



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 10:10 PM GMT

PDB ID : 1OFI  
Title : ASYMMETRIC COMPLEX BETWEEN HSLV AND I-DOMAIN DELETED  
HSLU (H. INFLUENZAE)  
Authors : Kwon, A.R.; Kessler, B.M.; Overkleeft, H.S.; Mckay, D.B.  
Deposited on : 2003-04-14  
Resolution : 3.20 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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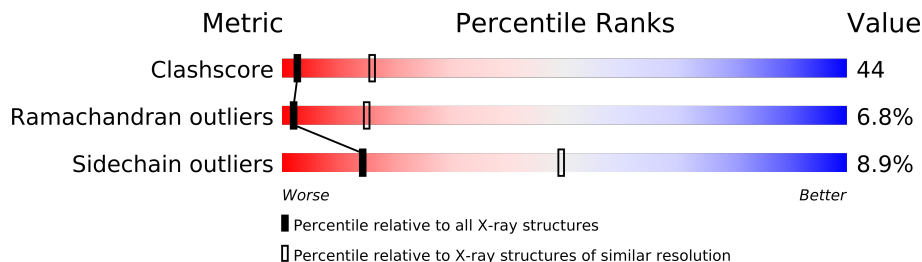
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.20 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	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	310	
1	B	310	
1	C	310	
2	G	174	
2	H	174	
2	I	174	
2	L	174	
2	M	174	
2	N	174	

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 15050 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

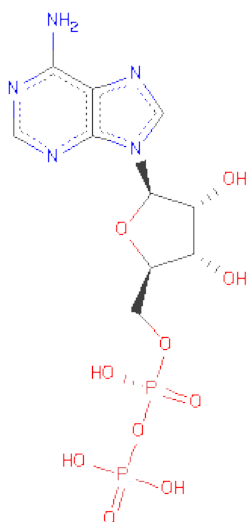
- Molecule 1 is a protein called ATP-DEPENDENT HSL PROTEASE ATP-BINDING SUB-UNIT HSLU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	299	Total	C	N	O	S	0	0	0
			2312	1446	411	446	9			
1	B	295	Total	C	N	O	S	0	0	0
			2284	1430	407	438	9			
1	C	296	Total	C	N	O	S	0	0	0
			2288	1431	407	441	9			

- Molecule 2 is a protein called ATP-DEPENDENT PROTEASE HSLV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	174	Total	C	N	O	S	0	0	1
			1319	826	236	253	4			
2	H	174	Total	C	N	O	S	0	0	1
			1319	826	236	253	4			
2	I	174	Total	C	N	O	S	0	0	1
			1319	826	236	253	4			
2	L	174	Total	C	N	O	S	0	0	1
			1319	826	236	253	4			
2	M	174	Total	C	N	O	S	0	0	1
			1319	826	236	253	4			
2	N	174	Total	C	N	O	S	0	0	1
			1319	826	236	253	4			

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).

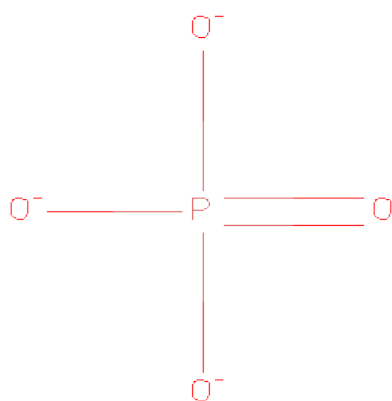


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

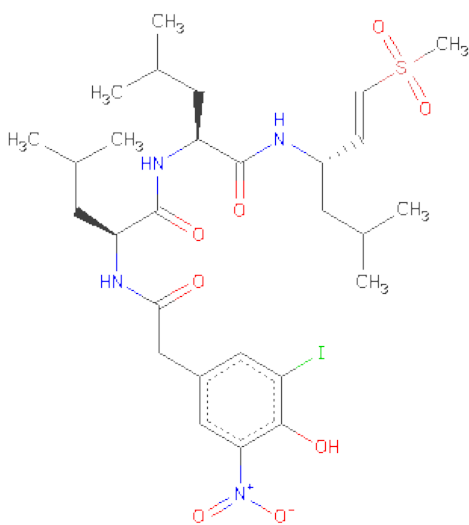
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total	Mg	0	0
			1	1		
4	H	1	Total	Mg	0	0
			1	1		
4	B	2	Total	Mg	0	0
			2	2		
4	I	1	Total	Mg	0	0
			1	1		
4	C	2	Total	Mg	0	0
			2	2		
4	A	2	Total	Mg	0	0
			2	2		
4	N	1	Total	Mg	0	0
			1	1		
4	L	1	Total	Mg	0	0
			1	1		
4	M	1	Total	Mg	0	0
			1	1		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula:  $\text{O}_4\text{P}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			5	4	1		
5	B	1	Total	O	P	0	0
			5	4	1		
5	C	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is 4-iodo-3-nitrophenyl acetyl-leucinyll-leucinyll-leucinyll-vinylsulfone (three-letter code: LVS) (formula:  $\text{C}_{28}\text{H}_{43}\text{IN}_4\text{O}_8\text{S}$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	G	1	Total 41	C 28	N 4	O 8	S 1	0	0
6	H	1	Total 41	C 28	N 4	O 8	S 1	0	0
6	I	1	Total 41	C 28	N 4	O 8	S 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	7	Total 7	O 7	0	0
7	B	7	Total 7	O 7	0	0
7	C	7	Total 7	O 7	0	0

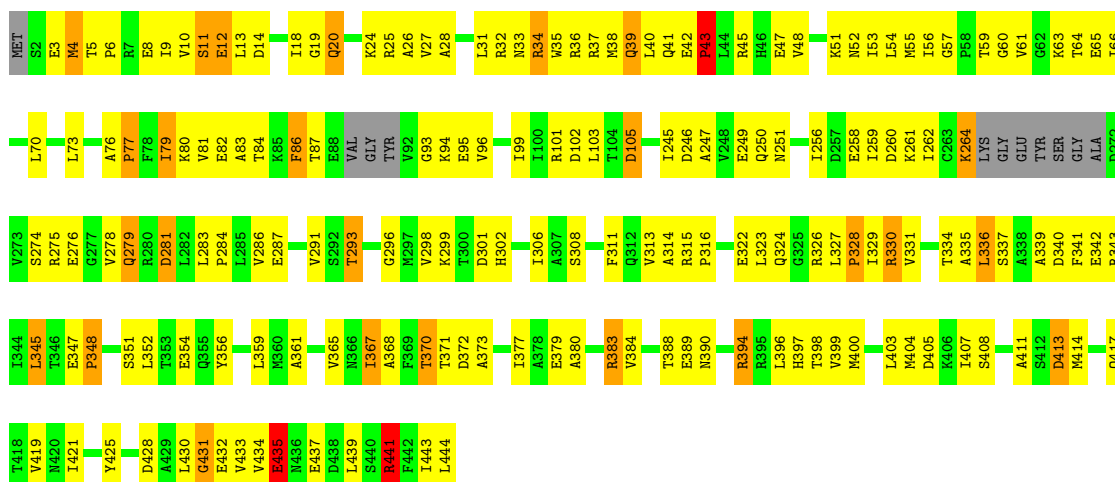
### 3 Residue-property plots

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

Note EDS was not executed.

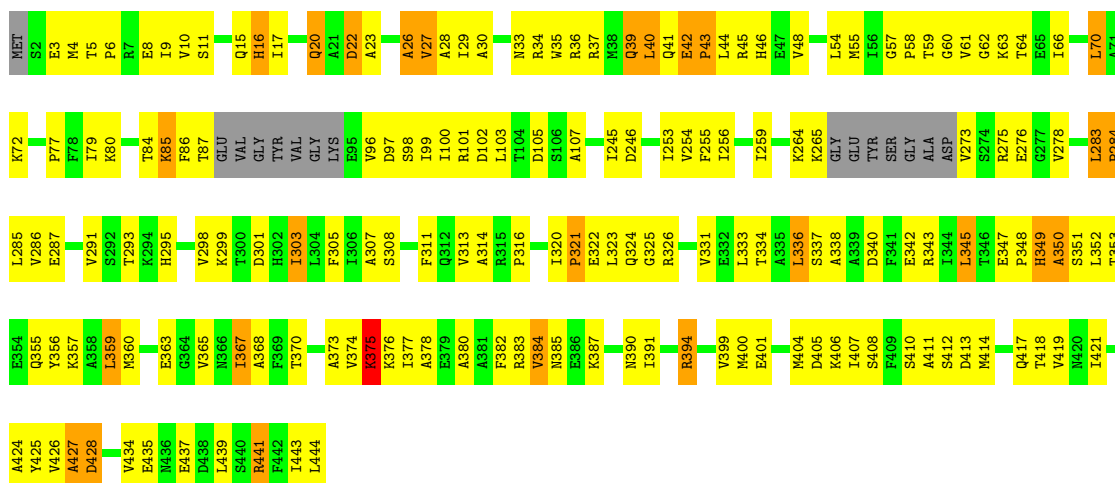
#### • Molecule 1: ATP-DEPENDENT HSL PROTEASE ATP-BINDING SUBUNIT HSLU

Chain A:



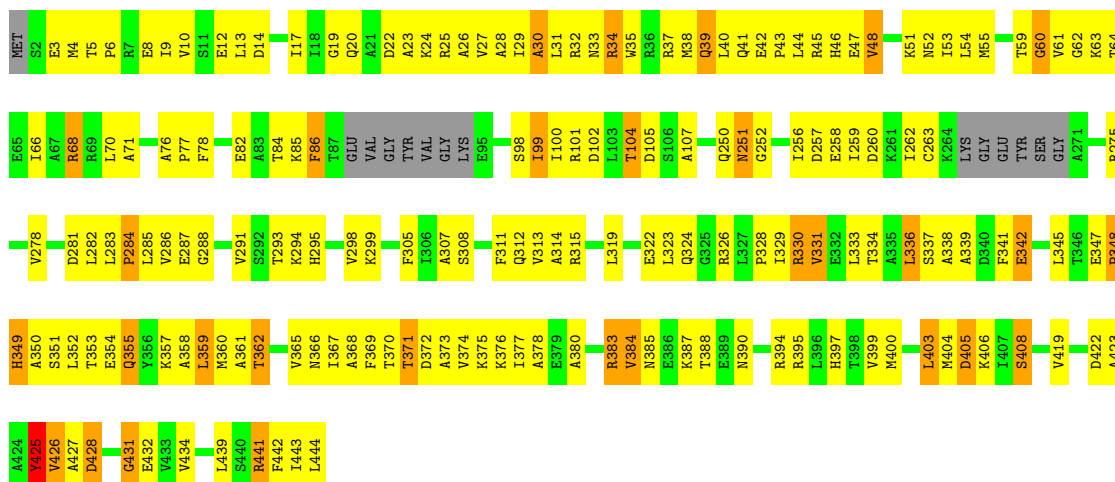
#### • Molecule 1: ATP-DEPENDENT HSL PROTEASE ATP-BINDING SUBUNIT HSLU

Chain B:



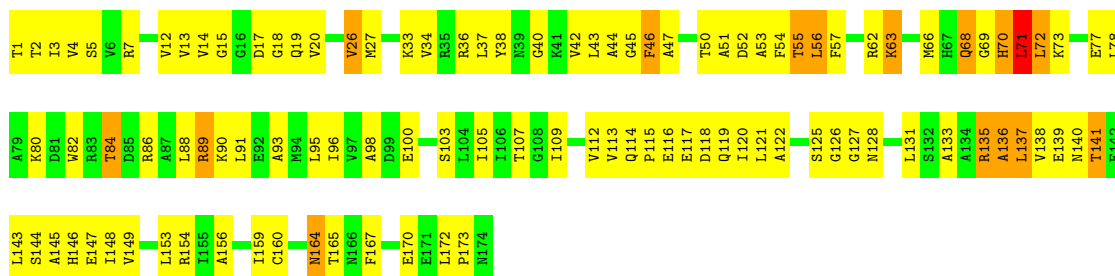
#### • Molecule 1: ATP-DEPENDENT HSL PROTEASE ATP-BINDING SUBUNIT HSLU

Chain C:



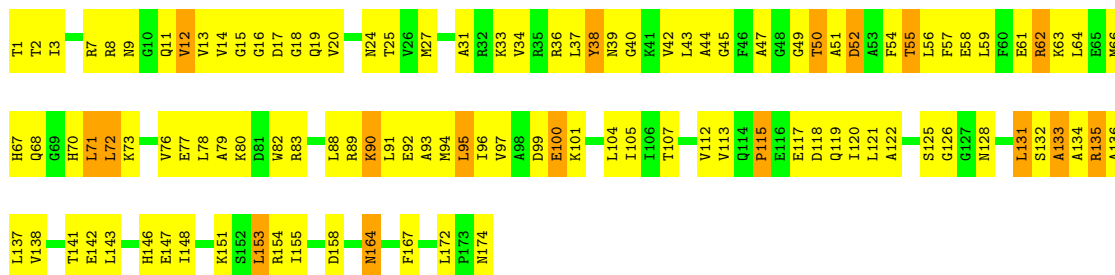
- Molecule 2: ATP-DEPENDENT PROTEASE HSLV

## Chain G:



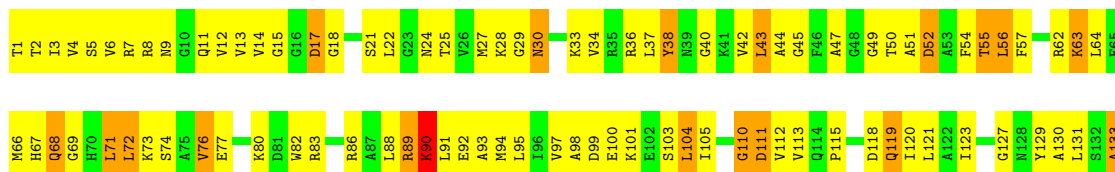
- Molecule 2: ATP-DEPENDENT PROTEASE HSLV

