695:LEU:HD21	2:C:833:LEU:HB3	1.73	0.70
3:D:502:PHE:HZ	3:D:511:TRP:HZ2	1.37	0.70
3:D:552:ASN:C	3:D:554:LEU:H	1.93	0.70
1:A:62:LEU:HD12	1:A:62:LEU:N	2.02	0.69
1:B:124:PRO:HG2	1:B:125:ASP:OD2	1.91	0.69
2:C:164:PRO:HG2	2:C:168:ARG:HB3	1.72	0.69
2:C:929:ARG:NH1	2:C:936:VAL:H	1.90	0.69
3:D:9:ARG:HA	3:D:1457:LYS:HA	1.72	0.69
3:D:25(U):UNK:HA	3:D:40(U):UNK:O	1.92	0.69
1:A:18:ASP:O	1:A:19:HIS:CG	2.45	0.69
3:D:1484:PHE:CZ	4:E:18:ARG:HG3	2.27	0.69
1:A:184:ARG:HE	1:A:193:LYS:HD2	1.56	0.69
2:C:62:GLY:C	2:C:103:LYS:HB2	2.13	0.69
3:D:1044:GLY:HA2	3:D:1058:VAL:HG23	1.72	0.69
3:D:1283:ARG:HG2	3:D:1283:ARG:HH11	1.57	0.69
3:D:1352:GLU:OE1	3:D:1355:LYS:HD2	1.92	0.69
3:D:601:ARG:NH1	3:D:601:ARG:HA	2.07	0.69
2:C:1107:ASN:N	2:C:1108:PRO:HD3	2.07	0.69
2:C:256:TYR:O	2:C:260:LEU:HD22	1.91	0.69
2:C:56:GLU:HB2	2:C:356:ARG:HH11	1.58	0.69
2:C:474:VAL:HG22	2:C:530:GLU:HA	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:753:ASP:O	2:C:791:ARG:HA	1.92	0.69
3:D:705:ALA:CB	3:D:706:PRO:CD	2.70	0.69
3:D:805:ALA:HB3	3:D:827:ILE:CB	2.22	0.69
3:D:807:ALA:C	3:D:809:PRO:HD3	2.13	0.69
1:B:41:ARG:HG2	1:B:176:VAL:HG12	1.73	0.69
2:C:129:ILE:CD1	2:C:386:PHE:HB3	2.23	0.69
2:C:95:TYR:CD2	2:C:114:PHE:HA	2.27	0.69
1:B:76:VAL:HA	1:B:79:ILE:HB	1.73	0.69
2:C:198:ARG:CG	2:C:228:ALA:HA	2.23	0.69
2:C:843:HIS:HD2	2:C:884:GLN:HA	1.56	0.69
3:D:997:TRP:CD2	3:D:1057:PRO:HG3	2.27	0.69
3:D:1430:LEU:HD13	3:D:1441:PHE:CD2	2.27	0.69
1:B:188:ARG:HD3	1:B:191:LEU:HD21	1.73	0.69
2:C:95:TYR:HD2	2:C:114:PHE:HA	1.57	0.69
1:A:41:ARG:HG2	1:A:176:VAL:CG1	2.23	0.69
2:C:1001:VAL:HG11	3:D:724:GLN:HB3	1.75	0.69
2:C:1008:ARG:HG3	2:C:1009:SER:H	1.57	0.69
2:C:676:ILE:O	2:C:677:MET:HB3	1.92	0.69
2:C:700:TYR:HB2	2:C:833:LEU:HD22	1.75	0.69
3:D:129:PHE:HA	3:D:454:ALA:CB	2.10	0.69
3:D:1206:TYR:CD1	3:D:1367:LYS:HD2	2.28	0.69
3:D:875:THR:HG23	3:D:879:ARG:HB3	1.75	0.69
3:D:986:ASP:O	3:D:989:ARG:HB3	1.92	0.69
1:B:14:THR:HB	1:B:22:GLU:N	2.07	0.69
2:C:13:ILE:CG2	2:C:14:PRO:HD2	2.20	0.69
2:C:603:VAL:HG23	2:C:604:VAL:H	1.57	0.69
2:C:397:GLU:HB2	2:C:633:GLN:HE21	1.58	0.69
2:C:852:ILE:H	2:C:852:ILE:HD13	1.56	0.69
3:D:1038:GLN:CG	3:D:1043:ARG:HD3	2.22	0.69
3:D:1139:SER:O	3:D:1142:GLU:HB3	1.93	0.69
3:D:1323:GLY:O	3:D:1324:GLN:HG2	1.91	0.69
2:C:202:TYR:HE1	2:C:304:LEU:HB3	1.58	0.69
2:C:328:LEU:C	2:C:467:ILE:HD13	2.13	0.69
3:D:699:VAL:HG12	3:D:717:GLN:HG3	1.75	0.69
1:A:130:THR:O	1:A:130:THR:HG22	1.93	0.68
1:B:114:THR:O	1:B:116:SER:N	2.22	0.68
1:B:175:ARG:HB3	1:B:199:TRP:HB2	1.73	0.68
2:C:17:PRO:HA	2:C:586:ARG:NH2	2.09	0.68
2:C:689:VAL:HG11	2:C:853:LEU:HD22	1.75	0.68
2:C:870:ILE:O	2:C:870:ILE:HG22	1.92	0.68
3:D:955:ALA:O	3:D:1063:ARG:HG3	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1354:GLN:HE21	3:D:1369:ILE:HD12	1.56	0.68
1:B:142:ARG:HG2	1:B:143:VAL:N	2.07	0.68
2:C:813:VAL:HG12	2:C:814:GLU:N	2.05	0.68
3:D:1005:THR:OG1	3:D:1037:ARG:HD2	1.93	0.68
3:D:808:THR:N	3:D:809:PRO:HD3	2.08	0.68
1:A:166:VAL:HG12	1:A:167:ASP:H	1.58	0.68
1:B:149:TYR:CE1	1:B:169:ILE:HG22	2.22	0.68
2:C:399:ASN:HB3	2:C:568:ALA:HB3	1.74	0.68
2:C:676:ILE:HG21	2:C:873:PRO:HB3	1.75	0.68
3:D:639:LEU:N	3:D:729:HIS:CD2	2.61	0.68
3:D:659:LYS:HZ3	3:D:663:GLU:HB2	1.59	0.68
1:B:168:ALA:HB1	1:B:170:PHE:CZ	2.28	0.68
2:C:1005:MET:HG2	3:D:724:GLN:HG3	1.76	0.68
2:C:110:GLU:HG2	2:C:369:PRO:CG	2.19	0.68
2:C:267:TYR:CD1	2:C:273:GLY:HA3	2.26	0.68
1:A:192:ASP:HB3	2:C:938:LYS:HD2	1.76	0.68
3:D:1058:VAL:HG12	3:D:1068:VAL:HG21	1.75	0.68
3:D:1108:VAL:HG21	3:D:1216:VAL:HG11	1.76	0.68
1:B:76:VAL:HB	3:D:872:ARG:HH22	1.58	0.68
2:C:843:HIS:CD2	2:C:884:GLN:HA	2.28	0.68
4:E:9:LEU:HD23	4:E:69:LEU:HD13	1.74	0.68
2:C:946:ARG:CZ	2:C:984:GLU:HB2	2.24	0.68
3:D:674:ARG:O	3:D:678:GLU:HB2	1.93	0.68
3:D:687:VAL:O	3:D:690:ALA:HB2	1.94	0.68
1:A:227:PRO:HA	1:B:11:PHE:O	1.94	0.68
2:C:1020:PRO:O	2:C:1021:LEU:HG	1.93	0.68
2:C:140:ILE:HD12	2:C:331:ARG:HD3	1.74	0.68
2:C:726:ILE:CD1	2:C:726:ILE:H	2.07	0.68
2:C:552:HIS:CD2	2:C:886:LEU:HD12	2.28	0.68
3:D:864:VAL:HA	3:D:875:THR:O	1.93	0.68
3:D:89:ARG:C	3:D:520:LEU:HD21	2.13	0.68
4:E:30:LEU:HD12	4:E:37:ASN:HB2	1.76	0.68
1:B:44:LEU:HD23	1:B:198:ILE:HD11	1.76	0.68
2:C:241:LEU:O	2:C:242:LEU:HD12	1.94	0.68
2:C:943:VAL:O	2:C:946:ARG:N	2.25	0.68
3:D:1253:ILE:C	3:D:1255:GLN:H	1.97	0.68
3:D:462:GLN:HA	3:D:512:MET:CE	2.24	0.68
4:E:13:VAL:HG21	4:E:19:LEU:HB2	1.75	0.68
1:A:187:GLN:O	1:A:188:ARG:HB3	1.93	0.68
1:B:103:GLU:O	1:B:135:GLY:HA3	1.94	0.68
1:A:194:LEU:CD2	1:A:195:THR:H	2.06	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:PHE:HB2	1:B:196:LEU:HD12	1.76	0.68
2:C:304:LEU:H	2:C:305:PRO:HD3	1.56	0.68
2:C:491:GLU:CG	2:C:510:THR:HB	2.24	0.68
2:C:682:TYR:CE1	2:C:851:LYS:HD2	2.29	0.68
3:D:1043:ARG:HH21	3:D:1066:LEU:CD2	2.05	0.68
3:D:1167:LEU:HB2	3:D:1171:ASP:CB	2.23	0.68
1:B:19:HIS:O	1:B:206:PRO:HG2	1.94	0.67
1:B:66:SER:OG	1:B:67:THR:N	2.27	0.67
2:C:1060:ILE:O	2:C:1061:GLU:C	2.33	0.67
2:C:1095:LEU:O	2:C:1096:ALA:HB3	1.94	0.67
2:C:184:MET:HE2	2:C:191:PHE:HZ	1.60	0.67
2:C:531:PHE:O	2:C:532:MET:HB2	1.93	0.67
2:C:761:PHE:O	2:C:762:LYS:O	2.12	0.67
3:D:1148:ARG:HD2	3:D:1189:VAL:HG21	1.77	0.67
3:D:14:SER:HA	3:D:510:GLU:OE1	1.94	0.67
3:D:644:LEU:HD21	3:D:747:VAL:HG21	1.76	0.67
2:C:14:PRO:O	2:C:15:LEU:HB3	1.94	0.67
2:C:181:VAL:HG12	2:C:182:VAL:H	1.59	0.67
3:D:1167:LEU:HB2	3:D:1171:ASP:HB2	1.75	0.67
3:D:1305:LYS:H	3:D:1305:LYS:HD3	1.57	0.67
3:D:1282:VAL:HG22	3:D:1315:LYS:CA	2.24	0.67
3:D:639:LEU:O	3:D:640:HIS:CB	2.42	0.67
2:C:946:ARG:HE	3:D:861:GLN:CD	1.98	0.67
4:E:6:ILE:HD12	4:E:10:PHE:CE1	2.29	0.67
1:A:106:LYS:HE3	1:A:108:VAL:HG22	1.77	0.67
2:C:1004:LYS:HD3	3:D:744:GLN:NE2	2.09	0.67
2:C:115:LEU:HD12	2:C:116:GLY:N	2.08	0.67
2:C:369:PRO:C	2:C:371:LYS:H	1.98	0.67
2:C:605:LYS:HD2	2:C:607:ASP:CG	2.13	0.67
2:C:807:ARG:HA	2:C:821:GLU:HA	1.76	0.67
3:D:795:VAL:HG22	3:D:876:ASN:OD1	1.95	0.67
1:A:98:LEU:O	1:A:99:ILE:HG13	1.94	0.67
1:B:89:PHE:CD1	1:B:94:TRP:HB3	2.29	0.67
2:C:872:ASN:HD21	2:C:874:LEU:CB	2.07	0.67
3:D:1283:ARG:HH21	3:D:1285:GLU:HG3	1.60	0.67
3:D:1348:TYR:O	3:D:1352:GLU:HB2	1.94	0.67
3:D:1460:LEU:HD13	3:D:1471:ARG:HH11	1.59	0.67
2:C:159:ILE:HD11	2:C:310:LEU:CD2	2.21	0.67
2:C:136:ILE:CG2	2:C:336:VAL:HG22	2.24	0.67
3:D:772:PRO:HD3	3:D:778:LEU:N	2.10	0.67
1:B:40:LEU:C	1:B:44:LEU:HD22	2.14	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:202:TYR:HE1	2:C:304:LEU:CB	2.06	0.67
2:C:688:ILE:HD12	2:C:871:LEU:HD12	1.76	0.67
2:C:839:LEU:O	2:C:994:ILE:HG22	1.95	0.67
3:D:538:SER:HA	3:D:541:ASN:ND2	2.08	0.67
3:D:589:SER:O	3:D:600:LEU:HG	1.95	0.67
1:B:86:VAL:N	1:B:123:ASN:HD21	1.92	0.67
1:B:78:ILE:CG1	1:B:129:ALA:HB2	2.24	0.67
2:C:157:ARG:HD3	2:C:157:ARG:H	1.59	0.67
1:A:111:VAL:CG2	1:A:125:ASP:H	2.06	0.67
1:B:151:PRO:HA	1:B:167:ASP:OD1	1.95	0.67
2:C:13:ILE:O	2:C:15:LEU:N	2.28	0.67
2:C:299:LYS:HD2	2:C:299:LYS:O	1.94	0.67
2:C:775:ARG:O	2:C:780:GLU:N	2.28	0.67
2:C:886:LEU:HD22	2:C:914:ILE:HD13	1.76	0.67
1:B:38:ASN:HB3	1:B:39:PRO:HD3	1.76	0.67
2:C:278:GLU:HG2	2:C:283:VAL:HG13	1.77	0.67
2:C:772:ARG:NH1	2:C:776:SER:HB3	2.10	0.67
3:D:1281:VAL:HG12	3:D:1282:VAL:H	1.60	0.67
2:C:654:LEU:HD22	2:C:664:GLY:N	2.10	0.67
3:D:1008:VAL:HG13	3:D:1009:PHE:N	2.10	0.67
3:D:1206:TYR:O	3:D:1207:GLY:O	2.12	0.67
1:A:150:VAL:O	1:A:168:ALA:HB3	1.95	0.66
1:A:88:ARG:HD3	1:A:120:GLU:CD	2.14	0.66
2:C:80:GLN:OE1	2:C:122:THR:HG23	1.95	0.66
2:C:304:LEU:N	2:C:305:PRO:CD	2.57	0.66
2:C:722:ILE:HA	2:C:758:ARG:HB2	1.77	0.66
3:D:1324:GLN:N	3:D:1325:PRO:CD	2.58	0.66
2:C:21:ILE:CD1	2:C:455:LEU:HD21	2.25	0.66
2:C:54:ILE:HG21	2:C:355:VAL:HG11	1.77	0.66
3:D:552:ASN:HA	3:D:555:LYS:HB3	1.76	0.66
3:D:669:ASN:OD1	3:D:671:LYS:HG2	1.94	0.66
1:A:221:LEU:HD11	1:B:217:LEU:HD23	1.76	0.66
1:B:30:ARG:HA	1:B:192:ASP:OD1	1.95	0.66
2:C:307:LEU:O	2:C:310:LEU:HB3	1.94	0.66
3:D:538:SER:HA	3:D:541:ASN:HD22	1.59	0.66
3:D:970:ARG:CZ	3:D:971:LYS:HE3	2.25	0.66
1:A:85:LEU:HA	1:A:123:ASN:HD21	1.59	0.66
2:C:13:ILE:C	2:C:15:LEU:H	1.98	0.66
2:C:446:GLY:HA2	2:C:449:ILE:CD1	2.26	0.66
2:C:813:VAL:HG11	2:C:815:LEU:HD11	1.77	0.66
1:A:15:THR:HG22	1:B:229:ALA:HB1	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:VAL:HG22	1:B:195:THR:HG23	1.78	0.66
3:D:1110:GLU:H	3:D:1218:ILE:HD12	1.61	0.66
3:D:648:MET:O	3:D:652:LEU:HD22	1.95	0.66
2:C:44:ILE:HD12	2:C:44:ILE:H	1.59	0.66
2:C:394:PHE:CE2	2:C:632:ASN:HB3	2.31	0.66
3:D:863:THR:O	3:D:864:VAL:HG23	1.96	0.66
2:C:9:ILE:HG22	2:C:10:ARG:H	1.61	0.66
2:C:468:ARG:HD2	2:C:468:ARG:H	1.60	0.66
2:C:889:HIS:HE1	3:D:951:GLY:N	1.91	0.66
3:D:1110:GLU:HG3	3:D:1111:ALA:N	2.10	0.66
3:D:1203:GLN:O	3:D:1204:LYS:HB2	1.96	0.66
3:D:688:TRP:HE3	3:D:688:TRP:HA	1.59	0.66
3:D:765:SER:O	3:D:769:LEU:HB2	1.96	0.66
4:E:14:ASP:CG	4:E:15:SER:H	1.99	0.66
1:A:6:LEU:C	1:A:8:ALA:H	1.99	0.66
1:B:172:PRO:HB3	1:B:204:VAL:HB	1.78	0.66
2:C:1113:GLU:C	2:C:1115:LEU:H	1.97	0.66
3:D:1093:GLY:HA2	3:D:1097:ARG:HH21	1.59	0.66
3:D:1156:ALA:HB1	3:D:1183:GLU:HB3	1.77	0.66
3:D:1150:LEU:O	3:D:1164:GLY:HA2	1.96	0.66
3:D:907:GLU:HB3	3:D:911:LEU:CD2	2.26	0.66
3:D:975:ILE:HD13	3:D:975:ILE:O	1.95	0.66
2:C:183:THR:CG2	2:C:190:LYS:HG3	2.26	0.66
2:C:270:GLY:HA3	2:C:274:ARG:HG2	1.78	0.66
2:C:676:ILE:O	2:C:677:MET:CB	2.44	0.66
2:C:691:SER:HB2	2:C:858:MET:CE	2.25	0.66
2:C:937:ASP:OD1	2:C:939:ARG:HD3	1.95	0.66
1:B:26:GLU:CB	1:B:27:PRO:CD	2.70	0.66
2:C:285:LEU:CD2	2:C:286:SER:H	2.09	0.66
2:C:728:HIS:C	2:C:730:SER:H	1.99	0.66
2:C:1026:GLN:HE21	3:D:674:ARG:HH21	1.43	0.66
2:C:149:THR:OG1	2:C:323:ASP:HA	1.96	0.65
2:C:101:ILE:CG2	2:C:102:HIS:H	2.07	0.65
2:C:211:LEU:HG	2:C:212:SER:N	2.08	0.65
2:C:605:LYS:CG	2:C:606:VAL:H	1.87	0.65
2:C:918:LEU:CD2	2:C:968:ASP:HA	2.25	0.65
3:D:1237:LEU:HD11	3:D:1357:TYR:HE2	1.61	0.65
3:D:1383:THR:HG23	3:D:1419:LYS:HE3	1.78	0.65
3:D:890:VAL:HG12	3:D:891:GLY:H	1.61	0.65
4:E:47:LYS:HE2	4:E:54:LEU:HD23	1.77	0.65
3:D:1016:TYR:CB	3:D:1020:PRO:HD3	2.22	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1157:LEU:HD12	3:D:1178:ALA:CA	2.23	0.65
3:D:1225:VAL:HG12	3:D:1225:VAL:O	1.96	0.65
3:D:477:LEU:HA	3:D:480:GLU:CB	2.27	0.65
3:D:710:ARG:NH1	3:D:768:ASN:HD21	1.94	0.65
2:C:149:THR:HB	2:C:158:TYR:CE1	2.32	0.65
2:C:21:ILE:HD11	2:C:455:LEU:HD21	1.77	0.65
2:C:222:LEU:O	2:C:225:ALA:N	2.29	0.65
2:C:352:ALA:HA	2:C:355:VAL:HG12	1.78	0.65
2:C:139:GLN:HA	2:C:411:SER:O	1.95	0.65
2:C:613:VAL:HG11	2:C:619:ARG:HA	1.78	0.65
2:C:873:PRO:O	2:C:877:PRO:HD2	1.97	0.65
3:D:1095:LEU:HD12	3:D:1099:LEU:HD13	1.76	0.65
2:C:1021:LEU:HD21	3:D:622:ARG:NE	2.12	0.65
3:D:769:LEU:HD22	3:D:779:ALA:HB2	1.78	0.65
3:D:906:GLN:OE1	3:D:906:GLN:N	2.29	0.65
3:D:911:LEU:HD22	3:D:911:LEU:H	1.61	0.65
1:A:109:ARG:HB2	1:A:125:ASP:O	1.96	0.65
2:C:1055:ILE:CG2	2:C:1066:ALA:HB2	2.26	0.65
2:C:266:ARG:C	2:C:268:ASP:H	1.99	0.65
3:D:1079:ARG:O	3:D:1081:GLY:N	2.30	0.65
1:A:183:THR:O	1:A:184:ARG:HD3	1.95	0.65
1:A:41:ARG:HH21	2:C:860:HIS:CD2	2.15	0.65
3:D:1110:GLU:H	3:D:1218:ILE:CD1	2.09	0.65
1:A:82:LEU:CD2	1:A:128:ILE:HD13	2.27	0.65
2:C:1034:GLU:O	2:C:1037:VAL:N	2.29	0.65
2:C:255:ALA:C	2:C:257:LEU:H	1.99	0.65
2:C:717:LEU:HD13	2:C:762:LYS:HA	1.77	0.65
2:C:903:SER:HB2	2:C:909:ALA:HB2	1.79	0.65
3:D:1272:LYS:HA	3:D:1331:ILE:HA	1.78	0.65
3:D:1432:THR:OG1	3:D:1433:LYS:HD3	1.96	0.65
3:D:465:LEU:HB2	3:D:512:MET:HE1	1.79	0.65
1:A:88:ARG:HB3	1:A:120:GLU:HB2	1.79	0.65
1:B:125:ASP:O	1:B:126:LEU:HB3	1.97	0.65
1:B:68:ILE:N	1:B:68:ILE:HD12	2.11	0.65
1:B:91:ASP:N	1:B:92:PRO:HD2	2.12	0.65
2:C:1012:PRO:HB3	2:C:1022:GLY:O	1.96	0.65
2:C:328:LEU:HB3	2:C:467:ILE:HG21	1.77	0.65
2:C:492:ASP:H	2:C:531:PHE:CB	2.09	0.65
2:C:1072:LYS:O	3:D:659:LYS:HE3	1.97	0.65
1:A:194:LEU:HD23	1:A:195:THR:N	2.10	0.65
1:B:213:ALA:HA	1:B:216:ILE:CD1	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1202:CYS:SG	3:D:1203:GLN:N	2.69	0.65
3:D:520:LEU:HB3	3:D:521:PRO:HD2	1.79	0.65
3:D:639:LEU:O	3:D:640:HIS:HB3	1.96	0.65
3:D:874:GLU:O	3:D:875:THR:O	2.15	0.65
2:C:970:GLY:HA3	3:D:950:ILE:HD13	1.78	0.65
3:D:1484:PHE:CE1	4:E:22:VAL:HG23	2.32	0.65
2:C:595:LEU:HG	2:C:655:LEU:CD2	2.27	0.65
2:C:892:LEU:HD12	2:C:967:PHE:CZ	2.33	0.65
3:D:1119:ILE:HD12	3:D:1119:ILE:N	2.12	0.65
3:D:890:VAL:HA	3:D:926:LYS:HZ1	1.60	0.65
1:A:194:LEU:O	1:A:195:THR:HB	1.97	0.64
2:C:1008:ARG:CG	2:C:1009:SER:H	2.10	0.64
2:C:164:PRO:HD3	2:C:267:TYR:CD2	2.32	0.64
2:C:759:THR:HB	2:C:785:VAL:HG22	1.79	0.64
2:C:987:ILE:HA	3:D:948:ILE:HG21	1.79	0.64
3:D:1016:TYR:CA	3:D:1019:ASN:HD22	2.05	0.64
3:D:1085:THR:C	3:D:1087:LEU:N	2.48	0.64
1:A:111:VAL:C	1:A:113:PHE:H	2.01	0.64
1:B:147:VAL:HG23	1:B:148:GLY:N	2.12	0.64
2:C:141:HIS:CE1	2:C:332:ARG:HD3	2.32	0.64
2:C:16:PRO:HA	2:C:586:ARG:NH2	2.12	0.64
3:D:1061:SER:C	3:D:1063:ARG:H	2.00	0.64
3:D:1167:LEU:H	3:D:1167:LEU:CD2	2.11	0.64
1:A:194:LEU:HD23	1:A:196:LEU:H	1.62	0.64
2:C:1067:TYR:O	2:C:1071:ILE:HD13	1.98	0.64
2:C:525:ALA:HB1	2:C:526:PRO:CD	2.27	0.64
3:D:1008:VAL:HG13	3:D:1009:PHE:H	1.61	0.64
3:D:1137:LYS:O	3:D:1139:SER:N	2.29	0.64
2:C:136:ILE:HB	2:C:336:VAL:HG22	1.80	0.64
2:C:603:VAL:HG21	2:C:645:VAL:HA	1.79	0.64
3:D:1048:LYS:HB3	3:D:1049:PRO:HD2	1.78	0.64
3:D:1134:ARG:HD2	3:D:1135:LEU:HD23	1.80	0.64
3:D:1238:THR:HG22	3:D:1240:ARG:H	1.62	0.64
3:D:638:LYS:O	3:D:639:LEU:HG	1.98	0.64
2:C:184:MET:HG2	2:C:193:LEU:HD23	1.80	0.64
2:C:218:VAL:O	2:C:221:LEU:N	2.31	0.64
2:C:710:ILE:HG13	2:C:790:LEU:HD13	1.80	0.64
3:D:729:HIS:NE2	3:D:731:LEU:HB2	2.13	0.64
1:A:102:ALA:HB3	1:A:137:LEU:HB3	1.80	0.64
2:C:495:THR:HG22	2:C:496:ILE:N	2.12	0.64
2:C:564:MET:SD	2:C:846:LYS:HB3	2.38	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:791:TYR:HE1	3:D:1024:MET:HG3	1.63	0.64
3:D:879:ARG:CG	3:D:904:VAL:HG22	2.16	0.64
3:D:790:TYR:CD2	3:D:906:GLN:HB3	2.33	0.64
2:C:889:HIS:CE1	3:D:950:ILE:HG22	2.32	0.64
2:C:140:ILE:CD1	2:C:331:ARG:HD3	2.28	0.64
2:C:64:LEU:HB3	2:C:359:MET:CE	2.28	0.64
2:C:875:GLY:CA	2:C:879:ARG:HG3	2.26	0.64
3:D:1104:HIS:HA	3:D:1223:GLY:HA3	1.80	0.64
3:D:499:VAL:O	3:D:503:LEU:N	2.29	0.64
3:D:558:LEU:CG	3:D:567:ILE:HD11	2.27	0.64
3:D:877:PRO:O	3:D:880:ILE:HB	1.97	0.64
1:B:215:ALA:O	1:B:219:GLU:HB2	1.97	0.64
2:C:1008:ARG:CG	2:C:1009:SER:N	2.61	0.64
2:C:1051:GLU:HA	2:C:1055:ILE:HD12	1.77	0.64
2:C:18:LEU:O	2:C:408:ARG:HD3	1.97	0.64
2:C:333:ILE:CD1	2:C:468:ARG:NE	2.61	0.64
2:C:605:LYS:HE2	2:C:611:ILE:HG23	1.79	0.64
2:C:7:GLY:O	2:C:8:ARG:HG3	1.97	0.64
3:D:1354:GLN:CD	3:D:1365:HIS:HB2	2.18	0.64
3:D:793:THR:HB	3:D:879:ARG:CZ	2.27	0.64
3:D:879:ARG:CZ	3:D:905:PRO:HD2	2.27	0.64
1:A:156:GLY:O	1:A:163:ALA:HB1	1.98	0.64
2:C:1011:GLY:O	2:C:1013:TYR:N	2.31	0.64
2:C:25:SER:O	2:C:28:LYS:HG2	1.97	0.64
2:C:322:VAL:O	2:C:322:VAL:HG13	1.98	0.64
1:A:120:GLU:O	1:A:121:ILE:HD13	1.98	0.64
2:C:94:LEU:HD23	2:C:344:PHE:HZ	1.63	0.64
3:D:836:VAL:HG11	3:D:858:LEU:CG	2.27	0.64
1:B:111:VAL:HG23	1:B:124:PRO:O	1.97	0.63
1:A:28:LEU:HD23	1:B:220:HIS:HE1	1.63	0.63
2:C:274:ARG:HG3	2:C:275:TYR:N	2.12	0.63
2:C:31:GLN:O	2:C:33:ASP:N	2.32	0.63
2:C:87:ASP:OD2	2:C:824:ARG:NH2	2.29	0.63
2:C:924:LEU:N	2:C:924:LEU:HD23	2.12	0.63
3:D:1081:GLY:O	3:D:1085:THR:HG23	1.97	0.63
3:D:1380:VAL:HG13	3:D:1397:GLU:HB2	1.80	0.63
1:A:184:ARG:NE	1:A:193:LYS:HD2	2.13	0.63
1:A:93:ARG:O	1:A:94:TRP:HB3	1.96	0.63
1:B:100:LEU:HD22	1:B:139:MET:HE1	1.80	0.63
2:C:148:PHE:HA	2:C:159:ILE:HA	1.80	0.63
2:C:460:ARG:HD2	2:C:464:LEU:HD22	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:441:VAL:HB	3:D:1075:SER:HB2	1.80	0.63
3:D:1108:VAL:HG13	3:D:1203:GLN:HA	1.79	0.63
3:D:1345:VAL:O	3:D:1348:TYR:N	2.31	0.63
3:D:638:LYS:CB	3:D:932:ASP:OD1	2.46	0.63
4:E:14:ASP:OD1	4:E:18:ARG:HD2	1.98	0.63
1:A:164:ILE:CG1	1:A:164:ILE:O	2.43	0.63
1:A:88:ARG:HD3	1:A:120:GLU:OE2	1.99	0.63
1:B:88:ARG:HB2	1:B:122:MET:SD	2.38	0.63
1:B:98:LEU:O	1:B:140:GLU:HA	1.98	0.63
1:B:44:LEU:CD2	1:B:198:ILE:HD11	2.27	0.63
2:C:1055:ILE:H	2:C:1055:ILE:CD1	2.07	0.63
2:C:246:ASP:O	2:C:248:PRO:HD3	1.97	0.63
2:C:110:GLU:CB	2:C:369:PRO:HG2	2.28	0.63
2:C:551:GLU:HA	2:C:906:PHE:CE2	2.30	0.63
2:C:149:THR:HG23	2:C:150:PRO:HD2	1.80	0.63
2:C:246:ASP:HB3	2:C:247:PRO:HD2	1.80	0.63
2:C:253:ALA:O	2:C:254:LEU:HB3	1.97	0.63
2:C:148:PHE:CE1	2:C:309:TYR:CD2	2.87	0.63
2:C:115:LEU:CG	2:C:378:LEU:HD22	2.29	0.63
2:C:734:LEU:O	2:C:737:LEU:O	2.17	0.63
3:D:627:GLY:O	3:D:747:VAL:HG12	1.99	0.63
1:A:223:TYR:CE1	1:B:9:PRO:HD2	2.33	0.63
2:C:1015:LEU:HD12	2:C:1016:ILE:HG12	1.80	0.63
2:C:141:HIS:NE2	2:C:332:ARG:HD3	2.14	0.63
2:C:439:CYS:CB	2:C:468:ARG:HH12	2.12	0.63
2:C:924:LEU:O	2:C:928:LYS:HG3	1.98	0.63
3:D:863:THR:C	3:D:864:VAL:HG23	2.19	0.63
4:E:38:THR:HG22	4:E:39:VAL:H	1.62	0.63
1:A:177:ALA:O	1:A:178:PHE:HB3	1.98	0.63
2:C:996:LYS:CE	2:C:1000:MET:HE3	2.27	0.63
2:C:333:ILE:HD11	2:C:468:ARG:NE	2.12	0.63
2:C:595:LEU:HD21	2:C:623:HIS:HB3	1.80	0.63
2:C:877:PRO:HG2	2:C:878:SER:H	1.64	0.63
2:C:862:PRO:HG3	2:C:925:TYR:OH	1.98	0.63
3:D:1208:TYR:HA	3:D:1215:PRO:HA	1.81	0.63
3:D:970:ARG:HG3	3:D:971:LYS:N	2.14	0.63
1:A:102:ALA:HA	1:A:106:LYS:NZ	2.14	0.63
1:A:19:HIS:HB2	1:A:200:THR:HA	1.81	0.63
1:A:57:TYR:CD2	1:A:57:TYR:C	2.71	0.63
2:C:1012:PRO:CB	2:C:1023:GLY:HA3	2.29	0.63
2:C:842:ARG:HH21	2:C:887:GLU:CD	2.01	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1081:GLY:HA2	3:D:1084:ASP:HB2	1.79	0.63
3:D:637:LEU:CB	3:D:641:GLN:HG3	2.29	0.63
1:A:56:VAL:HG11	1:A:82:LEU:CD1	2.28	0.63
1:B:193:LYS:O	1:B:193:LYS:HG2	1.98	0.63
2:C:212:SER:O	2:C:218:VAL:HG21	1.98	0.63
2:C:712:ALA:HB3	2:C:820:ARG:O	1.98	0.63
3:D:864:VAL:HG12	3:D:874:GLU:C	2.18	0.63
1:A:108:VAL:O	1:A:128:ILE:HB	1.98	0.63
2:C:605:LYS:HG2	2:C:607:ASP:N	2.10	0.63
2:C:969:LEU:HD13	3:D:952:ILE:CB	2.19	0.63
3:D:1267:ARG:O	3:D:1269:PRO:N	2.31	0.63
3:D:702:LEU:O	3:D:713:ILE:O	2.17	0.63
3:D:729:HIS:HE2	3:D:731:LEU:HB2	1.64	0.63
4:E:48:MET:O	4:E:54:LEU:HA	1.99	0.63
1:B:110:ALA:HA	1:B:113:PHE:HE1	1.63	0.62
1:B:99:ILE:HG12	1:B:140:GLU:HG2	1.81	0.62
2:C:1105:LYS:C	2:C:1108:PRO:HD3	2.18	0.62
2:C:852:ILE:N	2:C:852:ILE:HD13	2.13	0.62
2:C:861:LEU:HG	2:C:862:PRO:CD	2.27	0.62
3:D:103:TRP:O	3:D:104:PHE:CB	2.46	0.62
3:D:1066:LEU:O	3:D:1068:VAL:N	2.32	0.62
3:D:1106:ILE:HG23	3:D:1201:VAL:H	1.63	0.62
3:D:1402:GLU:C	3:D:1404:LEU:H	2.02	0.62
3:D:124:GLU:HA	3:D:456:MET:SD	2.40	0.62
3:D:770:LEU:HD12	3:D:770:LEU:N	2.14	0.62
3:D:866:THR:HA	3:D:873:LEU:O	1.98	0.62
1:A:126:LEU:HG	1:A:126:LEU:O	1.99	0.62
2:C:172:ILE:CD1	2:C:184:MET:SD	2.87	0.62
2:C:446:GLY:O	2:C:447:ALA:HB3	1.99	0.62
3:D:1087:LEU:HA	3:D:1090:ALA:HB3	1.80	0.62
3:D:1108:VAL:HG11	3:D:1216:VAL:HG12	1.79	0.62
3:D:1279:ASP:HA	3:D:1318:ASP:O	2.00	0.62
3:D:729:HIS:CE1	3:D:730:PRO:HG2	2.34	0.62
3:D:795:VAL:CG2	3:D:904:VAL:HG11	2.23	0.62
1:A:104:GLY:HA2	1:A:135:GLY:H	1.64	0.62
1:A:210:LEU:O	1:A:213:ALA:HB3	1.99	0.62
1:B:111:VAL:C	1:B:113:PHE:H	2.01	0.62
2:C:162:ILE:CA	2:C:171:TRP:HZ3	2.07	0.62
2:C:631:SER:CB	2:C:635:THR:H	2.09	0.62
2:C:859:PRO:HD2	2:C:867:VAL:HG21	1.82	0.62
2:C:984:GLU:CG	3:D:945:SER:HA	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1087:LEU:HD13	3:D:1239:MET:HB2	1.79	0.62
3:D:1354:GLN:OE1	3:D:1365:HIS:HB2	1.99	0.62
3:D:696:HIS:CE1	4:E:48:MET:HG3	2.34	0.62
4:E:38:THR:HG22	4:E:40:LEU:H	1.65	0.62
2:C:481:GLU:N	2:C:481:GLU:OE1	2.33	0.62
2:C:552:HIS:CE1	3:D:1065:GLY:HA2	2.33	0.62
2:C:760:SER:HB2	2:C:788:THR:HG21	1.80	0.62
2:C:881:ASN:N	2:C:881:ASN:ND2	2.46	0.62
2:C:1097:LEU:HD13	3:D:10:ILE:HD11	1.81	0.62
3:D:1322:ALA:O	3:D:1324:GLN:N	2.32	0.62
1:B:210:LEU:O	1:B:214:VAL:HG23	1.99	0.62
2:C:30:LEU:HA	2:C:44:ILE:HD13	1.80	0.62
2:C:632:ASN:HB2	2:C:633:GLN:HE22	1.63	0.62
2:C:84:ARG:HA	2:C:131:GLY:HA2	1.80	0.62
4:E:68:LEU:HA	4:E:73:LEU:CD1	2.28	0.62
1:A:100:LEU:C	1:A:100:LEU:HD12	2.19	0.62
1:A:44:LEU:HD13	1:A:198:ILE:HG13	1.82	0.62
1:B:56:VAL:HB	1:B:164:ILE:HD11	1.81	0.62
2:C:323:ASP:C	2:C:325:ILE:N	2.47	0.62
2:C:408:ARG:NH2	2:C:457:ALA:HA	2.15	0.62
3:D:1054:PHE:CE2	3:D:1073:ILE:HG13	2.34	0.62
3:D:1229:SER:O	3:D:1233:PRO:HD2	1.99	0.62
2:C:99:GLN:HA	2:C:108:ILE:O	1.98	0.62
2:C:159:ILE:HB	2:C:174:LEU:HB2	1.80	0.62
2:C:162:ILE:N	2:C:162:ILE:HD12	2.14	0.62
2:C:336:VAL:HA	2:C:339:LEU:HD13	1.80	0.62
2:C:605:LYS:HZ1	2:C:611:ILE:HG13	1.64	0.62
2:C:570:PRO:HB3	2:C:660:ALA:HB2	1.80	0.62
2:C:687:ALA:HB1	2:C:850:ALA:HB2	1.82	0.62
2:C:706:GLU:CD	2:C:707:ARG:H	2.02	0.62
2:C:839:LEU:HD23	2:C:849:VAL:HG23	1.80	0.62
2:C:579:VAL:HG23	2:C:842:ARG:HH22	1.64	0.62
2:C:981:GLU:HB3	2:C:982:PRO:HD2	1.81	0.62
2:C:1054:THR:HB	2:C:1055:ILE:HD12	1.81	0.62
2:C:20:GLU:OE1	2:C:461:VAL:HG22	2.00	0.62
2:C:707:ARG:HG3	2:C:707:ARG:O	1.98	0.62
3:D:1035:GLN:HE21	3:D:1035:GLN:CA	2.04	0.62
3:D:1284:ILE:O	3:D:1284:ILE:HG22	2.00	0.62
3:D:1484:PHE:CE2	4:E:18:ARG:HG3	2.34	0.62
3:D:795:VAL:HG22	3:D:876:ASN:ND2	2.14	0.62
3:D:880:ILE:O	3:D:883:ALA:HB3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:98:PRO:CB	3:D:574:LEU:HD23	2.30	0.62
1:B:150:VAL:HB	1:B:168:ALA:CB	2.30	0.62
1:B:176:VAL:HG13	1:B:198:ILE:HD12	1.81	0.62
2:C:1087:VAL:O	2:C:1091:GLU:HB2	1.99	0.62
2:C:352:ALA:O	2:C:355:VAL:HG12	2.00	0.62
2:C:21:ILE:HD12	2:C:460:ARG:HH21	1.63	0.62
2:C:540:PHE:CE1	2:C:906:PHE:HE1	2.17	0.62
2:C:944:LEU:HD21	2:C:963:LEU:HD22	1.81	0.62
3:D:1282:VAL:CG1	3:D:1315:LYS:HA	2.27	0.62
3:D:578:VAL:HG12	3:D:582:ILE:HD11	1.80	0.62
3:D:582:ILE:O	3:D:584:ASN:N	2.33	0.62
3:D:631:ILE:HG21	3:D:745:MET:CE	2.30	0.62
3:D:699:VAL:N	3:D:756:GLN:NE2	2.44	0.62
3:D:805:ALA:HB3	3:D:827:ILE:CA	2.29	0.62
1:A:157:ILE:HG23	1:A:158:LYS:N	2.07	0.62
1:A:161:ILE:HD13	1:A:162:ASN:HD21	1.65	0.62
1:A:191:LEU:HD23	1:A:191:LEU:H	1.65	0.62
1:B:91:ASP:N	1:B:92:PRO:CD	2.63	0.62
2:C:310:LEU:O	2:C:313:LEU:N	2.32	0.62
1:A:56:VAL:HG11	1:A:82:LEU:HD12	1.81	0.61
2:C:285:LEU:HD22	2:C:286:SER:H	1.63	0.61
2:C:497:ALA:HA	2:C:502:PRO:HG3	1.81	0.61
3:D:1044:GLY:HA2	3:D:1058:VAL:H	1.65	0.61
3:D:498:VAL:O	3:D:502:PHE:HB2	2.00	0.61
3:D:952:ILE:O	3:D:954:ASP:O	2.18	0.61
1:B:176:VAL:HG13	1:B:198:ILE:CD1	2.30	0.61
2:C:181:VAL:HG12	2:C:182:VAL:N	2.15	0.61
2:C:202:TYR:CE1	2:C:304:LEU:HD13	2.35	0.61
2:C:399:ASN:HD21	2:C:401:LEU:HB3	1.65	0.61
2:C:672:VAL:HG22	2:C:868:ASP:CG	2.20	0.61
2:C:813:VAL:CG1	2:C:815:LEU:HD11	2.31	0.61
3:D:691:LEU:C	3:D:693:GLU:N	2.52	0.61
3:D:701:LEU:HA	3:D:715:ALA:HB2	1.82	0.61
1:B:173:VAL:HA	1:B:200:THR:CG2	2.30	0.61
2:C:17:PRO:HG2	2:C:19:THR:N	2.06	0.61
2:C:363:SER:HB3	2:C:366:THR:HB	1.83	0.61
2:C:515:ALA:HB2	3:D:1070:GLU:OE2	2.00	0.61
2:C:754:ILE:HA	2:C:791:ARG:HG2	1.82	0.61
2:C:564:MET:SD	2:C:840:ALA:CB	2.87	0.61
3:D:1254:THR:HA	3:D:1259:ARG:HD2	1.81	0.61
3:D:566:ILE:HA	3:D:569:ASN:OD1	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:643:GLY:O	3:D:644:LEU:HB2	1.98	0.61
1:A:137:LEU:O	1:A:139:MET:HG3	2.00	0.61
1:B:55:SER:HA	1:B:165:PRO:HA	1.82	0.61
2:C:21:ILE:HD12	2:C:460:ARG:NH2	2.15	0.61
2:C:257:LEU:CD1	2:C:264:PRO:HG3	2.26	0.61
2:C:348:LEU:HD12	2:C:378:LEU:HD11	1.82	0.61
2:C:654:LEU:O	2:C:655:LEU:C	2.38	0.61
2:C:836:GLY:C	2:C:848:VAL:HG23	2.21	0.61
3:D:1464:LYS:O	3:D:1468:ILE:HG13	2.01	0.61
3:D:691:LEU:C	3:D:693:GLU:H	2.03	0.61
3:D:795:VAL:HG12	3:D:796:ARG:N	2.16	0.61
1:A:184:ARG:HH21	1:A:193:LYS:HE3	1.66	0.61
1:A:172:PRO:O	1:A:201:ASP:HA	2.00	0.61
1:B:212:GLN:O	1:B:215:ALA:HB3	2.00	0.61
2:C:1036:GLU:O	2:C:1039:ALA:HB3	2.00	0.61
2:C:285:LEU:HD11	2:C:302:VAL:CG2	2.31	0.61
2:C:421:GLU:HG2	2:C:424:GLY:N	2.15	0.61
2:C:65:VAL:HG23	2:C:101:ILE:HB	1.81	0.61
2:C:672:VAL:O	2:C:991:GLN:HA	2.01	0.61
2:C:682:TYR:CD1	2:C:851:LYS:HD2	2.35	0.61
3:D:1015:ASN:O	3:D:1016:TYR:CB	2.48	0.61
3:D:1069:LEU:C	3:D:1071:TYR:N	2.51	0.61
3:D:606:ILE:HD12	3:D:606:ILE:H	1.63	0.61
3:D:654:LYS:HB3	3:D:655:PRO:CD	2.26	0.61
2:C:196:LEU:HD11	2:C:200:LEU:HD21	1.82	0.61
2:C:439:CYS:HB2	2:C:468:ARG:HH12	1.64	0.61
2:C:588:VAL:HG23	2:C:666:LEU:HB2	1.83	0.61
2:C:759:THR:HB	2:C:785:VAL:CG2	2.30	0.61
3:D:1278:ILE:CG2	3:D:1279:ASP:N	2.64	0.61
3:D:1264:PHE:O	3:D:1425:VAL:HB	2.00	0.61
3:D:1460:LEU:CD1	3:D:1471:ARG:HH11	2.14	0.61
3:D:578:VAL:C	3:D:580:ALA:H	2.02	0.61
3:D:957:ILE:HG23	3:D:1040:CYS:O	2.01	0.61
1:A:124:PRO:HG2	1:A:125:ASP:OD1	2.01	0.61
2:C:204:GLN:HG3	2:C:205:GLU:HG2	1.82	0.61
2:C:354:GLY:O	2:C:358:ARG:HG2	2.01	0.61
2:C:457:ALA:O	2:C:459:ALA:N	2.34	0.61
2:C:922:PHE:C	2:C:924:LEU:H	2.02	0.61
3:D:1102:VAL:HG21	3:D:1425:VAL:CG1	2.30	0.61
3:D:1283:ARG:CG	3:D:1294:PHE:HB2	2.31	0.61
3:D:149:LYS:O	3:D:153:LEU:N	2.22	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:VAL:HG21	1:A:202:GLY:CA	2.30	0.61
2:C:128:ILE:N	2:C:128:ILE:HD12	2.14	0.61
2:C:185:LYS:HA	2:C:189:ARG:O	2.01	0.61
2:C:413:LEU:HD11	2:C:448:ASN:OD1	2.00	0.61
2:C:636:ALA:HB3	2:C:703:ILE:O	2.01	0.61
2:C:970:GLY:CA	3:D:950:ILE:HD13	2.31	0.61
3:D:625:TYR:HE1	3:D:751:LEU:HD21	1.66	0.61
2:C:491:GLU:CD	2:C:510:THR:HB	2.22	0.61
2:C:570:PRO:C	2:C:571:LEU:HD12	2.21	0.61
2:C:613:VAL:HG21	2:C:619:ARG:NE	2.16	0.61
2:C:691:SER:HB2	2:C:858:MET:HE1	1.82	0.61
2:C:859:PRO:HD2	2:C:867:VAL:CG2	2.31	0.61
3:D:1012:PHE:HA	3:D:1015:ASN:O	2.01	0.61
3:D:1087:LEU:HA	3:D:1090:ALA:CB	2.30	0.61
3:D:1482:VAL:CG1	4:E:21:VAL:HG21	2.30	0.61
3:D:849:ALA:O	3:D:853:VAL:HG23	2.00	0.61
3:D:961:LYS:CE	3:D:1042:MET:HB3	2.31	0.61
1:A:208:GLU:HB3	1:A:212:GLN:HE21	1.65	0.61
2:C:327:HIS:C	2:C:329:GLY:H	2.04	0.61
2:C:402:SER:O	2:C:403:SER:C	2.39	0.61
2:C:460:ARG:NH1	2:C:464:LEU:HD21	2.15	0.61
2:C:843:HIS:HD2	2:C:884:GLN:CA	2.14	0.61
3:D:1089:THR:HA	3:D:1092:SER:CB	2.30	0.61
3:D:1252:ASP:C	3:D:1254:THR:H	2.04	0.61
3:D:966:GLU:O	3:D:970:ARG:N	2.34	0.61
3:D:1487:VAL:HB	4:E:85:LEU:HD11	1.83	0.60
1:B:110:ALA:HB3	1:B:125:ASP:O	2.01	0.60
2:C:1043:TYR:CD2	3:D:763:MET:HG2	2.36	0.60
2:C:568:ALA:O	2:C:569:VAL:HG12	2.01	0.60
2:C:874:LEU:HD12	2:C:875:GLY:H	1.67	0.60
3:D:1123:LEU:HG	3:D:1141:ILE:HD13	1.82	0.60
3:D:1130:THR:O	3:D:1131:ARG:C	2.37	0.60
3:D:1146:TYR:CD2	3:D:1147:GLY:N	2.69	0.60
3:D:1330:ALA:O	3:D:1332:ASP:N	2.34	0.60
3:D:1379:TYR:CD1	3:D:1423:MET:HG3	2.36	0.60
3:D:705:ALA:HB3	3:D:706:PRO:CD	2.30	0.60
3:D:952:ILE:O	3:D:954:ASP:N	2.34	0.60
3:D:754:PHE:CD1	4:E:24:ALA:HB1	2.36	0.60
3:D:1473:ILE:O	3:D:1478:GLY:HA3	2.01	0.60
3:D:477:LEU:HD12	3:D:480:GLU:HB3	1.83	0.60
1:B:102:ALA:HB3	1:B:136:LYS:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:710:ILE:N	2:C:710:ILE:HD12	2.15	0.60
2:C:745:ILE:HA	2:C:800:VAL:HG12	1.83	0.60
3:D:777:PRO:HD2	3:D:912:LYS:HE3	1.82	0.60
1:A:109:ARG:H	1:A:109:ARG:CD	2.13	0.60
2:C:63:GLY:HA2	2:C:102:HIS:HA	1.82	0.60
2:C:86:LYS:HA	2:C:806:LEU:HD11	1.83	0.60
3:D:1293:VAL:HG23	3:D:1306:LEU:HD22	1.82	0.60
3:D:1381:GLU:HB3	3:D:1419:LYS:HD2	1.84	0.60
3:D:907:GLU:HB3	3:D:911:LEU:HD22	1.83	0.60
3:D:948:ILE:HD13	3:D:948:ILE:N	2.09	0.60
2:C:291:VAL:CB	2:C:299:LYS:HE3	2.32	0.60
2:C:328:LEU:HB3	2:C:467:ILE:CG2	2.31	0.60
2:C:502:PRO:HB2	2:C:507:ARG:NH2	2.17	0.60
3:D:1449:THR:O	3:D:1452:ALA:HB3	2.01	0.60
3:D:1476:GLY:C	3:D:1478:GLY:H	2.05	0.60
3:D:511:TRP:O	3:D:512:MET:HG3	2.02	0.60
1:B:184:ARG:CB	1:B:189:THR:HA	2.32	0.60
2:C:1020:PRO:HG2	3:D:624:ASP:HB2	1.82	0.60
2:C:63:GLY:CA	2:C:102:HIS:HA	2.31	0.60
2:C:568:ALA:O	2:C:569:VAL:CB	2.49	0.60
2:C:568:ALA:O	2:C:569:VAL:HB	2.01	0.60
2:C:613:VAL:HG13	2:C:620:LEU:N	2.15	0.60
2:C:950:LEU:O	2:C:951:GLY:C	2.40	0.60
3:D:1467:VAL:O	3:D:1470:GLY:N	2.33	0.60
3:D:752:SER:O	3:D:754:PHE:N	2.34	0.60
1:B:159:ASP:O	1:B:161:ILE:N	2.34	0.60
2:C:290:LEU:HD12	2:C:300:ASP:HA	1.84	0.60
2:C:981:GLU:H	2:C:981:GLU:CD	2.05	0.60
3:D:1138:ARG:HD2	3:D:1138:ARG:H	1.66	0.60
3:D:1281:VAL:HG12	3:D:1282:VAL:N	2.16	0.60
3:D:1354:GLN:O	3:D:1356:VAL:N	2.35	0.60
1:A:31:GLY:N	1:A:192:ASP:OD1	2.35	0.60
1:A:72:LYS:CA	2:C:607:ASP:HB3	2.31	0.60
1:B:25:LEU:HD11	1:B:28:LEU:CD1	2.30	0.60
2:C:1005:MET:CG	3:D:724:GLN:HG3	2.31	0.60
2:C:1107:ASN:N	2:C:1108:PRO:CD	2.65	0.60
2:C:30:LEU:O	2:C:31:GLN:C	2.41	0.60
2:C:396:ASP:HB3	2:C:402:SER:HB3	1.84	0.60
2:C:685:GLU:HB3	2:C:686:ASP:OD1	2.01	0.60
2:C:873:PRO:O	2:C:877:PRO:CD	2.50	0.60
3:D:1070:GLU:HG3	3:D:1073:ILE:CG1	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1111:ALA:HA	3:D:1203:GLN:O	2.01	0.60
3:D:1354:GLN:O	3:D:1355:LYS:C	2.38	0.60
2:C:984:GLU:O	3:D:945:SER:O	2.20	0.60
2:C:13:ILE:HG22	2:C:14:PRO:CD	2.28	0.60
2:C:565:GLN:HG3	2:C:668:LEU:CD1	2.32	0.60
2:C:588:VAL:HG12	2:C:588:VAL:O	2.00	0.60
3:D:616:GLN:O	3:D:617:ASN:HB2	2.00	0.60
3:D:638:LYS:CB	3:D:935:LYS:HD3	2.31	0.60
1:A:179:GLN:HE21	2:C:934:PHE:CB	2.11	0.59
1:B:58:ILE:CG2	1:B:139:MET:HG2	2.32	0.59
2:C:208:VAL:HG21	2:C:218:VAL:HG13	1.84	0.59
2:C:355:VAL:HG13	2:C:356:ARG:N	2.17	0.59
2:C:428:ARG:HA	2:C:431:HIS:HD2	1.65	0.59
2:C:460:ARG:O	2:C:461:VAL:HB	2.01	0.59
2:C:874:LEU:O	2:C:876:VAL:N	2.35	0.59
3:D:510:GLU:O	3:D:512:MET:N	2.35	0.59
1:B:93:ARG:O	1:B:94:TRP:O	2.20	0.59
2:C:502:PRO:HB2	2:C:507:ARG:NH1	2.16	0.59
2:C:772:ARG:HD3	2:C:772:ARG:O	2.02	0.59
2:C:837:ASP:N	2:C:837:ASP:OD2	2.35	0.59
2:C:673:LEU:CD2	2:C:867:VAL:HG12	2.32	0.59
2:C:958:SER:HB2	2:C:959:PRO:HD2	1.84	0.59
2:C:946:ARG:NH1	2:C:984:GLU:HB2	2.15	0.59
3:D:657:LEU:O	3:D:660:LYS:N	2.26	0.59
3:D:663:GLU:C	3:D:665:ALA:H	2.05	0.59
3:D:787:LEU:HD12	3:D:787:LEU:O	2.01	0.59
3:D:90:MET:N	3:D:520:LEU:HD21	2.16	0.59
1:A:114:THR:HG23	1:A:114:THR:O	2.03	0.59
1:B:41:ARG:HA	1:B:176:VAL:HG11	1.84	0.59
2:C:285:LEU:HD11	2:C:302:VAL:HG21	1.85	0.59
2:C:423:ALA:HA	2:C:427:VAL:HG21	1.84	0.59
2:C:21:ILE:CD1	2:C:460:ARG:HH21	2.15	0.59
2:C:803:ARG:HD2	2:C:803:ARG:O	2.01	0.59
2:C:551:GLU:CG	2:C:906:PHE:HD2	2.07	0.59
2:C:918:LEU:HD13	2:C:968:ASP:O	2.02	0.59
3:D:1018:PHE:HA	3:D:1024:MET:HE1	1.84	0.59
3:D:829:VAL:O	3:D:830:ALA:CB	2.50	0.59
3:D:1220:GLU:HA	4:E:17:TYR:OH	2.02	0.59
1:A:111:VAL:O	1:A:113:PHE:N	2.35	0.59
1:A:38:ASN:HB3	1:A:39:PRO:HD3	1.84	0.59
1:A:85:LEU:C	1:A:85:LEU:HD23	2.22	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:THR:HG21	1:B:43:ILE:HD11	1.83	0.59
2:C:497:ALA:C	2:C:502:PRO:HA	2.22	0.59
2:C:5:ARG:HH22	2:C:10:ARG:HH11	1.49	0.59
2:C:841:ASN:HD21	2:C:845:ASN:N	1.93	0.59
2:C:882:LEU:HD11	2:C:884:GLN:NE2	2.18	0.59
3:D:1364:LEU:CD2	3:D:1365:HIS:H	2.16	0.59
3:D:18:ILE:HD12	3:D:18:ILE:H	1.67	0.59
3:D:846:PRO:HG3	3:D:880:ILE:HD12	1.83	0.59
3:D:794:GLN:OE1	3:D:906:GLN:NE2	2.35	0.59
1:A:12:THR:HG22	1:A:13:ALA:H	1.66	0.59
1:A:84:GLU:O	1:A:85:LEU:C	2.40	0.59
1:A:98:LEU:HB3	1:A:113:PHE:HD2	1.66	0.59
2:C:613:VAL:HG22	2:C:620:LEU:C	2.21	0.59
2:C:764:GLU:OE2	2:C:786:LYS:HE3	2.03	0.59
3:D:1010:ASN:O	3:D:1013:GLU:HB3	2.03	0.59
3:D:1095:LEU:CD1	3:D:1099:LEU:HD13	2.30	0.59
3:D:514:LEU:O	3:D:515:GLU:CB	2.50	0.59
3:D:604:THR:O	3:D:608:SER:HB3	2.03	0.59
3:D:803:GLY:O	3:D:826:PRO:N	2.35	0.59
1:A:191:LEU:HD23	1:A:191:LEU:N	2.17	0.59
2:C:640:ARG:O	2:C:656:ALA:HB1	2.02	0.59
2:C:600:ASP:C	2:C:648:ARG:HB2	2.23	0.59
2:C:910:THR:HB	2:C:913:GLU:HG3	1.85	0.59
3:D:1097:ARG:NH1	3:D:1097:ARG:HG3	2.18	0.59
3:D:1332:ASP:C	3:D:1334:HIS:N	2.56	0.59
3:D:1433:LYS:CG	3:D:1434:SER:H	2.14	0.59
3:D:14:SER:O	3:D:17:LYS:N	2.33	0.59
3:D:979:TYR:C	3:D:981:MET:N	2.56	0.59
2:C:163:ILE:HG22	2:C:265:LYS:NZ	2.18	0.59
2:C:202:TYR:OH	2:C:304:LEU:HD22	2.03	0.59
2:C:376:ARG:N	2:C:377:PRO:CD	2.61	0.59
2:C:603:VAL:O	2:C:604:VAL:HB	2.02	0.59
2:C:842:ARG:NH2	2:C:887:GLU:OE1	2.34	0.59
2:C:872:ASN:ND2	2:C:874:LEU:N	2.51	0.59
3:D:1104:HIS:ND1	3:D:1105:GLU:N	2.50	0.59
3:D:1268:ARG:HH12	3:D:1331:ILE:CB	2.16	0.59
3:D:954:ASP:O	3:D:955:ALA:HB3	2.03	0.59
1:A:133:GLU:OE1	2:C:606:VAL:HB	2.02	0.59
1:B:105:PRO:HB3	1:B:132:GLU:HG3	1.85	0.59
1:B:173:VAL:HG12	1:B:200:THR:CG2	2.33	0.59
2:C:493:ARG:HH12	3:D:1070:GLU:CA	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:701:THR:HG22	2:C:832:LYS:CA	2.27	0.59
2:C:743:VAL:HG12	2:C:744:ARG:N	2.18	0.59
2:C:700:TYR:CB	2:C:833:LEU:HD22	2.32	0.59
3:D:601:ARG:HD3	3:D:605:ASP:CG	2.23	0.59
1:A:26:GLU:CB	1:A:27:PRO:CD	2.72	0.59
2:C:1034:GLU:HA	2:C:1037:VAL:HG23	1.84	0.59
2:C:257:LEU:O	2:C:259:GLY:N	2.36	0.59
2:C:344:PHE:O	2:C:346:VAL:N	2.36	0.59
2:C:565:GLN:HG3	2:C:668:LEU:HD13	1.84	0.59
3:D:616:GLN:O	3:D:617:ASN:CB	2.50	0.59
3:D:638:LYS:CB	3:D:729:HIS:CE1	2.86	0.59
3:D:719:VAL:O	3:D:721:VAL:HG23	2.03	0.59
1:A:23:PHE:CD2	1:A:210:LEU:HD22	2.37	0.59
2:C:1034:GLU:CG	2:C:1035:MET:N	2.66	0.59
2:C:196:LEU:O	2:C:200:LEU:HG	2.03	0.59
2:C:457:ALA:C	2:C:459:ALA:H	2.07	0.59
2:C:571:LEU:N	2:C:571:LEU:CD1	2.65	0.59
2:C:915:LYS:O	2:C:916:GLU:C	2.41	0.59
3:D:1482:VAL:HG13	3:D:1484:PHE:HE2	1.67	0.59
3:D:657:LEU:HD12	3:D:660:LYS:HB3	1.84	0.59
1:A:111:VAL:HG22	1:A:124:PRO:HB2	1.85	0.58
2:C:398:THR:OG1	2:C:633:GLN:HG3	2.02	0.58
2:C:613:VAL:HG21	2:C:619:ARG:HG3	1.85	0.58
2:C:54:ILE:O	2:C:65:VAL:O	2.21	0.58
2:C:682:TYR:HB3	2:C:689:VAL:HG22	1.85	0.58
2:C:845:ASN:HD21	2:C:876:VAL:HG11	1.68	0.58
2:C:881:ASN:C	2:C:882:LEU:HD23	2.23	0.58
2:C:901:TYR:O	2:C:902:ILE:HD12	2.03	0.58
3:D:1284:ILE:HG12	3:D:1293:VAL:HG13	1.85	0.58
1:A:38:ASN:O	1:A:41:ARG:N	2.36	0.58
2:C:40:GLU:HG2	2:C:41:ASN:ND2	2.18	0.58
2:C:642:ARG:H	2:C:656:ALA:HB2	1.68	0.58
2:C:772:ARG:HH11	2:C:776:SER:HB3	1.68	0.58
3:D:791:TYR:CE1	3:D:1024:MET:HG3	2.38	0.58
4:E:81:PRO:HB2	4:E:84:ARG:HB2	1.84	0.58
1:A:200:THR:HG22	1:A:201:ASP:N	2.18	0.58
2:C:115:LEU:CD1	2:C:116:GLY:H	2.15	0.58
2:C:308:ARG:O	2:C:310:LEU:N	2.37	0.58
2:C:54:ILE:HD13	2:C:355:VAL:HG13	1.84	0.58
2:C:501:THR:O	2:C:502:PRO:C	2.41	0.58
2:C:852:ILE:O	2:C:852:ILE:HG12	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1275:ILE:HA	3:D:1323:GLY:CA	2.33	0.58
3:D:1273:ALA:HB1	3:D:1325:PRO:HG2	1.85	0.58
3:D:564:GLU:HA	3:D:567:ILE:HG22	1.85	0.58
3:D:901:GLN:CB	3:D:905:PRO:HG3	2.27	0.58
1:B:117:ALA:O	1:B:119:VAL:N	2.36	0.58
2:C:290:LEU:HA	2:C:300:ASP:HA	1.83	0.58
2:C:362:GLY:HA3	2:C:367:LEU:HD23	1.84	0.58
2:C:570:PRO:CG	2:C:635:THR:HG23	2.33	0.58
3:D:1438:ALA:HA	3:D:1441:PHE:HD1	1.68	0.58
2:C:987:ILE:HA	3:D:948:ILE:HG23	1.85	0.58
1:A:224:PHE:HD2	1:B:11:PHE:CZ	2.21	0.58
1:B:194:LEU:HD11	1:B:196:LEU:HD13	1.86	0.58
1:B:24:VAL:HG22	1:B:195:THR:HA	1.86	0.58
2:C:290:LEU:HD11	2:C:298:PHE:HB3	1.84	0.58
2:C:360:VAL:O	2:C:361:MET:C	2.41	0.58
2:C:460:ARG:HH11	2:C:464:LEU:HD21	1.67	0.58
3:D:1257:LEU:HB3	3:D:1258:PRO:HD3	1.86	0.58
3:D:1295:VAL:O	3:D:1295:VAL:HG12	2.04	0.58
3:D:1305:LYS:N	3:D:1305:LYS:HD3	2.18	0.58
3:D:1379:TYR:CD1	3:D:1379:TYR:N	2.72	0.58
3:D:607:LEU:HD11	3:D:614:PHE:CZ	2.38	0.58
2:C:1055:ILE:N	2:C:1055:ILE:HD12	2.18	0.58
2:C:352:ALA:C	2:C:355:VAL:HG12	2.23	0.58
2:C:523:ILE:C	2:C:525:ALA:N	2.56	0.58
2:C:654:LEU:HD12	2:C:654:LEU:O	2.03	0.58
3:D:1043:ARG:NH2	3:D:1066:LEU:HD21	2.17	0.58
3:D:1104:HIS:O	3:D:1106:ILE:N	2.36	0.58
1:B:79:ILE:HD11	1:B:164:ILE:HD12	1.84	0.58
2:C:13:ILE:C	2:C:15:LEU:N	2.55	0.58
2:C:165:LEU:O	2:C:167:LYS:N	2.36	0.58
2:C:140:ILE:HB	2:C:332:ARG:O	2.04	0.58
2:C:605:LYS:HG3	2:C:612:ALA:N	2.05	0.58
3:D:711:LEU:HD12	3:D:778:LEU:HD23	1.86	0.58
1:B:41:ARG:HG2	1:B:176:VAL:CG1	2.33	0.58
2:C:1008:ARG:HD2	2:C:1029:GLY:N	2.17	0.58
2:C:112:GLU:O	2:C:113:VAL:HB	2.04	0.58
2:C:265:LYS:O	2:C:266:ARG:HB2	2.04	0.58
2:C:342:ASP:O	2:C:346:VAL:HG23	2.03	0.58
2:C:443:THR:O	2:C:444:PRO:O	2.22	0.58
2:C:443:THR:HB	2:C:444:PRO:HD3	1.86	0.58
2:C:573:ARG:O	2:C:575:GLN:HG3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:725:ASP:OD1	2:C:725:ASP:O	2.20	0.58
3:D:496:LEU:HG	3:D:500:ARG:HG2	1.85	0.58
3:D:654:LYS:O	3:D:657:LEU:N	2.37	0.58
3:D:859:ASP:OD1	3:D:861:GLN:NE2	2.36	0.58
3:D:1482:VAL:HG11	4:E:18:ARG:HA	1.84	0.58
2:C:163:ILE:HB	2:C:164:PRO:HD2	1.84	0.58
2:C:271:GLU:O	2:C:272:ALA:HB3	2.03	0.58
2:C:603:VAL:HG21	2:C:645:VAL:CA	2.34	0.58
2:C:600:ASP:HA	2:C:648:ARG:HD2	1.86	0.58
3:D:1068:VAL:CG1	3:D:1070:GLU:HB2	2.32	0.58
3:D:961:LYS:HE3	3:D:1042:MET:HB3	1.86	0.58
4:E:38:THR:HG22	4:E:39:VAL:N	2.19	0.58
1:A:91:ASP:HB3	1:A:94:TRP:NE1	2.19	0.58
2:C:552:HIS:ND1	3:D:1065:GLY:HA2	2.17	0.58
2:C:889:HIS:CE1	3:D:951:GLY:N	2.62	0.58
3:D:908:LYS:HD2	3:D:1028:GLY:HA3	1.86	0.58
3:D:501:ALA:HB1	3:D:1454:ALA:HA	1.86	0.58
3:D:704:ARG:HH11	3:D:704:ARG:HG2	1.67	0.58
3:D:853:VAL:HG13	3:D:858:LEU:O	2.04	0.58
3:D:925:GLU:O	3:D:928:ALA:HB3	2.04	0.58
3:D:979:TYR:C	3:D:981:MET:H	2.05	0.58
1:A:16:GLN:HG3	1:A:20:TYR:HB3	1.86	0.57
2:C:266:ARG:HG2	2:C:268:ASP:CA	2.34	0.57
2:C:509:ALA:O	2:C:515:ALA:O	2.22	0.57
2:C:642:ARG:O	2:C:643:VAL:HG23	2.04	0.57
2:C:795:GLY:O	2:C:797:GLY:N	2.37	0.57
2:C:710:ILE:HD12	2:C:823:VAL:O	2.03	0.57
2:C:679:PHE:HB2	2:C:870:ILE:HG21	1.86	0.57
2:C:936:VAL:HG13	2:C:940:GLU:HB2	1.86	0.57
3:D:1044:GLY:HA3	3:D:1058:VAL:H	1.69	0.57
3:D:1212:MET:C	3:D:1214:ARG:H	2.07	0.57
3:D:17:LYS:O	3:D:20:SER:N	2.34	0.57
4:E:50:THR:O	4:E:52:GLU:N	2.37	0.57
1:A:123:ASN:O	1:A:124:PRO:O	2.22	0.57
1:A:19:HIS:HA	1:A:201:ASP:OD1	2.03	0.57
1:A:39:PRO:HA	1:B:35:THR:HG23	1.86	0.57
1:B:86:VAL:H	1:B:123:ASN:HD21	1.52	0.57
2:C:1008:ARG:HD2	2:C:1029:GLY:H	1.69	0.57
2:C:102:HIS:HB3	2:C:104:ASP:OD1	2.04	0.57
2:C:139:GLN:NE2	2:C:334:ARG:HH21	2.02	0.57
2:C:163:ILE:HD12	2:C:163:ILE:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:541:SER:OG	2:C:544:THR:HB	2.04	0.57
2:C:892:LEU:HA	2:C:895:TYR:HB3	1.85	0.57
2:C:906:PHE:O	2:C:907:ASP:HB2	2.04	0.57
3:D:1238:THR:HG22	3:D:1239:MET:N	2.19	0.57
3:D:1221:ALA:HB2	3:D:1475:ALA:CB	2.32	0.57
3:D:770:LEU:CD1	3:D:770:LEU:N	2.66	0.57
2:C:946:ARG:HE	3:D:861:GLN:NE2	2.00	0.57
4:E:40:LEU:HB3	4:E:44:GLU:O	2.03	0.57
2:C:202:TYR:HB3	2:C:207:LEU:HD13	1.85	0.57
2:C:492:ASP:N	2:C:531:PHE:CB	2.66	0.57
2:C:848:VAL:HG12	3:D:740:PHE:O	2.04	0.57
2:C:552:HIS:NE2	2:C:886:LEU:HD12	2.19	0.57
3:D:1210:LEU:O	3:D:1210:LEU:HG	2.05	0.57
3:D:1434:SER:HB3	3:D:1465:GLU:OE2	2.03	0.57
2:C:1085:PHE:CD1	3:D:1469:LEU:HD22	2.39	0.57
3:D:660:LYS:O	3:D:664:LYS:N	2.28	0.57
3:D:728:LEU:CD2	3:D:745:MET:HE1	2.34	0.57
3:D:625:TYR:CE1	3:D:751:LEU:HD11	2.39	0.57
3:D:87:ARG:O	3:D:88:TYR:O	2.22	0.57
3:D:929:ARG:HH11	3:D:929:ARG:HG2	1.69	0.57
1:A:111:VAL:HG23	1:A:125:ASP:N	2.19	0.57
1:B:178:PHE:CB	1:B:196:LEU:HD12	2.34	0.57
2:C:1036:GLU:O	2:C:1040:LEU:HD23	2.03	0.57
2:C:291:VAL:HB	2:C:299:LYS:HE3	1.86	0.57
2:C:38:LYS:O	2:C:39:ARG:HB2	2.03	0.57
2:C:501:THR:O	2:C:507:ARG:NH2	2.37	0.57
2:C:642:ARG:H	2:C:656:ALA:CA	2.17	0.57
3:D:1077:GLY:HA2	3:D:1080:LYS:HG2	1.87	0.57
3:D:1262:GLU:CD	3:D:1269:PRO:HB3	2.25	0.57
3:D:1495:ALA:HB1	4:E:91:ARG:HD3	1.86	0.57
3:D:507:ASN:O	3:D:508:ARG:CG	2.52	0.57
3:D:793:THR:HG22	3:D:879:ARG:HA	1.86	0.57
3:D:1485:THR:HG23	4:E:85:LEU:HD22	1.86	0.57
1:B:70:GLY:O	1:B:131:LEU:HB2	2.04	0.57
2:C:1045:ALA:HB1	2:C:1048:THR:CB	2.29	0.57