## Chain H:



- Molecule 2: ATP-DEPENDENT PROTEASE HSLV

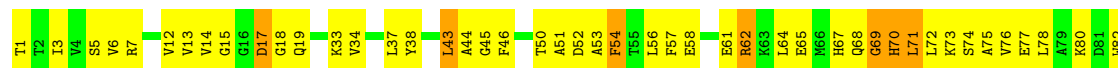
Chain I:





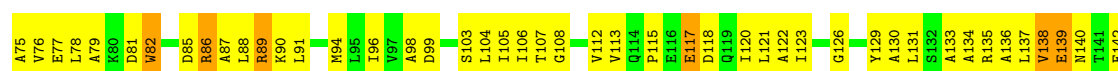
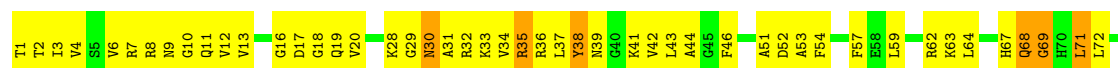
• Molecule 2: ATP-DEPENDENT PROTEASE HSLV

Chain L:



• Molecule 2: ATP-DEPENDENT PROTEASE HSLV

Chain M:



• Molecule 2: ATP-DEPENDENT PROTEASE HSLV

Chain N:



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 6	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	190.18Å 190.18Å 114.51Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.20	Depositor
% Data completeness (in resolution range)	96.7 (50.00-3.20)	Depositor
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.232 , 0.327	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	15050	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	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: MG, PO4, ADP, LVS

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	0.44	0/2339	0.71	0/3156
1	B	0.44	0/2311	0.70	0/3118
1	C	0.41	0/2315	0.69	1/3125 (0.0%)
2	G	0.38	0/1333	0.63	0/1798
2	H	0.38	0/1333	0.61	0/1798
2	I	0.36	0/1333	0.62	0/1798
2	L	0.34	0/1333	0.60	0/1798
2	M	0.33	0/1333	0.58	0/1798
2	N	0.34	0/1333	0.60	0/1798
All	All	0.39	0/14963	0.65	1/20187 (0.0%)

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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	345	LEU	CA-CB-CG	6.12	129.39	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	356	TYR	Sidechain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2312	0	2358	190	0
1	B	2284	0	2336	182	0
1	C	2288	0	2332	187	0
2	G	1319	0	1347	135	0
2	H	1319	0	1347	151	0
2	I	1319	0	1347	144	0
2	L	1319	0	1348	116	0
2	M	1319	0	1348	140	0
2	N	1319	0	1348	127	0
3	A	27	0	12	4	0
3	B	27	0	12	6	0
3	C	27	0	12	4	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	L	1	0	0	0	0
4	M	1	0	0	0	0
4	N	1	0	0	0	0
5	A	5	0	0	0	0
5	B	5	0	0	2	0
5	C	5	0	0	1	0
6	G	41	0	38	9	0
6	H	41	0	38	5	0
6	I	41	0	38	5	0
7	A	7	0	0	0	0
7	B	7	0	0	0	0
7	C	7	0	0	0	0
All	All	15050	0	15261	1331	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 44.

All (1331) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:3:GLU:HG3	1:C:4:MET:H	1.10	1.14
1:B:441:ARG:HH11	1:B:441:ARG:HB3	1.07	1.09
1:C:406:LYS:H	1:C:406:LYS:HD2	1.15	1.04
2:N:105:ILE:HG13	2:N:121:LEU:HD13	1.40	1.03
1:A:441:ARG:HH11	1:A:441:ARG:HB3	1.21	1.03
2:N:42:VAL:HG22	2:N:99:ASP:HB3	1.42	1.01
2:H:151:LYS:HE2	2:N:140:ASN:HD21	1.27	0.98
1:B:406:LYS:H	1:B:406:LYS:HD2	1.24	0.97
2:N:4:VAL:HG13	2:N:149:VAL:HG13	1.47	0.96
1:C:441:ARG:HB3	1:C:441:ARG:HH11	1.30	0.93
1:B:286:VAL:HG11	1:B:326:ARG:HB3	1.48	0.93
1:B:441:ARG:NH1	1:B:441:ARG:HB3	1.85	0.92
1:B:42:GLU:HB3	1:B:43:PRO:HD3	1.51	0.92
1:B:37:ARG:HA	1:B:40:LEU:HG	1.52	0.91
2:L:109:ILE:HG13	2:L:110:GLY:H	1.34	0.90
2:M:11:GLN:HA	2:M:173:PRO:HG2	1.53	0.90
2:H:141:THR:HG22	2:H:143:LEU:H	1.34	0.90
1:A:20:GLN:HA	1:A:20:GLN:HE21	1.36	0.90
2:H:45:GLY:O	2:H:95:LEU:HD23	1.71	0.90
1:C:330:ARG:HB3	1:C:330:ARG:HH11	1.34	0.90
1:A:441:ARG:HH11	1:A:441:ARG:CB	1.85	0.89
1:B:23:ALA:HA	1:B:331:VAL:HG21	1.55	0.88
2:I:56:LEU:HD13	2:I:95:LEU:HD22	1.54	0.88
1:A:27:VAL:HB	1:A:70:LEU:HD13	1.56	0.87
2:N:105:ILE:HB	2:N:113:VAL:HB	1.56	0.86
1:A:94:LYS:HG2	1:A:95:GLU:H	1.39	0.86
1:C:101:ARG:HG2	1:C:293:THR:HG22	1.55	0.86
2:G:105:ILE:HG23	2:G:121:LEU:HD13	1.58	0.86
2:N:12:VAL:HG11	2:N:172:LEU:HD12	1.54	0.86
2:I:17:ASP:HB2	2:I:164:ASN:ND2	1.91	0.85
1:B:27:VAL:HB	1:B:70:LEU:HD13	1.56	0.85
2:H:105:ILE:CG2	2:H:113:VAL:HB	2.06	0.85
2:L:88:LEU:HA	2:L:91:LEU:HD13	1.59	0.84
1:B:439:LEU:HD13	2:H:76:VAL:HG21	1.57	0.84
1:C:3:GLU:CG	1:C:4:MET:H	1.90	0.83
2:H:56:LEU:HD11	2:H:95:LEU:HB2	1.60	0.83
2:M:105:ILE:HG13	2:M:121:LEU:HD13	1.60	0.83
1:C:60:GLY:HA2	3:C:450:ADP:O3A	1.79	0.83
1:C:54:LEU:HD12	1:C:307:ALA:O	1.79	0.83

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:I:18:GLY:H	2:I:164:ASN:HD21	1.23	0.82
2:I:43:LEU:H	2:I:43:LEU:HD12	1.44	0.82
2:G:4:VAL:HG23	2:G:122:ALA:HB2	1.59	0.82
2:G:141:THR:OG1	2:G:143:LEU:HG	1.80	0.82
2:G:50:THR:HG21	6:G:0:LVS:HD12	1.62	0.81
1:A:4:MET:HB3	1:A:8:GLU:HB2	1.60	0.81
1:C:377:ILE:O	1:C:380:ALA:HB3	1.81	0.81
2:G:96:ILE:HG12	2:G:105:ILE:HG22	1.62	0.81
1:A:370:THR:HG23	1:A:421:ILE:O	1.80	0.81
1:B:20:GLN:HE21	1:B:20:GLN:HA	1.43	0.81
2:H:17:ASP:HB2	2:H:164:ASN:ND2	1.96	0.81
2:G:56:LEU:HD22	2:G:95:LEU:HD12	1.62	0.80
1:B:20:GLN:HE22	1:B:334:THR:H	1.28	0.80
1:C:403:LEU:HD23	1:C:404:MET:N	1.95	0.80
1:C:256:ILE:HD13	1:C:282:LEU:HD21	1.63	0.80
1:C:3:GLU:HG3	1:C:4:MET:N	1.93	0.80
1:C:98:SER:HA	1:C:101:ARG:HE	1.47	0.80
1:A:20:GLN:CA	1:A:20:GLN:HE21	1.94	0.79
1:C:42:GLU:HB3	1:C:43:PRO:HD3	1.64	0.79
2:I:37:LEU:HB2	2:I:42:VAL:HG23	1.64	0.79
2:I:1:THR:HG23	2:I:33:LYS:HD3	1.65	0.79
2:M:13:VAL:HG22	2:M:171:GLU:HG2	1.65	0.79
1:A:26:ALA:HB2	1:A:331:VAL:HG11	1.65	0.79
2:M:88:LEU:HA	2:M:91:LEU:HD13	1.65	0.78
1:C:441:ARG:NH1	1:C:441:ARG:HB3	1.98	0.78
1:A:262:ILE:HD12	1:A:278:VAL:HG23	1.64	0.78
2:G:38:TYR:CE1	2:G:69:GLY:HA3	2.18	0.78
6:G:0:LVS:HN1	6:G:0:LVS:HD13	1.48	0.78
2:G:131:LEU:HD11	2:G:135:ARG:NH1	1.99	0.78
2:H:136:ALA:HB2	2:N:155:ILE:HD13	1.66	0.78
2:I:17:ASP:HB2	2:I:164:ASN:HD22	1.47	0.78
2:M:71:LEU:H	2:M:71:LEU:HD12	1.47	0.78
2:N:1:THR:HG23	2:N:33:LYS:NZ	1.99	0.78
2:N:80:LYS:HB2	2:N:80:LYS:NZ	1.98	0.77
1:B:79:ILE:HG22	1:B:254:VAL:HG22	1.65	0.77
2:G:3:ILE:HG22	2:G:96:ILE:HD12	1.67	0.77
2:G:50:THR:HG23	2:G:51:ALA:N	2.00	0.77
1:B:299:LYS:HB3	1:B:301:ASP:OD1	1.86	0.76
2:N:19:GLN:HB2	2:N:164:ASN:HD22	1.50	0.76
2:N:19:GLN:HB2	2:N:164:ASN:ND2	2.00	0.76
1:C:19:GLY:O	1:C:24:LYS:NZ	2.17	0.76
2:L:96:ILE:HG12	2:L:105:ILE:HG12	1.67	0.76