2:C:72:ARG:HD3	2:C:112:GLU:OE1	2.04	0.57
2:C:283:VAL:CG1	2:C:284:GLY:H	2.17	0.57
2:C:389:SER:C	2:C:391:LEU:H	2.07	0.57
2:C:434:HIS:C	2:C:436:GLY:H	2.08	0.57
2:C:568:ALA:CB	2:C:668:LEU:HD22	2.33	0.57
3:D:1087:LEU:HD12	3:D:1090:ALA:CB	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:638:LYS:HA	3:D:729:HIS:CD2	2.39	0.57
3:D:642:CYS:SG	3:D:702:LEU:HD23	2.45	0.57
3:D:747:VAL:HG22	3:D:747:VAL:O	2.05	0.57
1:A:215:ALA:O	1:A:218:LYS:HB2	2.04	0.57
2:C:144:PRO:HA	2:C:162:ILE:HG22	1.87	0.57
2:C:910:THR:CG2	2:C:912:PRO:HD2	2.33	0.57
2:C:996:LYS:O	2:C:996:LYS:HG2	2.05	0.57
3:D:1020:PRO:C	3:D:1022:TYR:H	2.06	0.57
3:D:1426:THR:C	3:D:1428:SER:H	2.08	0.57
3:D:1102:VAL:HA	3:D:1429:ALA:HB2	1.86	0.57
3:D:642:CYS:O	3:D:719:VAL:HB	2.05	0.57
2:C:1034:GLU:O	2:C:1037:VAL:HG23	2.05	0.57
2:C:255:ALA:C	2:C:257:LEU:N	2.57	0.57
2:C:528:GLU:O	2:C:529:VAL:CB	2.53	0.57
2:C:839:LEU:HB3	2:C:994:ILE:HG21	1.86	0.57
2:C:959:PRO:HG2	2:C:960:GLU:H	1.70	0.57
3:D:582:ILE:HG22	3:D:583:ASP:H	1.70	0.57
3:D:808:THR:N	3:D:809:PRO:CD	2.67	0.57
4:E:82:GLU:O	4:E:85:LEU:HB3	2.05	0.57
2:C:313:LEU:O	2:C:313:LEU:HG	2.05	0.57
2:C:34:VAL:HG11	2:C:38:LYS:HG3	1.87	0.57
2:C:368:THR:HB	2:C:369:PRO:HD2	1.87	0.57
2:C:816:LYS:NZ	2:C:817:PRO:HG2	2.20	0.57
2:C:957:LYS:HB3	2:C:961:GLU:HB3	1.85	0.57
3:D:730:PRO:O	3:D:731:LEU:C	2.42	0.57
3:D:936:TYR:CD2	3:D:936:TYR:C	2.77	0.57
1:A:123:ASN:ND2	1:A:126:LEU:HD22	2.20	0.57
2:C:439:CYS:HA	2:C:455:LEU:HA	1.86	0.57
2:C:54:ILE:HD11	2:C:359:MET:SD	2.44	0.57
2:C:613:VAL:CG1	2:C:619:ARG:HA	2.33	0.57
2:C:698:ASP:OD2	2:C:701:THR:HG21	2.05	0.57
3:D:709:HIS:HA	3:D:1228:GLU:CB	2.35	0.57
3:D:607:LEU:O	3:D:608:SER:HB2	2.05	0.57
3:D:688:TRP:C	3:D:690:ALA:H	2.07	0.57
2:C:151:ASP:HA	2:C:158:TYR:CD2	2.37	0.57
2:C:176:VAL:HG11	2:C:311:PHE:HE2	1.69	0.57
2:C:580:MET:O	2:C:581:THR:CB	2.52	0.57
2:C:613:VAL:HG21	2:C:619:ARG:HE	1.70	0.57
3:D:1020:PRO:C	3:D:1022:TYR:N	2.55	0.57
3:D:1137:LYS:HE3	3:D:1140:ASP:OD1	2.05	0.57
3:D:768:ASN:HD22	4:E:16:LYS:NZ	2.02	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:987:ILE:HD11	3:D:946:GLY:CA	2.35	0.57
1:A:100:LEU:HD23	1:A:113:PHE:CE1	2.39	0.56
1:A:162:ASN:O	1:A:164:ILE:HG23	2.05	0.56
1:A:204:VAL:HG23	1:A:205:THR:N	2.19	0.56
1:A:67:THR:O	1:A:67:THR:HG23	2.05	0.56
2:C:1105:LYS:H	2:C:1108:PRO:HG2	1.70	0.56
2:C:502:PRO:O	2:C:507:ARG:NH2	2.37	0.56
2:C:845:ASN:ND2	2:C:884:GLN:NE2	2.42	0.56
3:D:1104:HIS:C	3:D:1106:ILE:N	2.57	0.56
3:D:1265:GLU:OE2	3:D:1424:GLY:O	2.23	0.56
3:D:1252:ASP:HB2	3:D:1270:LYS:NZ	2.19	0.56
3:D:1404:LEU:C	3:D:1408:LEU:HB2	2.25	0.56
3:D:586:ARG:O	3:D:588:GLY:N	2.38	0.56
3:D:95:LEU:O	3:D:96:ALA:HB2	2.04	0.56
1:A:15:THR:CG2	1:B:229:ALA:HB1	2.35	0.56
1:B:173:VAL:CA	1:B:200:THR:HG22	2.32	0.56
2:C:148:PHE:HE2	2:C:310:LEU:HB2	1.70	0.56
3:D:23(U):UNK:CB	3:D:43(U):UNK:N	2.69	0.56
3:D:486:ARG:CG	3:D:487:ALA:H	2.18	0.56
3:D:858:LEU:O	3:D:860:LEU:N	2.38	0.56
3:D:977:GLN:C	3:D:979:TYR:H	2.09	0.56
2:C:1060:ILE:O	2:C:1064:ASN:ND2	2.38	0.56
2:C:118:LEU:HD23	2:C:118:LEU:O	2.05	0.56
2:C:184:MET:CE	2:C:191:PHE:HZ	2.17	0.56
2:C:352:ALA:CA	2:C:355:VAL:HG12	2.34	0.56
2:C:549:PHE:CE2	2:C:886:LEU:HB3	2.41	0.56
3:D:1232:GLU:HB3	3:D:1233:PRO:CD	2.30	0.56
3:D:1400:ASP:OD2	3:D:1418:TRP:CE3	2.58	0.56
3:D:97:THR:O	3:D:571:LYS:HE2	2.05	0.56
4:E:27:ALA:HB1	4:E:60:ALA:HB1	1.86	0.56
1:A:58:ILE:HG23	1:A:139:MET:HG2	1.86	0.56
2:C:260:LEU:HD23	2:C:261:LEU:HB3	1.87	0.56
2:C:305:PRO:HB3	2:C:308:ARG:HH21	1.71	0.56
2:C:110:GLU:HG3	2:C:369:PRO:C	2.26	0.56
2:C:455:LEU:HD12	2:C:455:LEU:C	2.25	0.56
2:C:5:ARG:HG3	2:C:902:ILE:CG2	2.36	0.56
2:C:603:VAL:HG21	2:C:645:VAL:C	2.26	0.56
2:C:705:ILE:HD12	2:C:705:ILE:O	2.05	0.56
2:C:80:GLN:O	2:C:81:ASP:CB	2.50	0.56
2:C:860:HIS:H	2:C:977:GLY:H	1.53	0.56
3:D:1108:VAL:HG21	3:D:1216:VAL:CG1	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:709:HIS:CA	3:D:1228:GLU:HB3	2.35	0.56
3:D:795:VAL:HG22	3:D:876:ASN:CG	2.25	0.56
1:A:56:VAL:HG23	1:A:164:ILE:HD11	1.87	0.56
1:A:174:ARG:O	1:A:175:ARG:HB2	2.06	0.56
1:B:86:VAL:H	1:B:123:ASN:ND2	2.03	0.56
2:C:257:LEU:HB3	2:C:264:PRO:CG	2.35	0.56
2:C:344:PHE:C	2:C:346:VAL:N	2.58	0.56
2:C:421:GLU:HG3	2:C:422:ARG:N	2.20	0.56
2:C:642:ARG:H	2:C:656:ALA:CB	2.17	0.56
2:C:839:LEU:HD12	2:C:994:ILE:CG2	2.35	0.56
3:D:1093:GLY:HA2	3:D:1097:ARG:NH2	2.20	0.56
3:D:1108:VAL:HA	3:D:1202:CYS:O	2.06	0.56
3:D:1327:THR:C	3:D:1329:GLY:H	2.09	0.56
3:D:1418:TRP:HD1	3:D:1419:LYS:O	1.89	0.56
3:D:614:PHE:CD1	3:D:1439:ALA:HB1	2.39	0.56
3:D:544:TYR:OH	3:D:603:LEU:HD21	2.05	0.56
3:D:836:VAL:HG11	3:D:858:LEU:HD21	1.86	0.56
3:D:855:HIS:O	3:D:857:LEU:HD22	2.06	0.56
3:D:96:ALA:O	3:D:97:THR:C	2.43	0.56
4:E:81:PRO:CB	4:E:84:ARG:HD2	2.36	0.56
1:A:91:ASP:HB3	1:A:94:TRP:HE1	1.71	0.56
2:C:1062:GLY:O	2:C:1063:ARG:C	2.43	0.56
2:C:15:LEU:HD11	2:C:461:VAL:HG21	1.86	0.56
2:C:328:LEU:O	2:C:467:ILE:HD13	2.05	0.56
2:C:760:SER:CB	2:C:788:THR:HG21	2.35	0.56
2:C:547:ILE:HG23	2:C:843:HIS:CE1	2.40	0.56
2:C:876:VAL:HB	2:C:877:PRO:CD	2.35	0.56
2:C:493:ARG:NH2	3:D:1070:GLU:OE2	2.38	0.56
3:D:1155:GLU:CB	3:D:1160:ARG:HG2	2.35	0.56
3:D:1327:THR:O	3:D:1329:GLY:N	2.34	0.56
3:D:858:LEU:HB3	3:D:877:PRO:HG3	1.86	0.56
3:D:955:ALA:HA	3:D:1040:CYS:SG	2.46	0.56
3:D:975:ILE:HD12	3:D:989:ARG:HG3	1.86	0.56
4:E:59:ASN:ND2	4:E:62:THR:OG1	2.37	0.56
2:C:136:ILE:CB	2:C:336:VAL:HG22	2.34	0.56
2:C:249:LYS:O	2:C:250:LYS:C	2.44	0.56
2:C:35:PRO:O	2:C:37:GLU:N	2.31	0.56
3:D:1172:VAL:O	3:D:1176:ILE:HG12	2.06	0.56
3:D:1191:SER:H	3:D:1194:THR:HG22	1.70	0.56
3:D:1408:LEU:C	3:D:1410:ALA:N	2.58	0.56
3:D:1458:ASP:CG	3:D:1460:LEU:HD23	2.24	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1104:HIS:CE1	3:D:1463:LEU:H	2.18	0.56
3:D:948:ILE:CD1	3:D:948:ILE:H	2.09	0.56
4:E:26:ARG:HH21	4:E:67:GLU:CD	2.08	0.56
1:B:105:PRO:HB3	1:B:133:GLU:N	2.16	0.56
2:C:11:GLU:OE1	2:C:473:ARG:HG3	2.06	0.56
1:A:72:LYS:CB	2:C:607:ASP:HB3	2.35	0.56
2:C:722:ILE:HD13	2:C:823:VAL:CG2	2.34	0.56
3:D:1138:ARG:HD2	3:D:1138:ARG:N	2.20	0.56
3:D:548:ILE:C	3:D:550:ARG:H	2.09	0.56
3:D:728:LEU:HD22	3:D:745:MET:HE3	1.85	0.56
2:C:984:GLU:HG3	3:D:945:SER:HA	1.86	0.56
3:D:961:LYS:HE3	3:D:1042:MET:H	1.70	0.56
1:A:28:LEU:HD23	1:B:220:HIS:CE1	2.41	0.56
2:C:251:ASP:O	2:C:252:LYS:HB3	2.04	0.56
2:C:394:PHE:O	2:C:395:LYS:HB2	2.06	0.56
2:C:410:ILE:HD13	2:C:468:ARG:HH21	1.70	0.56
2:C:51:THR:OG1	2:C:348:LEU:HD23	2.05	0.56
2:C:523:ILE:O	2:C:525:ALA:N	2.39	0.56
2:C:545:ASN:HB2	2:C:583:LEU:HD12	1.86	0.56
3:D:508:ARG:O	3:D:508:ARG:HG3	2.06	0.56
3:D:860:LEU:HD12	3:D:878:GLY:HA2	1.88	0.56
1:A:161:ILE:CG2	1:A:162:ASN:N	2.69	0.56
1:A:196:LEU:HG	1:A:198:ILE:CD1	2.36	0.56
2:C:204:GLN:O	2:C:205:GLU:HB2	2.06	0.56
2:C:100:LEU:HD21	2:C:367:LEU:O	2.06	0.56
2:C:369:PRO:C	2:C:371:LYS:N	2.57	0.56
2:C:29:ALA:O	2:C:43:GLY:HA3	2.06	0.56
2:C:491:GLU:HG2	2:C:510:THR:O	2.05	0.56
2:C:401:LEU:CD2	2:C:543:ASN:HB2	2.30	0.56
1:A:133:GLU:HB3	2:C:606:VAL:HG23	1.88	0.56
2:C:648:ARG:HG2	2:C:648:ARG:HH11	1.70	0.56
2:C:758:ARG:NH1	2:C:758:ARG:HG3	2.19	0.56
2:C:872:ASN:HD21	2:C:874:LEU:CA	2.19	0.56
3:D:1063:ARG:HG3	3:D:1063:ARG:NH1	2.21	0.56
3:D:1127:ASP:OD1	3:D:1129:VAL:HB	2.06	0.56
3:D:518:PRO:HB3	3:D:544:TYR:CD1	2.41	0.56
3:D:551:ASN:HA	3:D:574:LEU:HD13	1.87	0.56
3:D:899:LEU:H	3:D:899:LEU:HD22	1.69	0.56
4:E:23:VAL:HG21	4:E:65:MET:HG2	1.87	0.56
4:E:8:LYS:NZ	4:E:69:LEU:HD21	2.20	0.56
1:A:198:ILE:O	1:A:198:ILE:HG22	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:VAL:HG12	1:A:123:ASN:CG	2.26	0.56
1:B:168:ALA:HB1	1:B:170:PHE:CE1	2.41	0.56
1:A:224:PHE:CE1	1:B:36:LEU:HD11	2.37	0.56
1:B:99:ILE:HA	1:B:139:MET:O	2.06	0.56
2:C:274:ARG:HG3	2:C:275:TYR:CD1	2.38	0.56
2:C:391:LEU:HD22	2:C:415:PRO:HD3	1.88	0.56
2:C:460:ARG:HD2	2:C:464:LEU:HD21	1.84	0.56
2:C:498:GLN:CB	2:C:503:LEU:H	2.19	0.56
2:C:869:VAL:CG2	2:C:871:LEU:HD13	2.36	0.56
2:C:428:ARG:CZ	3:D:1086:ALA:HB3	2.36	0.56
3:D:26:VAL:H	3:D:79:GLU:CB	2.19	0.56
1:B:172:PRO:O	1:B:200:THR:HB	2.06	0.55
2:C:149:THR:HB	2:C:158:TYR:CZ	2.41	0.55
2:C:193:LEU:HD13	2:C:193:LEU:O	2.06	0.55
2:C:136:ILE:HB	2:C:336:VAL:CG2	2.36	0.55
2:C:21:ILE:HG23	2:C:460:ARG:HH21	1.71	0.55
2:C:474:VAL:HG22	2:C:530:GLU:CA	2.36	0.55
1:A:70:GLY:HA2	2:C:606:VAL:CG2	2.36	0.55
2:C:640:ARG:NH1	2:C:640:ARG:HG3	2.21	0.55
3:D:1193:LEU:HD21	3:D:1370:GLU:HA	1.87	0.55
3:D:1195:CYS:SG	3:D:1202:CYS:HB2	2.46	0.55
3:D:126:VAL:H	3:D:456:MET:HE2	1.71	0.55
3:D:1354:GLN:HE21	3:D:1369:ILE:HD11	1.71	0.55
3:D:661:MET:CE	3:D:677:LEU:HD21	2.36	0.55
3:D:764:LEU:HG	3:D:766:ALA:H	1.70	0.55
4:E:30:LEU:O	4:E:32:ARG:N	2.36	0.55
2:C:683:ASN:ND2	2:C:870:ILE:HG22	2.22	0.55
2:C:745:ILE:HD12	2:C:802:GLY:HA2	1.87	0.55
2:C:902:ILE:O	2:C:902:ILE:HG22	2.05	0.55
3:D:1180:GLU:C	3:D:1182:GLY:H	2.08	0.55
3:D:127:LEU:O	3:D:145:VAL:HA	2.06	0.55
3:D:796:ARG:NH2	3:D:861:GLN:OE1	2.39	0.55
3:D:875:THR:CG2	3:D:876:ASN:N	2.69	0.55
3:D:899:LEU:O	3:D:900:ILE:CG1	2.55	0.55
3:D:908:LYS:HG2	3:D:909:ASN:N	2.21	0.55
1:A:131:LEU:HD21	1:A:137:LEU:HD22	1.88	0.55
2:C:878:SER:OG	2:C:879:ARG:N	2.38	0.55
2:C:80:GLN:HG3	2:C:90:TYR:CE1	2.41	0.55
2:C:674:VAL:N	2:C:990:GLY:O	2.36	0.55
3:D:1145:LEU:HD11	3:D:1187:VAL:HG21	1.88	0.55
3:D:1349:LEU:HG	3:D:1376:MET:HE3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1354:GLN:NE2	3:D:1369:ILE:HD11	2.21	0.55
3:D:87:ARG:CA	3:D:522:PRO:HG2	2.37	0.55
3:D:542:ASP:O	3:D:543:LEU:C	2.44	0.55
3:D:767:HIS:CE1	4:E:2:ALA:HB1	2.41	0.55
1:A:21:GLY:HA3	1:A:23:PHE:CZ	2.40	0.55
2:C:208:VAL:HG12	2:C:209:ARG:N	2.21	0.55
2:C:336:VAL:HA	2:C:339:LEU:CD1	2.37	0.55
2:C:841:ASN:C	2:C:841:ASN:HD22	2.09	0.55
2:C:987:ILE:HD11	3:D:946:GLY:HA3	1.88	0.55
2:C:987:ILE:HG22	2:C:987:ILE:O	2.04	0.55
3:D:654:LYS:O	3:D:657:LEU:HB3	2.07	0.55
3:D:662:GLU:HG3	3:D:670:VAL:CG2	2.36	0.55
1:A:163:ALA:O	1:A:164:ILE:C	2.45	0.55
1:B:150:VAL:CB	1:B:168:ALA:HB3	2.34	0.55
1:B:94:TRP:NE1	1:B:119:VAL:HG21	2.21	0.55
2:C:466:PHE:CD1	2:C:466:PHE:C	2.80	0.55
3:D:1203:GLN:O	3:D:1204:LYS:CB	2.54	0.55
3:D:1323:GLY:O	3:D:1324:GLN:CG	2.55	0.55
3:D:141:VAL:O	3:D:143:ASP:N	2.35	0.55
3:D:575:GLN:HG3	3:D:579:ASP:OD1	2.05	0.55
3:D:710:ARG:HG3	3:D:711:LEU:N	2.22	0.55
3:D:986:ASP:O	3:D:989:ARG:N	2.38	0.55
1:A:107:GLU:O	1:A:109:ARG:N	2.39	0.55
1:A:13:ALA:O	1:A:15:THR:N	2.40	0.55
1:B:100:LEU:HD22	1:B:139:MET:HE2	1.89	0.55
1:B:125:ASP:N	1:B:125:ASP:OD2	2.40	0.55
2:C:404:LEU:HD23	2:C:587:VAL:HG13	1.89	0.55
2:C:752:GLY:O	2:C:791:ARG:HD3	2.07	0.55
3:D:1167:LEU:HD22	3:D:1167:LEU:H	1.70	0.55
3:D:1148:ARG:CG	3:D:1189:VAL:HG21	2.36	0.55
3:D:1382:VAL:HG23	3:D:1393:GLY:H	1.71	0.55
3:D:1377:LEU:CD1	3:D:1422:LEU:HG	2.36	0.55
3:D:1438:ALA:HA	3:D:1441:PHE:CD1	2.42	0.55
3:D:604:THR:HG22	3:D:608:SER:HB3	1.88	0.55
3:D:764:LEU:HD12	3:D:765:SER:H	1.71	0.55
4:E:13:VAL:CG2	4:E:19:LEU:HB2	2.35	0.55
1:B:25:LEU:HD12	1:B:25:LEU:C	2.27	0.55
2:C:208:VAL:HG22	2:C:212:SER:OG	2.06	0.55
2:C:263:ASP:HB3	2:C:264:PRO:CD	2.32	0.55
2:C:380:ALA:O	2:C:384:GLU:N	2.40	0.55
2:C:675:ALA:HB2	2:C:989:VAL:HG22	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1108:VAL:HG11	3:D:1216:VAL:CG1	2.36	0.55
3:D:1126:MET:CG	3:D:1127:ASP:H	2.07	0.55
3:D:1278:ILE:CG2	3:D:1279:ASP:H	2.18	0.55
1:A:216:ILE:HG22	1:A:220:HIS:CD2	2.41	0.55
1:B:40:LEU:O	1:B:44:LEU:HB2	2.07	0.55
2:C:352:ALA:HA	2:C:355:VAL:CG1	2.36	0.55
2:C:889:HIS:C	2:C:891:GLY:N	2.59	0.55
3:D:483:HIS:N	3:D:484:PRO:CD	2.56	0.55
3:D:949:THR:HG22	3:D:949:THR:O	2.06	0.55
1:A:102:ALA:HB1	1:A:106:LYS:HE2	1.87	0.55
1:A:41:ARG:C	1:A:41:ARG:HD2	2.28	0.55
2:C:260:LEU:O	2:C:261:LEU:O	2.25	0.55
2:C:704:HIS:ND1	2:C:831:ARG:HD2	2.21	0.55
2:C:876:VAL:O	2:C:880:MET:HB2	2.06	0.55
2:C:882:LEU:CD2	2:C:882:LEU:N	2.62	0.55
3:D:1118:TYR:C	3:D:1119:ILE:HD12	2.28	0.55
3:D:496:LEU:HD11	3:D:500:ARG:CZ	2.36	0.55
3:D:497:GLU:HG2	3:D:1390:LEU:HD21	1.89	0.55
3:D:679:ARG:O	3:D:681:ARG:N	2.38	0.55
3:D:950:ILE:HD12	3:D:953:ASP:HB2	1.87	0.55
2:C:17:PRO:HD2	2:C:20:GLU:CB	2.36	0.55
2:C:312:ALA:HB1	2:C:318:PRO:CG	2.36	0.55
2:C:494:TYR:O	2:C:495:THR:CB	2.55	0.55
2:C:642:ARG:HD3	2:C:654:LEU:HD23	1.89	0.55
2:C:683:ASN:HA	2:C:687:ALA:O	2.07	0.55
1:A:41:ARG:NE	2:C:860:HIS:NE2	2.52	0.55
3:D:1104:HIS:CA	3:D:1223:GLY:HA3	2.36	0.55
3:D:691:LEU:HD12	3:D:692:GLU:H	1.70	0.55
3:D:752:SER:O	3:D:753:SER:C	2.46	0.55
3:D:795:VAL:HG22	3:D:876:ASN:HD21	1.70	0.55
3:D:903:ASP:OD1	3:D:903:ASP:O	2.24	0.55
1:A:100:LEU:HD23	1:A:113:PHE:CD1	2.42	0.54
1:A:82:LEU:HD23	1:A:128:ILE:HD13	1.88	0.54
1:B:131:LEU:HD23	1:B:131:LEU:O	2.07	0.54
2:C:150:PRO:HA	2:C:157:ARG:HA	1.89	0.54
2:C:194:VAL:O	2:C:197:LEU:HB2	2.06	0.54
2:C:340:MET:C	2:C:340:MET:SD	2.86	0.54
2:C:460:ARG:CG	2:C:461:VAL:H	2.20	0.54
2:C:729:LEU:HD23	2:C:734:LEU:CD2	2.37	0.54
2:C:831:ARG:HH12	2:C:1002:GLU:CB	2.18	0.54
3:D:1154:VAL:HG11	3:D:1175:LEU:HD21	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1205:CYS:C	3:D:1207:GLY:H	2.10	0.54
3:D:1486:GLN:HA	4:E:75:PHE:HA	1.88	0.54
3:D:664:LYS:O	3:D:665:ALA:HB3	2.07	0.54
3:D:965:LEU:O	3:D:967:GLU:N	2.38	0.54
4:E:22:VAL:HG12	4:E:23:VAL:N	2.23	0.54
1:A:131:LEU:CD2	1:A:137:LEU:HD22	2.37	0.54
1:B:102:ALA:HB3	1:B:137:LEU:O	2.07	0.54
1:B:73:GLU:OE2	1:B:73:GLU:N	2.40	0.54
2:C:389:SER:C	2:C:391:LEU:N	2.60	0.54
2:C:821:GLU:O	2:C:822:VAL:HG23	2.06	0.54
2:C:928:LYS:O	2:C:929:ARG:C	2.44	0.54
3:D:1220:GLU:O	3:D:1222:VAL:HG23	2.07	0.54
3:D:687:VAL:O	3:D:688:TRP:C	2.46	0.54
3:D:879:ARG:NH1	3:D:905:PRO:HD2	2.22	0.54
4:E:78:ASN:ND2	4:E:79:LEU:HG	2.22	0.54
1:B:102:ALA:CB	1:B:137:LEU:HB3	2.37	0.54
2:C:162:ILE:HG13	2:C:171:TRP:CZ3	2.42	0.54
2:C:22:GLN:NE2	2:C:336:VAL:HG21	2.15	0.54
2:C:434:HIS:O	2:C:436:GLY:N	2.40	0.54
2:C:394:PHE:HE2	2:C:632:ASN:HB3	1.72	0.54
2:C:729:LEU:HD23	2:C:734:LEU:HD23	1.90	0.54
2:C:569:VAL:HG11	2:C:996:LYS:O	2.08	0.54
3:D:1221:ALA:O	3:D:1225:VAL:HG23	2.08	0.54
3:D:1282:VAL:HG22	3:D:1315:LYS:HA	1.88	0.54
3:D:1354:GLN:O	3:D:1357:TYR:N	2.40	0.54
3:D:135:LEU:HA	3:D:139:GLY:O	2.07	0.54
1:A:103:GLU:H	1:A:106:LYS:HZ3	1.54	0.54
1:B:124:PRO:HG2	1:B:125:ASP:H	1.72	0.54
2:C:1012:PRO:HG3	2:C:1024:LYS:H	1.71	0.54
2:C:89:THR:HA	2:C:129:ILE:HA	1.89	0.54
2:C:177:GLU:HG2	2:C:181:VAL:N	2.19	0.54
2:C:203:ASP:O	2:C:206:THR:HG22	2.08	0.54
2:C:408:ARG:NH2	2:C:456:ALA:O	2.40	0.54
3:D:1235:THR:HG22	3:D:1235:THR:O	2.08	0.54
3:D:1292:SER:HA	3:D:1304:TYR:O	2.07	0.54
3:D:1436:LEU:HD22	3:D:1458:ASP:OD2	2.08	0.54
3:D:572:ARG:HG3	3:D:573:MET:HG3	1.89	0.54
3:D:801:GLY:O	3:D:802:ALA:HB2	2.08	0.54
3:D:899:LEU:C	3:D:900:ILE:HG13	2.28	0.54
1:A:24:VAL:HA	1:A:195:THR:HA	1.89	0.54
1:B:33:GLY:CA	1:B:194:LEU:HD23	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:VAL:O	1:B:79:ILE:HB	2.07	0.54
2:C:1030:GLN:HE22	3:D:628:ARG:HD3	1.73	0.54
2:C:743:VAL:CG1	2:C:800:VAL:HG21	2.36	0.54
3:D:661:MET:SD	3:D:677:LEU:HD21	2.46	0.54
3:D:703:ASN:OD1	3:D:704:ARG:N	2.41	0.54
3:D:849:ALA:O	3:D:852:ALA:HB3	2.07	0.54
3:D:958:PRO:HG3	3:D:1008:VAL:HB	1.89	0.54
1:A:62:LEU:CD1	1:A:62:LEU:H	1.93	0.54
2:C:312:ALA:HB1	2:C:318:PRO:HG3	1.90	0.54
2:C:544:THR:C	2:C:546:LEU:H	2.09	0.54
2:C:727:PRO:HG3	2:C:785:VAL:O	2.07	0.54
2:C:862:PRO:HA	2:C:975:TYR:CD1	2.42	0.54
3:D:1089:THR:HA	3:D:1092:SER:HB2	1.88	0.54
3:D:552:ASN:HA	3:D:555:LYS:CB	2.37	0.54
3:D:634:GLY:O	3:D:636:GLN:OE1	2.26	0.54
1:A:142:ARG:CG	1:A:143:VAL:H	2.20	0.54
1:A:170:PHE:O	1:A:171:SER:C	2.46	0.54
1:B:62:LEU:HD23	1:B:62:LEU:N	2.23	0.54
2:C:169:GLY:HA2	2:C:264:PRO:O	2.07	0.54
2:C:18:LEU:HD13	2:C:542:LEU:HD21	1.89	0.54
2:C:324:ASP:C	2:C:326:ASP:H	2.10	0.54
2:C:347:GLY:O	2:C:377:PRO:HB2	2.07	0.54
2:C:445:GLU:O	2:C:449:ILE:HD13	2.06	0.54
2:C:520:GLU:N	2:C:521:PRO:HD3	2.23	0.54
2:C:690:ILE:HD13	2:C:869:VAL:HA	1.89	0.54
2:C:701:THR:CG2	2:C:832:LYS:HA	2.27	0.54
3:D:1044:GLY:O	3:D:1058:VAL:HG23	2.08	0.54
3:D:1110:GLU:HG3	3:D:1111:ALA:H	1.70	0.54
3:D:1353:ILE:O	3:D:1354:GLN:C	2.46	0.54
3:D:542:ASP:O	3:D:545:ARG:N	2.40	0.54
3:D:597:GLU:HG2	3:D:598:ARG:H	1.72	0.54
2:C:648:ARG:NH1	2:C:653:ASP:OD2	2.38	0.54
2:C:642:ARG:H	2:C:656:ALA:HA	1.73	0.54
2:C:957:LYS:HB3	2:C:961:GLU:CB	2.38	0.54
3:D:663:GLU:C	3:D:665:ALA:N	2.60	0.54
3:D:729:HIS:ND1	3:D:730:PRO:HG2	2.23	0.54
3:D:904:VAL:HG12	3:D:906:GLN:OE1	2.08	0.54
1:A:30:ARG:HH11	1:A:191:LEU:H	1.56	0.54
1:A:35:THR:HG23	1:B:39:PRO:HB3	1.89	0.54
1:B:122:MET:O	1:B:124:PRO:HD3	2.08	0.54
2:C:110:GLU:O	2:C:113:VAL:HG23	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:203:ASP:O	2:C:204:GLN:C	2.45	0.54
2:C:17:PRO:CD	2:C:20:GLU:HB2	2.38	0.54
2:C:469:THR:HB	2:C:482:GLU:O	2.07	0.54
2:C:18:LEU:HD22	2:C:542:LEU:HD22	1.90	0.54
3:D:1253:ILE:O	3:D:1259:ARG:HB2	2.08	0.54
3:D:558:LEU:C	3:D:560:GLN:H	2.10	0.54
1:A:74:ASP:O	1:A:76:VAL:N	2.41	0.54
1:B:34:VAL:HG12	1:B:35:THR:N	2.23	0.54
1:B:86:VAL:N	1:B:123:ASN:ND2	2.56	0.54
2:C:165:LEU:C	2:C:167:LYS:H	2.11	0.54
2:C:261:LEU:HD21	2:C:263:ASP:HB3	1.89	0.54
2:C:267:TYR:N	2:C:267:TYR:CD2	2.73	0.54
2:C:731:GLU:O	2:C:733:ALA:N	2.41	0.54
2:C:745:ILE:HG22	2:C:746:GLY:N	2.23	0.54
3:D:1265:GLU:O	3:D:1266:ALA:HB3	2.08	0.54
3:D:733:CYS:O	3:D:736:PHE:HB2	2.08	0.54
1:A:157:ILE:HD11	1:A:160:ARG:NE	2.04	0.53
1:A:56:VAL:O	1:A:164:ILE:HG12	2.07	0.53
1:B:108:VAL:O	1:B:108:VAL:HG12	2.07	0.53
2:C:134:ARG:HH12	2:C:392:SER:CB	2.20	0.53
2:C:336:VAL:O	2:C:339:LEU:N	2.36	0.53
2:C:598:GLU:HG3	2:C:614:ARG:NH2	2.23	0.53
2:C:816:LYS:HZ2	2:C:817:PRO:HG2	1.74	0.53
3:D:1061:SER:C	3:D:1063:ARG:N	2.61	0.53
3:D:573:MET:HA	3:D:576:GLU:HB2	1.89	0.53
3:D:657:LEU:CD1	3:D:690:ALA:HB1	2.37	0.53
3:D:811:GLU:HA	3:D:814:ALA:CB	2.34	0.53
3:D:959:GLU:C	3:D:961:LYS:H	2.12	0.53
4:E:79:LEU:C	4:E:81:PRO:HD2	2.28	0.53
1:A:223:TYR:O	1:A:225:ALA:N	2.40	0.53
2:C:111:ASP:O	2:C:113:VAL:N	2.40	0.53
2:C:320:HIS:C	2:C:322:VAL:N	2.61	0.53
2:C:492:ASP:H	2:C:532:MET:H	1.56	0.53
2:C:556:ASN:O	2:C:559:LEU:HG	2.08	0.53
3:D:99:ALA:O	3:D:100:ALA:HB2	2.07	0.53
3:D:1354:GLN:NE2	3:D:1369:ILE:CD1	2.71	0.53
3:D:1381:GLU:OE1	3:D:1392:GLU:HG3	2.08	0.53
3:D:500:ARG:O	3:D:504:ASP:N	2.41	0.53
1:A:127:HIS:CE1	1:A:130:THR:HG1	2.26	0.53
1:A:181:GLU:O	1:A:193:LYS:HB3	2.08	0.53
1:A:37:GLY:CA	1:A:194:LEU:HD11	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:THR:HG21	1:B:22:GLU:HG3	1.90	0.53
2:C:1068:GLN:O	2:C:1072:LYS:HG3	2.09	0.53
2:C:433:THR:OG1	2:C:441:VAL:HG12	2.08	0.53
2:C:718:GLY:HA3	2:C:761:PHE:CD1	2.42	0.53
2:C:677:MET:H	2:C:873:PRO:HD3	1.73	0.53
2:C:914:ILE:O	2:C:918:LEU:HB2	2.08	0.53
1:A:197:ARG:HH12	2:C:932:GLU:CD	2.12	0.53
3:D:1060:SER:OG	3:D:1066:LEU:HD13	2.08	0.53
3:D:1148:ARG:HD2	3:D:1189:VAL:CG2	2.37	0.53
3:D:1236:GLN:O	3:D:1237:LEU:HD23	2.08	0.53
3:D:1385:PRO:HB2	3:D:1388:SER:O	2.09	0.53
3:D:1409:ILE:HG22	3:D:1409:ILE:O	2.08	0.53
3:D:936:TYR:CE2	3:D:940:THR:HG21	2.44	0.53
4:E:3:GLU:HB2	4:E:6:ILE:CG1	2.38	0.53
1:A:198:ILE:HG21	1:A:206:PRO:HA	1.89	0.53
1:B:117:ALA:C	1:B:119:VAL:H	2.12	0.53
1:B:203:SER:OG	1:B:204:VAL:N	2.40	0.53
2:C:996:LYS:HE2	2:C:1000:MET:CE	2.38	0.53
2:C:162:ILE:HG13	2:C:171:TRP:HH2	1.72	0.53
2:C:253:ALA:O	2:C:255:ALA:N	2.37	0.53
2:C:706:GLU:HA	2:C:706:GLU:OE1	2.09	0.53
2:C:815:LEU:N	2:C:815:LEU:HD12	2.23	0.53
2:C:840:ALA:HA	2:C:846:LYS:HA	1.90	0.53
2:C:903:SER:OG	2:C:909:ALA:HB3	2.08	0.53
2:C:922:PHE:C	2:C:924:LEU:N	2.62	0.53
3:D:1009:PHE:O	3:D:1009:PHE:CD2	2.61	0.53
3:D:1206:TYR:HD2	3:D:1216:VAL:HG21	1.73	0.53
3:D:647:ARG:O	3:D:650:LEU:HB3	2.07	0.53
3:D:761:ILE:HG21	4:E:20:THR:OG1	2.09	0.53
2:C:1076:VAL:O	2:C:1078:GLU:HG3	2.09	0.53
2:C:194:VAL:HG22	2:C:221:LEU:CD1	2.38	0.53
2:C:290:LEU:HG	2:C:291:VAL:N	2.24	0.53
2:C:628:TYR:N	2:C:628:TYR:CD1	2.76	0.53
2:C:890:LEU:O	2:C:890:LEU:HG	2.09	0.53
3:D:1402:GLU:C	3:D:1404:LEU:N	2.62	0.53
3:D:815:ALA:HB3	3:D:832:ARG:HD2	1.90	0.53
4:E:77:GLU:OE1	4:E:77:GLU:HA	2.09	0.53
1:A:122:MET:SD	1:A:122:MET:N	2.70	0.53
1:A:71:VAL:HA	1:A:131:LEU:HA	1.90	0.53
1:A:46:SER:OG	2:C:856:GLU:HG2	2.07	0.53
2:C:1005:MET:SD	3:D:724:GLN:HA	2.49	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:970:GLY:HA2	3:D:950:ILE:HG21	1.91	0.53
3:D:957:ILE:HD11	3:D:1063:ARG:HD2	1.91	0.53
3:D:1451:ALA:HA	3:D:1456:LYS:CG	2.36	0.53
3:D:660:LYS:O	3:D:664:LYS:HB2	2.08	0.53
3:D:691:LEU:HD12	3:D:691:LEU:N	2.23	0.53
1:A:199:TRP:O	1:A:200:THR:O	2.26	0.53
1:A:91:ASP:CG	1:A:92:PRO:HD2	2.29	0.53
2:C:1034:GLU:HG3	2:C:1035:MET:N	2.24	0.53
2:C:134:ARG:NH2	2:C:393:GLN:HA	2.24	0.53
2:C:399:ASN:HD22	2:C:401:LEU:H	1.53	0.53
2:C:42:VAL:HG12	2:C:43:GLY:H	1.74	0.53
2:C:491:GLU:O	2:C:509:ALA:CB	2.55	0.53
2:C:690:ILE:O	2:C:852:ILE:HA	2.09	0.53
2:C:816:LYS:HB3	2:C:819:VAL:HG21	1.89	0.53
3:D:1037:ARG:O	3:D:1041:GLY:O	2.27	0.53
3:D:1039:LEU:O	3:D:1061:SER:O	2.27	0.53
3:D:1106:ILE:HD12	3:D:1371:ILE:CG2	2.39	0.53
3:D:502:PHE:HZ	3:D:511:TRP:CZ2	2.23	0.53
3:D:661:MET:O	3:D:664:LYS:HB3	2.09	0.53
4:E:27:ALA:C	4:E:29:GLN:H	2.11	0.53
1:A:223:TYR:CD1	1:B:9:PRO:HD2	2.44	0.53
2:C:163:ILE:HG12	2:C:169:GLY:O	2.08	0.53
2:C:163:ILE:HG21	2:C:169:GLY:C	2.29	0.53
2:C:157:ARG:HG3	2:C:313:LEU:HG	1.91	0.53
2:C:136:ILE:HG22	2:C:336:VAL:HG22	1.90	0.53
2:C:613:VAL:HG11	2:C:619:ARG:CD	2.29	0.53
2:C:701:THR:HG22	2:C:832:LYS:HG2	1.91	0.53
3:D:1484:PHE:O	3:D:1485:THR:C	2.48	0.53
3:D:636:GLN:HE21	3:D:642:CYS:HA	1.73	0.53
3:D:681:ARG:O	3:D:682:ASP:HB3	2.09	0.53
3:D:862:ASP:CA	3:D:876:ASN:HB3	2.25	0.53
3:D:924:MET:O	3:D:927:THR:N	2.42	0.53
3:D:966:GLU:O	3:D:969:ASP:N	2.42	0.53
3:D:1484:PHE:HE1	4:E:22:VAL:HG23	1.74	0.53
2:C:257:LEU:HB3	2:C:264:PRO:HG3	1.90	0.53
2:C:614:ARG:NH1	2:C:623:HIS:HE1	2.05	0.53
3:D:636:GLN:HE21	3:D:642:CYS:CA	2.21	0.53
3:D:679:ARG:O	3:D:680:GLN:HG2	2.09	0.53
3:D:764:LEU:HD23	3:D:767:HIS:NE2	2.24	0.53
3:D:772:PRO:O	3:D:773:ALA:C	2.47	0.53
3:D:937:TYR:O	3:D:938:GLY:C	2.47	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:VAL:HG22	1:A:124:PRO:CB	2.38	0.53
1:A:57:TYR:HD2	1:A:57:TYR:C	2.11	0.53
1:A:98:LEU:HB3	1:A:113:PHE:CD2	2.43	0.53
2:C:1012:PRO:HG2	2:C:1027:PHE:HA	1.91	0.53
2:C:159:ILE:HD12	2:C:174:LEU:HB2	1.91	0.53
2:C:232:GLU:C	2:C:234:ALA:N	2.62	0.53
2:C:356:ARG:HA	2:C:359:MET:HG3	1.91	0.53
2:C:45:GLN:O	2:C:48:PHE:HB2	2.09	0.53
2:C:605:LYS:HZ3	2:C:611:ILE:HG13	1.70	0.53
2:C:689:VAL:CG1	2:C:853:LEU:HD22	2.39	0.53
2:C:897:LEU:O	2:C:899:GLN:HG3	2.09	0.53
3:D:1320:VAL:O	3:D:1321:GLU:C	2.47	0.53
3:D:617:ASN:O	3:D:619:LEU:O	2.27	0.53
2:C:21:ILE:HG23	2:C:460:ARG:HH22	1.73	0.52
2:C:258:PHE:N	2:C:258:PHE:CD1	2.77	0.52
2:C:342:ASP:O	2:C:345:ARG:HB2	2.09	0.52
2:C:723:THR:OG1	2:C:724:ARG:N	2.43	0.52
3:D:1481:PHE:CD2	3:D:1481:PHE:O	2.62	0.52
3:D:709:HIS:CD2	3:D:711:LEU:HB2	2.44	0.52
3:D:1219:GLY:C	4:E:17:TYR:HE2	2.12	0.52
1:A:102:ALA:CB	1:A:131:LEU:HD21	2.39	0.52
1:A:79:ILE:HG23	1:A:166:VAL:HG22	1.91	0.52
2:C:1030:GLN:CB	3:D:626:SER:HB3	2.39	0.52
2:C:1052:MET:CG	3:D:623:VAL:HG22	2.39	0.52
2:C:208:VAL:HG11	2:C:218:VAL:HG21	1.92	0.52
2:C:820:ARG:O	2:C:821:GLU:HB3	2.08	0.52
3:D:1048:LYS:HG2	3:D:1054:PHE:CZ	2.45	0.52
3:D:1070:GLU:C	3:D:1072:PHE:N	2.60	0.52
3:D:1410:ALA:O	3:D:1414:VAL:N	2.42	0.52
3:D:502:PHE:O	3:D:504:ASP:N	2.42	0.52
3:D:543:LEU:HB3	3:D:581:VAL:HG22	1.92	0.52
2:C:517:ARG:NH2	3:D:976:GLU:OE1	2.43	0.52
4:E:68:LEU:HA	4:E:73:LEU:HD11	1.90	0.52
1:A:205:THR:CG2	1:A:206:PRO:HD2	2.37	0.52
1:B:19:HIS:O	1:B:20:TYR:C	2.46	0.52
2:C:176:VAL:HG12	2:C:182:VAL:HG22	1.90	0.52
2:C:491:GLU:HG2	2:C:510:THR:HB	1.91	0.52
2:C:610:ARG:CB	2:C:624:PRO:HA	2.39	0.52
2:C:87:ASP:CG	2:C:824:ARG:HH22	2.12	0.52
2:C:890:LEU:HD11	2:C:901:TYR:CE2	2.44	0.52
3:D:1089:THR:HA	3:D:1092:SER:HB3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1358:ARG:HH22	3:D:1365:HIS:CD2	2.26	0.52
3:D:1494:LYS:C	3:D:1496:ILE:H	2.12	0.52
3:D:668:PRO:HG2	3:D:672:ALA:CB	2.40	0.52
3:D:645:PRO:HA	3:D:722:GLU:O	2.09	0.52
1:B:113:PHE:O	1:B:115:PRO:HD3	2.09	0.52
2:C:1005:MET:O	2:C:1005:MET:HG3	2.09	0.52
2:C:421:GLU:HG3	2:C:423:ALA:H	1.74	0.52
2:C:637:PHE:C	2:C:637:PHE:CD1	2.83	0.52
3:D:1060:SER:OG	3:D:1068:VAL:HG23	2.09	0.52
3:D:26:VAL:C	3:D:28:LYS:H	2.11	0.52
3:D:28(U):UNK:O	3:D:29(U):UNK:O	2.27	0.52
3:D:564:GLU:HA	3:D:567:ILE:CG2	2.39	0.52
3:D:747:VAL:O	3:D:748:HIS:O	2.28	0.52
3:D:767:HIS:NE2	4:E:6:ILE:HG13	2.23	0.52
3:D:855:HIS:O	3:D:857:LEU:CD2	2.57	0.52
3:D:795:VAL:CG2	3:D:876:ASN:HD21	2.23	0.52
3:D:969:ASP:O	3:D:970:ARG:C	2.47	0.52
1:A:181:GLU:OE2	2:C:934:PHE:HD2	1.92	0.52
1:A:199:TRP:HD1	1:A:200:THR:HG1	1.55	0.52
1:A:96:THR:OG1	1:A:97:THR:N	2.43	0.52
1:B:105:PRO:HD3	1:B:133:GLU:HA	1.91	0.52
2:C:202:TYR:O	2:C:203:ASP:HB3	2.09	0.52
2:C:332:ARG:HG2	2:C:333:ILE:N	2.23	0.52
2:C:662:GLU:O	2:C:664:GLY:N	2.42	0.52
2:C:8:ARG:C	2:C:9:ILE:HD12	2.30	0.52
3:D:1061:SER:O	3:D:1062:PHE:HB2	2.09	0.52
3:D:1152:ARG:N	3:D:1163:GLU:HG2	2.24	0.52
3:D:1259:ARG:C	3:D:1261:ILE:N	2.63	0.52
3:D:688:TRP:C	3:D:690:ALA:N	2.61	0.52
1:A:102:ALA:HB3	1:A:137:LEU:CB	2.39	0.52
1:B:59:GLU:O	1:B:60:ASP:HB2	2.09	0.52
2:C:1063:ARG:O	2:C:1066:ALA:HB3	2.09	0.52
2:C:559:LEU:HD12	2:C:560:MET:N	2.25	0.52
2:C:577:PRO:HA	2:C:671:ASN:HD22	1.73	0.52
2:C:593:ALA:HB1	2:C:659:PRO:HD3	1.90	0.52
3:D:590:PRO:O	3:D:600:LEU:HD21	2.09	0.52
3:D:792:ILE:HG23	3:D:792:ILE:O	2.10	0.52
3:D:815:ALA:O	3:D:817:GLU:N	2.43	0.52
2:C:1088:LEU:HD21	3:D:614:PHE:HE2	1.75	0.52
2:C:368:THR:OG1	2:C:371:LYS:HD2	2.09	0.52
3:D:1062:PHE:CE1	3:D:1066:LEU:HD23	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1070:GLU:HG3	3:D:1073:ILE:HB	1.92	0.52
3:D:1148:ARG:CD	3:D:1189:VAL:HG21	2.38	0.52
3:D:601:ARG:HH11	3:D:601:ARG:HA	1.73	0.52
3:D:628:ARG:O	3:D:629:SER:HB2	2.10	0.52
3:D:710:ARG:NH2	3:D:1220:GLU:OE2	2.42	0.52
1:A:11:PHE:HD1	1:A:25:LEU:HD23	1.75	0.52
1:B:37:GLY:HA3	1:B:194:LEU:HD21	1.90	0.52
2:C:184:MET:CG	2:C:193:LEU:HD23	2.40	0.52
2:C:34:VAL:HG13	2:C:35:PRO:HD2	1.92	0.52
2:C:134:ARG:HH12	2:C:392:SER:HB2	1.74	0.52
2:C:631:SER:CB	2:C:635:THR:HB	2.40	0.52
2:C:637:PHE:CG	2:C:637:PHE:O	2.62	0.52
2:C:974:LEU:HD23	2:C:987:ILE:CB	2.39	0.52
3:D:1052:GLU:O	3:D:1053:THR:O	2.28	0.52
3:D:1093:GLY:HA2	3:D:1097:ARG:HE	1.74	0.52
3:D:112:ILE:O	3:D:114:THR:N	2.42	0.52
3:D:1107:VAL:HG22	3:D:1221:ALA:HA	1.91	0.52
3:D:1315:LYS:O	3:D:1316:ASP:O	2.27	0.52
3:D:1404:LEU:CD2	3:D:1416:VAL:H	2.23	0.52
3:D:1466:ASN:HD21	3:D:1471:ARG:HH11	1.55	0.52
3:D:653:PHE:O	3:D:654:LYS:C	2.48	0.52
3:D:687:VAL:O	3:D:690:ALA:N	2.43	0.52
3:D:927:THR:HG22	3:D:931:LEU:HD23	1.92	0.52
1:A:142:ARG:HG3	1:A:143:VAL:H	1.74	0.52
1:A:30:ARG:CA	1:A:191:LEU:HA	2.40	0.52
2:C:1043:TYR:CE2	3:D:763:MET:HA	2.45	0.52
2:C:215:GLY:O	2:C:216:ASP:C	2.48	0.52
2:C:266:ARG:HG2	2:C:268:ASP:HA	1.92	0.52
2:C:283:VAL:CG1	2:C:284:GLY:N	2.71	0.52
2:C:427:VAL:C	2:C:429:ASP:H	2.13	0.52
2:C:872:ASN:OD1	2:C:873:PRO:HD2	2.09	0.52
2:C:912:PRO:O	2:C:915:LYS:HB2	2.10	0.52
3:D:1340:LYS:O	3:D:1340:LYS:HG3	2.10	0.52
3:D:1380:VAL:HG22	3:D:1395:VAL:O	2.10	0.52
3:D:1458:ASP:C	3:D:1460:LEU:H	2.13	0.52
3:D:575:GLN:O	3:D:579:ASP:N	2.32	0.52
1:A:26:GLU:HB3	1:A:27:PRO:HD2	1.86	0.52
2:C:163:ILE:HG22	2:C:265:LYS:HZ1	1.74	0.52
2:C:774:LEU:HA	2:C:777:ILE:HD12	1.92	0.52
2:C:837:ASP:O	2:C:848:VAL:HA	2.10	0.52
2:C:987:ILE:CA	3:D:948:ILE:HG21	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1018:PHE:HA	3:D:1024:MET:CE	2.40	0.52
3:D:1066:LEU:C	3:D:1068:VAL:H	2.13	0.52
3:D:1232:GLU:C	3:D:1234:GLY:H	2.13	0.52
3:D:1482:VAL:HG13	3:D:1484:PHE:CE2	2.45	0.52
3:D:836:VAL:HG11	3:D:858:LEU:HG	1.91	0.52
3:D:839:LEU:O	3:D:840:LYS:O	2.28	0.52
2:C:970:GLY:N	3:D:950:ILE:HG21	2.25	0.52
3:D:1482:VAL:CG1	4:E:18:ARG:HA	2.40	0.52
1:A:102:ALA:HB2	1:A:108:VAL:HG21	1.91	0.51
1:A:131:LEU:CD2	1:A:137:LEU:HB2	2.40	0.51
1:A:79:ILE:CG2	1:A:166:VAL:HG13	2.40	0.51
1:A:80:LEU:HD23	1:A:83:LYS:NZ	2.24	0.51
1:B:133:GLU:OE1	1:B:134:GLY:N	2.38	0.51
2:C:65:VAL:CG2	2:C:101:ILE:HB	2.39	0.51
2:C:110:GLU:HB2	2:C:369:PRO:HG2	1.91	0.51
2:C:172:ILE:HG13	2:C:186:VAL:HG22	1.92	0.51
2:C:569:VAL:O	2:C:569:VAL:CG1	2.52	0.51
2:C:642:ARG:CD	2:C:654:LEU:HD23	2.40	0.51
2:C:918:LEU:HD22	2:C:968:ASP:CA	2.30	0.51
2:C:77:PRO:CD	2:C:92:ALA:HA	2.40	0.51
3:D:1060:SER:OG	3:D:1066:LEU:HA	2.09	0.51
3:D:1259:ARG:O	3:D:1261:ILE:N	2.43	0.51
3:D:1281:VAL:CG1	3:D:1282:VAL:HG23	2.28	0.51
3:D:1273:ALA:HB2	3:D:1327:THR:CB	2.40	0.51
3:D:1271:ALA:CB	3:D:1329:GLY:HA3	2.35	0.51
3:D:1403:ALA:O	3:D:1416:VAL:HG21	2.10	0.51
3:D:772:PRO:CD	3:D:778:LEU:N	2.73	0.51
1:A:109:ARG:O	1:A:111:VAL:N	2.43	0.51
1:A:53:VAL:HG13	1:A:141:VAL:HG23	1.91	0.51
1:B:133:GLU:CG	1:B:134:GLY:N	2.72	0.51
1:B:98:LEU:HB2	1:B:141:VAL:O	2.10	0.51
1:A:35:THR:CG2	1:B:39:PRO:HB3	2.40	0.51
2:C:211:LEU:HD22	2:C:304:LEU:CD1	2.29	0.51
2:C:666:LEU:HD12	2:C:667:ALA:N	2.24	0.51
2:C:676:ILE:CG2	2:C:677:MET:N	2.73	0.51
2:C:743:VAL:CG1	2:C:744:ARG:N	2.73	0.51
2:C:549:PHE:CE2	2:C:886:LEU:HD13	2.46	0.51
2:C:987:ILE:O	2:C:988:VAL:C	2.48	0.51
3:D:1312:LEU:O	3:D:1313:LEU:O	2.27	0.51
3:D:502:PHE:C	3:D:504:ASP:N	2.64	0.51
3:D:578:VAL:HG12	3:D:582:ILE:CD1	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:691:LEU:O	3:D:693:GLU:N	2.43	0.51
3:D:773:ALA:O	3:D:774:SER:HB2	2.10	0.51
4:E:68:LEU:HA	4:E:73:LEU:HD12	1.92	0.51
2:C:163:ILE:C	2:C:163:ILE:HD12	2.31	0.51
2:C:208:VAL:O	2:C:209:ARG:HB2	2.10	0.51
2:C:64:LEU:HB3	2:C:359:MET:HE1	1.93	0.51
2:C:344:PHE:CE2	2:C:378:LEU:HD23	2.46	0.51
2:C:547:ILE:HG23	2:C:843:HIS:HE1	1.75	0.51
3:D:1149:VAL:O	3:D:1149:VAL:HG12	2.11	0.51
3:D:1193:LEU:HB3	3:D:1346:GLU:OE1	2.10	0.51
3:D:1479:SER:C	3:D:1481:PHE:N	2.60	0.51
3:D:35(U):UNK:O	3:D:36(U):UNK:CB	2.57	0.51
3:D:552:ASN:C	3:D:554:LEU:N	2.63	0.51
3:D:578:VAL:C	3:D:580:ALA:N	2.63	0.51
3:D:601:ARG:HD3	3:D:605:ASP:OD2	2.10	0.51
3:D:687:VAL:O	3:D:690:ALA:CB	2.56	0.51
3:D:699:VAL:HG22	3:D:756:GLN:HE21	1.74	0.51
3:D:927:THR:HG22	3:D:931:LEU:CD2	2.40	0.51
4:E:61:VAL:O	4:E:64:ALA:HB3	2.10	0.51
1:A:111:VAL:CG2	1:A:125:ASP:N	2.73	0.51
1:A:112:ASP:OD2	1:A:112:ASP:N	2.42	0.51
1:A:142:ARG:HH11	1:A:142:ARG:HG2	1.73	0.51
1:B:100:LEU:CD1	1:B:112:ASP:HB2	2.40	0.51
1:B:34:VAL:C	1:B:36:LEU:H	2.13	0.51
1:B:64:GLU:O	1:B:75:VAL:HB	2.10	0.51
2:C:162:ILE:HD12	2:C:162:ILE:H	1.74	0.51
2:C:14:PRO:HA	2:C:458:TYR:CD1	2.46	0.51
2:C:563:ASN:O	2:C:566:THR:N	2.43	0.51
2:C:572:ILE:O	2:C:573:ARG:HB2	2.09	0.51
2:C:836:GLY:O	2:C:848:VAL:HG23	2.10	0.51
2:C:839:LEU:O	2:C:995:MET:O	2.29	0.51
3:D:1232:GLU:O	3:D:1234:GLY:N	2.35	0.51
3:D:1401:VAL:HG12	3:D:1401:VAL:O	2.11	0.51
3:D:685:ASP:O	3:D:687:VAL:N	2.44	0.51
3:D:753:SER:O	3:D:754:PHE:C	2.47	0.51
3:D:776:GLU:HB3	3:D:912:LYS:CE	2.38	0.51
3:D:808:THR:O	3:D:808:THR:HG22	2.09	0.51
3:D:890:VAL:HG12	3:D:891:GLY:N	2.24	0.51
4:E:19:LEU:CD1	4:E:23:VAL:HG23	2.40	0.51
1:A:220:HIS:HA	1:A:223:TYR:HD2	1.75	0.51
1:A:74:ASP:OD2	2:C:627:ARG:NH2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:LEU:CD2	1:B:221:LEU:HD11	2.40	0.51
2:C:320:HIS:O	2:C:322:VAL:HG12	2.10	0.51
2:C:425:PHE:O	2:C:426:ASP:OD1	2.28	0.51
2:C:572:ILE:O	2:C:573:ARG:CB	2.58	0.51
2:C:577:PRO:CG	2:C:580:MET:HB3	2.35	0.51
2:C:655:LEU:O	2:C:656:ALA:HB3	2.09	0.51
2:C:675:ALA:CB	2:C:989:VAL:HG22	2.41	0.51
2:C:694:LEU:O	2:C:699:PHE:HB2	2.09	0.51
3:D:1138:ARG:H	3:D:1138:ARG:CD	2.18	0.51
3:D:1207:GLY:O	3:D:1208:TYR:O	2.29	0.51
2:C:1009:SER:HA	3:D:625:TYR:CD2	2.45	0.51
3:D:893:GLU:O	3:D:894:LYS:HB2	2.11	0.51
3:D:779:ALA:O	3:D:931:LEU:HD11	2.11	0.51
4:E:59:ASN:HB3	4:E:62:THR:OG1	2.10	0.51
1:A:134:GLY:O	1:A:136:LYS:N	2.44	0.51
1:A:163:ALA:O	1:A:164:ILE:HG12	2.10	0.51
1:A:196:LEU:N	1:A:196:LEU:HD23	2.26	0.51
1:A:42:ARG:NE	1:B:35:THR:OG1	2.40	0.51
1:B:125:ASP:O	1:B:126:LEU:CB	2.59	0.51
1:B:99:ILE:HD13	1:B:138:TYR:OH	2.11	0.51
1:B:154:ARG:O	1:B:155:HIS:HB2	2.11	0.51
2:C:455:LEU:HD12	2:C:456:ALA:O	2.10	0.51
2:C:531:PHE:O	2:C:532:MET:CB	2.59	0.51
2:C:774:LEU:HD23	2:C:777:ILE:HD12	1.91	0.51
2:C:877:PRO:O	2:C:881:ASN:N	2.43	0.51
2:C:970:GLY:CA	3:D:950:ILE:HG21	2.41	0.51
3:D:1320:VAL:HG21	3:D:1339:ALA:O	2.11	0.51
3:D:1353:ILE:HG22	3:D:1354:GLN:N	2.25	0.51
3:D:681:ARG:O	3:D:682:ASP:CB	2.58	0.51
3:D:902:MET:HE2	3:D:902:MET:O	2.10	0.51
1:A:22:GLU:HA	1:A:197:ARG:HA	1.92	0.51
1:A:86:VAL:HG21	1:A:202:GLY:HA3	1.92	0.51
2:C:1021:LEU:HD21	3:D:622:ARG:CZ	2.41	0.51
2:C:263:ASP:CB	2:C:264:PRO:CD	2.88	0.51
2:C:495:THR:CG2	2:C:496:ILE:H	2.21	0.51
2:C:692:GLU:HG2	2:C:696:LYS:HE3	1.92	0.51
2:C:882:LEU:HD11	2:C:884:GLN:HE21	1.75	0.51
3:D:1018:PHE:O	3:D:1020:PRO:N	2.43	0.51
3:D:628:ARG:HB3	3:D:628:ARG:HH11	1.76	0.51
3:D:683:ILE:CG2	3:D:687:VAL:HB	2.40	0.51
3:D:906:GLN:O	3:D:907:GLU:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:936:TYR:C	3:D:936:TYR:HD2	2.13	0.51
1:A:99:ILE:O	1:A:114:THR:CG2	2.58	0.51
1:A:79:ILE:HD11	1:A:164:ILE:CG1	2.40	0.51
1:A:82:LEU:HD21	1:A:128:ILE:HD13	1.92	0.51
2:C:1018:GLN:HE21	2:C:1060:ILE:HG12	1.76	0.51
2:C:474:VAL:CG1	2:C:530:GLU:HA	2.40	0.51
2:C:654:LEU:HD11	2:C:657:ASP:CA	2.30	0.51
2:C:843:HIS:HD2	2:C:884:GLN:CB	2.24	0.51
2:C:690:ILE:HG22	2:C:852:ILE:HG22	1.93	0.51
2:C:892:LEU:C	2:C:894:GLY:H	2.15	0.51
2:C:9:ILE:CG2	2:C:10:ARG:N	2.71	0.51
3:D:1095:LEU:HD22	3:D:1257:LEU:HD11	1.92	0.51
3:D:1257:LEU:O	3:D:1260:VAL:N	2.44	0.51
3:D:1283:ARG:HH21	3:D:1285:GLU:CG	2.22	0.51
3:D:1404:LEU:HD21	3:D:1416:VAL:N	2.25	0.51
3:D:520:LEU:HB3	3:D:521:PRO:CD	2.38	0.51
3:D:678:GLU:C	3:D:680:GLN:H	2.14	0.51
3:D:772:PRO:CB	3:D:778:LEU:HB2	2.38	0.51
3:D:829:VAL:O	3:D:830:ALA:HB2	2.11	0.51
3:D:907:GLU:HB3	3:D:911:LEU:HD21	1.93	0.51
4:E:21:VAL:O	4:E:24:ALA:HB3	2.11	0.51
4:E:9:LEU:CD2	4:E:69:LEU:HD13	2.41	0.51
1:A:156:GLY:O	1:A:163:ALA:CB	2.57	0.51
1:A:23:PHE:HZ	1:A:206:PRO:HB2	1.76	0.51
2:C:1108:PRO:O	2:C:1109:VAL:C	2.49	0.51
2:C:226:VAL:O	2:C:229:MET:HG2	2.11	0.51
2:C:391:LEU:HD22	2:C:415:PRO:CD	2.41	0.51
2:C:400:PRO:HG3	2:C:659:PRO:HG2	1.93	0.51
3:D:1282:VAL:HG22	3:D:1315:LYS:C	2.31	0.51
3:D:1342:PRO:O	3:D:1343:GLU:C	2.48	0.51
3:D:469:ASP:O	3:D:471:GLU:N	2.43	0.51
1:A:219:GLU:O	1:A:222:ASN:HB2	2.11	0.51
2:C:298:PHE:N	2:C:298:PHE:CD1	2.79	0.51
2:C:568:ALA:O	2:C:569:VAL:CG1	2.58	0.51
2:C:906:PHE:CD1	3:D:1069:LEU:HD12	2.45	0.51
2:C:953:VAL:HG13	2:C:965:GLU:OE1	2.10	0.51
2:C:97:ARG:HG2	2:C:112:GLU:N	2.17	0.51
3:D:1108:VAL:O	3:D:1218:ILE:HA	2.11	0.51
3:D:1220:GLU:O	3:D:1222:VAL:N	2.44	0.51
3:D:953:ASP:O	3:D:954:ASP:CB	2.59	0.51
3:D:989:ARG:O	3:D:993:VAL:HG23	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:ARG:NH1	1:A:144:ASP:OD1	2.44	0.50
2:C:1026:GLN:O	2:C:1027:PHE:CB	2.60	0.50
2:C:102:HIS:CD2	2:C:106:GLY:HA3	2.34	0.50
2:C:140:ILE:HD11	2:C:331:ARG:HH11	1.76	0.50
2:C:310:LEU:O	2:C:311:PHE:C	2.49	0.50
2:C:578:VAL:O	2:C:901:TYR:N	2.28	0.50
2:C:800:VAL:O	2:C:800:VAL:HG12	2.11	0.50
2:C:722:ILE:HD12	2:C:821:GLU:OE1	2.11	0.50
2:C:550:LEU:HB3	2:C:905:VAL:HG13	1.93	0.50
2:C:944:LEU:C	2:C:946:ARG:H	2.15	0.50
3:D:1083:ALA:O	3:D:1086:ALA:HB3	2.11	0.50
3:D:1373:VAL:HA	3:D:1376:MET:HE2	1.93	0.50
3:D:1426:THR:O	3:D:1428:SER:N	2.43	0.50
3:D:30(U):UNK:HA	3:D:35(U):UNK:O	2.11	0.50
3:D:659:LYS:HZ2	3:D:663:GLU:HB2	1.75	0.50
3:D:770:LEU:HB2	3:D:919:PHE:HE1	1.76	0.50
3:D:963:ARG:HG2	3:D:967:GLU:OE2	2.10	0.50
1:A:103:GLU:H	1:A:106:LYS:CE	2.25	0.50
1:A:157:ILE:HG12	1:A:158:LYS:N	2.26	0.50
1:B:100:LEU:HA	1:B:113:PHE:HA	1.94	0.50
1:B:175:ARG:HD3	1:B:199:TRP:CD1	2.46	0.50
2:C:1009:SER:HB2	3:D:651:GLU:OE1	2.12	0.50
2:C:153:ALA:O	2:C:154:ARG:HD3	2.12	0.50
2:C:540:PHE:CE1	2:C:906:PHE:CE1	2.98	0.50
2:C:544:THR:C	2:C:546:LEU:N	2.63	0.50
2:C:749:VAL:CG1	2:C:792:VAL:HG21	2.35	0.50
3:D:1148:ARG:O	3:D:1166:TYR:HA	2.11	0.50
3:D:115:LEU:C	3:D:117:ASP:H	2.14	0.50
3:D:1214:ARG:HG3	3:D:1215:PRO:N	2.26	0.50
3:D:657:LEU:O	3:D:658:LEU:C	2.49	0.50
3:D:631:ILE:HG21	3:D:745:MET:HE3	1.93	0.50
3:D:998:THR:O	3:D:1002:GLU:HG3	2.12	0.50
1:A:58:ILE:HG21	1:A:68:ILE:CD1	2.41	0.50
1:B:56:VAL:HG13	1:B:141:VAL:HG23	1.92	0.50
1:B:208:GLU:O	1:B:212:GLN:HB2	2.11	0.50
2:C:1095:LEU:O	2:C:1096:ALA:CB	2.57	0.50
2:C:139:GLN:HG3	2:C:140:ILE:N	2.24	0.50
2:C:17:PRO:O	2:C:18:LEU:HG	2.10	0.50
2:C:559:LEU:C	2:C:559:LEU:CD1	2.76	0.50
2:C:655:LEU:HD23	2:C:655:LEU:O	2.11	0.50
2:C:672:VAL:HG21	2:C:694:LEU:HD21	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1019:ASN:O	3:D:1021:LEU:N	2.43	0.50
2:C:881:ASN:HB3	3:D:1039:LEU:HG	1.92	0.50
3:D:644:LEU:O	3:D:645:PRO:C	2.48	0.50
3:D:92:HIS:HA	3:D:517:VAL:CG1	2.33	0.50
3:D:947:ILE:HG13	3:D:947:ILE:O	2.10	0.50
3:D:978:ALA:O	3:D:984:LEU:HD12	2.11	0.50
2:C:1071:ILE:O	3:D:659:LYS:CG	2.60	0.50
2:C:148:PHE:O	2:C:149:THR:CB	2.58	0.50
2:C:901:TYR:C	2:C:902:ILE:HD12	2.32	0.50
3:D:1012:PHE:CB	3:D:1020:PRO:HG2	2.40	0.50
3:D:1098:LYS:O	3:D:1102:VAL:HG23	2.11	0.50
3:D:1102:VAL:HG21	3:D:1425:VAL:CG2	2.37	0.50
3:D:1104:HIS:O	3:D:1105:GLU:HB3	2.12	0.50
3:D:1382:VAL:HG12	3:D:1383:THR:N	2.22	0.50
3:D:639:LEU:HD23	3:D:729:HIS:NE2	2.25	0.50
3:D:836:VAL:CB	3:D:858:LEU:HD21	2.42	0.50
3:D:865:THR:N	3:D:875:THR:O	2.45	0.50
3:D:935:LYS:HG2	3:D:939:PHE:CE1	2.47	0.50
1:A:111:VAL:C	1:A:113:PHE:N	2.64	0.50
1:A:191:LEU:CD2	1:A:191:LEU:H	2.24	0.50
1:B:132:GLU:HG2	1:B:133:GLU:N	2.26	0.50
1:B:40:LEU:HD22	1:B:40:LEU:N	2.26	0.50
2:C:140:ILE:HD11	2:C:331:ARG:NH1	2.26	0.50
2:C:151:ASP:HB2	2:C:156:GLY:O	2.12	0.50
2:C:291:VAL:HB	2:C:299:LYS:CG	2.38	0.50
2:C:291:VAL:HG21	2:C:299:LYS:NZ	2.26	0.50
2:C:399:ASN:HD22	2:C:400:PRO:N	2.10	0.50
2:C:544:THR:O	2:C:546:LEU:N	2.44	0.50
2:C:755:LEU:HD11	2:C:825:VAL:HB	1.93	0.50
2:C:964:LYS:NZ	2:C:964:LYS:HB2	2.26	0.50
3:D:1460:LEU:CD1	3:D:1471:ARG:NH1	2.75	0.50
3:D:637:LEU:O	3:D:638:LYS:C	2.49	0.50
1:B:133:GLU:O	1:B:135:GLY:N	2.39	0.50
2:C:1088:LEU:HD11	3:D:614:PHE:CE2	2.47	0.50
2:C:323:ASP:O	2:C:325:ILE:N	2.45	0.50
2:C:66:LEU:HD23	2:C:355:VAL:CG2	2.38	0.50
2:C:356:ARG:O	2:C:359:MET:HB2	2.11	0.50
1:A:77:GLU:OE2	2:C:640:ARG:NH1	2.45	0.50
2:C:603:VAL:HG13	2:C:646:GLY:O	2.12	0.50
2:C:754:ILE:HD13	2:C:791:ARG:HG2	1.92	0.50
2:C:863:ASP:OD2	2:C:863:ASP:C	2.48	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1043:ARG:O	3:D:1043:ARG:HG3	2.12	0.50
3:D:1066:LEU:C	3:D:1068:VAL:N	2.65	0.50
3:D:1145:LEU:N	3:D:1145:LEU:HD23	2.26	0.50
3:D:1381:GLU:CG	3:D:1392:GLU:HG3	2.41	0.50
3:D:494:LYS:O	3:D:495:ARG:C	2.50	0.50
1:A:142:ARG:HE	1:A:158:LYS:CE	2.24	0.50
1:A:142:ARG:CZ	1:A:144:ASP:OD1	2.59	0.50
1:A:194:LEU:CD2	1:A:196:LEU:HD22	2.42	0.50
1:B:193:LYS:O	1:B:194:LEU:O	2.29	0.50
2:C:11:GLU:OE2	2:C:473:ARG:NE	2.44	0.50
2:C:225:ALA:O	2:C:228:ALA:N	2.45	0.50
2:C:257:LEU:HB2	2:C:258:PHE:HD1	1.77	0.50
2:C:317:VAL:N	2:C:318:PRO:HD2	2.27	0.50
2:C:110:GLU:HG3	2:C:370:ALA:HB3	1.94	0.50
2:C:68:PHE:CD2	2:C:98:LEU:HD22	2.47	0.50
2:C:750:LYS:HB2	2:C:751:PRO:CD	2.36	0.50
2:C:77:PRO:HD2	2:C:92:ALA:HA	1.94	0.50
2:C:86:LYS:NZ	2:C:811:PRO:HG2	2.27	0.50
2:C:872:ASN:HD21	2:C:874:LEU:N	2.09	0.50
3:D:1060:SER:OG	3:D:1068:VAL:CG2	2.60	0.50
3:D:1122:PRO:C	3:D:1123:LEU:HD12	2.32	0.50
3:D:1385:PRO:HG3	3:D:1390:LEU:O	2.12	0.50
3:D:702:LEU:HD12	3:D:745:MET:SD	2.52	0.50
3:D:757:ALA:HB2	4:E:61:VAL:HG11	1.93	0.50
3:D:836:VAL:HG11	3:D:858:LEU:CD2	2.41	0.50
3:D:910:SER:HA	3:D:913:ASP:OD2	2.11	0.50
3:D:912:LYS:O	3:D:915:VAL:HB	2.12	0.50
3:D:966:GLU:O	3:D:967:GLU:C	2.48	0.50
4:E:26:ARG:NH2	4:E:30:LEU:HD13	2.26	0.50
1:A:217:LEU:O	1:A:221:LEU:HD23	2.11	0.50
1:A:221:LEU:HD21	1:B:217:LEU:HD23	1.92	0.50
1:A:221:LEU:O	1:A:224:PHE:HD1	1.94	0.50
1:B:100:LEU:HD12	1:B:112:ASP:C	2.32	0.50
1:B:173:VAL:HG12	1:B:200:THR:HG22	1.94	0.50
1:B:94:TRP:CD1	1:B:96:THR:HG23	2.47	0.50
1:B:97:THR:HG22	1:B:98:LEU:N	2.25	0.50
2:C:831:ARG:NH1	2:C:1002:GLU:HB2	2.22	0.50
2:C:64:LEU:N	2:C:101:ILE:O	2.41	0.50
2:C:487:THR:O	2:C:489:SER:N	2.45	0.50
2:C:570:PRO:HG3	2:C:635:THR:HG23	1.93	0.50
1:A:72:LYS:HB2	2:C:607:ASP:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:877:PRO:O	2:C:878:SER:C	2.50	0.50
3:D:1156:ALA:C	3:D:1158:GLY:H	2.15	0.50
3:D:1212:MET:HE2	4:E:16:LYS:HD2	1.94	0.50
3:D:566:ILE:O	3:D:566:ILE:CG2	2.60	0.50
3:D:674:ARG:NH1	3:D:678:GLU:HG3	2.27	0.50
3:D:703:ASN:CG	3:D:704:ARG:N	2.65	0.50
3:D:739:ASP:OD1	3:D:743:ASP:OD2	2.30	0.50
3:D:795:VAL:CA	3:D:862:ASP:CB	2.88	0.50
4:E:15:SER:O	4:E:18:ARG:N	2.45	0.50
4:E:26:ARG:NE	4:E:67:GLU:OE2	2.44	0.50
4:E:61:VAL:HA	4:E:64:ALA:HB3	1.94	0.50
1:A:102:ALA:HB3	1:A:131:LEU:HD21	1.93	0.50
1:A:89:PHE:HB2	1:A:145:ARG:NH2	2.26	0.50
2:C:1095:LEU:HD11	3:D:582:ILE:HG23	1.93	0.50
2:C:563:ASN:O	2:C:565:GLN:N	2.45	0.50
3:D:1157:LEU:O	3:D:1157:LEU:CD2	2.57	0.50
3:D:117:ASP:C	3:D:119:PHE:N	2.66	0.50
3:D:126:VAL:N	3:D:456:MET:HE2	2.26	0.50
3:D:897:GLN:OE1	3:D:902:MET:HG2	2.12	0.50
2:C:399:ASN:CB	2:C:568:ALA:HB3	2.42	0.49
2:C:566:THR:C	2:C:568:ALA:H	2.15	0.49
2:C:589:ARG:NH2	2:C:654:LEU:HD12	2.27	0.49
2:C:603:VAL:HG11	2:C:646:GLY:H	1.77	0.49
2:C:707:ARG:HB3	2:C:826:PHE:CD1	2.46	0.49
3:D:995:GLN:O	3:D:999:GLU:HG3	2.12	0.49
1:A:166:VAL:CG1	1:A:167:ASP:N	2.72	0.49
1:A:194:LEU:O	1:A:195:THR:CB	2.59	0.49
1:A:91:ASP:OD1	1:A:92:PRO:N	2.45	0.49
1:B:108:VAL:O	1:B:127:HIS:O	2.30	0.49
1:B:146:GLY:HA3	1:B:170:PHE:CE1	2.47	0.49
1:B:41:ARG:HD3	1:B:41:ARG:C	2.32	0.49
2:C:1030:GLN:OE1	3:D:628:ARG:CG	2.58	0.49
2:C:1030:GLN:NE2	2:C:1031:ARG:H	2.10	0.49
2:C:1043:TYR:HE2	3:D:763:MET:HA	1.76	0.49
2:C:91:GLN:HA	2:C:119:PRO:HA	1.94	0.49
2:C:12:VAL:CG1	2:C:13:ILE:N	2.53	0.49
2:C:493:ARG:HH22	3:D:1070:GLU:CD	2.16	0.49
2:C:598:GLU:HG3	2:C:614:ARG:CZ	2.42	0.49
2:C:755:LEU:O	2:C:755:LEU:HD13	2.12	0.49
2:C:910:THR:C	2:C:912:PRO:HD2	2.33	0.49
3:D:1196:GLN:O	3:D:1197:THR:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:461:ILE:HA	3:D:464:LEU:HD12	1.94	0.49
3:D:921:ARG:O	3:D:922:LEU:HD23	2.12	0.49
4:E:45:ARG:O	4:E:47:LYS:HG3	2.12	0.49
4:E:26:ARG:NH2	4:E:67:GLU:OE2	2.45	0.49
4:E:68:LEU:C	4:E:70:THR:H	2.15	0.49
1:A:56:VAL:CG2	1:A:164:ILE:HD11	2.43	0.49
1:A:221:LEU:HD12	1:B:214:VAL:HG13	1.94	0.49
1:A:85:LEU:O	1:A:85:LEU:HD23	2.11	0.49
1:B:25:LEU:CD1	1:B:28:LEU:CD1	2.90	0.49
1:B:73:GLU:OE1	1:B:127:HIS:NE2	2.45	0.49
2:C:115:LEU:HA	2:C:375:SER:OG	2.12	0.49
2:C:224:GLU:C	2:C:226:VAL:N	2.65	0.49
2:C:243:ARG:HG3	2:C:244:PRO:CA	2.42	0.49
2:C:342:ASP:HA	2:C:345:ARG:HB2	1.93	0.49
2:C:699:PHE:O	2:C:701:THR:N	2.45	0.49
2:C:875:GLY:O	2:C:876:VAL:C	2.49	0.49
2:C:540:PHE:CZ	2:C:906:PHE:HE1	2.31	0.49
3:D:1276:SER:OG	3:D:1295:VAL:HG11	2.11	0.49
3:D:1404:LEU:HD21	3:D:1416:VAL:H	1.77	0.49
3:D:492:ALA:O	3:D:495:ARG:HB2	2.12	0.49
3:D:558:LEU:C	3:D:560:GLN:N	2.66	0.49
1:A:166:VAL:CG1	1:A:167:ASP:H	2.25	0.49
1:A:196:LEU:N	1:A:196:LEU:CD2	2.75	0.49
1:A:19:HIS:ND1	1:A:19:HIS:C	2.65	0.49
1:A:220:HIS:O	1:A:221:LEU:C	2.50	0.49
1:A:30:ARG:NH1	1:A:191:LEU:HD22	2.28	0.49
1:B:14:THR:HB	1:B:22:GLU:H	1.76	0.49
1:B:58:ILE:HG12	1:B:139:MET:HB3	1.95	0.49
2:C:1051:GLU:HG2	2:C:1056:LYS:HE2	1.93	0.49
2:C:134:ARG:HH22	2:C:392:SER:C	2.14	0.49
2:C:207:LEU:HG	2:C:208:VAL:N	2.27	0.49
2:C:253:ALA:HA	2:C:256:TYR:CG	2.46	0.49
2:C:323:ASP:C	2:C:325:ILE:H	2.13	0.49
2:C:504:GLU:O	2:C:506:ASP:N	2.44	0.49
2:C:629:ALA:C	2:C:630:ARG:HD3	2.33	0.49
2:C:988:VAL:HG12	3:D:948:ILE:CG1	2.42	0.49
2:C:66:LEU:HD11	2:C:98:LEU:CB	2.43	0.49
3:D:1070:GLU:O	3:D:1073:ILE:N	2.46	0.49
1:B:187:GLN:HE22	3:D:646:LYS:NZ	2.11	0.49
3:D:669:ASN:OD1	3:D:670:VAL:N	2.45	0.49
4:E:67:GLU:O	4:E:70:THR:HB	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:PRO:O	1:A:125:ASP:C	2.51	0.49
1:A:206:PRO:O	1:A:207:LEU:C	2.50	0.49
2:C:1030:GLN:NE2	3:D:628:ARG:HD3	2.28	0.49
2:C:195:LEU:CD1	2:C:227:LEU:HD22	2.35	0.49
2:C:252:LYS:HZ3	2:C:293:PHE:HA	1.78	0.49
2:C:320:HIS:C	2:C:322:VAL:H	2.14	0.49
2:C:443:THR:H	2:C:444:PRO:HD2	1.77	0.49
2:C:15:LEU:HD11	2:C:461:VAL:HG11	1.93	0.49
2:C:439:CYS:SG	2:C:468:ARG:NH2	2.82	0.49
2:C:628:TYR:N	2:C:628:TYR:HD1	2.10	0.49
2:C:77:PRO:CD	2:C:93:PRO:HD3	2.32	0.49
3:D:1485:THR:O	3:D:1487:VAL:HG23	2.11	0.49
3:D:700:VAL:HG13	3:D:748:HIS:O	2.12	0.49
3:D:792:ILE:CG2	3:D:793:THR:HG23	2.42	0.49
1:B:36:LEU:O	1:B:40:LEU:HD23	2.13	0.49
1:B:58:ILE:HG12	1:B:139:MET:CB	2.43	0.49
2:C:134:ARG:HB3	2:C:134:ARG:NH1	2.28	0.49
2:C:215:GLY:O	2:C:216:ASP:O	2.31	0.49
2:C:642:ARG:N	2:C:656:ALA:HA	2.27	0.49
3:D:1435:TRP:CD1	3:D:1448:LEU:HD12	2.48	0.49
3:D:615:ARG:O	3:D:618:LEU:HB2	2.13	0.49
3:D:675:ARG:CA	3:D:678:GLU:HB3	2.37	0.49
3:D:810:GLU:C	3:D:812:ALA:N	2.65	0.49
3:D:94:GLU:O	3:D:95:LEU:C	2.51	0.49
1:A:142:ARG:HG2	1:A:144:ASP:OD1	2.12	0.49
1:A:174:ARG:HB2	1:A:200:THR:HB	1.93	0.49
1:B:62:LEU:O	1:B:63:HIS:C	2.50	0.49
2:C:291:VAL:HG11	2:C:299:LYS:HE3	1.94	0.49
2:C:673:LEU:HA	2:C:991:GLN:HA	1.95	0.49
2:C:729:LEU:O	2:C:729:LEU:HG	2.13	0.49
3:D:1458:ASP:O	3:D:1460:LEU:N	2.46	0.49
3:D:970:ARG:NH2	3:D:971:LYS:HE3	2.28	0.49
1:B:121:ILE:HG22	1:B:121:ILE:O	2.12	0.49
1:B:63:HIS:HB3	1:B:65:PHE:CE2	2.47	0.49
1:B:86:VAL:H	1:B:123:ASN:CG	2.16	0.49
2:C:1068:GLN:HG3	2:C:1072:LYS:HE3	1.94	0.49
2:C:115:LEU:CG	2:C:116:GLY:H	2.25	0.49
2:C:25:SER:HA	2:C:28:LYS:HE2	1.95	0.49
2:C:31:GLN:HG2	2:C:39:ARG:HD2	1.95	0.49
2:C:604:VAL:HG11	2:C:619:ARG:HH22	1.77	0.49
3:D:1015:ASN:C	3:D:1016:TYR:CG	2.83	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:483:HIS:CB	3:D:493:ARG:HH21	2.25	0.49
3:D:537:THR:HG22	3:D:537:THR:O	2.12	0.49
3:D:894:LYS:O	3:D:895:VAL:C	2.49	0.49
1:A:103:GLU:H	1:A:106:LYS:HE2	1.78	0.49
1:A:160:ARG:O	1:A:161:ILE:HB	2.13	0.49
1:A:38:ASN:HD21	1:A:41:ARG:HH22	1.61	0.49
1:A:98:LEU:C	1:A:99:ILE:HG13	2.33	0.49
1:B:30:ARG:NH1	2:C:854:PRO:HB3	2.28	0.49
1:B:81:ASN:HD21	1:B:127:HIS:HB3	1.77	0.49
2:C:1015:LEU:O	2:C:1016:ILE:HD13	2.13	0.49
2:C:253:ALA:HA	2:C:256:TYR:CD1	2.47	0.49
2:C:270:GLY:O	2:C:271:GLU:O	2.31	0.49
2:C:159:ILE:CD1	2:C:310:LEU:HD22	2.28	0.49
2:C:333:ILE:HD12	2:C:468:ARG:HE	1.74	0.49
2:C:728:HIS:O	2:C:730:SER:N	2.45	0.49
2:C:79:SER:N	2:C:82:GLU:OE1	2.43	0.49
3:D:1008:VAL:HG21	3:D:1040:CYS:CB	2.42	0.49
3:D:1009:PHE:CE1	3:D:1036:ILE:HG13	2.43	0.49
3:D:1200:GLY:O	3:D:1202:CYS:N	2.36	0.49
3:D:1271:ALA:HB1	3:D:1327:THR:CB	2.43	0.49
3:D:1424:GLY:O	3:D:1426:THR:N	2.39	0.49
3:D:476:GLU:O	3:D:480:GLU:HB2	2.13	0.49
3:D:636:GLN:NE2	3:D:642:CYS:HA	2.28	0.49
3:D:670:VAL:O	3:D:673:ALA:HB3	2.13	0.49
1:A:132:GLU:O	2:C:606:VAL:HG23	2.13	0.49
1:A:55:SER:HB2	1:A:156:GLY:HA3	1.94	0.49
1:B:180:VAL:O	1:B:180:VAL:HG13	2.13	0.49
1:B:34:VAL:O	1:B:36:LEU:N	2.42	0.49
2:C:274:ARG:HG3	2:C:275:TYR:H	1.77	0.49
2:C:259:GLY:HA2	2:C:289:THR:O	2.13	0.49
2:C:491:GLU:HA	2:C:531:PHE:CA	2.36	0.49
2:C:549:PHE:HD2	2:C:552:HIS:CD2	2.31	0.49
2:C:693:GLU:OE1	2:C:696:LYS:HD2	2.12	0.49
2:C:948:GLU:O	2:C:951:GLY:N	2.46	0.49
2:C:946:ARG:HH12	2:C:984:GLU:C	2.17	0.49
3:D:997:TRP:CD1	3:D:1057:PRO:HD3	2.48	0.49
3:D:1305:LYS:H	3:D:1305:LYS:CD	2.23	0.49
3:D:1263:LEU:CD2	3:D:1353:ILE:HA	2.43	0.49
3:D:1381:GLU:HG2	3:D:1392:GLU:HA	1.95	0.49
3:D:603:LEU:HA	3:D:606:ILE:HD13	1.94	0.49
3:D:691:LEU:HA	3:D:694:VAL:CB	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:VAL:O	1:A:218:LYS:HG3	2.13	0.48
1:B:70:GLY:O	1:B:71:VAL:HG23	2.13	0.48
2:C:11:GLU:OE1	2:C:479:VAL:HG12	2.13	0.48
2:C:32:ALA:O	2:C:34:VAL:N	2.46	0.48
2:C:601:GLY:O	2:C:602:GLU:CB	2.60	0.48
2:C:636:ALA:CB	2:C:703:ILE:O	2.61	0.48
3:D:1044:GLY:HA2	3:D:1058:VAL:N	2.28	0.48
3:D:952:ILE:HG12	3:D:1063:ARG:NH2	2.27	0.48
3:D:1104:HIS:N	3:D:1223:GLY:HA3	2.28	0.48
3:D:1273:ALA:O	3:D:1331:ILE:CB	2.61	0.48
3:D:680:GLN:O	3:D:681:ARG:HG3	2.12	0.48
3:D:70:GLY:C	3:D:72:VAL:H	2.16	0.48
3:D:995:GLN:HA	3:D:998:THR:HB	1.95	0.48
2:C:1060:ILE:CG2	2:C:1064:ASN:HD21	2.12	0.48
2:C:140:ILE:HG22	2:C:333:ILE:CG1	2.32	0.48
2:C:182:VAL:HG12	2:C:193:LEU:HG	1.95	0.48
2:C:198:ARG:HG3	2:C:228:ALA:HA	1.95	0.48
2:C:379:GLU:O	2:C:381:ALA:N	2.46	0.48
2:C:397:GLU:N	2:C:633:GLN:NE2	2.53	0.48
2:C:976:ASP:C	2:C:978:ARG:H	2.16	0.48
3:D:1104:HIS:H	3:D:1223:GLY:CA	2.26	0.48
3:D:1104:HIS:CG	3:D:1105:GLU:N	2.81	0.48
3:D:1126:MET:HG2	3:D:1127:ASP:N	2.15	0.48
3:D:722:GLU:HB3	3:D:723:GLY:H	1.44	0.48
3:D:806:PHE:HA	3:D:827:ILE:O	2.12	0.48
3:D:900:ILE:HG22	3:D:901:GLN:N	2.27	0.48
3:D:923:GLY:O	3:D:926:LYS:HB2	2.13	0.48
4:E:68:LEU:HD12	4:E:73:LEU:HD12	1.95	0.48
2:C:461:VAL:O	2:C:461:VAL:HG12	2.13	0.48
2:C:50:GLU:O	2:C:52:PHE:N	2.45	0.48
2:C:600:ASP:CA	2:C:648:ARG:HD2	2.44	0.48
2:C:679:PHE:O	2:C:681:GLY:N	2.46	0.48
2:C:774:LEU:O	2:C:777:ILE:HB	2.14	0.48
3:D:1124:PHE:HE2	3:D:1185:ARG:HA	1.77	0.48
3:D:1253:ILE:C	3:D:1255:GLN:N	2.65	0.48
3:D:1348:TYR:CZ	3:D:1352:GLU:HG2	2.48	0.48
3:D:88:TYR:O	3:D:520:LEU:HD13	2.13	0.48
3:D:564:GLU:O	3:D:568:ARG:HG2	2.13	0.48
3:D:643:GLY:HA3	3:D:727:GLN:N	2.25	0.48
1:A:222:ASN:C	1:A:224:PHE:N	2.67	0.48
2:C:95:TYR:HB3	2:C:114:PHE:HA	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:479:VAL:O	2:C:480:THR:HG22	2.13	0.48
2:C:568:ALA:HB2	2:C:668:LEU:HD22	1.94	0.48
2:C:728:HIS:C	2:C:730:SER:N	2.65	0.48
2:C:854:PRO:O	2:C:855:VAL:C	2.51	0.48
3:D:1012:PHE:O	3:D:1013:GLU:C	2.52	0.48
3:D:123:LEU:O	3:D:124:GLU:C	2.51	0.48
3:D:1357:TYR:HB3	3:D:1362:VAL:HB	1.96	0.48
3:D:149:LYS:O	3:D:150:ARG:C	2.51	0.48
3:D:765:SER:HB2	3:D:769:LEU:HD12	1.96	0.48
3:D:924:MET:O	3:D:925:GLU:C	2.51	0.48
4:E:18:ARG:O	4:E:21:VAL:HB	2.13	0.48
3:D:1484:PHE:CD1	4:E:75:PHE:HB2	2.49	0.48
1:A:30:ARG:CZ	1:A:190:ASP:HB3	2.43	0.48
1:A:6:LEU:O	1:A:7:LYS:HB2	2.13	0.48
1:B:173:VAL:HG12	1:B:200:THR:HG21	1.94	0.48
1:B:88:ARG:HB3	1:B:122:MET:HE1	1.95	0.48
2:C:100:LEU:O	2:C:101:ILE:HD13	2.13	0.48
2:C:389:SER:O	2:C:391:LEU:N	2.47	0.48
2:C:580:MET:CB	2:C:584:GLU:HG3	2.25	0.48
3:D:958:PRO:HD3	3:D:1008:VAL:HG23	1.96	0.48
3:D:1024:MET:SD	3:D:1024:MET:N	2.86	0.48
3:D:1104:HIS:H	3:D:1223:GLY:HA3	1.78	0.48
3:D:1222:VAL:O	3:D:1226:ALA:N	2.46	0.48
3:D:1084:ASP:OD2	3:D:1238:THR:HG23	2.13	0.48
3:D:777:PRO:CG	3:D:912:LYS:HG3	2.43	0.48
3:D:935:LYS:HG2	3:D:939:PHE:CD1	2.48	0.48
4:E:54:LEU:O	4:E:55:TYR:CB	2.60	0.48
4:E:23:VAL:HG12	4:E:61:VAL:HG12	1.95	0.48
1:A:175:ARG:HB3	1:A:199:TRP:HB3	1.95	0.48
1:A:217:LEU:HD23	1:B:221:LEU:HD11	1.96	0.48
1:B:64:GLU:HA	1:B:75:VAL:HG11	1.95	0.48
2:C:195:LEU:CB	2:C:227:LEU:HD13	2.28	0.48
2:C:335:THR:O	2:C:336:VAL:C	2.52	0.48
2:C:346:VAL:O	2:C:347:GLY:C	2.52	0.48
2:C:400:PRO:O	2:C:401:LEU:C	2.51	0.48
2:C:399:ASN:HD21	2:C:401:LEU:N	2.09	0.48
2:C:733:ALA:O	2:C:734:LEU:C	2.51	0.48
3:D:1079:ARG:O	3:D:1080:LYS:C	2.51	0.48
3:D:1156:ALA:C	3:D:1158:GLY:N	2.66	0.48
3:D:1257:LEU:O	3:D:1259:ARG:N	2.45	0.48
3:D:1344:ALA:O	3:D:1345:VAL:C	2.51	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:ILE:CD1	1:A:162:ASN:HD21	2.25	0.48
1:B:33:GLY:HA3	1:B:180:VAL:HG21	1.96	0.48
2:C:145:GLY:O	2:C:146:VAL:HG23	2.12	0.48
2:C:324:ASP:O	2:C:326:ASP:N	2.46	0.48
2:C:139:GLN:NE2	2:C:334:ARG:NH2	2.62	0.48
2:C:501:THR:HG23	2:C:524:VAL:CB	2.44	0.48
2:C:641:PRO:HA	2:C:656:ALA:CB	2.43	0.48
2:C:710:ILE:CG1	2:C:790:LEU:HD13	2.43	0.48
2:C:86:LYS:O	2:C:88:LEU:HG	2.14	0.48
2:C:963:LEU:O	2:C:965:GLU:N	2.47	0.48
3:D:1157:LEU:H	3:D:1183:GLU:CD	2.17	0.48
3:D:1422:LEU:HD23	3:D:1422:LEU:C	2.34	0.48
3:D:571:LYS:C	3:D:573:MET:N	2.66	0.48
3:D:656:PHE:CD2	3:D:698:LYS:NZ	2.82	0.48
3:D:1484:PHE:HE1	4:E:22:VAL:CG2	2.27	0.48
4:E:81:PRO:O	4:E:85:LEU:N	2.47	0.48
2:C:1042:ALA:HB2	3:D:1228:GLU:OE1	2.13	0.48
2:C:148:PHE:N	2:C:148:PHE:CD1	2.81	0.48
2:C:290:LEU:HD12	2:C:300:ASP:CA	2.43	0.48
2:C:327:HIS:O	2:C:330:ASN:N	2.47	0.48
2:C:38:LYS:O	2:C:39:ARG:O	2.32	0.48
2:C:466:PHE:HD1	2:C:466:PHE:C	2.17	0.48
2:C:596:TYR:O	2:C:655:LEU:HD13	2.13	0.48
2:C:575:GLN:O	2:C:667:ALA:HB1	2.13	0.48
2:C:840:ALA:HB3	2:C:997:LEU:HD11	1.96	0.48
3:D:1133:LEU:HD13	3:D:1185:ARG:HH12	1.78	0.48
3:D:1152:ARG:O	3:D:1153:GLU:C	2.51	0.48
3:D:545:ARG:CG	3:D:546:ARG:N	2.77	0.48
2:C:970:GLY:HA2	3:D:950:ILE:CG2	2.43	0.48
3:D:969:ASP:O	3:D:971:LYS:N	2.47	0.48
1:A:161:ILE:CG2	1:A:162:ASN:H	2.24	0.48
1:B:23:PHE:HD1	1:B:210:LEU:HD22	1.77	0.48
2:C:423:ALA:CA	2:C:427:VAL:HG21	2.44	0.48
2:C:6:PHE:HD1	2:C:902:ILE:O	1.97	0.48
2:C:736:ASP:O	2:C:737:LEU:HG	2.14	0.48
2:C:768:SER:O	2:C:769:PRO:O	2.32	0.48
2:C:876:VAL:HB	2:C:877:PRO:HD3	1.95	0.48
3:D:1330:ALA:O	3:D:1331:ILE:C	2.51	0.48
3:D:462:GLN:HA	3:D:512:MET:SD	2.54	0.48
2:C:750:LYS:HG3	3:D:680:GLN:NE2	2.29	0.48
3:D:698:LYS:O	3:D:718:PRO:HD2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:936:TYR:O	3:D:940:THR:HG22	2.13	0.48
3:D:979:TYR:CG	3:D:989:ARG:HD2	2.49	0.48
1:A:126:LEU:CG	1:A:126:LEU:O	2.61	0.48
1:A:76:VAL:O	1:A:77:GLU:C	2.52	0.48
1:A:221:LEU:HD21	1:B:217:LEU:CD2	2.43	0.48
1:B:58:ILE:HG22	1:B:58:ILE:O	2.14	0.48
1:B:71:VAL:HA	1:B:131:LEU:HA	1.95	0.48
2:C:149:THR:CG2	2:C:150:PRO:HD2	2.44	0.48
2:C:223:ASP:C	2:C:225:ALA:H	2.18	0.48
2:C:48:PHE:O	2:C:49:LYS:C	2.51	0.48
2:C:588:VAL:HG21	2:C:666:LEU:HA	1.96	0.48
3:D:1212:MET:CE	4:E:16:LYS:HD2	2.43	0.48
3:D:1328:ARG:O	3:D:1330:ALA:N	2.47	0.48
3:D:1336:LEU:C	3:D:1336:LEU:HD23	2.33	0.48
3:D:1426:THR:C	3:D:1428:SER:N	2.67	0.48
3:D:973:ARG:C	3:D:975:ILE:H	2.17	0.48
4:E:91:ARG:HB3	4:E:92:LEU:CD1	2.43	0.48
1:A:142:ARG:HE	1:A:158:LYS:HE2	1.79	0.47
1:A:187:GLN:O	1:A:188:ARG:CB	2.62	0.47
1:A:206:PRO:O	1:A:209:ALA:N	2.46	0.47
1:A:34:VAL:C	1:A:36:LEU:N	2.67	0.47
1:A:38:ASN:O	1:A:39:PRO:C	2.52	0.47
1:B:111:VAL:O	1:B:113:PHE:N	2.47	0.47
2:C:1072:LYS:O	3:D:659:LYS:HG3	2.14	0.47
2:C:1095:LEU:CD1	3:D:603:LEU:HD23	2.45	0.47
2:C:394:PHE:CD2	2:C:632:ASN:HB3	2.48	0.47
2:C:57:GLY:H	2:C:356:ARG:HH12	1.60	0.47
2:C:605:LYS:HD3	2:C:607:ASP:HA	1.95	0.47
2:C:693:GLU:OE1	2:C:693:GLU:HA	2.14	0.47
2:C:754:ILE:HD13	2:C:791:ARG:NE	2.29	0.47
2:C:915:LYS:O	2:C:918:LEU:N	2.47	0.47
3:D:997:TRP:CE3	3:D:1000:THR:HG21	2.48	0.47
3:D:1019:ASN:HB2	3:D:1020:PRO:HD3	1.96	0.47
3:D:1060:SER:CB	3:D:1066:LEU:HA	2.43	0.47
3:D:1062:PHE:CD1	3:D:1066:LEU:HD23	2.49	0.47
3:D:1167:LEU:HB2	3:D:1171:ASP:HB3	1.95	0.47
3:D:1329:GLY:O	3:D:1331:ILE:N	2.47	0.47
3:D:485:SER:OG	3:D:488:ARG:HD2	2.13	0.47
2:C:172:ILE:HD13	2:C:303:PHE:CZ	2.49	0.47
3:D:1230:ILE:HG22	3:D:1357:TYR:OH	2.13	0.47
3:D:1479:SER:O	3:D:1482:VAL:N	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:480:GLU:O	3:D:493:ARG:NH2	2.46	0.47
1:B:181:GLU:O	1:B:193:LYS:HB3	2.14	0.47
2:C:238:LEU:O	2:C:241:LEU:N	2.47	0.47
2:C:55:GLU:OE1	2:C:55:GLU:N	2.43	0.47
2:C:688:ILE:HG23	2:C:871:LEU:HD12	1.96	0.47
2:C:728:HIS:NE2	2:C:783:ARG:NH1	2.63	0.47
2:C:805:ARG:NH2	2:C:821:GLU:OE2	2.48	0.47
2:C:1042:ALA:HB1	3:D:1225:VAL:HG22	1.94	0.47
3:D:1315:LYS:O	3:D:1316:ASP:C	2.52	0.47
3:D:1431:SER:O	3:D:1432:THR:HB	2.15	0.47
3:D:1485:THR:HG21	4:E:79:LEU:HB2	1.96	0.47
3:D:653:PHE:O	3:D:656:PHE:N	2.48	0.47
3:D:760:ARG:O	3:D:761:ILE:HG13	2.15	0.47
3:D:901:GLN:O	3:D:905:PRO:HD3	2.14	0.47
3:D:925:GLU:OE1	4:E:7:ASP:OD2	2.32	0.47
1:A:222:ASN:O	1:A:223:TYR:C	2.53	0.47
1:B:144:ASP:CG	1:B:145:ARG:H	2.18	0.47
1:B:14:THR:O	1:B:15:THR:O	2.32	0.47
2:C:1018:GLN:HA	2:C:1018:GLN:OE1	2.13	0.47
2:C:177:GLU:CG	2:C:181:VAL:H	2.23	0.47
2:C:378:LEU:O	2:C:382:LEU:HB3	2.14	0.47
2:C:379:GLU:O	2:C:380:ALA:C	2.51	0.47
2:C:489:SER:O	2:C:490:GLU:CB	2.61	0.47
2:C:685:GLU:OE1	2:C:685:GLU:HA	2.13	0.47
2:C:882:LEU:CD1	2:C:884:GLN:HE21	2.27	0.47
2:C:963:LEU:O	2:C:964:LYS:C	2.52	0.47
3:D:1043:ARG:NH2	3:D:1062:PHE:CZ	2.82	0.47
2:C:1005:MET:HB2	3:D:629:SER:CB	2.44	0.47
3:D:704:ARG:HH11	3:D:704:ARG:CG	2.27	0.47
3:D:88:TYR:O	3:D:89:ARG:CB	2.61	0.47
1:A:102:ALA:HA	1:A:106:LYS:HZ1	1.79	0.47
1:A:127:HIS:CE1	1:A:130:THR:OG1	2.68	0.47
1:A:11:PHE:CD1	1:A:25:LEU:HD23	2.49	0.47
1:B:187:GLN:HG2	3:D:688:TRP:HD1	1.80	0.47
1:B:62:LEU:HB2	1:B:63:HIS:H	1.51	0.47
2:C:165:LEU:HD22	2:C:334:ARG:CD	2.42	0.47
2:C:26:TYR:HB2	2:C:121:MET:HE1	1.95	0.47
2:C:369:PRO:O	2:C:370:ALA:HB3	2.15	0.47
2:C:420:ARG:N	2:C:420:ARG:HD3	2.25	0.47
2:C:514:VAL:C	2:C:516:ARG:H	2.17	0.47
2:C:589:ARG:NH2	2:C:654:LEU:HA	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:713:ARG:HB2	2:C:720:GLU:OE1	2.14	0.47
2:C:768:SER:CB	2:C:769:PRO:HD2	2.34	0.47
2:C:876:VAL:HA	2:C:880:MET:SD	2.54	0.47
2:C:912:PRO:O	2:C:916:GLU:N	2.41	0.47
3:D:10:ILE:HG23	3:D:11:ALA:N	2.28	0.47
3:D:1484:PHE:CE1	4:E:75:PHE:HB2	2.50	0.47
3:D:121:THR:CB	3:D:461:ILE:HD11	2.45	0.47
3:D:551:ASN:HD22	3:D:574:LEU:HD13	1.79	0.47
2:C:1043:TYR:CE1	3:D:710:ARG:HB2	2.50	0.47
3:D:901:GLN:O	3:D:903:ASP:N	2.48	0.47
3:D:988:GLU:O	3:D:992:GLN:HB2	2.14	0.47
4:E:40:LEU:C	4:E:42:PRO:HD2	2.34	0.47
4:E:86:GLN:O	4:E:89:MET:HB2	2.13	0.47
1:A:83:LYS:HZ2	2:C:698:ASP:HB2	1.80	0.47
1:B:78:ILE:HG13	1:B:128:ILE:O	2.15	0.47
1:B:206:PRO:O	1:B:209:ALA:HB3	2.15	0.47
2:C:324:ASP:C	2:C:326:ASP:N	2.66	0.47
2:C:437:ARG:O	2:C:437:ARG:HG3	2.15	0.47
2:C:520:GLU:N	2:C:521:PRO:CD	2.77	0.47
2:C:650:LYS:O	2:C:651:LYS:CB	2.62	0.47
2:C:642:ARG:HB3	2:C:656:ALA:HA	1.96	0.47
2:C:713:ARG:CZ	2:C:819:VAL:HG22	2.45	0.47
2:C:762:LYS:HD2	2:C:786:LYS:CD	2.36	0.47
2:C:549:PHE:CE1	2:C:886:LEU:O	2.68	0.47
2:C:926:PHE:HE1	2:C:929:ARG:NH1	2.13	0.47
3:D:1200:GLY:C	3:D:1202:CYS:H	2.15	0.47
3:D:580:ALA:O	3:D:584:ASN:HB2	2.15	0.47
3:D:683:ILE:HG22	3:D:687:VAL:HB	1.96	0.47
1:B:187:GLN:CG	3:D:688:TRP:HD1	2.27	0.47
3:D:836:VAL:HG21	3:D:858:LEU:HD21	1.95	0.47
3:D:962:GLN:O	3:D:965:LEU:O	2.33	0.47
4:E:14:ASP:CG	4:E:15:SER:N	2.67	0.47
1:A:18:ASP:HA	1:A:205:THR:OG1	2.15	0.47
1:B:78:ILE:O	1:B:82:LEU:N	2.48	0.47
2:C:308:ARG:C	2:C:310:LEU:N	2.68	0.47
2:C:387:SER:O	2:C:388:ARG:HG3	2.14	0.47
2:C:581:THR:O	2:C:583:LEU:N	2.48	0.47
2:C:605:LYS:CE	2:C:611:ILE:HG13	2.45	0.47
2:C:683:ASN:ND2	2:C:870:ILE:O	2.39	0.47
2:C:845:ASN:ND2	2:C:876:VAL:HG11	2.30	0.47
2:C:1038:TRP:NE1	3:D:1100:VAL:HG11	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1379:TYR:O	3:D:1421:LEU:HB3	2.15	0.47
3:D:1460:LEU:HD13	3:D:1471:ARG:HD3	1.97	0.47
2:C:1046:ALA:CB	3:D:1473:ILE:HB	2.44	0.47
3:D:24(U):UNK:O	3:D:41(U):UNK:HA	2.15	0.47
3:D:630:VAL:O	3:D:725:SER:CA	2.59	0.47
3:D:657:LEU:HD11	3:D:690:ALA:HB1	1.96	0.47
3:D:810:GLU:O	3:D:812:ALA:N	2.48	0.47
3:D:947:ILE:O	3:D:947:ILE:CG1	2.63	0.47
2:C:969:LEU:HD12	3:D:950:ILE:CG2	2.45	0.47
1:B:31:GLY:H	1:B:192:ASP:CG	2.17	0.47
2:C:1113:GLU:C	2:C:1115:LEU:N	2.64	0.47
2:C:148:PHE:CD2	2:C:159:ILE:HG23	2.49	0.47
2:C:181:VAL:HG21	2:C:220:GLY:HA3	1.96	0.47
2:C:257:LEU:HD22	2:C:264:PRO:CD	2.38	0.47
2:C:332:ARG:HG2	2:C:333:ILE:H	1.79	0.47
2:C:430:VAL:O	2:C:431:HIS:C	2.53	0.47
2:C:572:ILE:HG13	2:C:572:ILE:O	2.14	0.47
2:C:605:LYS:HD2	2:C:607:ASP:OD2	2.14	0.47
2:C:754:ILE:CD1	2:C:791:ARG:NE	2.78	0.47
2:C:852:ILE:CD1	2:C:852:ILE:N	2.78	0.47
3:D:1156:ALA:O	3:D:1158:GLY:N	2.48	0.47
3:D:1214:ARG:HG3	3:D:1215:PRO:HD2	1.96	0.47
3:D:1257:LEU:O	3:D:1258:PRO:C	2.53	0.47
3:D:26:VAL:C	3:D:28:LYS:N	2.68	0.47
1:A:142:ARG:HG2	1:A:142:ARG:NH1	2.30	0.47
1:A:159:ASP:O	1:A:161:ILE:N	2.47	0.47
1:A:6:LEU:C	1:A:8:ALA:N	2.66	0.47
2:C:445:GLU:HB3	2:C:446:GLY:H	1.49	0.47
2:C:602:GLU:O	2:C:603:VAL:HG13	2.14	0.47
2:C:694:LEU:HD22	2:C:699:PHE:CD2	2.50	0.47
2:C:763:GLY:O	2:C:764:GLU:C	2.52	0.47
2:C:773:LEU:O	2:C:777:ILE:HG13	2.15	0.47
2:C:857:ASP:HB3	2:C:978:ARG:HG3	1.97	0.47
2:C:689:VAL:HB	2:C:870:ILE:HB	1.97	0.47
2:C:892:LEU:O	2:C:894:GLY:N	2.42	0.47
2:C:923:ASN:O	2:C:927:GLY:HA3	2.15	0.47
3:D:1214:ARG:HG3	3:D:1215:PRO:CD	2.45	0.47
3:D:1237:LEU:HD11	3:D:1357:TYR:CD2	2.48	0.47
3:D:1340:LYS:O	3:D:1340:LYS:CG	2.63	0.47
3:D:547:LEU:HD13	3:D:577:ALA:C	2.35	0.47
3:D:811:GLU:CA	3:D:814:ALA:HB3	2.36	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:836:VAL:HG11	3:D:858:LEU:HD11	1.95	0.47
3:D:911:LEU:N	3:D:911:LEU:HD22	2.30	0.47
3:D:1484:PHE:CZ	4:E:22:VAL:HG23	2.50	0.47
1:A:100:LEU:HD11	1:A:137:LEU:HD23	1.97	0.47
1:B:154:ARG:O	1:B:155:HIS:CB	2.62	0.47
1:B:159:ASP:OD2	1:B:161:ILE:O	2.33	0.47
1:B:23:PHE:CD1	1:B:210:LEU:HD22	2.50	0.47
2:C:14:PRO:HA	2:C:458:TYR:CE1	2.50	0.47
2:C:397:GLU:HB2	2:C:633:GLN:NE2	2.26	0.47
2:C:642:ARG:CB	2:C:656:ALA:HA	2.45	0.47
2:C:735:ARG:CA	2:C:737:LEU:O	2.58	0.47
2:C:953:VAL:HG11	2:C:962:GLN:HB3	1.96	0.47
3:D:1155:GLU:O	3:D:1156:ALA:HB2	2.15	0.47
3:D:1348:TYR:O	3:D:1352:GLU:CB	2.62	0.47
3:D:810:GLU:O	3:D:810:GLU:HG2	2.14	0.47
3:D:932:ASP:O	3:D:933:ALA:C	2.53	0.47
1:B:89:PHE:HZ	1:B:145:ARG:HE	1.55	0.47
2:C:208:VAL:CG1	2:C:218:VAL:HG21	2.45	0.47
2:C:261:LEU:HD11	2:C:263:ASP:HB2	1.96	0.47
2:C:434:HIS:C	2:C:436:GLY:N	2.68	0.47
2:C:727:PRO:HD2	2:C:759:THR:HG22	1.96	0.47
2:C:71:TYR:HA	2:C:96:ALA:HB2	1.97	0.47
3:D:1012:PHE:CE2	3:D:1023:VAL:HG11	2.50	0.47
2:C:432:ARG:NH1	3:D:1049:PRO:O	2.48	0.47
2:C:428:ARG:NH2	3:D:1086:ALA:O	2.48	0.47
3:D:1276:SER:H	3:D:1323:GLY:CA	2.18	0.47
3:D:1306:LEU:HD21	3:D:1311:ARG:CB	2.45	0.47
3:D:1345:VAL:O	3:D:1346:GLU:C	2.53	0.47
3:D:502:PHE:C	3:D:504:ASP:H	2.19	0.47
3:D:552:ASN:O	3:D:554:LEU:N	2.47	0.47
2:C:796:GLU:CG	3:D:681:ARG:HH12	2.13	0.47
3:D:760:ARG:NH2	4:E:3:GLU:OE2	2.48	0.47
3:D:87:ARG:CB	3:D:522:PRO:HG2	2.45	0.47
3:D:910:SER:O	3:D:911:LEU:C	2.54	0.47
3:D:916:TYR:O	3:D:919:PHE:HB3	2.15	0.47
3:D:997:TRP:HA	3:D:1000:THR:CG2	2.42	0.47
1:A:79:ILE:HD11	1:A:164:ILE:HG13	1.97	0.46
1:B:164:ILE:HG13	1:B:164:ILE:O	2.16	0.46
1:B:22:GLU:HA	1:B:196:LEU:O	2.15	0.46
2:C:1034:GLU:OE2	3:D:1097:ARG:NH1	2.46	0.46
2:C:22:GLN:O	2:C:24:GLU:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:269:LEU:O	2:C:274:ARG:NH2	2.49	0.46
2:C:359:MET:SD	2:C:372:LEU:HD11	2.55	0.46
2:C:378:LEU:O	2:C:382:LEU:CB	2.63	0.46
2:C:582:GLY:O	2:C:585:GLU:HG3	2.15	0.46
2:C:601:GLY:HA3	2:C:648:ARG:N	2.30	0.46
2:C:616:GLU:O	2:C:618:GLY:N	2.47	0.46
2:C:6:PHE:N	2:C:6:PHE:CD1	2.82	0.46
2:C:861:LEU:CD2	2:C:862:PRO:HD2	2.45	0.46
2:C:565:GLN:HB2	2:C:995:MET:SD	2.56	0.46
3:D:1282:VAL:HG13	3:D:1315:LYS:CA	2.36	0.46
3:D:465:LEU:CD2	3:D:509:PRO:HB3	2.41	0.46
3:D:543:LEU:HD21	3:D:600:LEU:HD12	1.98	0.46
3:D:772:PRO:HG3	3:D:778:LEU:HD22	1.97	0.46
3:D:795:VAL:N	3:D:862:ASP:CB	2.78	0.46
3:D:930:LEU:CD1	3:D:934:LEU:HG	2.45	0.46
1:A:89:PHE:HB2	1:A:145:ARG:HH21	1.79	0.46
1:A:79:ILE:HD11	1:A:164:ILE:HD11	1.95	0.46
2:C:1085:PHE:CE1	3:D:1469:LEU:HD22	2.49	0.46
2:C:252:LYS:HZ1	2:C:293:PHE:H	1.64	0.46
2:C:472:ARG:O	2:C:479:VAL:O	2.33	0.46
2:C:472:ARG:O	2:C:480:THR:HG22	2.14	0.46
2:C:881:ASN:ND2	3:D:1035:GLN:CG	2.78	0.46
3:D:546:ARG:HH21	3:D:577:ALA:HA	1.79	0.46
1:A:142:ARG:O	1:A:143:VAL:HG22	2.15	0.46
1:A:25:LEU:HB3	1:A:26:GLU:H	1.59	0.46
2:C:257:LEU:O	2:C:258:PHE:C	2.53	0.46
2:C:356:ARG:HD2	2:C:356:ARG:O	2.16	0.46
2:C:46:ALA:O	2:C:47:ALA:C	2.53	0.46
2:C:63:GLY:O	2:C:64:LEU:HB2	2.16	0.46
2:C:742:ILE:HG12	2:C:756:VAL:HG13	1.97	0.46
2:C:758:ARG:O	2:C:787:ASP:O	2.33	0.46
3:D:1050:SER:O	3:D:1051:GLY:C	2.54	0.46
3:D:477:LEU:CA	3:D:480:GLU:HB3	2.34	0.46
3:D:522:PRO:O	3:D:523:ASP:CB	2.63	0.46
3:D:645:PRO:HG3	3:D:724:GLN:O	2.14	0.46
3:D:710:ARG:C	3:D:712:GLY:H	2.19	0.46
3:D:718:PRO:O	3:D:719:VAL:HG23	2.15	0.46
1:B:110:ALA:CA	1:B:113:PHE:HE1	2.26	0.46
1:B:62:LEU:O	1:B:63:HIS:O	2.34	0.46
2:C:35:PRO:C	2:C:37:GLU:H	2.17	0.46
2:C:390:GLN:CD	2:C:413:LEU:O	2.53	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:420:ARG:CD	2:C:420:ARG:H	2.20	0.46
2:C:423:ALA:C	2:C:427:VAL:HG21	2.35	0.46
2:C:455:LEU:HD12	2:C:455:LEU:O	2.16	0.46
2:C:491:GLU:O	2:C:491:GLU:HG3	2.15	0.46
2:C:814:GLU:HG3	2:C:814:GLU:O	2.15	0.46
2:C:96:ALA:O	2:C:98:LEU:HG	2.16	0.46
3:D:1063:ARG:HD3	3:D:1064:GLU:N	2.30	0.46
3:D:1364:LEU:HG	3:D:1365:HIS:N	2.31	0.46
3:D:673:ALA:O	3:D:676:MET:N	2.48	0.46
3:D:724:GLN:O	3:D:725:SER:O	2.32	0.46
2:C:1051:GLU:OE2	3:D:752:SER:OG	2.30	0.46
4:E:87:LYS:O	4:E:90:GLU:HB3	2.15	0.46
1:B:172:PRO:CB	1:B:204:VAL:HB	2.45	0.46
2:C:1034:GLU:OE1	3:D:1097:ARG:NH1	2.49	0.46
2:C:128:ILE:CD1	2:C:128:ILE:N	2.79	0.46
2:C:262:ALA:HB1	2:C:266:ARG:CD	2.17	0.46
2:C:305:PRO:HB3	2:C:308:ARG:NH2	2.30	0.46
2:C:148:PHE:CE2	2:C:310:LEU:HA	2.50	0.46
2:C:54:ILE:HG12	2:C:355:VAL:CG1	2.45	0.46
2:C:795:GLY:O	2:C:796:GLU:C	2.54	0.46
2:C:833:LEU:C	2:C:834:GLN:HG3	2.35	0.46
2:C:857:ASP:O	2:C:858:MET:HB2	2.15	0.46
2:C:881:ASN:ND2	3:D:1035:GLN:OE1	2.49	0.46
2:C:996:LYS:NZ	2:C:1000:MET:HE3	2.31	0.46
3:D:1108:VAL:HG23	3:D:1222:VAL:HG23	1.97	0.46
3:D:131:LYS:O	3:D:132:TYR:C	2.54	0.46
3:D:21:TRP:O	3:D:23:TYR:N	2.48	0.46
3:D:566:ILE:O	3:D:570:GLU:HG3	2.16	0.46
3:D:590:PRO:HA	3:D:600:LEU:HD21	1.98	0.46
3:D:911:LEU:H	3:D:911:LEU:CD2	2.28	0.46
3:D:950:ILE:HB	3:D:953:ASP:HB3	1.98	0.46
1:A:205:THR:O	1:A:208:GLU:HB2	2.15	0.46
1:B:213:ALA:O	1:B:216:ILE:N	2.49	0.46
2:C:100:LEU:HD21	2:C:368:THR:CA	2.39	0.46
2:C:1080:SER:OG	2:C:1081:VAL:N	2.48	0.46
2:C:291:VAL:CG1	2:C:299:LYS:HE3	2.46	0.46
2:C:440:PRO:HD2	2:C:456:ALA:N	2.31	0.46
2:C:554:ASP:O	2:C:555:ALA:C	2.54	0.46
2:C:726:ILE:HB	2:C:729:LEU:HD23	1.96	0.46
2:C:794:PRO:HG2	2:C:1027:PHE:HB3	1.98	0.46
3:D:1016:TYR:CB	3:D:1019:ASN:HB2	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1084:ASP:O	3:D:1087:LEU:N	2.48	0.46
3:D:1155:GLU:CB	3:D:1160:ARG:HA	2.42	0.46
3:D:485:SER:OG	3:D:488:ARG:HB2	2.16	0.46
3:D:733:CYS:O	3:D:737:ASN:N	2.45	0.46
3:D:973:ARG:HA	3:D:976:GLU:HB2	1.97	0.46
4:E:68:LEU:CD1	4:E:73:LEU:HD12	2.46	0.46
1:A:18:ASP:O	1:A:19:HIS:CD2	2.69	0.46
1:B:225:ALA:O	1:B:227:PRO:HD3	2.15	0.46
1:B:58:ILE:O	1:B:59:GLU:O	2.34	0.46
2:C:439:CYS:O	2:C:440:PRO:O	2.34	0.46
2:C:44:ILE:HD12	2:C:44:ILE:N	2.29	0.46
2:C:613:VAL:HG12	2:C:615:TYR:CA	2.46	0.46
2:C:892:LEU:C	2:C:894:GLY:N	2.68	0.46
2:C:944:LEU:HD21	2:C:963:LEU:CD2	2.46	0.46
3:D:958:PRO:HG3	3:D:1008:VAL:CA	2.46	0.46
3:D:1131:ARG:H	3:D:1131:ARG:HD2	1.81	0.46
3:D:549:ASN:HD22	3:D:549:ASN:N	2.13	0.46
3:D:693:GLU:O	3:D:696:HIS:HB3	2.15	0.46
3:D:756:GLN:O	3:D:760:ARG:HG2	2.16	0.46
3:D:925:GLU:HG2	3:D:926:LYS:H	1.81	0.46
1:A:208:GLU:O	1:A:212:GLN:HG3	2.15	0.46
1:B:187:GLN:O	1:B:188:ARG:C	2.53	0.46
2:C:440:PRO:HG2	2:C:454:SER:O	2.16	0.46
2:C:766:GLU:O	2:C:768:SER:N	2.47	0.46
2:C:770:GLU:O	2:C:774:LEU:N	2.35	0.46
2:C:810:ASP:HB3	2:C:813:VAL:CG2	2.46	0.46
2:C:950:LEU:O	3:D:1019:ASN:OD1	2.34	0.46
3:D:1073:ILE:HD12	3:D:1073:ILE:N	2.31	0.46
3:D:1126:MET:CE	3:D:1133:LEU:HD21	2.45	0.46
3:D:1180:GLU:C	3:D:1182:GLY:N	2.70	0.46
3:D:1232:GLU:CB	3:D:1233:PRO:HD3	2.33	0.46
3:D:18:ILE:HA	3:D:21:TRP:CE3	2.51	0.46
3:D:538:SER:CA	3:D:541:ASN:HD22	2.25	0.46
3:D:878:GLY:O	3:D:880:ILE:N	2.48	0.46
3:D:98:PRO:O	3:D:99:ALA:HB2	2.16	0.46
4:E:4:PRO:CB	4:E:66:LYS:HE2	2.41	0.46
1:A:103:GLU:O	1:A:104:GLY:C	2.54	0.46
1:B:60:ASP:O	1:B:61:VAL:O	2.33	0.46
2:C:1040:LEU:N	2:C:1040:LEU:HD22	2.31	0.46
2:C:17:PRO:O	2:C:18:LEU:CB	2.63	0.46
2:C:323:ASP:O	2:C:324:ASP:C	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:31:GLN:NE2	2:C:39:ARG:CB	2.77	0.46
2:C:42:VAL:HG12	2:C:43:GLY:N	2.30	0.46
2:C:439:CYS:SG	2:C:453:THR:HG21	2.55	0.46
2:C:682:TYR:CB	2:C:689:VAL:HG22	2.45	0.46
2:C:814:GLU:C	2:C:815:LEU:HD12	2.36	0.46
2:C:837:ASP:H	2:C:1001:VAL:CG2	2.29	0.46
2:C:839:LEU:CD2	2:C:849:VAL:HG23	2.46	0.46
2:C:876:VAL:O	2:C:880:MET:SD	2.74	0.46
2:C:940:GLU:O	2:C:944:LEU:HG	2.16	0.46
3:D:1025:ALA:O	3:D:1028:GLY:N	2.43	0.46
3:D:1070:GLU:HG3	3:D:1073:ILE:HD13	1.98	0.46
3:D:477:LEU:O	3:D:477:LEU:HD12	2.16	0.46
3:D:547:LEU:HA	3:D:577:ALA:HB1	1.98	0.46
3:D:612:GLY:O	3:D:614:PHE:N	2.49	0.46
3:D:709:HIS:HD2	3:D:711:LEU:HB2	1.81	0.46
2:C:1043:TYR:CD1	3:D:710:ARG:HB2	2.51	0.46
3:D:930:LEU:HD12	3:D:934:LEU:HG	1.97	0.46
1:A:123:ASN:C	1:A:124:PRO:O	2.53	0.46
1:A:127:HIS:CD2	1:A:127:HIS:C	2.88	0.46
1:A:19:HIS:O	1:A:20:TYR:O	2.34	0.46
1:B:154:ARG:HD3	1:B:154:ARG:HA	1.71	0.46
2:C:145:GLY:O	2:C:162:ILE:N	2.45	0.46
2:C:399:ASN:HD21	2:C:401:LEU:CB	2.26	0.46
2:C:479:VAL:O	2:C:480:THR:O	2.33	0.46
2:C:714:ASP:O	2:C:715:THR:O	2.34	0.46
2:C:939:ARG:CZ	2:C:975:TYR:CE2	2.99	0.46
2:C:974:LEU:HD22	2:C:989:VAL:CG2	2.45	0.46
3:D:1173:HIS:O	3:D:1176:ILE:HB	2.16	0.46
3:D:1386:GLY:C	3:D:1388:SER:H	2.19	0.46
3:D:1460:LEU:HD13	3:D:1471:ARG:CD	2.46	0.46
3:D:1474:PRO:O	3:D:1479:SER:N	2.49	0.46
3:D:502:PHE:CD1	3:D:507:ASN:ND2	2.84	0.46
3:D:545:ARG:C	3:D:547:LEU:N	2.67	0.46
1:A:103:GLU:O	1:A:104:GLY:O	2.34	0.45
1:A:79:ILE:HG23	1:A:166:VAL:CG2	2.46	0.45
1:B:24:VAL:CG2	1:B:195:THR:HG23	2.45	0.45
2:C:1067:TYR:CZ	2:C:1071:ILE:HD11	2.51	0.45
2:C:1101:THR:HB	2:C:1110:ASP:CB	2.47	0.45
2:C:216:ASP:O	2:C:217:LEU:C	2.54	0.45
2:C:20:GLU:O	2:C:21:ILE:C	2.53	0.45
2:C:148:PHE:HE1	2:C:309:TYR:CD2	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:30:LEU:HG	2:C:30:LEU:O	2.16	0.45
2:C:327:HIS:C	2:C:329:GLY:N	2.69	0.45
2:C:408:ARG:HH22	2:C:457:ALA:HA	1.81	0.45
2:C:648:ARG:CG	2:C:648:ARG:HH11	2.28	0.45
2:C:744:ARG:O	2:C:747:ALA:HB2	2.16	0.45
2:C:92:ALA:HB2	2:C:120:LEU:HD11	1.97	0.45
1:A:179:GLN:NE2	2:C:934:PHE:HB3	2.19	0.45
3:D:1206:TYR:CD2	3:D:1216:VAL:HG21	2.50	0.45
3:D:1270:LYS:O	3:D:1271:ALA:C	2.54	0.45
3:D:1342:PRO:HD2	3:D:1343:GLU:OE1	2.16	0.45
3:D:496:LEU:HD11	3:D:500:ARG:NE	2.30	0.45
3:D:586:ARG:C	3:D:587:ARG:HD3	2.36	0.45
3:D:612:GLY:O	3:D:615:ARG:N	2.43	0.45
2:C:796:GLU:CG	3:D:681:ARG:NH1	2.73	0.45
3:D:792:ILE:HG22	3:D:793:THR:HG23	1.98	0.45
3:D:856:GLY:C	3:D:857:LEU:HD22	2.36	0.45
3:D:8:VAL:O	3:D:1435:TRP:CH2	2.69	0.45
3:D:965:LEU:O	3:D:966:GLU:HB3	2.17	0.45
1:A:142:ARG:C	1:A:143:VAL:HG22	2.36	0.45
1:A:151:PRO:O	1:A:153:GLU:N	2.49	0.45
1:A:32:PHE:N	1:A:32:PHE:CD1	2.84	0.45
1:A:80:LEU:HD23	1:A:83:LYS:HZ1	1.80	0.45
2:C:157:ARG:H	2:C:157:ARG:CD	2.21	0.45
2:C:203:ASP:H	2:C:207:LEU:HB2	1.81	0.45
2:C:325:ILE:C	2:C:327:HIS:N	2.70	0.45
2:C:380:ALA:O	2:C:384:GLU:HB2	2.17	0.45
2:C:460:ARG:O	2:C:461:VAL:CB	2.64	0.45
2:C:460:ARG:CG	2:C:461:VAL:N	2.78	0.45
2:C:653:ASP:O	2:C:653:ASP:OD1	2.34	0.45
2:C:897:LEU:HG	2:C:899:GLN:CD	2.36	0.45
3:D:1080:LYS:C	3:D:1082:GLY:N	2.70	0.45
3:D:1275:ILE:HD12	3:D:1275:ILE:O	2.16	0.45
3:D:1377:LEU:HD11	3:D:1422:LEU:HG	1.98	0.45
3:D:470:LEU:O	3:D:472:LYS:N	2.49	0.45
3:D:650:LEU:HD21	3:D:683:ILE:HD11	1.98	0.45
3:D:734:GLU:OE2	3:D:780:LYS:NZ	2.50	0.45
3:D:77:GLY:C	3:D:79:GLU:H	2.18	0.45
4:E:6:ILE:CG2	4:E:7:ASP:N	2.79	0.45
1:B:90:LEU:HG	1:B:118:ASP:O	2.17	0.45
2:C:837:ASP:N	2:C:1001:VAL:HG23	2.31	0.45
2:C:1008:ARG:CD	2:C:1029:GLY:H	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:144:PRO:HA	2:C:162:ILE:CG2	2.45	0.45
2:C:165:LEU:HD21	2:C:338:GLU:OE1	2.16	0.45
2:C:363:SER:O	2:C:367:LEU:N	2.40	0.45
2:C:497:ALA:HA	2:C:502:PRO:CB	2.47	0.45
2:C:564:MET:CE	2:C:846:LYS:HG2	2.46	0.45
2:C:918:LEU:CD1	2:C:968:ASP:O	2.65	0.45
2:C:959:PRO:HG2	2:C:960:GLU:N	2.32	0.45
3:D:10:ILE:HG12	3:D:11:ALA:N	2.26	0.45
3:D:1110:GLU:O	3:D:1203:GLN:CB	2.65	0.45
3:D:1205:CYS:C	3:D:1207:GLY:N	2.70	0.45
3:D:1278:ILE:HG22	3:D:1279:ASP:H	1.71	0.45
3:D:1345:VAL:O	3:D:1349:LEU:HD22	2.15	0.45
3:D:1364:LEU:CG	3:D:1365:HIS:N	2.79	0.45
2:C:1026:GLN:NE2	3:D:674:ARG:HH21	2.13	0.45
3:D:754:PHE:O	3:D:758:GLU:HG2	2.16	0.45
3:D:875:THR:HG23	3:D:879:ARG:CB	2.43	0.45
4:E:15:SER:O	4:E:18:ARG:HB3	2.16	0.45
1:A:85:LEU:CA	1:A:123:ASN:HD21	2.28	0.45
1:B:111:VAL:C	1:B:113:PHE:N	2.69	0.45
1:B:12:THR:O	1:B:24:VAL:N	2.48	0.45
1:B:59:GLU:O	1:B:60:ASP:CB	2.64	0.45
2:C:1107:ASN:H	2:C:1108:PRO:HD3	1.81	0.45
2:C:145:GLY:N	2:C:162:ILE:HB	2.32	0.45
2:C:281:LEU:C	2:C:283:VAL:H	2.20	0.45
2:C:159:ILE:HG21	2:C:306:THR:OG1	2.16	0.45
2:C:340:MET:O	2:C:340:MET:SD	2.74	0.45
2:C:520:GLU:O	2:C:521:PRO:C	2.54	0.45
2:C:708:TYR:N	2:C:708:TYR:CD1	2.84	0.45
2:C:80:GLN:HG3	2:C:90:TYR:CZ	2.52	0.45
2:C:906:PHE:O	2:C:907:ASP:CB	2.64	0.45
3:D:1008:VAL:CG1	3:D:1009:PHE:N	2.80	0.45
3:D:1077:GLY:O	3:D:1078:ALA:C	2.55	0.45
3:D:9(U):UNK:O	3:D:10(U):UNK:CB	2.63	0.45
3:D:709:HIS:H	3:D:1228:GLU:HB3	1.82	0.45
3:D:728:LEU:HD13	3:D:745:MET:CE	2.47	0.45
3:D:701:LEU:HD21	3:D:763:MET:HE1	1.98	0.45
3:D:794:GLN:HB3	3:D:1018:PHE:CZ	2.52	0.45
3:D:863:THR:C	3:D:864:VAL:CG2	2.85	0.45
3:D:958:PRO:O	3:D:959:GLU:C	2.54	0.45
3:D:975:ILE:HD11	3:D:984:LEU:HD13	1.99	0.45
3:D:1484:PHE:HB2	4:E:76:GLY:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:ILE:O	1:A:122:MET:C	2.55	0.45
1:B:41:ARG:HD3	1:B:41:ARG:O	2.17	0.45
2:C:328:LEU:CB	2:C:484:VAL:HG11	2.46	0.45
2:C:421:GLU:O	2:C:423:ALA:N	2.50	0.45
2:C:442:GLU:O	2:C:442:GLU:HG3	2.15	0.45
2:C:586:ARG:O	2:C:586:ARG:HG3	2.16	0.45
2:C:603:VAL:HG23	2:C:604:VAL:N	2.27	0.45
2:C:674:VAL:HG23	2:C:675:ALA:O	2.16	0.45
2:C:745:ILE:C	2:C:747:ALA:H	2.20	0.45
2:C:755:LEU:HD12	2:C:756:VAL:HG23	1.97	0.45
2:C:7:GLY:HA2	2:C:907:ASP:OD2	2.16	0.45
3:D:1085:THR:O	3:D:1087:LEU:N	2.50	0.45
3:D:1259:ARG:HG3	3:D:1259:ARG:NH1	2.31	0.45
3:D:1463:LEU:O	3:D:1464:LYS:C	2.55	0.45
3:D:469:ASP:O	3:D:470:LEU:C	2.55	0.45
3:D:890:VAL:CG1	3:D:891:GLY:H	2.25	0.45
3:D:985:THR:O	3:D:986:ASP:C	2.54	0.45
4:E:68:LEU:C	4:E:70:THR:N	2.69	0.45
1:A:77:GLU:O	1:A:78:ILE:C	2.54	0.45
1:A:78:ILE:O	1:A:81:ASN:N	2.50	0.45
1:B:36:LEU:O	1:B:39:PRO:HD2	2.16	0.45
2:C:142:ARG:NH1	2:C:142:ARG:HG2	2.32	0.45
2:C:200:LEU:HD23	2:C:200:LEU:N	2.30	0.45
2:C:384:GLU:OE2	2:C:388:ARG:HD2	2.17	0.45
2:C:442:GLU:OE2	2:C:544:THR:HG21	2.17	0.45
1:A:65:PHE:HD2	2:C:628:TYR:CE2	2.35	0.45
2:C:688:ILE:HD12	2:C:871:LEU:CD1	2.46	0.45
3:D:1252:ASP:C	3:D:1254:THR:N	2.70	0.45
3:D:899:LEU:O	3:D:900:ILE:HG13	2.16	0.45
3:D:993:VAL:O	3:D:996:LEU:HB3	2.17	0.45
1:B:122:MET:N	1:B:122:MET:HE3	2.32	0.45
1:B:85:LEU:C	1:B:123:ASN:HD21	2.19	0.45
1:B:97:THR:HA	1:B:142:ARG:HA	1.98	0.45
2:C:1026:GLN:O	2:C:1027:PHE:HB2	2.17	0.45
2:C:1008:ARG:HB2	2:C:1029:GLY:H	1.81	0.45
2:C:194:VAL:HG22	2:C:221:LEU:HD12	1.97	0.45
2:C:335:THR:O	2:C:338:GLU:N	2.45	0.45
2:C:969:LEU:HD11	3:D:953:ASP:N	2.20	0.45
3:D:1080:LYS:C	3:D:1082:GLY:H	2.19	0.45
3:D:462:GLN:O	3:D:463:GLU:C	2.54	0.45
3:D:507:ASN:ND2	3:D:508:ARG:H	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:696:HIS:CD2	4:E:57:ASP:HB2	2.51	0.45
1:A:180:VAL:O	1:A:181:GLU:C	2.55	0.45
1:B:56:VAL:HG11	1:B:58:ILE:HD11	1.99	0.45
2:C:63:GLY:HA2	2:C:102:HIS:CA	2.46	0.45
2:C:15:LEU:HD21	2:C:461:VAL:HG23	1.96	0.45
2:C:164:PRO:HD3	2:C:267:TYR:HD2	1.78	0.45
2:C:274:ARG:O	2:C:278:GLU:HB2	2.17	0.45
2:C:321:GLU:O	2:C:322:VAL:C	2.56	0.45
2:C:564:MET:CG	2:C:997:LEU:HD11	2.46	0.45
2:C:659:PRO:HG2	2:C:660:ALA:N	2.28	0.45
2:C:703:ILE:HA	2:C:829:GLN:O	2.16	0.45
3:D:1070:GLU:HG3	3:D:1073:ILE:CB	2.46	0.45
3:D:1093:GLY:HA2	3:D:1097:ARG:NE	2.32	0.45
3:D:1126:MET:CG	3:D:1127:ASP:N	2.78	0.45
3:D:1195:CYS:SG	3:D:1202:CYS:CB	3.04	0.45
3:D:15:PRO:HD3	3:D:510:GLU:HB3	1.98	0.45
3:D:625:TYR:CE1	3:D:751:LEU:HD21	2.48	0.45
3:D:633:VAL:O	3:D:633:VAL:HG13	2.16	0.45
3:D:701:LEU:HA	3:D:715:ALA:CB	2.45	0.45
3:D:806:PHE:CA	3:D:827:ILE:O	2.65	0.45
1:A:200:THR:CG2	1:A:201:ASP:N	2.80	0.45
2:C:1030:GLN:HE21	2:C:1031:ARG:H	1.63	0.45
2:C:1037:VAL:O	2:C:1041:GLU:HG3	2.17	0.45
2:C:1045:ALA:CB	2:C:1048:THR:HB	2.33	0.45
2:C:163:ILE:HG21	2:C:170:PRO:N	2.32	0.45
2:C:204:GLN:O	2:C:205:GLU:CB	2.65	0.45
2:C:461:VAL:O	2:C:462:ASP:CB	2.65	0.45
2:C:559:LEU:HA	2:C:562:SER:HB3	1.99	0.45
2:C:742:ILE:HD13	2:C:823:VAL:HG13	1.99	0.45
2:C:874:LEU:CD1	2:C:875:GLY:H	2.30	0.45
2:C:981:GLU:HB3	2:C:982:PRO:CD	2.47	0.45
3:D:1252:ASP:O	3:D:1254:THR:N	2.44	0.45
3:D:1320:VAL:O	3:D:1322:ALA:N	2.50	0.45
3:D:1268:ARG:NH1	3:D:1331:ILE:CB	2.80	0.45
3:D:130:ASN:CB	3:D:464:LEU:HD21	2.47	0.45
3:D:699:VAL:HA	3:D:716:PHE:O	2.17	0.45
3:D:770:LEU:O	3:D:771:SER:HB2	2.16	0.45
1:B:30:ARG:O	1:B:30:ARG:HG3	2.17	0.45
2:C:1092:LEU:HD22	2:C:1097:LEU:HD12	1.99	0.45
2:C:157:ARG:HD3	2:C:157:ARG:N	2.28	0.45
2:C:212:SER:HB2	2:C:218:VAL:CG2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:589:ARG:HH12	2:C:596:TYR:HA	1.81	0.45
2:C:614:ARG:O	2:C:615:TYR:CB	2.65	0.45
3:D:1146:TYR:HD2	3:D:1147:GLY:N	2.13	0.45
3:D:1317:GLY:O	3:D:1318:ASP:CB	2.64	0.45
3:D:1421:LEU:HD12	3:D:1422:LEU:H	1.82	0.45
3:D:1466:ASN:HD21	3:D:1471:ARG:NH1	2.15	0.45
3:D:104:PHE:O	3:D:511:TRP:HZ3	2.00	0.45
3:D:638:LYS:O	3:D:639:LEU:CB	2.65	0.45
3:D:728:LEU:HD13	3:D:745:MET:HE3	1.98	0.45
1:A:44:LEU:O	1:A:173:VAL:HG21	2.18	0.44
1:A:214:VAL:HG23	1:A:215:ALA:N	2.31	0.44
1:A:30:ARG:HD2	1:A:190:ASP:HB3	1.99	0.44
1:A:66:SER:CB	1:A:75:VAL:HG21	2.44	0.44
1:B:133:GLU:CD	1:B:134:GLY:H	2.19	0.44
1:B:138:TYR:CE2	1:B:140:GLU:HG3	2.52	0.44
1:B:56:VAL:O	1:B:163:ALA:O	2.35	0.44
1:B:147:VAL:O	1:B:170:PHE:O	2.34	0.44
2:C:1004:LYS:O	2:C:1005:MET:HB3	2.17	0.44
2:C:1042:ALA:CB	3:D:1228:GLU:OE1	2.66	0.44
2:C:196:LEU:O	2:C:199:VAL:HB	2.17	0.44
2:C:231:PRO:HA	2:C:234:ALA:HB2	1.98	0.44
2:C:552:HIS:CE1	3:D:1065:GLY:CA	3.00	0.44
2:C:610:ARG:O	2:C:611:ILE:C	2.54	0.44
2:C:684:PHE:O	2:C:685:GLU:HB2	2.17	0.44
2:C:86:LYS:CE	2:C:811:PRO:HG2	2.47	0.44
3:D:1031:GLY:O	3:D:1032:ASN:CB	2.55	0.44
3:D:1155:GLU:HB3	3:D:1160:ARG:HG2	1.98	0.44
3:D:1463:LEU:O	3:D:1465:GLU:N	2.50	0.44
3:D:151:GLN:O	3:D:152:LEU:C	2.55	0.44
3:D:17:LYS:O	3:D:18:ILE:C	2.54	0.44
3:D:805:ALA:HB1	3:D:809:PRO:HD2	1.99	0.44
3:D:972:LEU:O	3:D:976:GLU:HG2	2.17	0.44
1:A:161:ILE:HG23	1:A:162:ASN:ND2	2.31	0.44
2:C:1055:ILE:HG21	2:C:1077:PRO:HB3	1.99	0.44
2:C:17:PRO:HA	2:C:586:ARG:HH21	1.82	0.44
2:C:9:ILE:HD13	2:C:494:TYR:CE1	2.52	0.44
2:C:18:LEU:HD13	2:C:542:LEU:CD2	2.47	0.44
2:C:589:ARG:HH21	2:C:654:LEU:CD1	2.30	0.44
2:C:729:LEU:CD2	2:C:734:LEU:HD23	2.47	0.44
2:C:677:MET:N	2:C:873:PRO:HD3	2.32	0.44