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:M:3:ILE:HB	2:M:123:ILE:HG13	1.67	0.76
2:L:141:THR:CG2	2:L:143:LEU:HG	2.16	0.76
2:L:141:THR:HG21	2:L:143:LEU:HG	1.65	0.76
1:A:20:GLN:HE22	1:A:334:THR:H	1.34	0.76
1:A:264:LYS:N	1:A:264:LYS:HD2	2.00	0.76
1:A:330:ARG:HH11	1:A:330:ARG:HB3	1.50	0.75
2:G:51:ALA:O	2:G:55:THR:HG22	1.86	0.75
2:I:67:HIS:NE2	2:I:77:GLU:HG3	2.00	0.75
1:B:359:LEU:HD13	1:C:40:LEU:HD11	1.69	0.75
1:C:27:VAL:HG23	1:C:70:LEU:HD13	1.69	0.75
1:B:443:ILE:HG12	2:H:112:VAL:CG2	2.17	0.74
1:C:76:ALA:HB1	1:C:251:ASN:O	1.87	0.74
2:H:83:ARG:HH11	2:I:54:PHE:HB3	1.51	0.74
2:H:131:LEU:HD11	2:H:135:ARG:NH1	2.02	0.74
2:L:19:GLN:HB2	2:L:164:ASN:ND2	2.02	0.74
2:H:94:MET:HG2	2:H:107:THR:HG22	1.70	0.74
2:G:18:GLY:H	2:G:164:ASN:HD21	1.36	0.74
2:G:52:ASP:HA	2:G:55:THR:CG2	2.18	0.74
2:N:85:ASP:HB3	2:N:88:LEU:HD23	1.70	0.74
2:M:6:VAL:HG12	2:M:7:ARG:H	1.53	0.73
1:A:278:VAL:HA	1:A:281:ASP:HB2	1.70	0.73
1:C:17:ILE:HG12	1:C:66:ILE:HD13	1.69	0.73
1:A:249:GLU:OE1	1:A:299:LYS:HG2	1.89	0.73
2:H:136:ALA:HB2	2:N:155:ILE:CD1	2.19	0.73
2:M:32:ARG:HH21	2:M:35:ARG:HA	1.52	0.73
1:B:443:ILE:HG22	1:B:444:LEU:N	2.04	0.72
2:H:143:LEU:HD11	2:N:140:ASN:ND2	2.04	0.72
2:N:88:LEU:HA	2:N:91:LEU:HD13	1.71	0.72
2:M:4:VAL:HG13	2:M:149:VAL:HG13	1.69	0.72
2:H:56:LEU:CD1	2:H:95:LEU:HD12	2.19	0.72
2:G:37:LEU:HD21	2:G:57:PHE:CZ	2.25	0.72
1:B:37:ARG:HD2	1:B:48:VAL:HG13	1.72	0.72
1:B:367:ILE:HG12	1:B:368:ALA:N	2.03	0.72
2:L:80:LYS:HB3	2:L:80:LYS:NZ	2.04	0.72
2:I:5:SER:HB2	2:I:14:VAL:HG22	1.72	0.72
2:H:37:LEU:HB2	2:H:42:VAL:HG23	1.71	0.72
2:N:52:ASP:O	2:N:56:LEU:HD23	1.89	0.72
2:L:33:LYS:HA	2:L:46:PHE:CE1	2.24	0.72
2:I:52:ASP:HA	2:I:55:THR:HG23	1.72	0.72
2:M:2:THR:HG22	2:M:126:GLY:HA3	1.72	0.71
1:B:63:LYS:HD2	1:B:308:SER:HB2	1.70	0.71
2:N:46:PHE:CZ	2:N:50:THR:HG22	2.24	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:42:GLU:HB3	1:A:43:PRO:HD3	1.70	0.71
2:H:56:LEU:HD13	2:H:95:LEU:HD12	1.71	0.71
2:I:5:SER:CB	2:I:14:VAL:HG22	2.21	0.71
1:A:37:ARG:O	1:A:38:MET:HB3	1.90	0.71
2:H:151:LYS:HE2	2:N:140:ASN:ND2	2.05	0.71
1:B:390:ASN:HB2	2:H:68:GLN:NE2	2.06	0.71
1:A:293:THR:HG23	1:A:296:GLY:O	1.90	0.71
2:N:1:THR:HG23	2:N:33:LYS:HZ2	1.54	0.71
2:I:52:ASP:HA	2:I:55:THR:CG2	2.20	0.71
1:B:79:ILE:CG2	1:B:254:VAL:HG22	2.22	0.70
1:B:20:GLN:HE21	1:B:20:GLN:CA	2.03	0.70
1:B:283:LEU:HB2	1:B:284:PRO:HD3	1.74	0.70
2:H:105:ILE:HG23	2:H:113:VAL:HB	1.73	0.70
2:H:18:GLY:H	2:H:164:ASN:HD21	1.40	0.70
2:M:71:LEU:HD11	2:M:99:ASP:OD1	1.90	0.70
2:M:32:ARG:NH2	2:M:35:ARG:HA	2.06	0.70
2:H:12:VAL:HG23	2:H:172:LEU:HB3	1.72	0.70
2:G:37:LEU:HB2	2:G:42:VAL:HG23	1.73	0.70
2:I:37:LEU:HD21	2:I:57:PHE:CZ	2.26	0.70
2:H:115:PRO:HG3	2:H:121:LEU:HD21	1.72	0.70
1:B:85:LYS:HG2	1:B:85:LYS:O	1.92	0.70
1:B:303:ILE:HG22	1:B:305:PHE:CE1	2.26	0.70
2:I:56:LEU:HD13	2:I:95:LEU:CD2	2.23	0.69
2:M:133:ALA:O	2:M:136:ALA:HB3	1.92	0.69
2:H:125:SER:H	6:H:0:LVS:C1'	2.05	0.69
2:L:64:LEU:HA	2:L:74:SER:OG	1.92	0.69
2:G:89:ARG:HG2	2:G:89:ARG:HH11	1.58	0.69
1:B:55:MET:CE	1:B:333:LEU:HD11	2.23	0.69
1:C:390:ASN:HB2	2:I:68:GLN:NE2	2.08	0.69
2:L:131:LEU:HD11	2:L:135:ARG:NE	2.08	0.68
1:A:37:ARG:HD2	1:A:48:VAL:HG13	1.75	0.68
2:N:46:PHE:HZ	2:N:50:THR:HG22	1.59	0.68
2:H:154:ARG:HA	2:H:167:PHE:HZ	1.58	0.68
2:I:1:THR:HB	6:I:0:LVS:H1'2	1.76	0.68
1:A:283:LEU:O	1:A:284:PRO:C	2.31	0.68
2:L:109:ILE:HG13	2:L:110:GLY:N	2.08	0.68
1:C:35:TRP:O	1:C:39:GLN:NE2	2.26	0.68
1:B:5:THR:OG1	1:B:8:GLU:HG3	1.94	0.68
1:C:62:GLY:O	1:C:66:ILE:HG12	1.94	0.67
2:L:50:THR:O	2:L:53:ALA:HB3	1.94	0.67
2:G:46:PHE:HB3	2:G:95:LEU:HD21	1.74	0.67
2:H:172:LEU:HD23	2:H:174:ASN:N	2.09	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:313:VAL:HG23	1:C:314:ALA:H	1.57	0.67
1:B:365:VAL:HG22	1:B:414:MET:HB2	1.75	0.67
1:A:330:ARG:HH11	1:A:330:ARG:CB	2.08	0.67
2:L:1:THR:HG23	2:L:33:LYS:HE3	1.75	0.67
2:N:104:LEU:CD1	2:N:114:GLN:HG2	2.24	0.67
2:H:19:GLN:H	2:H:33:LYS:HZ3	1.42	0.67
2:M:106:ILE:N	2:M:106:ILE:HD12	2.09	0.67
2:H:51:ALA:O	2:H:55:THR:HG22	1.95	0.67
2:I:67:HIS:HE2	2:I:77:GLU:HG3	1.57	0.67
1:B:286:VAL:HG12	1:B:287:GLU:N	2.08	0.67
1:B:347:GLU:HB2	1:B:348:PRO:HD3	1.76	0.67
2:M:86:ARG:HA	2:M:86:ARG:HH11	1.59	0.67
1:B:100:ILE:HB	1:B:291:VAL:HG21	1.77	0.66
1:B:39:GLN:HE21	1:B:39:GLN:N	1.94	0.66
1:C:63:LYS:HG2	1:C:333:LEU:HD22	1.77	0.66
2:H:52:ASP:HA	2:H:55:THR:CG2	2.25	0.66
2:L:70:HIS:HB3	2:L:73:LYS:HD3	1.77	0.66
2:M:41:LYS:O	2:M:172:LEU:HD11	1.95	0.66
1:B:61:VAL:HB	1:B:336:LEU:HD13	1.78	0.66
1:C:34:ARG:HH11	1:C:34:ARG:HG3	1.60	0.66
1:C:41:GLN:HE21	1:C:41:GLN:HA	1.60	0.66
1:C:250:GLN:HE21	1:C:250:GLN:HA	1.60	0.66
1:B:64:THR:HB	3:B:450:ADP:O1A	1.95	0.66
1:A:20:GLN:HE22	1:A:334:THR:HG22	1.61	0.66
1:B:439:LEU:HD22	2:H:76:VAL:HG11	1.76	0.65
1:C:34:ARG:HH21	1:C:251:ASN:C	2.00	0.65
2:N:104:LEU:HD12	2:N:114:GLN:HG2	1.76	0.65
2:M:160:CYS:SG	2:M:162:PHE:HB2	2.35	0.65
1:A:396:LEU:O	1:A:400:MET:HB2	1.97	0.65
2:H:52:ASP:OD2	2:H:91:LEU:HA	1.96	0.65
2:N:71:LEU:HD23	2:N:102:GLU:HG3	1.79	0.65
2:H:20:VAL:HG12	2:H:27:MET:HB3	1.77	0.65
2:N:3:ILE:HB	2:N:123:ILE:HG12	1.79	0.65
1:B:342:GLU:OE2	1:B:375:LYS:HG3	1.97	0.65
1:A:34:ARG:HH11	1:A:34:ARG:CG	2.10	0.65
2:N:131:LEU:HD11	2:N:135:ARG:HE	1.60	0.65
1:A:101:ARG:HG3	1:A:293:THR:HB	1.77	0.65
2:I:83:ARG:HH21	2:I:111:ASP:HA	1.62	0.65
1:C:360:MET:HG3	1:C:367:ILE:HD13	1.78	0.65
2:M:6:VAL:HG12	2:M:7:ARG:N	2.11	0.64
2:M:72:LEU:HD13	2:M:104:LEU:HD21	1.79	0.64
2:I:42:VAL:HG12	2:I:99:ASP:HB3	1.79	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:L:76:VAL:O	2:L:80:LYS:HG2	1.96	0.64
1:C:357:LYS:HE3	1:C:369:PHE:HD1	1.62	0.64
1:A:13:LEU:HD12	1:A:24:LYS:HG2	1.78	0.64
1:C:100:ILE:O	1:C:104:THR:OG1	2.14	0.64
1:B:313:VAL:HG23	1:B:314:ALA:H	1.60	0.64
1:C:34:ARG:NH2	1:C:251:ASN:HA	2.12	0.64
2:M:2:THR:HG23	2:M:163:THR:OG1	1.97	0.64
2:I:52:ASP:OD2	2:I:91:LEU:HA	1.97	0.64
1:C:101:ARG:HG2	1:C:293:THR:CG2	2.27	0.64
1:B:55:MET:HE2	1:B:333:LEU:HD11	1.78	0.64
2:I:131:LEU:HD11	2:I:135:ARG:NH1	2.12	0.64
2:M:20:VAL:HB	2:M:28:LYS:H	1.62	0.64
2:M:3:ILE:HD13	2:M:16:GLY:HA3	1.79	0.64
2:M:71:LEU:HD21	2:M:99:ASP:HB3	1.80	0.64
2:H:7:ARG:HH11	2:H:7:ARG:HG3	1.61	0.64
2:N:133:ALA:O	2:N:136:ALA:HB3	1.97	0.64
2:N:17:ASP:CG	2:N:163:THR:HG23	2.18	0.64
2:H:72:LEU:HD22	2:H:104:LEU:HD11	1.80	0.64
2:H:19:GLN:H	2:H:33:LYS:NZ	1.95	0.64
1:B:353:THR:O	1:B:357:LYS:HB2	1.97	0.63
2:G:37:LEU:HD21	2:G:57:PHE:CE2	2.34	0.63
2:M:155:ILE:C	2:M:157:GLY:H	1.99	0.63
2:M:2:THR:HG22	2:M:126:GLY:CA	2.28	0.63
1:C:41:GLN:NE2	1:C:41:GLN:HA	2.12	0.63
1:C:59:THR:HA	5:C:452:PO4:O2	1.98	0.63
2:G:115:PRO:HG3	2:G:121:LEU:HD11	1.79	0.63
2:N:4:VAL:HG13	2:N:149:VAL:CG1	2.27	0.62
2:G:2:THR:OG1	2:G:126:GLY:HA3	1.99	0.62
1:A:407:ILE:O	1:A:411:ALA:HB2	1.99	0.62
1:C:250:GLN:NE2	1:C:250:GLN:HA	2.15	0.62
1:C:313:VAL:HG23	1:C:314:ALA:N	2.14	0.62
2:H:141:THR:HG22	2:H:142:GLU:N	2.13	0.62
2:G:136:ALA:O	2:G:137:LEU:C	2.37	0.62
2:H:131:LEU:HD11	2:H:135:ARG:HH11	1.64	0.62
1:C:371:THR:CG2	1:C:375:LYS:HE2	2.30	0.62
1:B:313:VAL:HG23	1:B:314:ALA:N	2.14	0.62
2:H:131:LEU:HD21	2:H:135:ARG:NH1	2.14	0.62
1:B:365:VAL:CG2	1:B:414:MET:HB2	2.29	0.62
1:A:79:ILE:HG22	1:A:103:LEU:HD13	1.81	0.62
1:C:406:LYS:HD2	1:C:406:LYS:N	1.99	0.62
2:N:87:ALA:C	2:N:88:LEU:HD22	2.20	0.62
2:M:131:LEU:HD11	2:M:135:ARG:NE	2.14	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:L:7:ARG:HB3	2:L:119:GLN:HB3	1.82	0.62
2:H:155:ILE:HA	2:H:158:ASP:OD1	1.99	0.62
2:G:78:LEU:HG	2:G:82:TRP:HZ3	1.65	0.62
1:A:326:ARG:C	1:A:328:PRO:HD3	2.20	0.61
1:C:27:VAL:CG2	1:C:70:LEU:HD13	2.29	0.61