3:D:117:ASP:C	3:D:119:PHE:H	2.19	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1312:LEU:O	3:D:1324:GLN:OE1	2.34	0.44
3:D:1340:LYS:HA	3:D:1340:LYS:HD2	1.84	0.44
3:D:575:GLN:O	3:D:578:VAL:N	2.47	0.44
3:D:603:LEU:O	3:D:606:ILE:HD13	2.17	0.44
3:D:606:ILE:CD1	3:D:606:ILE:N	2.75	0.44
3:D:773:ALA:O	3:D:774:SER:CB	2.65	0.44
3:D:896:ALA:O	3:D:899:LEU:N	2.48	0.44
3:D:954:ASP:HA	3:D:956:VAL:HG23	2.00	0.44
4:E:57:ASP:HA	4:E:58:PRO:HD3	1.81	0.44
3:D:1487:VAL:O	4:E:79:LEU:CD1	2.65	0.44
1:A:196:LEU:H	1:A:196:LEU:CD2	2.31	0.44
1:A:24:VAL:HG12	1:A:25:LEU:O	2.17	0.44
1:B:105:PRO:CA	1:B:132:GLU:HA	2.43	0.44
2:C:22:GLN:HA	2:C:25:SER:HB3	1.99	0.44
2:C:377:PRO:HG2	2:C:378:LEU:H	1.82	0.44
2:C:474:VAL:HG12	2:C:526:PRO:HB3	1.99	0.44
2:C:501:THR:N	2:C:502:PRO:CD	2.80	0.44
2:C:474:VAL:HA	2:C:527:GLU:CB	2.47	0.44
2:C:603:VAL:O	2:C:613:VAL:O	2.35	0.44
2:C:48:PHE:HE2	2:C:71:TYR:HB3	1.80	0.44
2:C:873:PRO:O	2:C:877:PRO:CG	2.65	0.44
3:D:1282:VAL:HB	3:D:1283:ARG:H	1.29	0.44
3:D:1276:SER:N	3:D:1323:GLY:HA2	2.19	0.44
3:D:1381:GLU:O	3:D:1419:LYS:N	2.50	0.44
3:D:131:LYS:CB	3:D:454:ALA:HA	2.47	0.44
3:D:628:ARG:HB3	3:D:628:ARG:NH1	2.32	0.44
3:D:657:LEU:HD13	3:D:690:ALA:HB1	1.99	0.44
3:D:642:CYS:SG	3:D:702:LEU:CD2	3.05	0.44
3:D:925:GLU:HG2	3:D:926:LYS:N	2.33	0.44
1:A:65:PHE:HD2	2:C:628:TYR:HE2	1.65	0.44
1:A:75:VAL:HA	1:A:78:ILE:CD1	2.36	0.44
1:B:141:VAL:O	1:B:141:VAL:HG13	2.17	0.44
1:B:159:ASP:O	1:B:160:ARG:C	2.56	0.44
2:C:1032:PHE:HB2	3:D:623:VAL:CG2	2.43	0.44
2:C:1054:THR:O	2:C:1056:LYS:N	2.50	0.44
2:C:243:ARG:CG	2:C:244:PRO:HA	2.44	0.44
2:C:141:HIS:HE2	2:C:332:ARG:HD3	1.82	0.44
2:C:526:PRO:O	2:C:527:GLU:C	2.55	0.44
2:C:473:ARG:O	2:C:531:PHE:O	2.34	0.44
2:C:882:LEU:CD1	2:C:884:GLN:NE2	2.80	0.44
2:C:987:ILE:HD11	3:D:946:GLY:C	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:9:ILE:HD13	2:C:494:TYR:HE1	1.82	0.44
3:D:1167:LEU:HD23	3:D:1167:LEU:O	2.18	0.44
3:D:1349:LEU:HG	3:D:1376:MET:CE	2.47	0.44
3:D:37(U):UNK:O	3:D:38(U):UNK:CB	2.65	0.44
3:D:550:ARG:NH2	3:D:573:MET:SD	2.90	0.44
3:D:694:VAL:O	3:D:695:ILE:C	2.56	0.44
3:D:845:ASN:CB	3:D:846:PRO:HD2	2.48	0.44
1:A:102:ALA:CB	1:A:108:VAL:HG21	2.47	0.44
1:A:180:VAL:HG23	2:C:939:ARG:HH11	1.83	0.44
1:B:100:LEU:HD21	1:B:108:VAL:HG13	1.99	0.44
1:B:136:LYS:HG2	1:B:137:LEU:N	2.32	0.44
1:B:50:GLY:HA3	1:B:172:PRO:HD3	2.00	0.44
2:C:1054:THR:HG22	2:C:1055:ILE:N	2.33	0.44
2:C:218:VAL:O	2:C:219:GLN:C	2.55	0.44
2:C:494:TYR:O	2:C:495:THR:OG1	2.33	0.44
2:C:815:LEU:HD23	2:C:822:VAL:CG2	2.48	0.44
2:C:843:HIS:CD2	2:C:884:GLN:CA	2.96	0.44
2:C:918:LEU:O	2:C:918:LEU:HD23	2.18	0.44
2:C:920:GLU:C	2:C:922:PHE:N	2.68	0.44
2:C:949:LYS:C	2:C:951:GLY:H	2.19	0.44
3:D:1224:VAL:C	3:D:1226:ALA:H	2.21	0.44
3:D:1283:ARG:HG2	3:D:1283:ARG:NH1	2.26	0.44
3:D:1379:TYR:OH	3:D:1432:THR:HB	2.17	0.44
3:D:1444:THR:O	3:D:1448:LEU:HB2	2.18	0.44
3:D:480:GLU:HA	3:D:493:ARG:NH1	2.32	0.44
3:D:794:GLN:O	3:D:795:VAL:HG23	2.18	0.44
3:D:805:ALA:O	3:D:806:PHE:CB	2.66	0.44
3:D:916:TYR:CE2	3:D:920:LEU:HD21	2.52	0.44
2:C:100:LEU:HD12	2:C:100:LEU:C	2.38	0.44
2:C:1059:ASP:OD1	2:C:1062:GLY:N	2.38	0.44
2:C:141:HIS:CE1	2:C:334:ARG:HG3	2.53	0.44
2:C:31:GLN:CG	2:C:39:ARG:HD2	2.48	0.44
2:C:355:VAL:CG1	2:C:356:ARG:N	2.80	0.44
2:C:457:ALA:C	2:C:459:ALA:N	2.70	0.44
2:C:525:ALA:O	2:C:526:PRO:C	2.56	0.44
2:C:569:VAL:O	2:C:571:LEU:HD12	2.17	0.44
1:A:70:GLY:HA2	2:C:606:VAL:HG22	2.00	0.44
2:C:676:ILE:O	2:C:677:MET:HG2	2.17	0.44
2:C:780:GLU:O	2:C:781:LYS:C	2.55	0.44
2:C:860:HIS:CD2	2:C:977:GLY:CA	2.95	0.44
2:C:674:VAL:HB	2:C:869:VAL:HG13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:870:ILE:CG2	2:C:870:ILE:O	2.63	0.44
2:C:885:ILE:C	2:C:887:GLU:H	2.21	0.44
2:C:925:TYR:OH	2:C:972:VAL:HG21	2.16	0.44
3:D:1070:GLU:HG3	3:D:1073:ILE:HG12	2.00	0.44
3:D:1283:ARG:HB3	3:D:1294:PHE:HB2	1.99	0.44
3:D:1373:VAL:HG22	3:D:1376:MET:CE	2.47	0.44
2:C:835:VAL:CG1	3:D:632:VAL:HG21	2.48	0.44
3:D:752:SER:O	3:D:755:ALA:N	2.48	0.44
3:D:711:LEU:HD21	3:D:768:ASN:O	2.18	0.44
3:D:935:LYS:CG	3:D:939:PHE:HE1	2.30	0.44
3:D:977:GLN:OE1	3:D:980:GLU:OE1	2.35	0.44
3:D:758:GLU:HB3	4:E:20:THR:CG2	2.48	0.44
1:A:102:ALA:O	1:A:135:GLY:O	2.36	0.44
1:A:156:GLY:H	1:A:165:PRO:HB3	1.83	0.44
1:A:32:PHE:HD1	1:A:32:PHE:N	2.16	0.44
1:A:94:TRP:CZ3	1:A:96:THR:HB	2.53	0.44
1:B:19:HIS:H	1:B:19:HIS:CD2	2.35	0.44
1:B:86:VAL:HG23	1:B:123:ASN:OD1	2.16	0.44
2:C:1092:LEU:CD2	2:C:1097:LEU:HD12	2.48	0.44
2:C:129:ILE:HG21	2:C:387:SER:HB2	2.00	0.44
2:C:482:GLU:CB	2:C:486:MET:SD	3.06	0.44
2:C:572:ILE:O	2:C:573:ARG:HG3	2.18	0.44
2:C:580:MET:CB	2:C:584:GLU:OE1	2.66	0.44
2:C:601:GLY:CA	2:C:648:ARG:N	2.80	0.44
2:C:641:PRO:HA	2:C:656:ALA:HB2	1.98	0.44
2:C:87:ASP:O	2:C:88:LEU:HD23	2.17	0.44
2:C:984:GLU:HG2	3:D:944:THR:O	2.17	0.44
3:D:1018:PHE:O	3:D:1019:ASN:C	2.55	0.44
3:D:1167:LEU:CD2	3:D:1167:LEU:N	2.77	0.44
3:D:1238:THR:HG22	3:D:1239:MET:H	1.81	0.44
3:D:482:LYS:HD3	3:D:492:ALA:HB3	2.00	0.44
3:D:704:ARG:O	3:D:705:ALA:O	2.35	0.44
3:D:831:GLY:C	3:D:833:GLU:H	2.21	0.44
3:D:787:LEU:CD2	3:D:947:ILE:HD11	2.37	0.44
3:D:950:ILE:H	3:D:950:ILE:HG13	1.63	0.44
1:A:102:ALA:CB	1:A:137:LEU:HB3	2.47	0.44
1:A:93:ARG:O	1:A:94:TRP:CB	2.63	0.44
1:B:184:ARG:C	1:B:186:GLY:N	2.70	0.44
1:B:53:VAL:CG2	1:B:85:LEU:HD23	2.48	0.44
2:C:110:GLU:HB3	2:C:370:ALA:HB2	2.00	0.44
2:C:234:ALA:O	2:C:235:MET:C	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:427:VAL:HG12	2:C:431:HIS:NE2	2.33	0.44
2:C:474:VAL:HG12	2:C:526:PRO:CA	2.47	0.44
2:C:536:PRO:O	2:C:537:LYS:C	2.56	0.44
2:C:563:ASN:O	2:C:564:MET:C	2.55	0.44
2:C:567:GLN:O	2:C:568:ALA:O	2.35	0.44
2:C:706:GLU:CG	2:C:707:ARG:H	2.31	0.44
2:C:78:PHE:HD2	2:C:82:GLU:OE1	2.01	0.44
2:C:845:ASN:ND2	2:C:876:VAL:CG1	2.81	0.44
3:D:1042:MET:HG2	3:D:1043:ARG:N	2.33	0.44
3:D:1179:ALA:HA	3:D:1184:VAL:O	2.18	0.44
3:D:1259:ARG:C	3:D:1261:ILE:H	2.19	0.44
3:D:1473:ILE:HA	3:D:1473:ILE:HD13	1.89	0.44
3:D:543:LEU:C	3:D:545:ARG:H	2.20	0.44
3:D:657:LEU:O	3:D:659:LYS:N	2.50	0.44
3:D:674:ARG:NH1	3:D:678:GLU:CG	2.80	0.44
3:D:699:VAL:HG22	3:D:756:GLN:NE2	2.33	0.44
3:D:760:ARG:HH11	4:E:59:ASN:HD21	1.66	0.44
3:D:81:THR:O	3:D:82:ARG:CB	2.66	0.44
3:D:1490:GLN:CB	4:E:72:ARG:HD2	2.48	0.44
4:E:80:VAL:N	4:E:81:PRO:HD2	2.32	0.44
1:B:180:VAL:HG22	1:B:180:VAL:O	2.16	0.44
1:B:221:LEU:O	1:B:224:PHE:HD1	2.01	0.44
1:B:53:VAL:HG12	1:B:54:THR:N	2.32	0.44
2:C:97:ARG:NH2	2:C:109:LYS:NZ	2.66	0.44
2:C:208:VAL:HG12	2:C:209:ARG:H	1.82	0.44
2:C:165:LEU:HD11	2:C:338:GLU:OE1	2.18	0.44
2:C:425:PHE:O	2:C:426:ASP:CB	2.65	0.44
2:C:699:PHE:C	2:C:701:THR:H	2.21	0.44
3:D:108:VAL:O	3:D:110:SER:N	2.51	0.44
3:D:1107:VAL:HG12	3:D:1109:ARG:HG3	2.00	0.44
3:D:1109:ARG:O	3:D:1110:GLU:CB	2.65	0.44
3:D:1142:GLU:C	3:D:1144:GLY:H	2.22	0.44
3:D:1239:MET:HG3	3:D:1239:MET:O	2.18	0.44
3:D:131:LYS:O	3:D:133:ILE:N	2.51	0.44
3:D:1433:LYS:HG2	3:D:1434:SER:H	1.80	0.44
3:D:495:ARG:O	3:D:496:LEU:C	2.56	0.44
3:D:659:LYS:C	3:D:659:LYS:HD3	2.38	0.44
3:D:711:LEU:HB3	3:D:735:ALA:HB1	1.99	0.44
3:D:794:GLN:O	3:D:795:VAL:CB	2.66	0.44
2:C:1112:PHE:C	2:C:1114:GLY:N	2.71	0.43
2:C:258:PHE:HD1	2:C:258:PHE:N	2.15	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:442:GLU:O	2:C:559:LEU:HB2	2.18	0.43
2:C:574:ALA:O	2:C:575:GLN:O	2.35	0.43
2:C:735:ARG:C	2:C:737:LEU:N	2.62	0.43
2:C:862:PRO:HA	2:C:975:TYR:HE1	1.77	0.43
2:C:89:THR:HG23	2:C:129:ILE:HG12	2.00	0.43
3:D:1337:LEU:O	3:D:1341:GLY:N	2.51	0.43
3:D:618:LEU:HA	3:D:618:LEU:HD23	1.77	0.43
3:D:795:VAL:H	3:D:862:ASP:CB	2.31	0.43
3:D:8:VAL:HG12	3:D:8:VAL:O	2.17	0.43
4:E:39:VAL:HG12	4:E:39:VAL:O	2.17	0.43
1:A:103:GLU:H	1:A:106:LYS:NZ	2.16	0.43
1:A:26:GLU:OE2	1:A:184:ARG:NE	2.50	0.43
1:A:80:LEU:HD11	2:C:572:ILE:HD12	1.99	0.43
1:A:9:PRO:HG3	1:A:25:LEU:HD13	2.00	0.43
1:B:111:VAL:CG2	1:B:124:PRO:HA	2.48	0.43
1:B:58:ILE:HA	1:B:138:TYR:O	2.18	0.43
1:B:89:PHE:CG	1:B:89:PHE:O	2.71	0.43
2:C:112:GLU:O	2:C:113:VAL:CB	2.65	0.43
2:C:159:ILE:HD12	2:C:174:LEU:CB	2.47	0.43
2:C:396:ASP:O	2:C:403:SER:N	2.51	0.43
2:C:525:ALA:CB	2:C:526:PRO:CD	2.94	0.43
2:C:474:VAL:CG2	2:C:530:GLU:HA	2.45	0.43
2:C:6:PHE:CD2	2:C:909:ALA:N	2.81	0.43
2:C:738:ASP:HA	2:C:743:VAL:HA	1.99	0.43
2:C:836:GLY:O	2:C:837:ASP:O	2.37	0.43
2:C:837:ASP:O	2:C:848:VAL:HG23	2.18	0.43
2:C:94:LEU:HD23	2:C:344:PHE:CZ	2.50	0.43
3:D:1016:TYR:HB3	3:D:1020:PRO:CD	2.30	0.43
3:D:1196:GLN:O	3:D:1197:THR:OG1	2.36	0.43
3:D:578:VAL:O	3:D:582:ILE:HG13	2.19	0.43
3:D:601:ARG:O	3:D:602:SER:O	2.37	0.43
3:D:645:PRO:HG3	3:D:724:GLN:C	2.38	0.43
3:D:638:LYS:CA	3:D:729:HIS:CD2	3.01	0.43
3:D:767:HIS:O	3:D:769:LEU:N	2.47	0.43
3:D:810:GLU:C	3:D:812:ALA:H	2.20	0.43
3:D:815:ALA:CB	3:D:832:ARG:HD2	2.48	0.43
3:D:948:ILE:HG12	3:D:950:ILE:HG13	1.99	0.43
4:E:59:ASN:O	4:E:62:THR:HB	2.17	0.43
1:A:125:ASP:HB2	1:A:126:LEU:H	1.55	0.43
2:C:66:LEU:CA	2:C:100:LEU:HA	2.45	0.43
2:C:9:ILE:O	2:C:10:ARG:CB	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:16:PRO:HA	2:C:17:PRO:HA	1.52	0.43
2:C:261:LEU:HD21	2:C:263:ASP:CB	2.48	0.43
2:C:310:LEU:HA	2:C:313:LEU:CD2	2.48	0.43
2:C:54:ILE:HG12	2:C:355:VAL:HG11	2.00	0.43
2:C:115:LEU:CD2	2:C:378:LEU:HD22	2.49	0.43
2:C:399:ASN:HD22	2:C:401:LEU:N	2.12	0.43
2:C:439:CYS:HA	2:C:440:PRO:HD2	1.80	0.43
2:C:446:GLY:O	2:C:447:ALA:CB	2.63	0.43
2:C:328:LEU:HD21	2:C:468:ARG:NH1	2.33	0.43
2:C:654:LEU:HD21	2:C:657:ASP:CG	2.38	0.43
2:C:681:GLY:O	2:C:684:PHE:HB2	2.18	0.43
2:C:679:PHE:CE2	2:C:978:ARG:NH2	2.86	0.43
3:D:1004:VAL:O	3:D:1007:ALA:HB3	2.17	0.43
3:D:1015:ASN:O	3:D:1016:TYR:HB2	2.16	0.43
3:D:1100:VAL:O	3:D:1104:HIS:HB3	2.18	0.43
3:D:1145:LEU:HB2	3:D:1172:VAL:CG1	2.44	0.43
3:D:1327:THR:C	3:D:1329:GLY:N	2.71	0.43
3:D:1366:ASP:O	3:D:1367:LYS:HB2	2.18	0.43
3:D:1423:MET:HB3	3:D:1428:SER:HB2	2.00	0.43
3:D:100:ALA:HA	3:D:575:GLN:OE1	2.18	0.43
3:D:710:ARG:O	3:D:712:GLY:N	2.51	0.43
3:D:729:HIS:ND1	3:D:730:PRO:CD	2.81	0.43
3:D:880:ILE:O	3:D:883:ALA:N	2.50	0.43
1:A:158:LYS:O	1:A:160:ARG:N	2.49	0.43
1:A:183:THR:O	1:A:183:THR:HG23	2.18	0.43
1:A:72:LYS:O	1:A:73:GLU:O	2.36	0.43
1:B:65:PHE:CD1	1:B:65:PHE:O	2.71	0.43
2:C:1051:GLU:OE2	3:D:751:LEU:CB	2.66	0.43
2:C:1112:PHE:C	2:C:1114:GLY:H	2.22	0.43
2:C:160:ALA:HA	2:C:173:ASP:OD1	2.19	0.43
2:C:193:LEU:HD13	2:C:193:LEU:C	2.38	0.43
2:C:721:ARG:O	2:C:758:ARG:HB2	2.19	0.43
2:C:759:THR:HA	2:C:786:LYS:O	2.18	0.43
2:C:83:CYS:SG	2:C:90:TYR:HA	2.57	0.43
3:D:1012:PHE:CD2	3:D:1023:VAL:HG11	2.53	0.43
3:D:1094:TYR:HE2	3:D:1098:LYS:HE3	1.83	0.43
3:D:1214:ARG:HD2	3:D:1215:PRO:HD2	1.99	0.43
3:D:1276:SER:HA	3:D:1304:TYR:CE1	2.52	0.43
3:D:1344:ALA:O	3:D:1346:GLU:N	2.52	0.43
3:D:502:PHE:CD1	3:D:1453:ILE:HG23	2.52	0.43
3:D:482:LYS:HE2	3:D:488:ARG:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:104:PHE:O	3:D:511:TRP:CZ3	2.71	0.43
3:D:571:LYS:C	3:D:573:MET:H	2.21	0.43
4:E:9:LEU:C	4:E:11:GLY:N	2.71	0.43
1:A:55:SER:O	1:A:141:VAL:HA	2.18	0.43
1:A:59:GLU:OE2	1:A:136:LYS:HE3	2.18	0.43
1:B:23:PHE:O	1:B:195:THR:HA	2.18	0.43
1:B:79:ILE:HG22	1:B:80:LEU:N	2.34	0.43
1:B:89:PHE:CZ	1:B:145:ARG:NE	2.77	0.43
2:C:104:ASP:O	2:C:105:THR:O	2.36	0.43
2:C:168:ARG:NH1	2:C:268:ASP:OD2	2.51	0.43
2:C:304:LEU:H	2:C:305:PRO:HD2	1.78	0.43
2:C:551:GLU:CD	2:C:906:PHE:H	2.22	0.43
3:D:1077:GLY:CA	3:D:1080:LYS:HG2	2.48	0.43
2:C:1005:MET:HB2	3:D:629:SER:HB2	2.01	0.43
1:A:146:GLY:HA3	1:A:170:PHE:CZ	2.53	0.43
1:B:86:VAL:N	1:B:123:ASN:OD1	2.51	0.43
1:B:133:GLU:CG	1:B:134:GLY:H	2.31	0.43
2:C:1011:GLY:O	2:C:1012:PRO:C	2.56	0.43
2:C:1053:LEU:HD12	3:D:621:LYS:HD2	2.01	0.43
2:C:1109:VAL:O	2:C:1109:VAL:HG13	2.17	0.43
2:C:161:SER:OG	2:C:172:ILE:HG22	2.19	0.43
2:C:327:HIS:O	2:C:329:GLY:N	2.38	0.43
2:C:439:CYS:CB	2:C:468:ARG:NH1	2.70	0.43
2:C:514:VAL:C	2:C:516:ARG:N	2.72	0.43
2:C:521:PRO:O	2:C:522:VAL:C	2.56	0.43
2:C:676:ILE:O	2:C:677:MET:CG	2.67	0.43
2:C:821:GLU:O	2:C:822:VAL:CG2	2.66	0.43
2:C:920:GLU:HG2	2:C:921:ALA:N	2.21	0.43
3:D:1023:VAL:HA	3:D:1026:GLN:CB	2.49	0.43
3:D:1049:PRO:HD3	3:D:1076:HIS:CE1	2.54	0.43
3:D:1374:ARG:O	3:D:1377:LEU:N	2.52	0.43
3:D:899:LEU:O	3:D:900:ILE:HG12	2.18	0.43
3:D:990:TYR:HD2	3:D:991:ASP:OD1	2.01	0.43
1:B:159:ASP:O	1:B:159:ASP:CG	2.57	0.43
1:B:19:HIS:N	1:B:19:HIS:CD2	2.86	0.43
1:B:218:LYS:O	1:B:219:GLU:C	2.57	0.43
2:C:91:GLN:HB3	2:C:117:HIS:HB3	2.01	0.43
2:C:406:HIS:ND1	2:C:406:HIS:O	2.51	0.43
2:C:421:GLU:H	2:C:424:GLY:HA3	1.84	0.43
2:C:555:ALA:O	2:C:556:ASN:C	2.57	0.43
2:C:922:PHE:CE2	2:C:964:LYS:HB2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:971:LYS:O	2:C:972:VAL:O	2.36	0.43
3:D:1017:PRO:HG2	3:D:1018:PHE:CD1	2.54	0.43
3:D:1262:GLU:CD	3:D:1269:PRO:CB	2.87	0.43
3:D:637:LEU:O	3:D:639:LEU:O	2.36	0.43
3:D:643:GLY:CA	3:D:727:GLN:HB2	2.49	0.43
3:D:683:ILE:HG22	3:D:684:LYS:N	2.33	0.43
3:D:817:GLU:O	3:D:818:ARG:HB3	2.19	0.43
3:D:836:VAL:HG21	3:D:858:LEU:CD2	2.47	0.43
3:D:940:THR:O	3:D:943:THR:HB	2.19	0.43
1:B:132:GLU:CG	1:B:133:GLU:N	2.82	0.43
2:C:304:LEU:HD23	2:C:305:PRO:HG3	2.01	0.43
2:C:352:ALA:O	2:C:355:VAL:CG1	2.67	0.43
2:C:91:GLN:HE22	2:C:383:ARG:HD2	1.83	0.43
2:C:668:LEU:HD23	2:C:668:LEU:HA	1.79	0.43
2:C:735:ARG:C	2:C:737:LEU:H	2.13	0.43
2:C:754:ILE:HD13	2:C:791:ARG:CG	2.48	0.43
2:C:920:GLU:C	2:C:922:PHE:H	2.22	0.43
2:C:964:LYS:HZ3	2:C:964:LYS:HB2	1.84	0.43
3:D:1291:LEU:HB3	3:D:1306:LEU:HB3	2.00	0.43
3:D:638:LYS:C	3:D:729:HIS:CD2	2.92	0.43
3:D:886:VAL:HG22	3:D:930:LEU:HD11	2.01	0.43
3:D:95:LEU:O	3:D:96:ALA:CB	2.64	0.43
1:A:110:ALA:N	1:A:128:ILE:HG13	2.34	0.43
1:A:157:ILE:HG13	1:A:160:ARG:HG2	2.00	0.43
1:B:16:GLN:HB2	1:B:20:TYR:O	2.19	0.43
1:B:170:PHE:O	1:B:171:SER:OG	2.36	0.43
1:B:86:VAL:HG13	1:B:202:GLY:HA2	2.01	0.43
2:C:304:LEU:HD23	2:C:305:PRO:CD	2.49	0.43
2:C:421:GLU:CG	2:C:423:ALA:H	2.32	0.43
2:C:445:GLU:O	2:C:449:ILE:CD1	2.67	0.43
1:A:83:LYS:NZ	2:C:698:ASP:HB2	2.34	0.43
2:C:710:ILE:CD1	2:C:823:VAL:HB	2.35	0.43
2:C:911:GLU:N	2:C:912:PRO:HD2	2.34	0.43
2:C:918:LEU:O	2:C:920:GLU:O	2.37	0.43
3:D:1033:PRO:O	3:D:1034:GLN:C	2.57	0.43
3:D:1347:ARG:HA	3:D:1347:ARG:HD2	1.87	0.43
3:D:1397:GLU:O	3:D:1400:ASP:HB3	2.18	0.43
1:A:36:LEU:O	1:A:40:LEU:HG	2.19	0.43
1:B:47:SER:O	1:B:48:ILE:HG12	2.19	0.43
2:C:1089:VAL:O	2:C:1093:GLN:HG3	2.18	0.43
2:C:222:LEU:O	2:C:223:ASP:C	2.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:257:LEU:C	2:C:259:GLY:N	2.69	0.43
2:C:290:LEU:HD12	2:C:300:ASP:N	2.34	0.43
2:C:412:ALA:C	2:C:414:GLY:H	2.21	0.43
2:C:801:VAL:CG2	2:C:828:ALA:CB	2.91	0.43
2:C:918:LEU:HD13	2:C:968:ASP:HA	2.00	0.43
3:D:704:ARG:CG	3:D:704:ARG:NH1	2.82	0.43
3:D:861:GLN:O	3:D:862:ASP:CB	2.67	0.43
3:D:882:PHE:C	3:D:884:ARG:N	2.71	0.43
3:D:899:LEU:C	3:D:900:ILE:CG1	2.88	0.43
1:A:217:LEU:HG	1:A:221:LEU:HD23	2.01	0.42
1:B:123:ASN:OD1	1:B:123:ASN:N	2.38	0.42
2:C:1021:LEU:HG	3:D:622:ARG:HG3	2.00	0.42
2:C:1050:GLN:HG2	2:C:1054:THR:OG1	2.19	0.42
2:C:298:PHE:N	2:C:298:PHE:HD1	2.16	0.42
2:C:443:THR:N	2:C:444:PRO:HD2	2.34	0.42
2:C:42:VAL:N	2:C:46:ALA:HB2	2.33	0.42
2:C:706:GLU:CD	2:C:707:ARG:N	2.71	0.42
2:C:731:GLU:C	2:C:733:ALA:N	2.72	0.42
2:C:910:THR:CB	2:C:912:PRO:HD2	2.49	0.42
3:D:1364:LEU:CG	3:D:1365:HIS:H	2.32	0.42
3:D:1102:VAL:HG12	3:D:1375:GLN:HB3	2.01	0.42
3:D:486:ARG:HG3	3:D:487:ALA:H	1.84	0.42
3:D:653:PHE:CD1	3:D:653:PHE:N	2.87	0.42
3:D:795:VAL:CG1	3:D:796:ARG:N	2.82	0.42
1:A:109:ARG:H	1:A:109:ARG:HD2	1.83	0.42
1:A:58:ILE:HG21	1:A:68:ILE:HD13	2.00	0.42
1:B:99:ILE:O	1:B:114:THR:N	2.52	0.42
2:C:21:ILE:O	2:C:335:THR:HG21	2.19	0.42
2:C:225:ALA:O	2:C:229:MET:HG2	2.20	0.42
2:C:360:VAL:HG12	2:C:361:MET:N	2.35	0.42
2:C:394:PHE:O	2:C:395:LYS:CB	2.67	0.42
2:C:414:GLY:C	2:C:419:THR:HG21	2.39	0.42
2:C:549:PHE:O	2:C:550:LEU:C	2.58	0.42
2:C:872:ASN:ND2	2:C:874:LEU:H	2.17	0.42
2:C:6:PHE:CE2	2:C:909:ALA:HA	2.54	0.42
3:D:100:ALA:HB2	3:D:575:GLN:HG3	2.01	0.42
3:D:1195:CYS:SG	3:D:1202:CYS:SG	3.17	0.42
3:D:477:LEU:CD1	3:D:480:GLU:HB3	2.46	0.42
3:D:490:ALA:O	3:D:491:LYS:C	2.58	0.42
3:D:844:ALA:O	3:D:845:ASN:CB	2.67	0.42
3:D:855:HIS:O	3:D:856:GLY:C	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:836:VAL:CG1	3:D:858:LEU:HD21	2.47	0.42
3:D:875:THR:HG22	3:D:876:ASN:O	2.19	0.42
3:D:876:ASN:HD21	3:D:904:VAL:HG21	1.84	0.42
3:D:936:TYR:O	3:D:937:TYR:C	2.57	0.42
1:A:109:ARG:HD3	1:A:112:ASP:OD2	2.20	0.42
1:A:142:ARG:NE	1:A:158:LYS:HE2	2.34	0.42
1:A:153:GLU:O	1:A:155:HIS:N	2.50	0.42
1:A:161:ILE:HG12	1:A:162:ASN:ND2	2.34	0.42
1:A:184:ARG:HE	1:A:193:LYS:CD	2.27	0.42
1:A:95:ARG:HD3	1:A:95:ARG:H	1.84	0.42
1:B:117:ALA:C	1:B:119:VAL:N	2.73	0.42
1:B:159:ASP:O	1:B:161:ILE:O	2.38	0.42
1:B:201:ASP:O	1:B:203:SER:N	2.48	0.42
1:B:198:ILE:HG22	1:B:206:PRO:HB3	2.00	0.42
1:B:76:VAL:CA	1:B:79:ILE:HB	2.46	0.42
2:C:12:VAL:CG1	2:C:13:ILE:HD12	2.49	0.42
2:C:25:SER:O	2:C:26:TYR:C	2.57	0.42
2:C:325:ILE:O	2:C:326:ASP:C	2.57	0.42
2:C:355:VAL:HG13	2:C:356:ARG:H	1.81	0.42
2:C:428:ARG:NH1	3:D:1083:ALA:O	2.53	0.42
2:C:583:LEU:O	2:C:584:GLU:C	2.57	0.42
2:C:688:ILE:CG2	2:C:869:VAL:HG23	2.49	0.42
2:C:858:MET:HE3	2:C:867:VAL:HG23	2.01	0.42
2:C:939:ARG:NH2	2:C:975:TYR:CZ	2.87	0.42
2:C:66:LEU:HD11	2:C:98:LEU:HB3	2.01	0.42
3:D:1061:SER:O	3:D:1063:ARG:N	2.40	0.42
3:D:1060:SER:C	3:D:1062:PHE:H	2.23	0.42
3:D:1063:ARG:CG	3:D:1063:ARG:NH1	2.82	0.42
3:D:1084:ASP:O	3:D:1086:ALA:N	2.51	0.42
3:D:538:SER:O	3:D:539:ASP:C	2.57	0.42
3:D:647:ARG:HA	3:D:647:ARG:HD2	1.82	0.42
3:D:772:PRO:HG3	3:D:778:LEU:CD2	2.49	0.42
3:D:92:HIS:O	3:D:93:ILE:C	2.58	0.42
1:A:104:GLY:N	1:A:135:GLY:HA3	2.34	0.42
1:A:109:ARG:H	1:A:109:ARG:HD3	1.85	0.42
1:A:99:ILE:O	1:A:114:THR:HG22	2.19	0.42
1:A:26:GLU:OE1	1:A:184:ARG:HG3	2.19	0.42
1:B:86:VAL:HG11	1:B:201:ASP:O	2.19	0.42
1:B:47:SER:O	1:B:216:ILE:HD13	2.20	0.42
1:B:82:LEU:HD21	1:B:141:VAL:CG2	2.49	0.42
2:C:181:VAL:O	2:C:182:VAL:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:201:GLY:O	2:C:202:TYR:O	2.37	0.42
2:C:253:ALA:C	2:C:255:ALA:N	2.73	0.42
2:C:497:ALA:HA	2:C:502:PRO:CG	2.45	0.42
2:C:56:GLU:HG2	2:C:57:GLY:N	2.34	0.42
2:C:672:VAL:HG13	2:C:868:ASP:HB2	2.01	0.42
2:C:920:GLU:O	2:C:921:ALA:C	2.58	0.42
3:D:100:ALA:HB1	3:D:579:ASP:OD1	2.19	0.42
3:D:1060:SER:HG	3:D:1068:VAL:CG2	2.32	0.42
3:D:472:LYS:C	3:D:474:GLU:N	2.73	0.42
3:D:554:LEU:O	3:D:558:LEU:HB2	2.19	0.42
3:D:583:ASP:O	3:D:585:GLY:N	2.41	0.42
2:C:1047:HIS:CD2	3:D:754:PHE:CD2	3.07	0.42
3:D:864:VAL:HA	3:D:875:THR:C	2.40	0.42
3:D:696:HIS:HD2	4:E:57:ASP:HB2	1.83	0.42
1:A:186:GLY:O	1:A:187:GLN:HG3	2.19	0.42
1:B:213:ALA:HA	1:B:216:ILE:CG1	2.49	0.42
2:C:232:GLU:O	2:C:233:GLU:C	2.58	0.42
2:C:46:ALA:O	2:C:50:GLU:N	2.42	0.42
2:C:745:ILE:C	2:C:747:ALA:N	2.73	0.42
2:C:920:GLU:CG	2:C:921:ALA:N	2.82	0.42
2:C:969:LEU:HG	2:C:970:GLY:H	1.85	0.42
3:D:1044:GLY:HA3	3:D:1057:PRO:HB2	2.00	0.42
3:D:1070:GLU:C	3:D:1072:PHE:H	2.23	0.42
3:D:1087:LEU:CA	3:D:1090:ALA:HB3	2.49	0.42
3:D:1232:GLU:OE1	3:D:1233:PRO:HG3	2.19	0.42
3:D:485:SER:CB	3:D:488:ARG:HB2	2.49	0.42
3:D:473:LEU:HD23	3:D:503:LEU:HD11	2.02	0.42
3:D:545:ARG:HG2	3:D:546:ARG:N	2.34	0.42
3:D:634:GLY:N	3:D:728:LEU:O	2.47	0.42
3:D:875:THR:HG22	3:D:876:ASN:N	2.33	0.42
3:D:896:ALA:O	3:D:897:GLN:C	2.57	0.42
3:D:970:ARG:NH2	3:D:971:LYS:NZ	2.68	0.42
1:B:158:LYS:HB3	1:B:159:ASP:H	1.55	0.42
1:B:194:LEU:O	1:B:195:THR:CB	2.67	0.42
2:C:1070:ILE:HD12	2:C:1070:ILE:N	2.33	0.42
2:C:197:LEU:HD22	2:C:202:TYR:CD1	2.54	0.42
2:C:100:LEU:CG	2:C:369:PRO:HD3	2.44	0.42
2:C:140:ILE:HG23	2:C:410:ILE:CG2	2.50	0.42
2:C:421:GLU:C	2:C:423:ALA:N	2.73	0.42
2:C:764:GLU:N	2:C:764:GLU:OE1	2.52	0.42
2:C:857:ASP:OD1	2:C:978:ARG:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1084:ASP:C	3:D:1086:ALA:N	2.73	0.42
3:D:1109:ARG:O	3:D:1110:GLU:HB3	2.20	0.42
3:D:129:PHE:O	3:D:130:ASN:CB	2.67	0.42
3:D:1382:VAL:HG23	3:D:1393:GLY:N	2.33	0.42
3:D:557:LEU:HG	3:D:557:LEU:O	2.20	0.42
3:D:730:PRO:O	3:D:732:VAL:N	2.53	0.42
3:D:836:VAL:HG11	3:D:858:LEU:CD1	2.48	0.42
3:D:896:ALA:O	3:D:898:GLU:N	2.52	0.42
3:D:758:GLU:HB3	4:E:20:THR:HG21	2.00	0.42
4:E:50:THR:HG22	4:E:50:THR:O	2.20	0.42
1:A:32:PHE:O	1:A:34:VAL:N	2.53	0.42
1:A:38:ASN:CG	1:A:41:ARG:HH12	2.23	0.42
2:C:317:VAL:N	2:C:318:PRO:CD	2.82	0.42
2:C:609:THR:O	2:C:609:THR:HG22	2.20	0.42
2:C:758:ARG:HG2	2:C:758:ARG:O	2.18	0.42
2:C:935:GLY:O	2:C:936:VAL:O	2.37	0.42
3:D:1021:LEU:HD23	3:D:1021:LEU:HA	1.83	0.42
3:D:1035:GLN:O	3:D:1038:GLN:HB3	2.20	0.42
3:D:1067:THR:O	3:D:1068:VAL:C	2.57	0.42
2:C:493:ARG:NH2	3:D:1070:GLU:CD	2.73	0.42
3:D:1121:VAL:HA	3:D:1122:PRO:HD2	1.92	0.42
3:D:709:HIS:N	3:D:1228:GLU:HB3	2.35	0.42
3:D:1408:LEU:O	3:D:1410:ALA:N	2.53	0.42
3:D:1480:ASP:C	3:D:1482:VAL:H	2.23	0.42
3:D:465:LEU:HB3	3:D:509:PRO:HB2	2.02	0.42
3:D:485:SER:HB3	3:D:488:ARG:HB2	2.01	0.42
3:D:685:ASP:C	3:D:687:VAL:N	2.72	0.42
3:D:643:GLY:HA2	3:D:721:VAL:HG21	2.01	0.42
3:D:639:LEU:HD21	3:D:731:LEU:HB2	2.02	0.42
1:A:103:GLU:C	1:A:135:GLY:HA3	2.40	0.42
1:A:34:VAL:O	1:A:35:THR:C	2.57	0.42
1:B:80:LEU:C	1:B:82:LEU:N	2.73	0.42
2:C:351:LEU:HD11	2:C:373:VAL:HG22	2.00	0.42
2:C:410:ILE:CD1	2:C:468:ARG:HH21	2.31	0.42
2:C:595:LEU:HD21	2:C:623:HIS:CB	2.48	0.42
2:C:611:ILE:HD11	2:C:641:PRO:HA	2.02	0.42
2:C:755:LEU:HD11	2:C:825:VAL:CG1	2.50	0.42
2:C:943:VAL:O	2:C:944:LEU:C	2.56	0.42
3:D:1087:LEU:O	3:D:1087:LEU:HG	2.19	0.42
3:D:1095:LEU:O	3:D:1096:THR:C	2.57	0.42
3:D:1110:GLU:OE2	3:D:1197:THR:HG21	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1476:GLY:C	3:D:1478:GLY:N	2.71	0.42
3:D:462:GLN:O	3:D:465:LEU:N	2.52	0.42
3:D:502:PHE:CG	3:D:507:ASN:ND2	2.87	0.42
3:D:699:VAL:N	3:D:756:GLN:HE22	2.18	0.42
3:D:700:VAL:N	3:D:716:PHE:O	2.46	0.42
3:D:959:GLU:O	3:D:961:LYS:N	2.49	0.42
4:E:13:VAL:HG12	4:E:75:PHE:CZ	2.55	0.42
1:A:108:VAL:HG21	1:A:137:LEU:CD2	2.49	0.42
1:A:16:GLN:HE21	1:A:17:GLY:N	1.91	0.42
1:A:193:LYS:O	1:A:193:LYS:HG2	2.19	0.42
1:A:194:LEU:CG	1:A:195:THR:H	2.31	0.42
1:A:199:TRP:HD1	1:A:200:THR:OG1	2.03	0.42
1:B:105:PRO:O	1:B:106:LYS:HD3	2.19	0.42
1:B:194:LEU:HD22	1:B:194:LEU:HA	1.90	0.42
2:C:1008:ARG:HG2	2:C:1009:SER:N	2.32	0.42
2:C:1075:ASP:OD1	2:C:1076:VAL:N	2.50	0.42
2:C:1091:GLU:OE1	3:D:606:ILE:CG2	2.67	0.42
2:C:1111:ILE:O	2:C:1112:PHE:O	2.37	0.42
2:C:184:MET:SD	2:C:303:PHE:HE2	2.43	0.42
2:C:274:ARG:NE	2:C:275:TYR:CE1	2.88	0.42
2:C:391:LEU:HD12	2:C:391:LEU:HA	1.84	0.42
2:C:474:VAL:O	2:C:526:PRO:HA	2.20	0.42
2:C:692:GLU:O	2:C:693:GLU:C	2.59	0.42
2:C:816:LYS:HB3	2:C:819:VAL:CG2	2.50	0.42
3:D:1170:GLU:O	3:D:1173:HIS:HB2	2.20	0.42
3:D:1200:GLY:C	3:D:1202:CYS:N	2.72	0.42
3:D:1294:PHE:HA	3:D:1302:LYS:O	2.19	0.42
3:D:1279:ASP:CA	3:D:1318:ASP:O	2.68	0.42
3:D:1433:LYS:CG	3:D:1434:SER:N	2.83	0.42
3:D:628:ARG:CB	3:D:628:ARG:NH1	2.83	0.42
3:D:691:LEU:HD12	3:D:692:GLU:N	2.35	0.42
3:D:643:GLY:O	3:D:719:VAL:O	2.37	0.42
3:D:772:PRO:CG	3:D:778:LEU:HD22	2.50	0.42
4:E:3:GLU:HB2	4:E:6:ILE:HG12	2.02	0.42
1:A:208:GLU:HB3	1:A:212:GLN:NE2	2.34	0.42
1:A:38:ASN:HA	1:A:178:PHE:CE2	2.55	0.42
1:A:48:ILE:HA	1:A:49:PRO:HD3	1.92	0.42
2:C:1042:ALA:O	3:D:1225:VAL:CG2	2.68	0.42
2:C:1055:ILE:CD1	2:C:1055:ILE:N	2.80	0.42
2:C:224:GLU:C	2:C:226:VAL:H	2.23	0.42
2:C:253:ALA:C	2:C:256:TYR:H	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:384:GLU:O	2:C:388:ARG:HB2	2.20	0.42
2:C:580:MET:O	2:C:581:THR:HB	2.19	0.42
2:C:5:ARG:HG3	2:C:902:ILE:HG21	2.01	0.42
2:C:709:GLU:O	2:C:710:ILE:HG13	2.19	0.42
2:C:872:ASN:ND2	2:C:874:LEU:HB3	2.24	0.42
3:D:1148:ARG:NH1	3:D:1191:SER:HB2	2.29	0.42
3:D:1278:ILE:CD1	3:D:1302:LYS:HD3	2.49	0.42
3:D:496:LEU:O	3:D:500:ARG:HG2	2.20	0.42
3:D:636:GLN:C	3:D:638:LYS:H	2.24	0.42
3:D:638:LYS:O	3:D:639:LEU:CG	2.66	0.42
3:D:631:ILE:CD1	3:D:745:MET:HE2	2.35	0.42
3:D:824:ASN:O	3:D:825:ALA:O	2.38	0.42
3:D:856:GLY:O	3:D:857:LEU:HD22	2.20	0.42
3:D:941:LEU:C	3:D:943:THR:N	2.73	0.42
3:D:954:ASP:O	3:D:955:ALA:CB	2.68	0.42
4:E:9:LEU:C	4:E:11:GLY:H	2.22	0.42
1:B:94:TRP:NE1	1:B:119:VAL:CG2	2.83	0.41
2:C:232:GLU:O	2:C:234:ALA:N	2.52	0.41
2:C:480:THR:HG23	2:C:480:THR:O	2.20	0.41
2:C:541:SER:O	2:C:545:ASN:ND2	2.53	0.41
2:C:581:THR:O	2:C:582:GLY:C	2.58	0.41
2:C:59:LYS:O	2:C:61:LYS:HE2	2.20	0.41
2:C:768:SER:HB2	2:C:769:PRO:CD	2.36	0.41
2:C:792:VAL:HA	2:C:793:PRO:HD2	1.74	0.41
2:C:813:VAL:CG1	2:C:814:GLU:H	2.05	0.41
2:C:755:LEU:HD11	2:C:825:VAL:CB	2.50	0.41
3:D:997:TRP:CE2	3:D:1057:PRO:HG3	2.53	0.41
3:D:500:ARG:HG3	3:D:1389:PRO:HG3	2.02	0.41
3:D:645:PRO:HG2	3:D:724:GLN:HA	2.02	0.41
3:D:662:GLU:OE1	3:D:662:GLU:C	2.58	0.41
3:D:761:ILE:HG22	3:D:762:GLN:N	2.35	0.41
3:D:903:ASP:O	3:D:905:PRO:HD3	2.20	0.41
3:D:905:PRO:O	3:D:906:GLN:CB	2.58	0.41
4:E:38:THR:HG22	4:E:41:GLU:H	1.85	0.41
1:A:15:THR:HG22	1:B:230:SER:H	1.85	0.41
1:A:30:ARG:HH22	1:A:188:ARG:HB3	1.84	0.41
1:A:31:GLY:C	1:A:33:GLY:H	2.23	0.41
1:B:128:ILE:O	1:B:129:ALA:HB2	2.20	0.41
1:B:26:GLU:O	1:B:27:PRO:C	2.58	0.41
2:C:165:LEU:C	2:C:167:LYS:N	2.73	0.41
2:C:257:LEU:HD22	2:C:263:ASP:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:54:ILE:CD1	2:C:355:VAL:HG13	2.50	0.41
2:C:437:ARG:C	2:C:438:ILE:HG12	2.40	0.41
2:C:20:GLU:OE2	2:C:461:VAL:HG22	2.20	0.41
2:C:401:LEU:HD21	2:C:543:ASN:HD22	1.84	0.41
2:C:662:GLU:O	2:C:663:GLU:C	2.57	0.41
2:C:677:MET:CA	2:C:873:PRO:HD3	2.49	0.41
2:C:705:ILE:HD12	2:C:705:ILE:C	2.40	0.41
2:C:787:ASP:C	2:C:787:ASP:OD1	2.58	0.41
2:C:841:ASN:ND2	2:C:843:HIS:H	2.17	0.41
2:C:910:THR:O	2:C:913:GLU:N	2.53	0.41
3:D:1337:LEU:HB2	3:D:1345:VAL:HG21	2.02	0.41
3:D:1463:LEU:C	3:D:1465:GLU:N	2.73	0.41
3:D:452:ILE:O	3:D:453:ASP:C	2.57	0.41
3:D:789:LEU:HD23	3:D:789:LEU:HA	1.69	0.41
3:D:853:VAL:HG22	3:D:858:LEU:HB2	2.02	0.41
3:D:896:ALA:HA	3:D:899:LEU:CD2	2.50	0.41
3:D:92:HIS:O	3:D:94:GLU:N	2.53	0.41
4:E:48:MET:HB3	4:E:55:TYR:O	2.20	0.41
1:A:58:ILE:HG21	1:A:68:ILE:HD11	2.02	0.41
1:A:64:GLU:CG	1:A:65:PHE:H	2.33	0.41
1:A:64:GLU:OE2	1:A:76:VAL:HG13	2.20	0.41
2:C:184:MET:HB3	2:C:191:PHE:CE2	2.55	0.41
2:C:202:TYR:O	2:C:203:ASP:CB	2.68	0.41
2:C:614:ARG:NH2	2:C:623:HIS:CE1	2.88	0.41
2:C:69:LEU:HB3	2:C:70:GLU:H	1.54	0.41
2:C:722:ILE:HA	2:C:758:ARG:CB	2.48	0.41
2:C:841:ASN:C	2:C:841:ASN:ND2	2.71	0.41
2:C:903:SER:CB	2:C:909:ALA:HB2	2.48	0.41
3:D:1141:ILE:O	3:D:1145:LEU:N	2.46	0.41
3:D:1144:GLY:C	3:D:1145:LEU:HD23	2.41	0.41
3:D:492:ALA:O	3:D:493:ARG:C	2.59	0.41
3:D:563:PRO:O	3:D:564:GLU:HB3	2.20	0.41
3:D:575:GLN:O	3:D:578:VAL:HB	2.20	0.41
3:D:636:GLN:HB3	3:D:641:GLN:HB2	2.01	0.41
2:C:1071:ILE:O	3:D:659:LYS:HG2	2.20	0.41
3:D:953:ASP:O	3:D:953:ASP:OD1	2.37	0.41
4:E:82:GLU:HA	4:E:85:LEU:HB3	2.02	0.41
1:A:103:GLU:N	1:A:106:LYS:HE2	2.34	0.41
1:A:18:ASP:O	1:A:19:HIS:CB	2.68	0.41
1:A:99:ILE:HG23	1:A:138:TYR:CE1	2.55	0.41
1:B:142:ARG:O	1:B:143:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:101:ILE:CG2	2:C:102:HIS:N	2.69	0.41
2:C:103:LYS:HD3	2:C:103:LYS:HA	1.87	0.41
2:C:1054:THR:HG21	2:C:1079:PRO:HB3	2.02	0.41
2:C:224:GLU:O	2:C:226:VAL:N	2.53	0.41
2:C:233:GLU:OE2	2:C:237:ARG:NE	2.52	0.41
2:C:159:ILE:CD1	2:C:310:LEU:HB2	2.50	0.41
2:C:54:ILE:CD1	2:C:359:MET:HE2	2.50	0.41
2:C:367:LEU:CD1	2:C:372:LEU:HG	2.50	0.41
2:C:419:THR:O	2:C:420:ARG:C	2.58	0.41
2:C:44:ILE:CD1	2:C:44:ILE:H	2.28	0.41
2:C:468:ARG:HD3	2:C:468:ARG:H	1.80	0.41
2:C:52:PHE:O	2:C:53:PRO:C	2.56	0.41
2:C:32:ALA:CB	2:C:73:ILE:HD13	2.43	0.41
3:D:1156:ALA:CB	3:D:1183:GLU:HB3	2.48	0.41
3:D:1232:GLU:C	3:D:1234:GLY:N	2.73	0.41
3:D:1252:ASP:HB2	3:D:1270:LYS:HZ3	1.83	0.41
3:D:1281:VAL:CG1	3:D:1282:VAL:H	2.32	0.41
3:D:1479:SER:O	3:D:1480:ASP:C	2.59	0.41
3:D:643:GLY:HA3	3:D:727:GLN:HB2	2.01	0.41
3:D:794:GLN:O	3:D:795:VAL:HB	2.21	0.41
3:D:841:PHE:O	3:D:845:ASN:N	2.44	0.41
3:D:855:HIS:O	3:D:857:LEU:N	2.53	0.41
3:D:899:LEU:N	3:D:899:LEU:HD13	2.35	0.41
1:A:168:ALA:O	1:A:169:ILE:HD13	2.20	0.41
1:A:41:ARG:O	1:A:41:ARG:HD2	2.20	0.41
1:B:64:GLU:HG3	1:B:79:ILE:HG13	2.02	0.41
2:C:148:PHE:CE2	2:C:159:ILE:HG23	2.56	0.41
2:C:149:THR:HG23	2:C:323:ASP:HA	2.03	0.41
2:C:142:ARG:NE	2:C:324:ASP:HA	2.23	0.41
2:C:34:VAL:CG1	2:C:35:PRO:N	2.83	0.41
2:C:129:ILE:HD11	2:C:386:PHE:CD2	2.56	0.41
2:C:743:VAL:CG2	2:C:755:LEU:O	2.66	0.41
2:C:758:ARG:CG	2:C:758:ARG:NH1	2.83	0.41
2:C:703:ILE:HG13	2:C:830:LYS:HG3	2.01	0.41
3:D:1015:ASN:O	3:D:1016:TYR:CD2	2.73	0.41
3:D:1135:LEU:N	3:D:1135:LEU:HD23	2.29	0.41
3:D:492:ALA:O	3:D:495:ARG:N	2.54	0.41
3:D:516:ALA:O	3:D:517:VAL:HG13	2.21	0.41
3:D:590:PRO:HA	3:D:600:LEU:CD2	2.50	0.41
3:D:666:PHE:O	3:D:667:ALA:O	2.38	0.41
1:B:72:LYS:HB3	1:B:130:THR:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:VAL:HA	1:B:143:VAL:HA	2.02	0.41
2:C:284:GLY:O	2:C:285:LEU:HB2	2.19	0.41
2:C:200:LEU:HD13	2:C:300:ASP:HB3	2.03	0.41
2:C:394:PHE:HB3	2:C:395:LYS:H	1.52	0.41
2:C:577:PRO:HA	2:C:671:ASN:ND2	2.36	0.41
2:C:613:VAL:O	2:C:614:ARG:C	2.58	0.41
2:C:750:LYS:HE2	2:C:753:ASP:OD1	2.21	0.41
3:D:1119:ILE:CD1	3:D:1119:ILE:N	2.81	0.41
3:D:1386:GLY:C	3:D:1388:SER:N	2.74	0.41
3:D:1467:VAL:O	3:D:1468:ILE:C	2.59	0.41
3:D:663:GLU:O	3:D:665:ALA:N	2.53	0.41
3:D:930:LEU:HD11	3:D:934:LEU:HD11	2.02	0.41
4:E:91:ARG:C	4:E:92:LEU:HD12	2.41	0.41
1:A:181:GLU:OE2	2:C:934:PHE:CD2	2.73	0.41
1:B:94:TRP:HE1	1:B:119:VAL:HG21	1.84	0.41
1:B:149:TYR:HE1	1:B:169:ILE:CG2	2.17	0.41
1:B:205:THR:OG1	1:B:208:GLU:HB2	2.21	0.41
2:C:278:GLU:HG3	2:C:284:GLY:N	2.35	0.41
2:C:755:LEU:HD11	2:C:825:VAL:HG11	2.03	0.41
2:C:840:ALA:CA	2:C:846:LYS:HA	2.50	0.41
3:D:1120:SER:HB3	3:D:1186:GLU:HB3	2.03	0.41
3:D:1458:ASP:OD1	3:D:1458:ASP:O	2.39	0.41
3:D:590:PRO:CA	3:D:600:LEU:HD21	2.50	0.41
3:D:732:VAL:O	3:D:733:CYS:C	2.59	0.41
3:D:734:GLU:O	3:D:735:ALA:C	2.57	0.41
1:B:170:PHE:C	1:B:171:SER:OG	2.59	0.41
1:B:94:TRP:NE1	1:B:96:THR:HG23	2.36	0.41
2:C:271:GLU:O	2:C:272:ALA:CB	2.68	0.41
2:C:285:LEU:HD11	2:C:302:VAL:HG22	2.01	0.41
2:C:555:ALA:O	2:C:558:ALA:HB3	2.21	0.41
2:C:565:GLN:HB2	2:C:995:MET:CE	2.50	0.41
2:C:610:ARG:O	2:C:612:ALA:N	2.53	0.41
2:C:649:VAL:CB	2:C:653:ASP:HB3	2.50	0.41
2:C:684:PHE:O	2:C:686:ASP:N	2.54	0.41
2:C:701:THR:HA	2:C:832:LYS:HA	2.03	0.41
2:C:773:LEU:O	2:C:774:LEU:C	2.59	0.41
2:C:845:ASN:HD21	2:C:876:VAL:CG1	2.33	0.41
1:A:42:ARG:HH12	2:C:857:ASP:CG	2.24	0.41
3:D:1068:VAL:C	3:D:1070:GLU:H	2.22	0.41
3:D:1102:VAL:HG22	3:D:1425:VAL:O	2.21	0.41
3:D:1119:ILE:HG22	3:D:1120:SER:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1146:TYR:HD2	3:D:1147:GLY:H	1.68	0.41
3:D:1222:VAL:O	3:D:1223:GLY:C	2.59	0.41
3:D:1479:SER:O	3:D:1481:PHE:N	2.54	0.41
3:D:630:VAL:HG12	3:D:631:ILE:O	2.20	0.41
3:D:633:VAL:N	3:D:740:PHE:CE2	2.89	0.41
3:D:772:PRO:HD2	3:D:777:PRO:HA	2.03	0.41
4:E:6:ILE:HG22	4:E:7:ASP:N	2.36	0.41
1:A:175:ARG:NH2	1:A:199:TRP:CH2	2.89	0.41
1:B:108:VAL:HB	1:B:129:ALA:O	2.21	0.41
2:C:1114:GLY:O	2:C:1115:LEU:HB2	2.20	0.41
2:C:399:ASN:ND2	2:C:399:ASN:O	2.53	0.41
2:C:15:LEU:CD1	2:C:461:VAL:HG11	2.50	0.41
2:C:613:VAL:HG21	2:C:619:ARG:CD	2.50	0.41
2:C:635:THR:HG23	2:C:635:THR:O	2.20	0.41
2:C:676:ILE:HG22	2:C:677:MET:N	2.36	0.41
2:C:744:ARG:O	2:C:747:ALA:CB	2.69	0.41
2:C:95:TYR:HB3	2:C:113:VAL:O	2.21	0.41
2:C:915:LYS:CD	2:C:968:ASP:HB3	2.38	0.41
3:D:1212:MET:O	3:D:1213:ALA:HB3	2.20	0.41
3:D:127:LEU:HA	3:D:456:MET:CB	2.38	0.41
3:D:1282:VAL:HG22	3:D:1315:LYS:CB	2.51	0.41
3:D:1438:ALA:O	3:D:1441:PHE:HB2	2.21	0.41
3:D:1494:LYS:O	3:D:1496:ILE:N	2.53	0.41
1:B:80:LEU:HD13	3:D:839:LEU:HA	2.03	0.41
1:A:11:PHE:HZ	1:A:210:LEU:HD21	1.86	0.41
1:A:19:HIS:H	1:A:206:PRO:CD	2.33	0.41
1:B:40:LEU:N	1:B:40:LEU:CD2	2.84	0.41
2:C:11:GLU:HB3	2:C:534:VAL:HG12	2.03	0.41
2:C:332:ARG:NH1	2:C:465:GLY:O	2.51	0.41
2:C:547:ILE:O	2:C:547:ILE:HG22	2.20	0.41
2:C:576:ALA:HB3	2:C:900:ARG:HH11	1.86	0.41
2:C:924:LEU:O	2:C:925:TYR:C	2.59	0.41
2:C:994:ILE:N	2:C:994:ILE:HD13	2.36	0.41
3:D:633:VAL:HA	3:D:740:PHE:CZ	2.56	0.41
3:D:865:THR:O	3:D:866:THR:C	2.58	0.41
3:D:8:VAL:O	3:D:1435:TRP:CZ3	2.74	0.41
3:D:976:GLU:OE1	3:D:989:ARG:NH2	2.54	0.41
4:E:92:LEU:HD12	4:E:92:LEU:N	2.36	0.41
1:A:89:PHE:CB	1:A:145:ARG:NH2	2.84	0.41
1:A:41:ARG:HD3	1:A:176:VAL:O	2.21	0.41
1:A:80:LEU:HA	1:A:83:LYS:HE3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:363:SER:HB3	2:C:366:THR:CB	2.49	0.41
2:C:378:LEU:N	2:C:378:LEU:HD12	2.36	0.41
2:C:642:ARG:HB3	2:C:656:ALA:H	1.86	0.41
2:C:73:ILE:HD12	2:C:94:LEU:HD13	2.03	0.41
2:C:870:ILE:HD13	2:C:870:ILE:HA	1.80	0.41
2:C:892:LEU:HA	2:C:895:TYR:CB	2.50	0.41
2:C:905:VAL:O	2:C:906:PHE:HB2	2.21	0.41
2:C:915:LYS:NZ	3:D:952:ILE:HD11	2.36	0.41
3:D:1066:LEU:O	3:D:1066:LEU:HD12	2.21	0.41
3:D:1367:LYS:O	3:D:1369:ILE:N	2.54	0.41
3:D:1334:HIS:CE1	3:D:1422:LEU:HB3	2.55	0.41
3:D:482:LYS:HD3	3:D:492:ALA:CB	2.51	0.41
3:D:642:CYS:HB2	3:D:716:PHE:HB2	2.03	0.41
3:D:876:ASN:O	3:D:877:PRO:C	2.59	0.41
3:D:924:MET:N	4:E:7:ASP:OD2	2.54	0.41
4:E:34:ARG:O	4:E:35:PHE:CB	2.69	0.41
1:A:12:THR:O	1:A:13:ALA:HB2	2.21	0.40
1:A:21:GLY:O	1:A:23:PHE:CE2	2.75	0.40
1:B:78:ILE:CD1	1:B:129:ALA:HB2	2.51	0.40
1:B:157:ILE:O	1:B:158:LYS:C	2.59	0.40
1:B:29:GLU:OE1	1:B:188:ARG:NH2	2.54	0.40
2:C:1036:GLU:CD	2:C:1036:GLU:N	2.75	0.40
2:C:1052:MET:HG3	3:D:623:VAL:HG22	2.02	0.40
2:C:181:VAL:CG1	2:C:182:VAL:H	2.30	0.40
2:C:252:LYS:NZ	2:C:293:PHE:H	2.18	0.40
2:C:467:ILE:CG2	2:C:484:VAL:HG21	2.47	0.40
2:C:603:VAL:HG22	2:C:646:GLY:O	2.21	0.40
2:C:648:ARG:CG	2:C:648:ARG:NH1	2.82	0.40
2:C:578:VAL:HG23	2:C:671:ASN:ND2	2.36	0.40
2:C:874:LEU:O	2:C:875:GLY:C	2.59	0.40
2:C:880:MET:C	2:C:881:ASN:ND2	2.75	0.40
2:C:969:LEU:HD12	3:D:950:ILE:HG21	2.03	0.40
3:D:961:LYS:NZ	3:D:1042:MET:HB3	2.36	0.40
3:D:1097:ARG:NH1	3:D:1097:ARG:CG	2.81	0.40
3:D:521:PRO:O	3:D:523:ASP:N	2.53	0.40
3:D:603:LEU:HA	3:D:606:ILE:CD1	2.50	0.40
3:D:653:PHE:O	3:D:656:PHE:HB2	2.21	0.40
3:D:721:VAL:CG1	3:D:722:GLU:N	2.61	0.40
3:D:797:LYS:C	3:D:798:GLU:HG2	2.41	0.40
3:D:928:ALA:O	3:D:931:LEU:HB2	2.21	0.40
1:A:142:ARG:HD2	1:A:158:LYS:HE3	2.01	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:VAL:O	1:B:71:VAL:HG12	2.20	0.40
1:B:56:VAL:HG21	1:B:82:LEU:CD2	2.51	0.40
2:C:1106:ASP:OD2	3:D:1457:LYS:NZ	2.55	0.40
2:C:200:LEU:HD22	2:C:290:LEU:HD11	2.03	0.40
2:C:266:ARG:NE	2:C:268:ASP:HA	2.36	0.40
2:C:707:ARG:HB3	2:C:826:PHE:HD1	1.87	0.40
2:C:750:LYS:HG2	2:C:753:ASP:OD2	2.21	0.40
2:C:876:VAL:HA	2:C:880:MET:CE	2.50	0.40
2:C:842:ARG:NH2	2:C:887:GLU:CD	2.72	0.40
3:D:1012:PHE:O	3:D:1014:GLU:N	2.54	0.40
3:D:1062:PHE:HA	3:D:1062:PHE:HD1	1.76	0.40
2:C:1099:VAL:HA	3:D:10:ILE:HA	2.02	0.40
3:D:1175:LEU:HD23	3:D:1175:LEU:HA	1.92	0.40
3:D:1337:LEU:HD22	3:D:1422:LEU:HD12	2.03	0.40
3:D:1458:ASP:C	3:D:1460:LEU:N	2.73	0.40
3:D:14:SER:C	3:D:17:LYS:H	2.23	0.40
3:D:543:LEU:HB3	3:D:581:VAL:CG2	2.51	0.40
3:D:583:ASP:C	3:D:585:GLY:H	2.23	0.40
3:D:879:ARG:HD2	3:D:904:VAL:N	2.36	0.40
1:A:63:HIS:CD2	1:A:164:ILE:HG22	2.56	0.40
1:A:148:GLY:O	1:A:170:PHE:HB2	2.22	0.40
1:A:180:VAL:O	1:A:180:VAL:HG12	2.22	0.40
1:A:21:GLY:O	1:A:23:PHE:CD2	2.75	0.40
1:A:90:LEU:HD21	1:A:120:GLU:OE2	2.22	0.40
1:B:20:TYR:HE2	1:B:197:ARG:HB3	1.86	0.40
2:C:142:ARG:CZ	2:C:147:TYR:HE1	2.35	0.40
2:C:187:ASN:OD1	2:C:188:LYS:N	2.46	0.40
2:C:209:ARG:O	2:C:210:GLU:HB2	2.21	0.40
2:C:30:LEU:O	2:C:32:ALA:N	2.54	0.40
2:C:536:PRO:O	2:C:538:GLN:HG2	2.22	0.40
2:C:552:HIS:NE2	2:C:886:LEU:CD1	2.82	0.40
2:C:605:LYS:CG	2:C:607:ASP:H	2.20	0.40
2:C:609:THR:CG2	2:C:609:THR:O	2.70	0.40
2:C:756:VAL:H	2:C:790:LEU:HB3	1.87	0.40
2:C:813:VAL:HG12	2:C:815:LEU:CD1	2.51	0.40
2:C:811:PRO:O	2:C:813:VAL:N	2.54	0.40
2:C:837:ASP:HB3	2:C:1000:MET:HA	2.03	0.40
2:C:875:GLY:O	2:C:877:PRO:N	2.54	0.40
2:C:987:ILE:C	3:D:948:ILE:HG21	2.41	0.40
2:C:839:LEU:HD12	2:C:994:ILE:HG21	2.01	0.40
2:C:998:TYR:O	2:C:998:TYR:CG	2.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1006:GLN:O	3:D:1010:ASN:HB3	2.22	0.40
3:D:1102:VAL:HG11	3:D:1425:VAL:HG22	2.03	0.40
3:D:1197:THR:O	3:D:1199:TYR:N	2.54	0.40
3:D:1282:VAL:HG13	3:D:1314:VAL:O	2.21	0.40
3:D:1403:ALA:HB1	3:D:1416:VAL:HG21	2.03	0.40
3:D:1403:ALA:CB	3:D:1416:VAL:HG11	2.52	0.40
3:D:586:ARG:C	3:D:588:GLY:H	2.24	0.40
3:D:645:PRO:HD2	3:D:648:MET:HG2	2.03	0.40
3:D:767:HIS:HE1	4:E:2:ALA:HB1	1.84	0.40
3:D:973:ARG:C	3:D:975:ILE:N	2.75	0.40
4:E:5:GLY:O	4:E:9:LEU:HG	2.21	0.40
1:A:179:GLN:HG3	2:C:934:PHE:CG	2.55	0.40
1:A:216:ILE:HG22	1:A:220:HIS:HD2	1.86	0.40
1:A:64:GLU:HG3	1:A:65:PHE:H	1.86	0.40
1:A:77:GLU:O	1:A:80:LEU:N	2.55	0.40
1:B:178:PHE:CG	1:B:178:PHE:O	2.74	0.40
1:B:194:LEU:O	1:B:195:THR:OG1	2.34	0.40
1:B:40:LEU:H	1:B:40:LEU:CD2	2.34	0.40
1:B:40:LEU:HD12	1:B:214:VAL:HG22	2.04	0.40
2:C:1107:ASN:OD1	2:C:1107:ASN:O	2.39	0.40
2:C:124:ASP:OD1	2:C:124:ASP:C	2.60	0.40
2:C:171:TRP:CE3	2:C:171:TRP:HA	2.57	0.40
2:C:32:ALA:C	2:C:34:VAL:N	2.73	0.40
2:C:580:MET:HB3	2:C:584:GLU:OE1	2.22	0.40
2:C:629:ALA:O	2:C:705:ILE:HG12	2.21	0.40
2:C:686:ASP:N	2:C:686:ASP:OD1	2.54	0.40
2:C:691:SER:HB2	2:C:858:MET:HE2	2.03	0.40
2:C:729:LEU:O	2:C:734:LEU:HG	2.20	0.40
2:C:760:SER:N	2:C:785:VAL:HG22	2.37	0.40
2:C:79:SER:O	2:C:80:GLN:C	2.58	0.40
1:B:30:ARG:CZ	2:C:854:PRO:HB3	2.52	0.40
2:C:976:ASP:C	2:C:978:ARG:N	2.74	0.40
3:D:964:TYR:HE2	3:D:1003:LYS:HB3	1.86	0.40
3:D:1446:HIS:CD2	3:D:1446:HIS:C	2.94	0.40
3:D:1458:ASP:OD1	3:D:1460:LEU:HA	2.22	0.40
3:D:477:LEU:O	3:D:478:LEU:C	2.59	0.40
2:C:684:PHE:HB3	3:D:633:VAL:HG21	2.03	0.40
3:D:806:PHE:H	3:D:827:ILE:CA	2.31	0.40
3:D:841:PHE:C	3:D:843:PHE:H	2.25	0.40
3:D:879:ARG:HH11	3:D:904:VAL:CA	2.17	0.40
3:D:990:TYR:CE1	3:D:994:ILE:HD11	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:97:GLU:C	4:E:98:GLU:HG3	2.42	0.40
1:A:109:ARG:HA	1:A:128:ILE:H	1.87	0.40
1:A:31:GLY:H	1:A:192:ASP:CG	2.23	0.40
1:A:64:GLU:CG	1:A:65:PHE:N	2.84	0.40
2:C:1108:PRO:HB3	3:D:3:LYS:NZ	2.37	0.40
2:C:127:PHE:CE2	2:C:386:PHE:CE2	3.10	0.40
2:C:196:LEU:CD1	2:C:200:LEU:HD21	2.50	0.40
2:C:508:ILE:HA	2:C:517:ARG:O	2.21	0.40
2:C:565:GLN:CG	2:C:565:GLN:O	2.69	0.40
2:C:612:ALA:O	2:C:613:VAL:O	2.40	0.40
3:D:1135:LEU:O	3:D:1135:LEU:HG	2.21	0.40
3:D:1156:ALA:HB1	3:D:1183:GLU:CB	2.46	0.40
3:D:1283:ARG:CG	3:D:1283:ARG:NH1	2.82	0.40
3:D:1443:ASN:OD1	3:D:1443:ASN:N	2.54	0.40
3:D:23:TYR:O	3:D:24:GLY:C	2.59	0.40
3:D:573:MET:O	3:D:574:LEU:C	2.58	0.40
3:D:669:ASN:CG	3:D:671:LYS:HG2	2.41	0.40
3:D:806:PHE:N	3:D:827:ILE:HA	2.30	0.40
3:D:934:LEU:HA	3:D:934:LEU:HD23	1.86	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	221/313 (71%)	98 (44%)	68 (31%)	55 (25%)	0	0
1	B	227/313 (72%)	109 (48%)	61 (27%)	57 (25%)	0	0
2	C	1111/1119 (99%)	559 (50%)	300 (27%)	252 (23%)	0	0
3	D	1127/1265 (89%)	543 (48%)	319 (28%)	265 (24%)	0	0
4	E	96/99 (97%)	49 (51%)	22 (23%)	25 (26%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2782/3109 (90%)	1358 (49%)	770 (28%)	654 (24%)	<b>0</b> <b>0</b>