2:I:5:SER:OG	2:I:14:VAL:HG22	2.00	0.61
2:H:1:THR:HG23	2:H:33:LYS:HD3	1.82	0.61
1:A:250:GLN:NE2	1:A:250:GLN:HA	2.14	0.61
2:M:115:PRO:HG3	2:M:121:LEU:CD1	2.30	0.61
1:C:425:TYR:O	1:C:428:ASP:N	2.23	0.61
1:A:377:ILE:O	1:A:380:ALA:HB3	2.01	0.61
1:C:98:SER:HB3	1:C:101:ARG:HH21	1.66	0.61
1:B:311:PHE:CE1	1:B:316:PRO:HA	2.35	0.61
2:M:63:LYS:NZ	2:M:77:GLU:HB3	2.14	0.61
2:I:27:MET:CE	2:I:27:MET:HA	2.31	0.61
1:B:84:THR:O	1:B:86:PHE:N	2.32	0.61
2:N:12:VAL:CG1	2:N:172:LEU:HB2	2.31	0.61
1:B:367:ILE:HD11	1:B:421:ILE:HD12	1.81	0.61
1:C:55:MET:O	1:C:308:SER:HA	2.00	0.61
2:H:125:SER:H	6:H:0:LVS:H1'1	1.66	0.61
2:L:134:ALA:O	2:L:135:ARG:C	2.37	0.61
1:C:312:GLN:HE21	2:I:66:MET:HG2	1.66	0.61
2:L:5:SER:HB2	2:L:14:VAL:HG22	1.83	0.61
2:N:161:VAL:HG23	2:N:162:PHE:CD2	2.36	0.61
2:I:62:ARG:HB3	2:I:62:ARG:NH1	2.16	0.61
2:L:64:LEU:HD21	2:L:69:GLY:HA2	1.83	0.60
2:I:1:THR:HB	6:I:0:LVS:C1'	2.31	0.60
2:G:50:THR:CG2	2:G:51:ALA:N	2.64	0.60
1:A:258:GLU:O	1:A:261:LYS:HB2	2.01	0.60
1:B:98:SER:HA	1:B:101:ARG:NH1	2.16	0.60
1:C:443:ILE:HG12	2:I:112:VAL:CG2	2.31	0.60
1:A:6:PRO:HD3	1:A:32:ARG:HD3	1.84	0.60
1:C:372:ASP:O	1:C:376:LYS:HB2	2.01	0.60
2:M:131:LEU:HD11	2:M:135:ARG:HE	1.64	0.60
2:M:79:ALA:HB2	2:M:112:VAL:HG23	1.83	0.60
2:I:37:LEU:HD21	2:I:57:PHE:CE2	2.36	0.60
2:G:13:VAL:HG21	2:G:146:HIS:N	2.16	0.60
1:C:444:LEU:HB3	2:I:113:VAL:HG22	1.84	0.60
2:L:88:LEU:CA	2:L:91:LEU:HD13	2.30	0.60
2:N:91:LEU:N	2:N:91:LEU:HD12	2.16	0.60
2:N:28:LYS:HE3	2:N:30:ASN:O	2.02	0.60
1:A:250:GLN:HE21	1:A:250:GLN:HA	1.67	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:337:SER:O	1:B:340:ASP:HB2	2.02	0.60
1:A:322:GLU:N	1:A:322:GLU:OE2	2.35	0.60
2:H:44:ALA:HA	2:H:96:ILE:O	2.02	0.60
1:A:73:LEU:O	1:A:73:LEU:HD12	2.02	0.60
1:C:342:GLU:OE2	1:C:375:LYS:HG2	2.02	0.60
2:H:72:LEU:O	2:H:76:VAL:HG23	2.01	0.59
2:G:91:LEU:N	2:G:91:LEU:HD12	2.17	0.59
2:H:17:ASP:HB2	2:H:164:ASN:HD21	1.66	0.59
1:B:407:ILE:HD11	1:B:425:TYR:HE1	1.67	0.59
1:C:25:ARG:O	1:C:28:ALA:HB3	2.02	0.59
2:L:95:LEU:HB2	2:L:106:ILE:HB	1.83	0.59
1:A:441:ARG:NH1	1:A:441:ARG:CB	2.61	0.59
1:C:360:MET:HA	1:C:360:MET:HE2	1.83	0.59
2:M:37:LEU:HD11	2:M:57:PHE:HB3	1.84	0.59
2:I:9:ASN:O	2:I:11:GLN:HG2	2.02	0.59
2:M:6:VAL:HG21	2:M:148:ILE:HG22	1.83	0.59
1:A:34:ARG:NH1	1:A:34:ARG:HG2	2.18	0.59
1:C:360:MET:HA	1:C:360:MET:CE	2.31	0.59
2:M:78:LEU:O	2:M:78:LEU:HD12	2.02	0.59
2:N:30:ASN:HA	2:N:166:ASN:ND2	2.17	0.59
2:L:15:GLY:HA2	2:L:34:VAL:HG21	1.84	0.59
2:I:89:ARG:O	2:I:90:LYS:HB3	2.01	0.59
1:C:347:GLU:HB2	1:C:348:PRO:HD3	1.84	0.59
2:N:11:GLN:OE1	2:N:173:PRO:HD2	2.02	0.59
2:M:87:ALA:O	2:M:88:LEU:HD12	2.02	0.59
1:B:35:TRP:O	1:B:39:GLN:NE2	2.35	0.59
2:N:4:VAL:HG12	2:N:153:LEU:HD21	1.84	0.59
1:A:262:ILE:HD12	1:A:278:VAL:CG2	2.30	0.59
1:B:443:ILE:HG12	2:H:112:VAL:HG21	1.84	0.59
1:C:34:ARG:CZ	1:C:251:ASN:HA	2.33	0.59
2:I:115:PRO:HG3	2:I:121:LEU:CG	2.33	0.59
1:A:94:LYS:HG2	1:A:95:GLU:N	2.14	0.59
2:N:133:ALA:O	2:N:137:LEU:HD22	2.01	0.59
2:N:108:GLY:C	2:N:110:GLY:H	2.05	0.59
2:G:137:LEU:O	2:G:141:THR:HG22	2.02	0.59
6:G:0:LVS:HD42	6:G:0:LVS:HN2	1.68	0.59
1:B:20:GLN:NE2	1:B:334:THR:H	1.99	0.59
1:C:9:ILE:HD13	1:C:31:LEU:HD23	1.85	0.59
1:B:84:THR:C	1:B:86:PHE:H	2.06	0.59
1:C:283:LEU:O	1:C:285:LEU:N	2.36	0.59
1:A:390:ASN:HB2	2:G:68:GLN:HE21	1.66	0.59
2:M:103:SER:C	2:M:104:LEU:HD12	2.24	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:390:ASN:HB2	2:I:68:GLN:HE21	1.67	0.58
2:N:58:GLU:C	2:N:60:PHE:H	2.06	0.58
1:B:406:LYS:HD2	1:B:406:LYS:N	2.07	0.58
2:L:67:HIS:CD2	2:L:77:GLU:HG3	2.38	0.58
2:L:18:GLY:HA2	2:L:33:LYS:HZ3	1.67	0.58
1:A:37:ARG:HA	1:A:40:LEU:HG	1.86	0.58
2:N:60:PHE:HB2	2:N:78:LEU:HD22	1.85	0.58
2:L:43:LEU:CD2	2:L:43:LEU:H	2.16	0.58
2:L:120:ILE:HD11	2:L:138:VAL:HG11	1.85	0.58
2:H:43:LEU:HD12	2:H:43:LEU:N	2.18	0.58
2:H:37:LEU:HB2	2:H:42:VAL:CG2	2.32	0.58
1:A:26:ALA:CB	1:A:331:VAL:HG11	2.32	0.58
1:C:312:GLN:NE2	2:I:66:MET:HG2	2.17	0.58
1:B:80:LYS:HG3	1:B:255:PHE:HD2	1.69	0.58
2:N:131:LEU:HD11	2:N:135:ARG:NE	2.18	0.58
1:A:34:ARG:HH11	1:A:34:ARG:CB	2.17	0.58
2:L:161:VAL:HG23	2:L:162:PHE:CD1	2.39	0.58
2:L:43:LEU:H	2:L:43:LEU:HD23	1.68	0.58
1:C:84:THR:O	1:C:86:PHE:N	2.36	0.58
1:C:9:ILE:CD1	1:C:31:LEU:HD23	2.34	0.58
1:B:443:ILE:CG2	1:B:444:LEU:N	2.67	0.58
2:I:71:LEU:HD21	2:I:97:VAL:CG2	2.34	0.58
1:C:293:THR:C	1:C:295:HIS:H	2.07	0.58
2:G:46:PHE:HB3	2:G:95:LEU:CD2	2.33	0.57
1:B:55:MET:O	1:B:308:SER:HA	2.04	0.57
1:B:62:GLY:O	1:B:66:ILE:HG13	2.03	0.57
2:N:80:LYS:HB2	2:N:80:LYS:HZ2	1.66	0.57
2:I:141:THR:CG2	2:I:143:LEU:HG	2.33	0.57
2:M:172:LEU:HB3	2:M:173:PRO:HD3	1.86	0.57
2:H:42:VAL:HG12	2:H:99:ASP:HB3	1.85	0.57
1:C:17:ILE:HG21	1:C:66:ILE:HD11	1.86	0.57
2:H:83:ARG:HG2	2:I:55:THR:HB	1.85	0.57
2:M:28:LYS:HG2	2:M:29:GLY:N	2.19	0.57
2:M:38:TYR:CE2	2:M:64:LEU:HD22	2.38	0.57
1:C:63:LYS:HB2	3:C:450:ADP:O2B	2.04	0.57
1:A:443:ILE:HD11	2:G:72:LEU:HD11	1.85	0.57
2:H:115:PRO:HG3	2:H:121:LEU:HD11	1.87	0.57
2:G:37:LEU:HB2	2:G:42:VAL:CG2	2.34	0.57
2:I:134:ALA:C	2:I:136:ALA:H	2.07	0.57
2:L:116:GLU:C	2:L:118:ASP:H	2.07	0.57
2:N:148:ILE:HG22	2:N:149:VAL:N	2.19	0.57
2:N:12:VAL:O	2:N:12:VAL:HG13	2.04	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:68:ARG:HG2	1:C:68:ARG:HH11	1.69	0.57
2:N:137:LEU:HD22	2:N:137:LEU:H	1.69	0.57
2:M:59:LEU:O	2:M:63:LYS:HB2	2.05	0.57
2:N:6:VAL:HG13	2:N:120:ILE:HG12	1.86	0.57
1:B:338:ALA:O	1:B:342:GLU:HG3	2.04	0.57
1:C:352:LEU:HD13	1:C:400:MET:HG3	1.85	0.57
2:H:67:HIS:HD2	2:H:73:LYS:HD3	1.68	0.57
1:C:370:THR:O	1:C:373:ALA:N	2.36	0.57
2:M:72:LEU:CD1	2:M:104:LEU:HD21	2.35	0.57
2:H:7:ARG:NH1	2:H:12:VAL:HG13	2.20	0.57
2:M:130:ALA:N	2:M:156:ALA:HB2	2.20	0.57
2:L:3:ILE:HG22	2:L:96:ILE:HD12	1.87	0.57
2:I:51:ALA:O	2:I:55:THR:HG22	2.05	0.57
1:B:311:PHE:HD1	1:B:314:ALA:O	1.88	0.57
2:G:91:LEU:CD1	2:G:91:LEU:H	2.18	0.56
2:G:19:GLN:HE21	2:G:164:ASN:HB3	1.70	0.56
2:N:60:PHE:O	2:N:63:LYS:HB2	2.05	0.56
1:A:18:ILE:HD13	1:A:348:PRO:HG3	1.85	0.56
2:H:136:ALA:C	2:H:138:VAL:H	2.08	0.56
2:N:38:TYR:CD1	2:N:41:LYS:HD3	2.41	0.56
2:G:98:ALA:HB2	2:G:103:SER:HA	1.87	0.56
2:L:172:LEU:HD23	2:L:173:PRO:CA	2.35	0.56
1:C:330:ARG:HH11	1:C:330:ARG:CB	2.14	0.56
2:I:22:LEU:O	2:I:25:THR:HG22	2.06	0.56
2:L:64:LEU:HG	2:L:74:SER:OG	2.05	0.56
2:I:67:HIS:HD2	2:I:73:LYS:HG2	1.71	0.56
2:L:73:LYS:O	2:L:76:VAL:HG22	2.05	0.56
2:I:90:LYS:HG2	2:I:90:LYS:O	2.05	0.56
2:H:61:GLU:O	2:H:63:LYS:N	2.38	0.56
2:H:141:THR:CG2	2:H:142:GLU:N	2.68	0.56
2:H:38:TYR:C	2:H:40:GLY:H	2.08	0.56
1:C:330:ARG:HB3	1:C:330:ARG:NH1	2.13	0.56
2:L:103:SER:O	2:L:104:LEU:HD23	2.05	0.56
1:C:32:ARG:O	1:C:35:TRP:HB3	2.06	0.56
1:B:59:THR:HA	5:B:452:PO4:P	2.46	0.56
2:H:131:LEU:O	2:H:132:SER:C	2.43	0.56
1:B:351:SER:O	1:B:355:GLN:HG3	2.06	0.56
1:A:339:ALA:O	1:A:343:ARG:HG3	2.06	0.56
2:L:144:SER:H	2:L:147:GLU:HB2	1.70	0.56
1:C:384:VAL:O	1:C:385:ASN:C	2.42	0.56
1:C:102:ASP:O	1:C:105:ASP:HB2	2.05	0.56
1:A:26:ALA:HB2	1:A:331:VAL:CG1	2.36	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:N:72:LEU:HD12	2:N:104:LEU:HG	1.88	0.56
1:C:41:GLN:HE21	1:C:41:GLN:CA	2.16	0.56
2:G:62:ARG:O	2:G:66:MET:HG3	2.05	0.56
1:B:342:GLU:OE1	1:B:375:LYS:HE2	2.06	0.56
2:H:19:GLN:N	2:H:33:LYS:NZ	2.54	0.55
2:G:146:HIS:ND1	2:G:146:HIS:O	2.40	0.55
2:G:50:THR:HG23	2:G:51:ALA:H	1.68	0.55
1:C:46:HIS:O	1:C:48:VAL:N	2.39	0.55
1:C:275:ARG:O	1:C:278:VAL:HG23	2.06	0.55
2:H:76:VAL:O	2:H:79:ALA:HB3	2.06	0.55
2:M:164:ASN:ND2	2:M:166:ASN:HB2	2.20	0.55
2:L:5:SER:CB	2:L:14:VAL:HG22	2.37	0.55
2:L:144:SER:HB3	2:L:147:GLU:HG3	1.88	0.55
2:L:148:ILE:HG22	2:L:149:VAL:N	2.21	0.55
1:A:57:GLY:O	1:A:63:LYS:HE2	2.07	0.55
2:G:77:GLU:O	2:G:80:LYS:HB3	2.05	0.55
2:L:17:ASP:HB3	2:L:163:THR:HG23	1.87	0.55
1:B:57:GLY:N	1:B:63:LYS:HE2	2.21	0.55
2:I:97:VAL:HG22	2:I:104:LEU:HD12	1.89	0.55
1:C:358:ALA:O	1:C:361:ALA:HB3	2.07	0.55
2:L:13:VAL:HG22	2:L:171:GLU:HG3	1.89	0.55
2:H:36:ARG:O	2:H:37:LEU:HD23	2.07	0.55
2:H:56:LEU:CD1	2:H:95:LEU:HB2	2.32	0.55
1:B:61:VAL:C	3:B:450:ADP:N7	2.60	0.55
1:C:257:ASP:OD1	1:C:258:GLU:N	2.40	0.55
2:H:100:GLU:O	2:H:101:LYS:HD3	2.06	0.55
2:H:71:LEU:HD11	2:H:97:VAL:HG23	1.89	0.55
1:A:443:ILE:HG12	2:G:112:VAL:CG2	2.36	0.55
1:A:37:ARG:O	1:A:38:MET:CB	2.49	0.55
2:H:153:LEU:HD22	2:H:167:PHE:CD2	2.41	0.55
1:B:23:ALA:CA	1:B:331:VAL:HG21	2.32	0.55
2:G:1:THR:H3	6:G:0:LVS:C2'	2.20	0.55
1:C:104:THR:HG21	1:C:298:VAL:HG11	1.89	0.55
2:H:143:LEU:HD22	2:H:147:GLU:OE1	2.06	0.55
1:B:367:ILE:HA	1:B:419:VAL:O	2.07	0.55
2:M:106:ILE:HG22	2:M:107:THR:N	2.21	0.55
2:M:71:LEU:N	2:M:71:LEU:HD12	2.18	0.55
2:L:115:PRO:HB2	2:L:119:GLN:OE1	2.07	0.55
2:I:5:SER:HA	2:I:13:VAL:O	2.06	0.55
2:H:47:ALA:O	2:H:93:ALA:HB1	2.06	0.55
2:H:3:ILE:HG22	2:H:96:ILE:HD12	1.89	0.54
2:G:86:ARG:HH11	2:G:86:ARG:HB2	1.71	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:82:TRP:HZ2	2:H:91:LEU:HD23	1.71	0.54
1:C:82:GLU:OE2	1:C:258:GLU:HG3	2.07	0.54
2:I:145:ALA:O	2:I:149:VAL:HG23	2.07	0.54
2:N:73:LYS:HA	2:N:73:LYS:HE3	1.88	0.54
2:M:126:GLY:HA2	2:M:129:TYR:CD2	2.42	0.54
2:N:157:GLY:HA2	2:N:163:THR:HB	1.90	0.54
2:G:117:GLU:C	2:G:119:GLN:H	2.10	0.54
1:B:352:LEU:HD13	1:B:400:MET:HG3	1.88	0.54
2:G:144:SER:HB3	2:G:147:GLU:HG3	1.89	0.54
2:L:77:GLU:O	2:L:80:LYS:HB2	2.08	0.54
1:A:311:PHE:HB3	1:A:314:ALA:O	2.07	0.54
1:B:286:VAL:HG11	1:B:326:ARG:CB	2.29	0.54
2:M:3:ILE:HB	2:M:123:ILE:CG1	2.36	0.54
1:A:264:LYS:HE2	1:A:276:GLU:CD	2.27	0.54
1:C:283:LEU:HB2	1:C:284:PRO:HD3	1.89	0.54
2:I:134:ALA:O	2:I:136:ALA:N	2.40	0.54
1:B:380:ALA:O	1:B:383:ARG:HB3	2.07	0.54
1:A:41:GLN:HA	1:A:41:GLN:HE21	1.71	0.54
2:I:1:THR:HA	2:I:33:LYS:NZ	2.22	0.54
2:H:44:ALA:HB1	2:H:95:LEU:HD21	1.88	0.54
2:L:38:TYR:CE2	2:L:64:LEU:HD22	2.42	0.54
1:A:37:ARG:HH21	1:A:302:HIS:CD2	2.24	0.54
2:M:67:HIS:O	2:M:68:GLN:HB3	2.06	0.54
2:G:33:LYS:HA	2:G:46:PHE:CE2	2.43	0.54
1:C:404:MET:O	1:C:408:SER:HB2	2.08	0.54
2:H:16:GLY:HA2	2:H:153:LEU:HD21	1.87	0.54
1:B:16:HIS:C	1:B:17:ILE:HD12	2.27	0.54
1:B:434:VAL:HG12	1:B:435:GLU:N	2.23	0.54
2:N:109:ILE:O	2:N:109:ILE:HG22	2.07	0.54
1:B:283:LEU:O	1:B:285:LEU:N	2.41	0.54
2:M:17:ASP:OD2	2:M:33:LYS:HE3	2.08	0.54
2:I:89:ARG:HG2	2:I:90:LYS:HD3	1.89	0.54
2:I:147:GLU:O	2:I:151:LYS:HB2	2.08	0.54
2:N:135:ARG:HB3	2:N:139:GLU:OE2	2.07	0.53
1:A:443:ILE:HG22	1:A:444:LEU:N	2.22	0.53
2:H:33:LYS:HE3	6:H:0:LVS:HB32	1.89	0.53
2:M:135:ARG:O	2:M:139:GLU:HB2	2.08	0.53
1:A:286:VAL:HG11	1:A:326:ARG:HB3	1.90	0.53
2:L:34:VAL:HA	2:L:45:GLY:HA2	1.90	0.53
1:B:9:ILE:HG21	1:B:28:ALA:HA	1.90	0.53
1:C:77:PRO:HG3	1:C:107:ALA:HB2	1.88	0.53
1:A:63:LYS:HZ2	1:A:308:SER:HB2	1.72	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:L:58:GLU:O	2:L:62:ARG:HD3	2.07	0.53
2:M:144:SER:HB3	2:M:147:GLU:HB2	1.90	0.53
2:G:91:LEU:HD12	2:G:91:LEU:H	1.73	0.53
1:C:439:LEU:HD13	2:I:72:LEU:HD12	1.91	0.53
2:M:129:TYR:HB2	2:M:156:ALA:CB	2.38	0.53
1:B:367:ILE:HD11	1:B:421:ILE:CD1	2.38	0.53
2:L:161:VAL:HG23	2:L:162:PHE:CE1	2.44	0.53
2:M:148:ILE:HG22	2:M:149:VAL:N	2.22	0.53
2:M:147:GLU:O	2:M:151:LYS:HG3	2.09	0.53
2:M:2:THR:HG21	2:M:156:ALA:O	2.09	0.53
2:H:151:LYS:CE	2:N:140:ASN:HD21	2.13	0.53
2:M:7:ARG:HA	2:M:11:GLN:O	2.09	0.53
2:I:38:TYR:C	2:I:40:GLY:H	2.11	0.53
2:H:71:LEU:HB2	2:H:99:ASP:OD1	2.07	0.53
2:G:50:THR:CG2	2:G:51:ALA:H	2.20	0.53
2:I:71:LEU:HD21	2:I:97:VAL:HG23	1.89	0.53
1:A:367:ILE:HG12	1:A:368:ALA:N	2.24	0.53
2:I:38:TYR:CE1	2:I:69:GLY:HA3	2.43	0.53
1:A:79:ILE:HG21	1:A:103:LEU:HB2	1.90	0.53
2:M:72:LEU:O	2:M:76:VAL:HG23	2.09	0.53
1:C:17:ILE:HB	1:C:24:LYS:HE3	1.90	0.53
2:L:80:LYS:HB3	2:L:80:LYS:HZ3	1.71	0.53
2:G:5:SER:HB2	2:G:14:VAL:HG22	1.91	0.53
1:A:25:ARG:O	1:A:28:ALA:HB3	2.09	0.53
1:B:105:ASP:C	1:B:107:ALA:H	2.12	0.53
2:N:33:LYS:HA	2:N:46:PHE:CE1	2.44	0.53
2:L:5:SER:HB3	2:L:121:LEU:HB2	1.89	0.53
2:G:105:ILE:CG2	2:G:121:LEU:HD13	2.36	0.52
2:G:156:ALA:O	2:G:159:ILE:N	2.36	0.52
2:I:91:LEU:O	2:I:93:ALA:N	2.41	0.52
2:L:67:HIS:NE2	2:L:77:GLU:HG3	2.24	0.52
2:I:115:PRO:HG3	2:I:121:LEU:HG	1.91	0.52
2:L:146:HIS:O	2:L:146:HIS:ND1	2.42	0.52
2:M:81:ASP:O	2:M:82:TRP:HB2	2.09	0.52
2:G:46:PHE:O	2:G:46:PHE:HD2	1.92	0.52
1:A:370:THR:O	1:A:373:ALA:N	2.40	0.52
1:B:443:ILE:HG23	2:H:112:VAL:HG23	1.92	0.52
2:L:46:PHE:CE2	2:L:50:THR:HA	2.44	0.52
1:B:245:ILE:O	1:B:246:ASP:C	2.46	0.52
1:B:410:SER:O	1:B:412:SER:N	2.42	0.52
2:H:7:ARG:NH1	2:H:7:ARG:HG3	2.23	0.52
2:I:6:VAL:HG12	2:I:7:ARG:N	2.25	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:N:58:GLU:O	2:N:60:PHE:N	2.36	0.52
1:B:61:VAL:O	1:B:61:VAL:HG23	2.09	0.52
1:A:34:ARG:HH11	1:A:34:ARG:HB2	1.74	0.52
2:G:14:VAL:O	2:G:34:VAL:HG11	2.09	0.52
2:N:43:LEU:HD11	2:N:171:GLU:O	2.08	0.52
2:M:76:VAL:O	2:M:79:ALA:HB3	2.10	0.52
1:A:6:PRO:O	1:A:10:VAL:HG23	2.09	0.52
1:B:356:TYR:O	1:B:359:LEU:N	2.43	0.52
2:L:73:LYS:HA	2:L:76:VAL:HG22	1.91	0.52
2:M:34:VAL:HG13	2:M:44:ALA:O	2.10	0.52
2:M:146:HIS:O	2:M:148:ILE:N	2.43	0.52
1:C:293:THR:O	1:C:295:HIS:N	2.43	0.52
2:M:96:ILE:HG12	2:M:105:ILE:HG12	1.91	0.52
1:A:245:ILE:O	1:A:247:ALA:N	2.43	0.52
1:C:406:LYS:H	1:C:406:LYS:CD	2.01	0.52
1:B:41:GLN:HE21	1:B:42:GLU:H	1.58	0.52
2:H:76:VAL:HG12	2:H:80:LYS:HE2	1.92	0.52
2:H:61:GLU:C	2:H:63:LYS:N	2.61	0.52
2:H:13:VAL:HG21	2:H:146:HIS:N	2.25	0.52
2:M:91:LEU:HD12	2:M:91:LEU:N	2.24	0.52
2:H:1:THR:HG23	2:H:33:LYS:CD	2.40	0.52
2:G:34:VAL:HA	2:G:44:ALA:O	2.10	0.52
1:A:315:ARG:HE	1:A:316:PRO:HD3	1.75	0.52
1:B:54:LEU:HD12	1:B:307:ALA:O	2.10	0.52
1:C:23:ALA:HA	1:C:331:VAL:HG11	1.92	0.52
2:H:136:ALA:O	2:H:138:VAL:N	2.36	0.51
2:L:64:LEU:CD2	2:L:69:GLY:HA2	2.40	0.51
2:M:28:LYS:HD3	2:M:31:ALA:HB2	1.91	0.51
2:I:27:MET:HE3	2:I:27:MET:HA	1.91	0.51
2:M:64:LEU:HD23	2:M:64:LEU:O	2.11	0.51
1:A:313:VAL:HG23	1:A:314:ALA:N	2.26	0.51
2:I:155:ILE:O	2:I:158:ASP:HB2	2.11	0.51
2:H:76:VAL:O	2:H:80:LYS:HD3	2.10	0.51
2:G:33:LYS:HE2	6:G:0:LVS:HB32	1.92	0.51
2:M:88:LEU:CA	2:M:91:LEU:HD13	2.38	0.51
1:B:5:THR:O	1:B:6:PRO:C	2.48	0.51
1:C:22:ASP:O	1:C:25:ARG:HB2	2.10	0.51
2:M:36:ARG:O	2:M:37:LEU:HD23	2.09	0.51
1:B:383:ARG:NH2	1:B:387:LYS:HE3	2.25	0.51
1:A:352:LEU:HD21	1:A:397:HIS:CE1	2.45	0.51
1:A:12:GLU:HA	1:A:12:GLU:OE1	2.09	0.51
2:M:79:ALA:HB2	2:M:112:VAL:CG2	2.41	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:444:LEU:OXT	2:G:113:VAL:HG13	2.11	0.51
2:N:88:LEU:CA	2:N:91:LEU:HD13	2.41	0.51
2:I:97:VAL:CG2	2:I:104:LEU:HD12	2.41	0.51
2:G:80:LYS:NZ	2:G:84:THR:HG22	2.26	0.51
1:C:359:LEU:O	1:C:362:THR:OG1	2.25	0.51
2:I:18:GLY:O	2:I:29:GLY:HA2	2.10	0.51
2:G:141:THR:HG21	2:G:143:LEU:HD12	1.92	0.51
2:L:6:VAL:HG12	2:L:7:ARG:N	2.25	0.51
2:M:63:LYS:HZ2	2:M:77:GLU:HB3	1.74	0.51
2:N:13:VAL:HG22	2:N:171:GLU:HG2	1.91	0.51
2:L:56:LEU:HD13	2:L:95:LEU:HD11	1.91	0.51
1:A:43:PRO:O	1:A:47:GLU:HG2	2.10	0.51
1:B:101:ARG:HG3	1:B:293:THR:HG22	1.92	0.51
2:M:138:VAL:O	2:M:140:ASN:N	2.43	0.51
2:M:12:VAL:HG21	2:M:98:ALA:HB1	1.93	0.51
2:H:37:LEU:HD21	2:H:57:PHE:CZ	2.46	0.51
2:M:19:GLN:HE22	2:M:162:PHE:HA	1.75	0.51
1:A:327:LEU:N	1:A:328:PRO:HD3	2.23	0.51
1:C:405:ASP:HB3	1:C:406:LYS:HD2	1.91	0.51
2:M:2:THR:CG2	2:M:126:GLY:HA3	2.39	0.51
2:G:141:THR:HG1	2:G:143:LEU:HG	1.71	0.51
1:C:20:GLN:HE22	1:C:334:THR:N	2.09	0.51
1:B:17:ILE:HG23	3:B:450:ADP:N6	2.26	0.51
2:M:20:VAL:CG2	2:M:28:LYS:HB3	2.41	0.51