All (654) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	26	GLU
1	A	59	GLU
1	A	64	GLU
1	A	73	GLU
1	A	75	VAL
1	A	108	VAL
1	A	110	ALA
1	A	114	THR
1	A	143	VAL
1	A	157	ILE
1	A	160	ARG
1	A	161	ILE
1	A	195	THR
1	A	200	THR
1	A	223	TYR
1	B	15	THR
1	B	26	GLU
1	B	47	SER
1	B	59	GLU
1	B	61	VAL
1	B	63	HIS
1	B	66	SER
1	B	91	ASP
1	B	92	PRO
1	B	94	TRP
1	B	95	ARG
1	B	118	ASP
1	B	157	ILE
1	B	160	ARG
1	B	187	GLN
1	B	189	THR
1	B	194	LEU
1	B	195	THR
2	C	10	ARG
2	C	18	LEU
2	C	31	GLN
2	C	32	ALA

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Mol	Chain	Res	Type
2	C	42	VAL
2	C	81	ASP
2	C	105	THR
2	C	149	THR
2	C	153	ALA
2	C	155	PRO
2	C	164	PRO
2	C	181	VAL
2	C	182	VAL
2	C	202	TYR
2	C	210	GLU
2	C	216	ASP
2	C	258	PHE
2	C	261	LEU
2	C	271	GLU
2	C	283	VAL
2	C	322	VAL
2	C	326	ASP
2	C	360	VAL
2	C	361	MET
2	C	375	SER
2	C	388	ARG
2	C	394	PHE
2	C	395	LYS
2	C	402	SER
2	C	425	PHE
2	C	426	ASP
2	C	431	HIS
2	C	438	ILE
2	C	440	PRO
2	C	444	PRO
2	C	449	ILE
2	C	457	ALA
2	C	458	TYR
2	C	461	VAL
2	C	462	ASP
2	C	467	ILE
2	C	468	ARG
2	C	480	THR
2	C	488	ALA
2	C	495	THR
2	C	502	PRO