2:M:33:LYS:HA	2:M:46:PHE:CE1	2.46	0.51
1:B:9:ILE:HG21	1:B:28:ALA:CB	2.40	0.51
2:M:126:GLY:HA2	2:M:129:TYR:CE2	2.46	0.51
2:G:50:THR:O	2:G:54:PHE:HD1	1.93	0.51
1:A:443:ILE:HG12	2:G:112:VAL:HG21	1.93	0.51
1:A:19:GLY:O	1:A:24:LYS:NZ	2.41	0.51
1:A:245:ILE:C	1:A:247:ALA:H	2.14	0.51
1:B:55:MET:HE1	1:B:333:LEU:HD11	1.93	0.51
2:N:20:VAL:CG2	2:N:28:LYS:HB3	2.41	0.51
2:N:20:VAL:HG23	2:N:28:LYS:HB3	1.93	0.51
1:B:356:TYR:O	1:B:357:LYS:C	2.49	0.51
1:A:53:ILE:CG2	1:A:54:LEU:N	2.73	0.51
2:G:1:THR:HB	6:G:0:LVS:C1'	2.41	0.50
2:G:33:LYS:HA	2:G:46:PHE:HE2	1.76	0.50
2:G:52:ASP:HA	2:G:55:THR:HG22	1.92	0.50
1:A:73:LEU:C	1:A:73:LEU:HD12	2.32	0.50
1:B:443:ILE:HG12	2:H:112:VAL:HG23	1.93	0.50
2:M:1:THR:HG23	2:M:17:ASP:OD1	2.11	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:M:51:ALA:O	2:M:52:ASP:C	2.49	0.50
2:N:126:GLY:O	2:N:127:GLY:C	2.49	0.50
2:G:13:VAL:HG21	2:G:146:HIS:CA	2.41	0.50
2:L:141:THR:HG22	2:L:143:LEU:HG	1.93	0.50
1:C:100:ILE:HB	1:C:291:VAL:HG21	1.93	0.50
2:H:67:HIS:NE2	2:H:77:GLU:HG3	2.25	0.50
1:A:102:ASP:O	1:A:105:ASP:HB2	2.11	0.50
2:G:4:VAL:HG12	2:G:153:LEU:CD2	2.41	0.50
1:A:249:GLU:HG3	1:A:298:VAL:HG13	1.94	0.50
2:I:141:THR:HB	2:I:143:LEU:HG	1.93	0.50
2:H:61:GLU:C	2:H:63:LYS:H	2.15	0.50
2:G:144:SER:O	2:G:148:ILE:HG13	2.11	0.50
2:N:149:VAL:O	2:N:149:VAL:HG12	2.12	0.50
1:B:15:GLN:O	1:B:16:HIS:CG	2.64	0.50
2:M:87:ALA:C	2:M:88:LEU:HD12	2.32	0.50
2:L:37:LEU:HD11	2:L:57:PHE:HB3	1.92	0.50
2:N:11:GLN:HE22	2:N:173:PRO:HB2	1.75	0.50
2:N:110:GLY:O	2:N:111:ASP:HB3	2.12	0.50
2:I:2:THR:HB	2:I:163:THR:HG21	1.93	0.50
2:G:172:LEU:O	2:G:173:PRO:C	2.50	0.50
2:N:138:VAL:HG23	2:N:148:ILE:HD13	1.94	0.50
1:B:42:GLU:CB	1:B:43:PRO:HD3	2.32	0.50
2:G:115:PRO:HG3	2:G:121:LEU:CD1	2.42	0.50
2:H:155:ILE:O	2:H:158:ASP:HB2	2.12	0.50
1:A:245:ILE:C	1:A:247:ALA:N	2.64	0.50
1:C:341:PHE:HB2	1:C:378:ALA:HB1	1.92	0.50
2:N:44:ALA:HB1	2:N:57:PHE:CE1	2.46	0.50
2:M:155:ILE:O	2:M:157:GLY:N	2.45	0.49
2:I:36:ARG:HH11	2:I:170:GLU:HB3	1.77	0.49
1:A:83:ALA:HB1	1:A:262:ILE:HD13	1.94	0.49
2:L:18:GLY:CA	2:L:33:LYS:HZ3	2.25	0.49
1:C:29:ILE:O	1:C:32:ARG:N	2.43	0.49
2:N:169:ILE:N	2:N:169:ILE:HD12	2.27	0.49
2:I:2:THR:HG22	2:I:153:LEU:HD22	1.93	0.49
2:I:94:MET:SD	2:I:105:ILE:HD11	2.52	0.49
1:A:443:ILE:CG2	1:A:444:LEU:N	2.75	0.49
2:N:52:ASP:OD2	2:N:91:LEU:HD23	2.11	0.49
2:H:7:ARG:NH2	2:H:12:VAL:HG11	2.27	0.49
1:A:56:ILE:HD11	1:A:316:PRO:HG2	1.93	0.49
2:H:58:GLU:O	2:H:61:GLU:HB3	2.12	0.49
1:A:313:VAL:HG23	1:A:314:ALA:H	1.76	0.49
2:M:12:VAL:HG13	2:M:12:VAL:O	2.13	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:11:SER:HA	1:A:14:ASP:HB2	1.95	0.49
2:H:2:THR:O	2:H:3:ILE:HD13	2.12	0.49
2:I:43:LEU:HD12	2:I:98:ALA:O	2.12	0.49
1:A:32:ARG:O	1:A:35:TRP:HB3	2.11	0.49
2:N:80:LYS:HB2	2:N:80:LYS:HZ3	1.73	0.49
1:C:26:ALA:HB2	1:C:331:VAL:CG1	2.43	0.49
1:A:345:LEU:HD13	1:A:396:LEU:HD13	1.93	0.49
1:A:250:GLN:HE21	1:A:250:GLN:CA	2.25	0.49
1:B:273:VAL:HA	1:B:276:GLU:HB3	1.94	0.49
1:B:286:VAL:CG1	1:B:326:ARG:HB3	2.31	0.49
2:I:43:LEU:HD12	2:I:43:LEU:N	2.19	0.49
2:I:99:ASP:HA	2:I:172:LEU:CD1	2.43	0.49
1:A:42:GLU:CB	1:A:43:PRO:HD3	2.41	0.49
2:I:24:ASN:O	2:N:161:VAL:HG13	2.13	0.49
2:N:82:TRP:CD2	2:N:108:GLY:HA2	2.47	0.49
2:L:148:ILE:O	2:L:149:VAL:C	2.50	0.49
2:G:47:ALA:O	2:G:93:ALA:HB1	2.13	0.49
2:I:15:GLY:HA2	2:I:34:VAL:HG21	1.95	0.49
2:M:6:VAL:HG21	2:M:148:ILE:CG2	2.42	0.49
1:C:34:ARG:NH2	1:C:251:ASN:C	2.65	0.49
1:A:37:ARG:HG2	1:A:38:MET:N	2.26	0.49
1:B:26:ALA:O	1:B:28:ALA:N	2.46	0.49
1:C:383:ARG:O	1:C:387:LYS:HG2	2.12	0.49
1:C:53:ILE:HG12	1:C:329:ILE:HG21	1.94	0.49
2:I:36:ARG:HD2	2:I:170:GLU:OE2	2.13	0.49
1:B:355:GLN:O	1:B:356:TYR:C	2.50	0.49
2:G:18:GLY:H	2:G:164:ASN:ND2	2.06	0.49
1:A:437:GLU:O	1:A:437:GLU:HG3	2.12	0.49
2:H:76:VAL:HG12	2:H:80:LYS:CE	2.43	0.49
2:H:120:ILE:HD12	2:H:135:ARG:HA	1.94	0.49
1:C:20:GLN:HE22	1:C:334:THR:H	1.59	0.49
2:L:115:PRO:HG3	2:L:121:LEU:HD21	1.94	0.49
2:H:125:SER:H	6:H:0:LVS:H1'3	1.75	0.49
2:M:86:ARG:HH11	2:M:86:ARG:CA	2.26	0.49
2:I:153:LEU:O	2:I:156:ALA:N	2.45	0.49
1:C:3:GLU:OE1	1:C:3:GLU:HA	2.12	0.49
2:N:115:PRO:HG3	2:N:121:LEU:HD21	1.95	0.49
1:B:48:VAL:HG13	1:B:48:VAL:O	2.12	0.49
2:I:127:GLY:O	2:I:131:LEU:N	2.36	0.49
2:G:7:ARG:HB3	2:G:119:GLN:HB3	1.95	0.49
2:I:36:ARG:O	2:I:37:LEU:HD23	2.13	0.49
2:G:1:THR:HB	6:G:0:LVS:H1'2	1.95	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:357:LYS:HE2	1:C:368:ALA:HA	1.94	0.49
1:C:395:ARG:O	1:C:399:VAL:HG23	2.13	0.49
1:C:439:LEU:C	1:C:441:ARG:H	2.16	0.48
1:C:68:ARG:HG2	1:C:68:ARG:NH1	2.28	0.48
2:G:56:LEU:HD22	2:G:95:LEU:CD1	2.39	0.48
1:A:76:ALA:HB1	1:A:251:ASN:O	2.12	0.48
2:I:3:ILE:HB	2:I:123:ILE:HG13	1.94	0.48
2:G:26:VAL:O	2:G:26:VAL:HG12	2.12	0.48
1:A:287:GLU:O	1:A:287:GLU:HG2	2.12	0.48
2:G:33:LYS:O	2:G:45:GLY:HA2	2.13	0.48
2:H:7:ARG:CZ	2:H:12:VAL:HG13	2.43	0.48
1:A:390:ASN:HB2	2:G:68:GLN:NE2	2.27	0.48
1:C:5:THR:HG23	1:C:8:GLU:OE1	2.12	0.48
1:A:51:LYS:O	1:A:329:ILE:HD12	2.14	0.48
1:B:37:ARG:HB3	1:B:48:VAL:HG11	1.94	0.48
2:H:3:ILE:O	2:H:122:ALA:HA	2.13	0.48
1:A:370:THR:O	1:A:371:THR:C	2.51	0.48
2:N:17:ASP:OD2	2:N:163:THR:HG23	2.13	0.48
2:L:105:ILE:HD12	2:L:121:LEU:HD22	1.96	0.48
1:C:40:LEU:HD12	1:C:48:VAL:HG11	1.94	0.48
1:A:38:MET:HA	1:A:45:ARG:HD2	1.96	0.48
2:G:13:VAL:HG21	2:G:145:ALA:C	2.33	0.48
2:I:71:LEU:HD13	2:I:71:LEU:C	2.34	0.48
2:G:144:SER:HB3	2:G:147:GLU:CG	2.44	0.48
2:N:57:PHE:O	2:N:61:GLU:HG2	2.13	0.48
1:B:256:ILE:HG21	1:B:259:ILE:HD13	1.94	0.48
1:B:360:MET:HE1	1:B:408:SER:HA	1.95	0.48
1:B:401:GLU:OE1	1:C:51:LYS:HG3	2.12	0.48
1:B:443:ILE:CG2	1:B:444:LEU:H	2.26	0.48
2:M:28:LYS:NZ	2:M:30:ASN:ND2	2.60	0.48
2:G:13:VAL:HG11	2:G:146:HIS:HA	1.94	0.48
2:N:146:HIS:CD2	2:N:169:ILE:HG21	2.49	0.48
2:M:105:ILE:HD12	2:M:121:LEU:HD22	1.96	0.48
2:G:136:ALA:O	2:G:139:GLU:N	2.47	0.48
1:C:374:VAL:O	1:C:376:LYS:N	2.47	0.48
2:H:120:ILE:HD13	2:H:134:ALA:HB1	1.96	0.48
2:N:155:ILE:O	2:N:159:ILE:HG13	2.13	0.48
1:A:79:ILE:HD12	1:A:80:LYS:H	1.79	0.48
2:I:120:ILE:O	2:I:121:LEU:HD23	2.14	0.48
2:G:36:ARG:NH1	2:G:170:GLU:OE2	2.47	0.48
2:M:155:ILE:C	2:M:157:GLY:N	2.66	0.48
1:A:81:VAL:HG21	1:A:99:ILE:HD13	1.96	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:330:ARG:NH1	1:A:330:ARG:CB	2.75	0.48
2:H:15:GLY:C	2:H:153:LEU:HD11	2.34	0.48
1:B:37:ARG:HD2	1:B:48:VAL:CG1	2.41	0.48
2:G:4:VAL:HG12	2:G:153:LEU:HD21	1.95	0.48
2:L:91:LEU:HD12	2:L:91:LEU:N	2.28	0.48
2:M:112:VAL:HG12	2:M:113:VAL:N	2.28	0.48
1:A:421:ILE:HG23	1:A:425:TYR:CD2	2.48	0.48
1:A:37:ARG:C	1:A:39:GLN:H	2.17	0.48
1:B:414:MET:O	1:B:417:GLN:HG3	2.13	0.48
1:A:54:LEU:HD13	1:A:327:LEU:HD13	1.94	0.48
2:G:107:THR:OG1	2:G:109:ILE:HG12	2.14	0.48
1:B:3:GLU:HA	1:B:3:GLU:OE1	2.12	0.48
2:N:42:VAL:HA	2:N:98:ALA:O	2.13	0.48
2:G:128:ASN:O	2:G:131:LEU:HB3	2.13	0.48
1:B:377:ILE:O	1:B:380:ALA:HB3	2.13	0.48
1:C:349:HIS:O	1:C:350:ALA:HB3	2.13	0.48
1:B:72:LYS:C	1:B:72:LYS:HD2	2.34	0.48
2:H:25:THR:HA	2:M:159:ILE:O	2.13	0.48
1:A:20:GLN:NE2	1:A:334:THR:HG22	2.28	0.48
2:I:73:LYS:HA	2:I:76:VAL:HG23	1.95	0.48
2:N:104:LEU:HD12	2:N:114:GLN:HA	1.94	0.48
2:M:59:LEU:HD12	2:M:59:LEU:O	2.15	0.47
1:A:315:ARG:HG3	1:A:316:PRO:HD2	1.96	0.47
1:B:426:VAL:C	1:B:428:ASP:H	2.18	0.47
2:N:5:SER:OG	2:N:14:VAL:HG22	2.13	0.47
1:C:63:LYS:HD2	1:C:308:SER:HB2	1.95	0.47
1:C:23:ALA:O	1:C:27:VAL:HG13	2.14	0.47
1:C:425:TYR:O	1:C:426:VAL:C	2.52	0.47
2:N:116:GLU:O	2:N:118:ASP:N	2.47	0.47
2:G:115:PRO:HG3	2:G:121:LEU:CG	2.44	0.47
2:N:50:THR:C	2:N:52:ASP:H	2.16	0.47
1:B:367:ILE:CG1	1:B:368:ALA:N	2.75	0.47
2:G:88:LEU:O	2:G:90:LYS:N	2.47	0.47
2:N:3:ILE:O	2:N:122:ALA:HA	2.13	0.47
2:G:78:LEU:HG	2:G:82:TRP:CZ3	2.48	0.47
2:G:5:SER:HA	2:G:13:VAL:O	2.14	0.47
2:I:7:ARG:HH11	2:I:7:ARG:HG3	1.79	0.47
1:C:52:ASN:ND2	1:C:305:PHE:H	2.12	0.47
2:H:59:LEU:HB3	2:H:78:LEU:HD11	1.96	0.47
2:I:21:SER:O	6:I:0:LVS:HD42	2.14	0.47
2:M:115:PRO:HG3	2:M:121:LEU:HG	1.97	0.47
1:C:63:LYS:CG	1:C:333:LEU:HD22	2.44	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:L:71:LEU:HD22	2:L:99:ASP:OD2	2.15	0.47
2:L:94:MET:O	2:L:95:LEU:HD23	2.14	0.47
2:I:115:PRO:HG3	2:I:121:LEU:HD11	1.96	0.47
1:B:391:ILE:O	1:B:394:ARG:HB2	2.14	0.47
2:I:1:THR:H3	6:I:0:LVS:C2'	2.27	0.47
2:M:96:ILE:CD1	2:M:123:ILE:HG12	2.44	0.47
1:A:36:ARG:C	1:A:37:ARG:O	2.51	0.47
1:A:86:PHE:HB2	1:A:278:VAL:HG11	1.97	0.47
2:I:67:HIS:CD2	2:I:77:GLU:HG3	2.49	0.47
1:A:13:LEU:HD12	1:A:24:LYS:CG	2.44	0.47
1:C:37:ARG:O	1:C:45:ARG:HD3	2.14	0.47
2:H:8:ARG:O	2:H:11:GLN:HB2	2.15	0.47
1:B:42:GLU:HB3	1:B:43:PRO:CD	2.35	0.47
1:C:98:SER:O	1:C:101:ARG:N	2.48	0.47
1:C:64:THR:HB	3:C:450:ADP:O1A	2.15	0.47
1:B:66:ILE:HD12	1:B:333:LEU:HD21	1.95	0.47
2:G:120:ILE:CD1	2:G:135:ARG:HA	2.44	0.47
2:L:19:GLN:HB2	2:L:164:ASN:HD22	1.79	0.47
2:L:134:ALA:O	2:L:137:LEU:N	2.47	0.47
2:L:133:ALA:HB1	2:L:155:ILE:HD12	1.96	0.47
2:H:49:GLY:O	2:H:50:THR:C	2.52	0.47
2:N:83:ARG:O	2:N:89:ARG:HD3	2.15	0.47
2:I:34:VAL:HA	2:I:45:GLY:HA2	1.97	0.47
2:I:3:ILE:HB	2:I:123:ILE:CG1	2.44	0.47
2:N:10:GLY:O	2:N:11:GLN:HG2	2.14	0.47
2:I:164:ASN:HD22	2:I:164:ASN:H	1.63	0.47
2:H:115:PRO:HG3	2:H:121:LEU:CD2	2.41	0.47
2:M:71:LEU:O	2:M:75:ALA:N	2.39	0.47
2:N:85:ASP:CB	2:N:88:LEU:HD23	2.44	0.47
1:B:443:ILE:HG22	1:B:444:LEU:H	1.75	0.47
1:A:37:ARG:NH2	1:A:302:HIS:CD2	2.83	0.47
2:I:133:ALA:O	2:I:136:ALA:N	2.46	0.47
1:B:320:ILE:O	1:B:320:ILE:HG13	2.15	0.47
1:B:441:ARG:HH11	1:B:441:ARG:CB	2.00	0.47
1:B:441:ARG:NH1	1:B:441:ARG:CB	2.70	0.47
1:B:41:GLN:HA	1:B:41:GLN:NE2	2.30	0.47
1:C:98:SER:HA	1:C:101:ARG:NE	2.23	0.47
1:C:61:VAL:HA	1:C:336:LEU:CD2	2.45	0.47
2:G:1:THR:HG23	2:G:33:LYS:HD3	1.97	0.47
2:G:118:ASP:O	2:G:120:ILE:HG13	2.15	0.47
1:A:52:ASN:O	1:A:328:PRO:HD2	2.15	0.47
2:L:138:VAL:O	2:L:138:VAL:HG22	2.14	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:I:144:SER:OG	2:I:147:GLU:HG3	2.15	0.47
2:M:167:PHE:CD2	2:M:167:PHE:N	2.83	0.47
1:B:370:THR:O	1:B:373:ALA:HB3	2.15	0.47
2:I:172:LEU:HD23	2:I:172:LEU:HA	1.79	0.47
1:A:439:LEU:HD23	2:G:72:LEU:HD12	1.97	0.47
2:N:17:ASP:O	2:N:33:LYS:HD2	2.15	0.47
1:B:61:VAL:HA	1:B:336:LEU:HD22	1.97	0.47
2:I:137:LEU:N	2:I:137:LEU:HD12	2.29	0.47
2:H:54:PHE:O	2:H:58:GLU:HG3	2.15	0.47
2:N:6:VAL:HG22	2:N:120:ILE:HG23	1.97	0.46
2:L:104:LEU:HD23	2:L:115:PRO:HD3	1.95	0.46
1:B:17:ILE:HG23	3:B:450:ADP:C6	2.50	0.46
1:C:367:ILE:HG22	1:C:419:VAL:HB	1.96	0.46
2:G:5:SER:CB	2:G:14:VAL:HG22	2.45	0.46
2:N:60:PHE:CD1	2:N:78:LEU:HD22	2.50	0.46
2:L:1:THR:HG23	2:L:33:LYS:CE	2.44	0.46
1:A:53:ILE:HG12	1:A:329:ILE:CG2	2.46	0.46
2:I:118:ASP:O	2:I:119:GLN:C	2.54	0.46
1:B:360:MET:O	1:B:363:GLU:N	2.43	0.46
1:B:426:VAL:O	1:B:428:ASP:N	2.49	0.46
2:M:10:GLY:O	2:M:11:GLN:NE2	2.49	0.46
1:A:20:GLN:CA	1:A:20:GLN:NE2	2.68	0.46
2:G:15:GLY:HA2	2:G:34:VAL:HG21	1.97	0.46
1:B:29:ILE:HG22	1:B:30:ALA:N	2.30	0.46
1:C:3:GLU:CG	1:C:4:MET:N	2.62	0.46
2:M:6:VAL:HG23	2:M:149:VAL:HG22	1.98	0.46
2:G:140:ASN:O	2:G:141:THR:HB	2.15	0.46
1:B:57:GLY:CA	1:B:63:LYS:HE2	2.46	0.46
1:C:20:GLN:HA	1:C:20:GLN:HE21	1.81	0.46
2:M:86:ARG:HB3	2:M:86:ARG:NH1	2.30	0.46
2:N:38:TYR:O	2:N:39:ASN:HB3	2.15	0.46
2:M:8:ARG:HH12	2:M:142:GLU:HA	1.79	0.46
2:N:71:LEU:HB2	2:N:99:ASP:OD2	2.15	0.46
2:G:167:PHE:N	2:G:167:PHE:CD2	2.82	0.46
1:B:20:GLN:NE2	1:B:20:GLN:HA	2.22	0.46
2:H:14:VAL:O	2:H:34:VAL:HG11	2.15	0.46
1:A:407:ILE:HD11	1:A:419:VAL:HG11	1.97	0.46
2:I:7:ARG:HA	2:I:11:GLN:O	2.16	0.46
2:M:89:ARG:HH11	2:M:89:ARG:HG3	1.80	0.46
2:L:75:ALA:O	2:L:78:LEU:N	2.48	0.46
2:G:3:ILE:O	2:G:122:ALA:HA	2.16	0.46
2:I:37:LEU:N	2:I:42:VAL:O	2.45	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:13:LEU:HB2	1:C:24:LYS:HD3	1.96	0.46
2:L:7:ARG:NH2	2:L:99:ASP:O	2.44	0.46
2:H:83:ARG:HG2	2:I:55:THR:CB	2.46	0.46
2:G:13:VAL:HB	2:G:149:VAL:HG21	1.97	0.46
2:G:138:VAL:HG22	2:G:148:ILE:CD1	2.46	0.46
2:N:143:LEU:HD22	2:N:147:GLU:OE1	2.16	0.46
2:M:2:THR:HG22	2:M:126:GLY:C	2.36	0.46
1:C:61:VAL:C	3:C:450:ADP:N7	2.69	0.46
1:C:14:ASP:HA	1:C:24:LYS:HE2	1.97	0.46
2:I:7:ARG:NH1	2:I:12:VAL:HG22	2.30	0.46
2:I:134:ALA:C	2:I:136:ALA:N	2.69	0.46
1:B:322:GLU:N	1:B:322:GLU:OE2	2.46	0.46
1:B:86:PHE:O	1:B:87:THR:OG1	2.25	0.46
1:A:20:GLN:NE2	1:A:334:THR:H	2.07	0.46
1:C:101:ARG:HA	1:C:293:THR:HG21	1.97	0.46
1:C:63:LYS:HE3	1:C:308:SER:HB2	1.97	0.46
1:C:55:MET:HB3	1:C:63:LYS:HD2	1.98	0.46
1:C:374:VAL:C	1:C:376:LYS:N	2.68	0.46
2:H:115:PRO:HG3	2:H:121:LEU:CG	2.46	0.46
2:N:56:LEU:HD12	2:N:95:LEU:HD11	1.98	0.46
2:N:90:LYS:C	2:N:91:LEU:HD12	2.37	0.46
1:B:342:GLU:CD	1:B:375:LYS:HE2	2.36	0.46
1:A:63:LYS:NZ	1:A:308:SER:HB2	2.31	0.46
2:H:89:ARG:O	2:H:90:LYS:HB2	2.16	0.46
1:A:430:LEU:O	1:A:431:GLY:C	2.54	0.46
1:A:31:LEU:O	1:A:31:LEU:HG	2.16	0.46
1:C:84:THR:C	1:C:86:PHE:N	2.70	0.46
2:G:117:GLU:C	2:G:119:GLN:N	2.69	0.46
1:B:276:GLU:C	1:B:278:VAL:H	2.18	0.46
1:A:61:VAL:HA	1:A:336:LEU:HD22	1.98	0.46
1:C:4:MET:HA	1:C:8:GLU:OE1	2.16	0.45
1:A:361:ALA:HA	1:A:365:VAL:O	2.16	0.45
2:L:83:ARG:HA	2:L:89:ARG:HD3	1.97	0.45
1:B:343:ARG:HE	1:B:347:GLU:CD	2.19	0.45
1:C:84:THR:C	1:C:86:PHE:H	2.19	0.45
2:M:164:ASN:HD21	2:M:166:ASN:HB2	1.81	0.45
1:A:41:GLN:CA	1:A:41:GLN:HE21	2.28	0.45
1:C:61:VAL:HG23	1:C:333:LEU:HD23	1.98	0.45
2:H:138:VAL:HG22	2:H:148:ILE:HD13	1.98	0.45
2:I:47:ALA:O	2:I:93:ALA:HB1	2.16	0.45
1:B:59:THR:HA	5:B:452:PO4:O2	2.17	0.45
1:A:315:ARG:HG3	1:A:316:PRO:CD	2.46	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:G:46:PHE:HB2	2:G:53:ALA:HB1	1.98	0.45
2:G:55:THR:HG23	2:G:91:LEU:HD23	1.98	0.45
2:L:6:VAL:CG1	2:L:7:ARG:N	2.79	0.45
1:C:360:MET:CA	1:C:360:MET:CE	2.95	0.45
2:L:144:SER:C	2:L:146:HIS:N	2.68	0.45
2:I:153:LEU:O	2:I:154:ARG:C	2.54	0.45
1:C:52:ASN:HB2	1:C:326:ARG:O	2.16	0.45
2:N:172:LEU:CB	2:N:173:PRO:HD3	2.47	0.45
2:M:90:LYS:C	2:M:91:LEU:HD12	2.37	0.45
2:I:73:LYS:O	2:I:74:SER:C	2.54	0.45
2:M:20:VAL:HG21	2:M:28:LYS:HB3	1.97	0.45
2:L:172:LEU:HD23	2:L:173:PRO:HA	1.97	0.45
1:C:322:GLU:OE2	1:C:322:GLU:N	2.46	0.45
2:H:18:GLY:HA2	2:H:31:ALA:HB3	1.98	0.45
1:A:286:VAL:CG1	1:A:326:ARG:HB3	2.46	0.45
2:N:58:GLU:C	2:N:60:PHE:N	2.70	0.45
2:I:71:LEU:HD13	2:I:71:LEU:O	2.17	0.45
1:C:427:ALA:O	1:C:431:GLY:HA2	2.17	0.45
1:C:337:SER:O	1:C:339:ALA:N	2.50	0.45
2:N:8:ARG:HH22	2:N:142:GLU:HA	1.82	0.45
2:G:91:LEU:N	2:G:91:LEU:CD1	2.77	0.45
2:I:115:PRO:HB2	2:I:119:GLN:HA	1.99	0.45
2:I:154:ARG:HH11	2:I:154:ARG:HG3	1.80	0.45
2:N:66:MET:HG3	2:N:67:HIS:HD2	1.82	0.45
1:A:64:THR:N	3:A:450:ADP:O2B	2.50	0.45
1:A:82:GLU:HG2	1:A:84:THR:OG1	2.16	0.45
1:C:422:ASP:O	1:C:423:ALA:C	2.55	0.45
2:M:137:LEU:N	2:M:137:LEU:HD22	2.31	0.45
2:L:109:ILE:CG1	2:L:110:GLY:H	2.18	0.45
2:G:133:ALA:O	2:G:136:ALA:HB3	2.16	0.45
2:H:94:MET:CG	2:H:107:THR:HG22	2.44	0.45
2:L:67:HIS:HB3	2:L:73:LYS:HE2	1.98	0.45
1:A:38:MET:HA	1:A:45:ARG:CG	2.47	0.45
1:B:85:LYS:CG	1:B:85:LYS:O	2.65	0.45
1:A:283:LEU:HB2	1:A:284:PRO:HD3	1.98	0.45
2:N:104:LEU:N	2:N:104:LEU:HD22	2.32	0.45
1:C:357:LYS:HA	1:C:367:ILE:HD11	1.99	0.45
1:B:424:ALA:C	1:B:426:VAL:N	2.69	0.45
2:H:141:THR:CG2	2:H:143:LEU:HG	2.47	0.45
1:A:27:VAL:HB	1:A:70:LEU:CD1	2.39	0.45
2:I:22:LEU:HD13	6:I:0:LVS:HD13	1.98	0.45
2:G:13:VAL:HG21	2:G:146:HIS:HA	1.98	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:G:125:SER:H	6:G:0:LVS:H1'3	1.81	0.45