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Mol	Chain	Res	Type
2	C	513	VAL
2	C	516	ARG
2	C	517	ARG
2	C	520	GLU
2	C	524	VAL
2	C	526	PRO
2	C	529	VAL
2	C	537	LYS
2	C	564	MET
2	C	568	ALA
2	C	569	VAL
2	C	573	ARG
2	C	575	GLN
2	C	600	ASP
2	C	605	LYS
2	C	613	VAL
2	C	643	VAL
2	C	648	ARG
2	C	657	ASP
2	C	659	PRO
2	C	663	GLU
2	C	677	MET
2	C	680	ASP
2	C	715	THR
2	C	731	GLU
2	C	732	ALA
2	C	734	LEU
2	C	762	LYS
2	C	764	GLU
2	C	777	ILE
2	C	796	GLU
2	C	800	VAL
2	C	811	PRO
2	C	814	GLU
2	C	837	ASP
2	C	840	ALA
2	C	876	VAL
2	C	881	ASN
2	C	907	ASP
2	C	921	ALA
2	C	936	VAL
2	C	963	LEU

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Mol	Chain	Res	Type
2	C	969	LEU
2	C	972	VAL
2	C	977	GLY
2	C	998	TYR
2	C	1012	PRO
2	C	1025	ALA
2	C	1043	TYR
2	C	1055	ILE
2	C	1059	ASP
2	C	1109	VAL
2	C	1110	ASP
2	C	1112	PHE
3	D	72	VAL
3	D	76	CYS
3	D	78	VAL
3	D	81	THR
3	D	84	ILE
3	D	88	TYR
3	D	93	ILE
3	D	96	ALA
3	D	98	PRO
3	D	99	ALA
3	D	104	PHE
3	D	112	ILE
3	D	113	GLY
3	D	124	GLU
3	D	126	VAL
3	D	132	TYR
3	D	133	ILE
3	D	137	PRO
3	D	453	ASP
3	D	468	LEU
3	D	483	HIS
3	D	486	ARG
3	D	491	LYS
3	D	509	PRO
3	D	511	TRP
3	D	512	MET
3	D	515	GLU
3	D	539	ASP
3	D	582	ILE
3	D	583	ASP

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Mol	Chain	Res	Type
3	D	587	ARG
3	D	602	SER
3	D	617	ASN
3	D	625	TYR
3	D	658	LEU
3	D	705	ALA
3	D	709	HIS
3	D	725	SER
3	D	748	HIS
3	D	753	SER
3	D	773	ALA
3	D	774	SER
3	D	783	ARG
3	D	795	VAL
3	D	798	GLU
3	D	800	LYS
3	D	802	ALA
3	D	817	GLU
3	D	828	VAL
3	D	830	ALA
3	D	840	LYS
3	D	859	ASP
3	D	869	LEU
3	D	875	THR
3	D	892	ASP
3	D	902	MET
3	D	953	ASP
3	D	1016	TYR
3	D	1029	ALA
3	D	1032	ASN
3	D	1053	THR
3	D	1080	LYS
3	D	1110	GLU
3	D	1112	ASP
3	D	1115	THR
3	D	1129	VAL
3	D	1138	ARG
3	D	1197	THR
3	D	1204	LYS
3	D	1207	GLY
3	D	1208	TYR
3	D	1268	ARG

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Mol	Chain	Res	Type
3	D	1280	GLY
3	D	1282	VAL
3	D	1313	LEU
3	D	1314	VAL
3	D	1316	ASP
3	D	1318	ASP
3	D	1321	GLU
3	D	1323	GLY
3	D	1324	GLN
3	D	1330	ALA
3	D	1331	ILE
3	D	1340	LYS
3	D	1345	VAL
3	D	1355	LYS
3	D	1365	HIS
3	D	1443	ASN
3	D	1453	ILE
3	D	1456	LYS
3	D	1489	ASP
4	E	2	ALA
4	E	12	MET
4	E	30	LEU
4	E	38	THR
4	E	42	PRO
4	E	51	LEU
4	E	55	TYR
4	E	56	ASP
4	E	72	ARG
4	E	94	PRO
4	E	95	THR
1	A	11	PHE
1	A	13	ALA
1	A	14	THR
1	A	19	HIS
1	A	20	TYR
1	A	25	LEU
1	A	30	ARG
1	A	47	SER
1	A	78	ILE
1	A	85	LEU
1	A	94	TRP
1	A	104	GLY

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Mol	Chain	Res	Type
1	A	112	ASP
1	A	124	PRO
1	A	127	HIS
1	A	135	GLY
1	A	142	ARG
1	A	152	ALA
1	A	153	GLU
1	A	194	LEU
1	B	5	LYS
1	B	18	ASP
1	B	35	THR
1	B	53	VAL
1	B	62	LEU
1	B	90	LEU
1	B	112	ASP
1	B	117	ALA
1	B	125	ASP
1	B	136	LYS
1	B	137	LEU
1	B	158	LYS
2	C	23	VAL
2	C	33	ASP
2	C	36	PRO
2	C	56	GLU
2	C	66	LEU
2	C	112	GLU
2	C	166	PRO
2	C	168	ARG
2	C	223	ASP
2	C	232	GLU
2	C	266	ARG
2	C	273	GLY
2	C	295	ASP
2	C	309	TYR
2	C	315	ALA
2	C	319	GLY
2	C	336	VAL
2	C	345	ARG
2	C	362	GLY
2	C	386	PHE
2	C	403	SER
2	C	424	GLY

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Mol	Chain	Res	Type
2	C	435	TYR
2	C	439	CYS
2	C	463	ALA
2	C	498	GLN
2	C	505	GLY
2	C	527	GLU
2	C	555	ALA
2	C	582	GLY
2	C	603	VAL
2	C	629	ALA
2	C	700	TYR
2	C	713	ARG
2	C	716	LYS
2	C	729	LEU
2	C	770	GLU
2	C	788	THR
2	C	791	ARG
2	C	812	GLY
2	C	813	VAL
2	C	822	VAL
2	C	857	ASP
2	C	875	GLY
2	C	920	GLU
2	C	970	GLY
2	C	988	VAL
2	C	993	PHE
2	C	1033	GLY
2	C	1057	SER
2	C	1080	SER
2	C	1096	ALA
3	D	22	SER
3	D	26	VAL
3	D	29	PRO
3	D	82	ARG
3	D	85	VAL
3	D	95	LEU
3	D	125	GLN
3	D	129	PHE
3	D	136	ASP
3	D	141	VAL
3	D	142	LEU
3	D	143	ASP

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Mol	Chain	Res	Type
3	D	454	ALA
3	D	466	LYS
3	D	470	LEU
3	D	503	LEU
3	D	505	SER
3	D	507	ASN
3	D	520	LEU
3	D	549	ASN
3	D	584	ASN
3	D	588	GLY
3	D	590	PRO
3	D	613	ARG
3	D	629	SER
3	D	636	GLN
3	D	638	LYS
3	D	680	GLN
3	D	682	ASP
3	D	686	GLU
3	D	711	LEU
3	D	730	PRO
3	D	761	ILE
3	D	784	ASP
3	D	803	GLY
3	D	809	PRO
3	D	816	TYR
3	D	823	LEU
3	D	825	ALA
3	D	827	ILE
3	D	838	ARG
3	D	856	GLY
3	D	861	GLN
3	D	893	GLU
3	D	924	MET
3	D	946	GLY
3	D	996	LEU
3	D	1007	ALA
3	D	1066	LEU
3	D	1067	THR
3	D	1095	LEU
3	D	1103	ALA
3	D	1113	CYS
3	D	1198	ARG

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Mol	Chain	Res	Type
3	D	1201	VAL
3	D	1202	CYS
3	D	1221	ALA
3	D	1256	GLY
3	D	1283	ARG
3	D	1307	PRO
3	D	1311	ARG
3	D	1322	ALA
3	D	1341	GLY
3	D	1427	LYS
3	D	1459	GLU
3	D	1462	GLY
4	E	35	PHE
4	E	64	ALA
1	A	18	ASP
1	A	74	ASP
1	A	93	ARG
1	A	117	ALA
1	A	122	MET
1	A	151	PRO
1	A	178	PHE
1	A	181	GLU
1	B	20	TYR
1	B	60	ASP
1	B	126	LEU
1	B	127	HIS
1	B	135	GLY
1	B	188	ARG
1	B	203	SER
1	B	210	LEU
2	C	9	ILE
2	C	38	LYS
2	C	77	PRO
2	C	187	ASN
2	C	204	GLN
2	C	250	LYS
2	C	285	LEU
2	C	302	VAL
2	C	325	ILE
2	C	380	ALA
2	C	385	PHE
2	C	398	THR

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Mol	Chain	Res	Type
2	C	420	ARG
2	C	428	ARG
2	C	432	ARG
2	C	490	GLU
2	C	499	ALA
2	C	528	GLU
2	C	574	ALA
2	C	581	THR
2	C	589	ARG
2	C	606	VAL
2	C	645	VAL
2	C	685	GLU
2	C	699	PHE
2	C	756	VAL
2	C	768	SER
2	C	769	PRO
2	C	793	PRO
2	C	877	PRO
2	C	964	LYS
2	C	992	MET
2	C	1009	SER
2	C	1020	PRO
2	C	1026	GLN
3	D	11	ALA
3	D	94	GLU
3	D	105	VAL
3	D	153	LEU
3	D	485	SER
3	D	502	PHE
3	D	553	ARG
3	D	599	PRO
3	D	667	ALA
3	D	714	GLN
3	D	722	GLU
3	D	768	ASN
3	D	806	PHE
3	D	808	THR
3	D	824	ASN
3	D	862	ASP
3	D	879	ARG
3	D	897	GLN
3	D	969	ASP

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Mol	Chain	Res	Type
3	D	970	ARG
3	D	1009	PHE
3	D	1131	ARG
3	D	1157	LEU
3	D	1288	GLU
3	D	1315	LYS
3	D	1344	ALA
3	D	1368	HIS
3	D	1475	ALA
3	D	1483	ARG
3	D	1485	THR
3	D	1495	ALA
1	A	9	PRO
1	A	15	THR
1	A	16	GLN
1	B	75	VAL
1	B	115	PRO
1	B	155	HIS
1	B	206	PRO
1	B	229	ALA
2	C	14	PRO
2	C	39	ARG
2	C	231	PRO
2	C	264	PRO
2	C	290	LEU
2	C	308	ARG
2	C	367	LEU
2	C	422	ARG
2	C	469	THR
2	C	506	ASP
2	C	532	MET
2	C	545	ASN
2	C	567	GLN
2	C	596	TYR
2	C	602	GLU
2	C	607	ASP
2	C	743	VAL
2	C	973	VAL
2	C	974	LEU
2	C	978	ARG
2	C	1027	PHE
3	D	75	ARG

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Mol	Chain	Res	Type
3	D	100	ALA
3	D	144	GLY
3	D	538	SER
3	D	657	LEU
3	D	696	HIS
3	D	811	GLU
3	D	890	VAL
3	D	904	VAL
3	D	907	GLU
3	D	954	ASP
3	D	960	GLU
3	D	978	ALA
3	D	1019	ASN
3	D	1104	HIS
3	D	1152	ARG
3	D	1254	THR
3	D	1271	ALA
3	D	1354	GLN
3	D	1441	PHE
3	D	1454	ALA
3	D	1477	THR
4	E	4	PRO
4	E	31	LEU
4	E	39	VAL
4	E	60	ALA
4	E	93	TYR
1	A	171	SER
1	A	175	ARG
1	A	188	ARG
1	A	206	PRO
1	B	36	LEU
1	B	119	VAL
1	B	148	GLY
1	B	151	PRO
1	B	162	ASN
1	B	163	ALA
1	B	172	PRO
1	B	230	SER
2	C	116	GLY
2	C	157	ARG
2	C	203	ASP
2	C	205	GLU

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Mol	Chain	Res	Type
2	C	297	GLU
2	C	443	THR
2	C	460	ARG
2	C	483	VAL
2	C	536	PRO
2	C	556	ASN
2	C	619	ARG
2	C	717	LEU
2	C	858	MET
2	C	859	PRO
2	C	938	LYS
2	C	1035	MET
2	C	1113	GLU
3	D	80	VAL
3	D	127	LEU
3	D	154	THR
3	D	490	ALA
3	D	508	ARG
3	D	639	LEU
3	D	640	HIS
3	D	644	LEU
3	D	668	PRO
3	D	731	LEU
3	D	776	GLU
3	D	799	LYS
3	D	857	LEU
3	D	894	LYS
3	D	984	LEU
3	D	1044	GLY
3	D	1045	LEU
3	D	1085	THR
3	D	1267	ARG
3	D	1329	GLY
3	D	1367	LYS
3	D	1389	PRO
3	D	1415	PRO
4	E	41	GLU
4	E	50	THR
4	E	70	THR
1	A	32	PHE
1	B	71	VAL
1	B	111	VAL

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Mol	Chain	Res	Type
1	B	133	GLU
1	B	192	ASP
2	C	113	VAL
2	C	114	PHE
2	C	156	GLY
2	C	234	ALA
2	C	243	ARG
2	C	304	LEU
2	C	390	GLN
2	C	416	GLY
2	C	535	SER
2	C	1099	VAL
2	C	1107	ASN
3	D	134	VAL
3	D	145	VAL
3	D	544	TYR
3	D	654	LYS
3	D	673	ALA
3	D	864	VAL
3	D	1051	GLY
3	D	1156	ALA
3	D	1253	ILE
3	D	1258	PRO
3	D	1276	SER
3	D	1333	PRO
3	D	1420	PRO
3	D	1425	VAL
3	D	1465	GLU
4	E	28	GLN
4	E	96	GLU
1	A	37	GLY
1	A	204	VAL
1	B	134	GLY
1	B	169	ILE
2	C	12	VAL
2	C	75	ASP
2	C	474	VAL
2	C	894	GLY
2	C	1079	PRO
3	D	109	PRO
3	D	484	PRO
3	D	1108	VAL

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Mol	Chain	Res	Type
3	D	1216	VAL
3	D	1260	VAL
3	D	1320	VAL
3	D	1353	ILE
2	C	501	THR
2	C	855	VAL
3	D	147	VAL
3	D	1409	ILE
3	D	1447	VAL
4	E	71	GLY
1	A	198	ILE
2	C	263	ASP
2	C	376	ARG
2	C	604	VAL
2	C	987	ILE
1	A	33	GLY
2	C	1022	GLY
3	D	772	PRO
3	D	821	VAL
3	D	845	ASN
4	E	80	VAL
2	C	867	VAL
2	C	1077	PRO
3	D	10	ILE
3	D	948	ILE
3	D	994	ILE
3	D	1023	VAL
2	C	17	PRO
2	C	244	PRO

### 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	190/271 (70%)	163 (86%)	27 (14%)	3	17
1	B	191/271 (70%)	171 (90%)	20 (10%)	7	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	869/936 (93%)	747 (86%)	122 (14%)	4	18
3	D	782/1036 (76%)	693 (89%)	89 (11%)	6	25
4	E	67/88 (76%)	64 (96%)	3 (4%)	30	63
All	All	2099/2602 (81%)	1838 (88%)	261 (12%)	5	22

All (261) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	19	HIS
1	A	20	TYR
1	A	25	LEU
1	A	30	ARG
1	A	41	ARG
1	A	47	SER
1	A	57	TYR
1	A	62	LEU
1	A	63	HIS
1	A	95	ARG
1	A	100	LEU
1	A	109	ARG
1	A	112	ASP
1	A	113	PHE
1	A	122	MET
1	A	125	ASP
1	A	142	ARG
1	A	143	VAL
1	A	192	ASP
1	A	194	LEU
1	A	196	LEU
1	A	199	TRP
1	A	201	ASP
1	A	204	VAL
1	A	206	PRO
1	A	221	LEU
1	B	18	ASP
1	B	19	HIS
1	B	36	LEU
1	B	44	LEU
1	B	56	VAL
1	B	57	TYR

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Mol	Chain	Res	Type
1	B	62	LEU
1	B	86	VAL
1	B	89	PHE
1	B	122	MET
1	B	125	ASP
1	B	127	HIS
1	B	131	LEU
1	B	133	GLU
1	B	170	PHE
1	B	171	SER
1	B	187	GLN
1	B	194	LEU
1	B	196	LEU
1	B	220	HIS
2	C	13	ILE
2	C	36	PRO
2	C	54	ILE
2	C	56	GLU
2	C	67	ASP
2	C	70	GLU
2	C	75	ASP
2	C	95	TYR
2	C	115	LEU
2	C	118	LEU
2	C	139	GLN
2	C	142	ARG
2	C	147	TYR
2	C	155	PRO
2	C	171	TRP
2	C	172	ILE
2	C	177	GLU
2	C	198	ARG
2	C	206	THR
2	C	212	SER
2	C	214	TYR
2	C	216	ASP
2	C	232	GLU
2	C	256	TYR
2	C	258	PHE
2	C	261	LEU
2	C	264	PRO
2	C	267	TYR

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Mol	Chain	Res	Type
2	C	285	LEU
2	C	298	PHE
2	C	299	LYS
2	C	303	PHE
2	C	304	LEU
2	C	306	THR
2	C	313	LEU
2	C	324	ASP
2	C	335	THR
2	C	344	PHE
2	C	350	ARG
2	C	356	ARG
2	C	367	LEU
2	C	372	LEU
2	C	391	LEU
2	C	393	GLN
2	C	394	PHE
2	C	399	ASN
2	C	421	GLU
2	C	429	ASP
2	C	434	HIS
2	C	435	TYR
2	C	441	VAL
2	C	443	THR
2	C	448	ASN
2	C	466	PHE
2	C	468	ARG
2	C	502	PRO
2	C	508	ILE
2	C	526	PRO
2	C	534	VAL
2	C	535	SER
2	C	544	THR
2	C	559	LEU
2	C	571	LEU
2	C	579	VAL
2	C	580	MET
2	C	584	GLU
2	C	627	ARG
2	C	630	ARG
2	C	633	GLN
2	C	635	THR

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Mol	Chain	Res	Type
2	C	637	PHE
2	C	672	VAL
2	C	674	VAL
2	C	676	ILE
2	C	680	ASP
2	C	686	ASP
2	C	690	ILE
2	C	693	GLU
2	C	698	ASP
2	C	699	PHE
2	C	710	ILE
2	C	723	THR
2	C	739	GLU
2	C	750	LYS
2	C	755	LEU
2	C	758	ARG
2	C	764	GLU
2	C	770	GLU
2	C	772	ARG
2	C	810	ASP
2	C	834	GLN
2	C	837	ASP
2	C	841	ASN
2	C	846	LYS
2	C	852	ILE
2	C	853	LEU
2	C	861	LEU
2	C	867	VAL
2	C	869	VAL
2	C	873	PRO
2	C	880	MET
2	C	881	ASN
2	C	882	LEU
2	C	892	LEU
2	C	924	LEU
2	C	952	LEU
2	C	964	LYS
2	C	978	ARG
2	C	983	PHE
2	C	1000	MET
2	C	1005	MET
2	C	1010	THR

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Mol	Chain	Res	Type
2	C	1012	PRO
2	C	1015	LEU
2	C	1017	THR
2	C	1018	GLN
2	C	1031	ARG
2	C	1052	MET
2	C	1055	ILE
2	C	1106	ASP
2	C	1112	PHE
2	C	1115	LEU
3	D	462	GLN
3	D	486	ARG
3	D	502	PHE
3	D	509	PRO
3	D	511	TRP
3	D	517	VAL
3	D	550	ARG
3	D	567	ILE
3	D	587	ARG
3	D	601	ARG
3	D	625	TYR
3	D	651	GLU
3	D	652	LEU
3	D	662	GLU
3	D	674	ARG
3	D	688	TRP
3	D	691	LEU
3	D	702	LEU
3	D	722	GLU
3	D	751	LEU
3	D	752	SER
3	D	754	PHE
3	D	770	LEU
3	D	772	PRO
3	D	778	LEU
3	D	791	TYR
3	D	792	ILE
3	D	794	GLN
3	D	834	THR
3	D	860	LEU
3	D	864	VAL
3	D	879	ARG

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Mol	Chain	Res	Type
3	D	899	LEU
3	D	906	GLN
3	D	914	LEU
3	D	925	GLU
3	D	936	TYR
3	D	941	LEU
3	D	948	ILE
3	D	957	ILE
3	D	965	LEU
3	D	969	ASP
3	D	972	LEU
3	D	975	ILE
3	D	984	LEU
3	D	985	THR
3	D	988	GLU
3	D	1001	THR
3	D	1010	ASN
3	D	1012	PHE
3	D	1032	ASN
3	D	1034	GLN
3	D	1035	GLN
3	D	1039	LEU
3	D	1042	MET
3	D	1045	LEU
3	D	1046	MET
3	D	1053	THR
3	D	1058	VAL
3	D	1062	PHE
3	D	1063	ARG
3	D	1066	LEU
3	D	1091	ASP
3	D	1094	TYR
3	D	1104	HIS
3	D	1106	ILE
3	D	1109	ARG
3	D	1124	PHE
3	D	1131	ARG
3	D	1138	ARG
3	D	1167	LEU
3	D	1195	CYS
3	D	1197	THR
3	D	1254	THR

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Mol	Chain	Res	Type
3	D	1265	GLU
3	D	1269	PRO
3	D	1274	VAL
3	D	1282	VAL
3	D	1289	ASP
3	D	1292	SER
3	D	1300	PHE
3	D	1305	LYS
3	D	1316	ASP
3	D	1364	LEU
3	D	1383	THR
3	D	1433	LYS
3	D	1435	TRP
3	D	1445	THR
3	D	1448	LEU
4	E	6	ILE
4	E	7	ASP
4	E	32	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	162	ASN
1	A	179	GLN
1	A	212	GLN
1	A	220	HIS
1	A	226	ASN
1	B	19	HIS
1	B	155	HIS
1	B	187	GLN
1	B	212	GLN
1	B	220	HIS
1	B	222	ASN
2	C	22	GLN
2	C	31	GLN
2	C	91	GLN
2	C	102	HIS
2	C	139	GLN
2	C	374	ASN
2	C	399	ASN
2	C	538	GLN

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Mol	Chain	Res	Type
2	C	543	ASN
2	C	563	ASN
2	C	565	GLN
2	C	623	HIS
2	C	632	ASN
2	C	633	GLN
2	C	671	ASN
2	C	704	HIS
2	C	841	ASN
2	C	843	HIS
2	C	845	ASN
2	C	860	HIS
2	C	872	ASN
2	C	881	ASN
2	C	889	HIS
2	C	991	GLN
2	C	1006	HIS
2	C	1018	GLN
2	C	1026	GLN
2	C	1030	GLN
2	C	1047	HIS
2	C	1064	ASN
2	C	1107	ASN
3	D	507	ASN
3	D	541	ASN
3	D	549	ASN
3	D	551	ASN
3	D	552	ASN
3	D	584	ASN
3	D	636	GLN
3	D	680	GLN
3	D	696	HIS
3	D	727	GLN
3	D	737	ASN
3	D	756	GLN
3	D	762	GLN
3	D	768	ASN
3	D	917	GLN
3	D	977	GLN
3	D	1038	GLN
3	D	1125	GLN
3	D	1354	GLN

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Mol	Chain	Res	Type
3	D	1368	HIS
3	D	1375	GLN
3	D	1442	GLN
3	D	1446	HIS
3	D	1466	ASN
4	E	59	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

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

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

There are no such residues in this entry.



## 5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	D	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	155:ASP	C	2(U):UNK	N	55.17
1	D	46(U):UNK	C	452:ILE	N	46.65
1	D	10(U):UNK	C	20(U):UNK	N	14.79

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.