2:L:104:LEU:HD21	2:L:114:GLN:HG2	1.99	0.45
1:C:33:ASN:O	1:C:34:ARG:C	2.52	0.45
2:I:52:ASP:CA	2:I:55:THR:HG23	2.45	0.45
2:L:133:ALA:O	2:L:134:ALA:C	2.55	0.45
1:A:343:ARG:HH21	1:A:347:GLU:CD	2.19	0.45
1:A:4:MET:HE2	1:A:73:LEU:HD13	1.99	0.44
1:A:86:PHE:CZ	1:A:99:ILE:HD11	2.52	0.44
2:G:112:VAL:HG23	2:G:112:VAL:O	2.17	0.44
2:L:71:LEU:HB2	2:L:99:ASP:OD2	2.18	0.44
1:C:31:LEU:HD22	1:C:70:LEU:HD11	1.99	0.44
2:H:91:LEU:HD22	2:H:91:LEU:N	2.32	0.44
1:B:60:GLY:HA2	3:B:450:ADP:PB	2.57	0.44
2:H:62:ARG:O	2:H:66:MET:HG3	2.17	0.44
2:L:90:LYS:C	2:L:91:LEU:HD12	2.38	0.44
2:G:38:TYR:C	2:G:40:GLY:H	2.21	0.44
2:M:28:LYS:NZ	2:M:30:ASN:HD21	2.14	0.44
2:M:37:LEU:HD11	2:M:57:PHE:CB	2.46	0.44
2:I:156:ALA:O	2:I:159:ILE:N	2.46	0.44
2:N:6:VAL:HG23	2:N:149:VAL:HG22	2.00	0.44
2:M:103:SER:O	2:M:115:PRO:HD3	2.17	0.44
2:N:63:LYS:NZ	2:N:81:ASP:OD1	2.47	0.44
2:N:8:ARG:NH2	2:N:142:GLU:HA	2.32	0.44
1:C:328:PRO:HG2	1:C:329:ILE:H	1.82	0.44
2:I:36:ARG:NH1	2:I:43:LEU:HD23	2.33	0.44
1:A:5:THR:H	1:A:8:GLU:HB2	1.81	0.44
1:C:403:LEU:CD2	1:C:404:MET:HG2	2.47	0.44
2:N:17:ASP:OD2	2:N:163:THR:HA	2.17	0.44
1:A:249:GLU:OE1	1:A:299:LYS:N	2.38	0.44
2:I:62:ARG:NH1	2:I:62:ARG:CB	2.81	0.44
2:G:68:GLN:HB2	2:G:70:HIS:CD2	2.52	0.44
2:I:1:THR:HA	2:I:33:LYS:HZ2	1.83	0.44
2:L:3:ILE:CG2	2:L:96:ILE:HD12	2.47	0.44
1:B:283:LEU:O	1:B:284:PRO:C	2.55	0.44
2:H:7:ARG:HB3	2:H:119:GLN:HB3	2.00	0.44
2:H:15:GLY:HA2	2:H:34:VAL:HG21	1.98	0.44
1:B:60:GLY:HA2	3:B:450:ADP:O3A	2.16	0.44
2:I:6:VAL:CG1	2:I:7:ARG:N	2.80	0.44
1:B:9:ILE:HG22	1:B:10:VAL:N	2.32	0.44
2:I:154:ARG:HG3	2:I:154:ARG:NH1	2.33	0.44
1:A:256:ILE:O	1:A:256:ILE:HG22	2.17	0.44
1:A:404:MET:O	1:A:408:SER:HB2	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:86:PHE:HB2	1:A:278:VAL:CG1	2.48	0.44
1:C:44:LEU:O	1:C:48:VAL:HG12	2.18	0.44
2:H:141:THR:CG2	2:H:142:GLU:H	2.31	0.44
2:I:110:GLY:O	2:I:111:ASP:HB3	2.18	0.44
2:I:8:ARG:O	2:I:11:GLN:HB2	2.18	0.44
2:I:138:VAL:HG12	2:I:138:VAL:O	2.18	0.44
1:C:98:SER:O	1:C:99:ILE:C	2.55	0.44
2:G:125:SER:H	6:G:0:LVS:C1'	2.31	0.44
1:B:374:VAL:O	1:B:375:LYS:C	2.56	0.44
1:C:312:GLN:NE2	2:I:66:MET:HA	2.33	0.44
2:I:137:LEU:HB3	2:I:143:LEU:HD12	1.99	0.44
2:L:57:PHE:O	2:L:61:GLU:HG2	2.18	0.44
2:G:43:LEU:HD13	2:G:170:GLU:O	2.17	0.44
1:B:34:ARG:NH2	1:B:253:ILE:HD13	2.32	0.44
2:H:42:VAL:HG21	2:H:64:LEU:HD13	2.00	0.44
1:B:27:VAL:HB	1:B:70:LEU:CD1	2.37	0.44
2:G:71:LEU:O	2:G:72:LEU:C	2.56	0.44
2:L:104:LEU:CD2	2:L:114:GLN:HA	2.48	0.44
2:I:62:ARG:HB3	2:I:62:ARG:CZ	2.48	0.44
1:B:102:ASP:O	1:B:105:ASP:HB2	2.17	0.44
2:H:141:THR:HG22	2:H:143:LEU:N	2.17	0.43
2:M:172:LEU:CB	2:M:173:PRO:HD3	2.46	0.43
2:L:128:ASN:HA	2:L:131:LEU:HB3	2.00	0.43
1:A:286:VAL:HG11	1:A:326:ARG:CB	2.47	0.43
1:A:65:GLU:HG3	3:A:450:ADP:H2'	1.99	0.43
1:A:87:THR:O	1:A:274:SER:HB2	2.18	0.43
1:B:44:LEU:O	1:B:45:ARG:C	2.55	0.43
2:M:157:GLY:HA2	2:M:163:THR:CG2	2.48	0.43
1:A:367:ILE:HD11	1:A:421:ILE:HD12	1.99	0.43
2:H:120:ILE:O	2:H:121:LEU:HD23	2.18	0.43
2:I:34:VAL:HG22	2:I:45:GLY:HA3	1.99	0.43
1:A:323:LEU:O	1:A:324:GLN:C	2.56	0.43
2:M:115:PRO:HG3	2:M:121:LEU:HD11	2.00	0.43
2:M:105:ILE:CG1	2:M:121:LEU:HD13	2.40	0.43
1:C:63:LYS:CE	1:C:308:SER:HB2	2.47	0.43
2:N:91:LEU:N	2:N:91:LEU:CD1	2.82	0.43
1:C:10:VAL:HG12	1:C:14:ASP:OD2	2.18	0.43
2:L:69:GLY:O	2:L:71:LEU:N	2.51	0.43
1:A:13:LEU:HD13	1:A:66:ILE:HG23	1.99	0.43
2:M:64:LEU:HD21	2:M:69:GLY:HA2	2.00	0.43
2:I:133:ALA:O	2:I:134:ALA:C	2.57	0.43
1:A:260:ASP:HB3	1:A:311:PHE:CE2	2.53	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:41:GLN:NE2	1:B:41:GLN:CA	2.81	0.43
2:G:153:LEU:O	2:G:156:ALA:HB3	2.18	0.43
1:C:256:ILE:CD1	1:C:282:LEU:HD21	2.42	0.43
2:H:131:LEU:HD21	2:H:135:ARG:HH12	1.81	0.43
2:H:132:SER:O	2:H:133:ALA:C	2.57	0.43
2:M:42:VAL:HG22	2:M:99:ASP:HB3	1.99	0.43
2:G:89:ARG:O	2:G:90:LYS:HB3	2.19	0.43
2:I:88:LEU:O	2:I:89:ARG:HB2	2.17	0.43
1:A:398:THR:O	1:A:399:VAL:C	2.56	0.43
2:H:141:THR:HG21	2:H:143:LEU:HG	2.01	0.43
2:G:114:GLN:HA	2:G:115:PRO:HD3	1.82	0.43
2:M:94:MET:HB2	2:M:123:ILE:HD12	2.00	0.43
1:A:4:MET:HB3	1:A:8:GLU:CB	2.41	0.43
2:H:17:ASP:HB2	2:H:164:ASN:HD22	1.75	0.43
2:L:82:TRP:CD2	2:L:108:GLY:HA2	2.53	0.43
2:L:82:TRP:O	2:L:82:TRP:HD1	2.01	0.43
1:A:337:SER:O	1:A:340:ASP:HB2	2.18	0.43
1:A:388:THR:OG1	1:A:389:GLU:N	2.50	0.43
2:N:121:LEU:HA	2:N:121:LEU:HD23	1.78	0.43
1:B:41:GLN:HE21	1:B:42:GLU:N	2.16	0.43
1:B:27:VAL:CB	1:B:70:LEU:HD13	2.36	0.43
1:A:4:MET:CE	1:A:73:LEU:HD13	2.48	0.43
2:M:71:LEU:H	2:M:71:LEU:CD1	2.18	0.43
1:B:299:LYS:C	1:B:301:ASP:H	2.21	0.43
2:L:133:ALA:O	2:L:134:ALA:O	2.37	0.43
1:A:390:ASN:H	2:G:68:GLN:NE2	2.16	0.43
1:A:84:THR:O	1:A:87:THR:HG23	2.18	0.43
2:M:2:THR:O	2:M:16:GLY:HA2	2.19	0.43
1:A:439:LEU:HD21	2:G:73:LYS:HA	2.01	0.43
1:A:37:ARG:HB2	1:A:48:VAL:HG11	2.01	0.43
2:M:28:LYS:HZ2	2:M:30:ASN:CG	2.21	0.43
2:N:13:VAL:HG21	2:N:146:HIS:N	2.34	0.43
1:A:352:LEU:HA	1:A:352:LEU:HD23	1.73	0.43
2:G:100:GLU:OE1	2:G:172:LEU:HD22	2.18	0.43
1:B:275:ARG:O	1:B:278:VAL:HG23	2.18	0.43
1:B:256:ILE:CG2	1:B:259:ILE:HD13	2.48	0.43
2:L:89:ARG:HG3	2:L:89:ARG:HH11	1.84	0.43
1:B:384:VAL:HG22	1:B:385:ASN:N	2.34	0.43
2:M:9:ASN:O	2:M:11:GLN:HG2	2.18	0.43
2:H:128:ASN:HA	2:H:131:LEU:HB3	2.00	0.43
2:G:164:ASN:HD22	2:G:164:ASN:C	2.22	0.43
2:G:86:ARG:O	2:G:88:LEU:HD22	2.19	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:426:VAL:C	1:B:428:ASP:N	2.70	0.43
1:A:324:GLN:HE21	1:A:324:GLN:HB2	1.66	0.43
2:I:49:GLY:O	2:I:50:THR:C	2.55	0.43
2:N:148:ILE:C	2:N:150:GLU:H	2.21	0.43
2:I:36:ARG:HA	2:I:43:LEU:HA	1.99	0.43
2:L:64:LEU:HA	2:L:74:SER:CB	2.49	0.43
2:I:67:HIS:O	2:I:69:GLY:N	2.51	0.43
2:I:7:ARG:NH2	2:I:103:SER:OG	2.51	0.43
1:B:33:ASN:HA	1:B:36:ARG:HB2	1.99	0.43
1:C:365:VAL:HG12	1:C:366:ASN:N	2.33	0.43
1:B:41:GLN:HE21	1:B:41:GLN:CA	2.30	0.43
2:L:18:GLY:HA2	2:L:33:LYS:NZ	2.33	0.43
2:H:38:TYR:C	2:H:40:GLY:N	2.69	0.43
1:C:384:VAL:HG23	1:C:388:THR:OG1	2.19	0.43
1:B:424:ALA:C	1:B:426:VAL:H	2.22	0.43
1:B:96:VAL:HG13	1:B:99:ILE:HD12	2.00	0.43
1:C:53:ILE:HG22	1:C:54:LEU:N	2.33	0.42
2:M:120:ILE:O	2:M:121:LEU:HD23	2.18	0.42
1:A:275:ARG:O	1:A:278:VAL:HG22	2.19	0.42
2:H:120:ILE:HD13	2:H:134:ALA:CB	2.48	0.42
1:C:34:ARG:HH21	1:C:252:GLY:N	2.17	0.42
2:G:86:ARG:NH1	2:G:86:ARG:HB2	2.33	0.42
2:H:52:ASP:HA	2:H:91:LEU:HD12	2.01	0.42
1:B:374:VAL:O	1:B:376:LYS:N	2.52	0.42
1:A:76:ALA:HA	1:A:77:PRO:HD3	1.93	0.42
1:C:283:LEU:O	1:C:284:PRO:C	2.58	0.42
2:I:137:LEU:N	2:I:137:LEU:CD1	2.82	0.42
2:H:38:TYR:O	2:H:40:GLY:N	2.51	0.42
1:C:287:GLU:O	1:C:287:GLU:HG2	2.19	0.42
1:A:413:ASP:OD2	1:A:413:ASP:N	2.51	0.42
2:I:42:VAL:HG21	2:I:64:LEU:HD13	2.02	0.42
2:L:53:ALA:O	2:L:56:LEU:HB2	2.17	0.42
1:B:39:GLN:NE2	1:B:39:GLN:N	2.65	0.42
2:N:2:THR:O	2:N:3:ILE:HD13	2.18	0.42
2:I:155:ILE:O	2:I:159:ILE:HG13	2.18	0.42
2:N:44:ALA:HA	2:N:96:ILE:O	2.19	0.42
1:B:276:GLU:C	1:B:278:VAL:N	2.72	0.42
2:L:51:ALA:O	2:L:52:ASP:C	2.57	0.42
1:C:299:LYS:HD2	1:C:299:LYS:N	2.34	0.42
2:M:37:LEU:HD21	2:M:57:PHE:HB3	2.00	0.42
2:L:116:GLU:C	2:L:118:ASP:N	2.71	0.42
1:B:72:LYS:O	1:B:72:LYS:HD2	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:M:6:VAL:CG1	2:M:7:ARG:H	2.29	0.42
2:M:6:VAL:CG1	2:M:7:ARG:N	2.82	0.42
2:H:76:VAL:CG1	2:H:80:LYS:HE2	2.48	0.42
1:A:5:THR:HA	1:A:32:ARG:HH11	1.84	0.42
1:B:20:GLN:HG3	1:B:333:LEU:HD23	2.02	0.42
2:M:71:LEU:HD21	2:M:99:ASP:CB	2.47	0.42
2:H:154:ARG:O	2:H:155:ILE:C	2.58	0.42
2:I:141:THR:CB	2:I:143:LEU:HG	2.50	0.42
2:L:12:VAL:HG13	2:L:12:VAL:O	2.19	0.42
1:C:384:VAL:HG22	1:C:385:ASN:N	2.33	0.42
2:G:20:VAL:HB	2:G:27:MET:HB3	2.01	0.42
2:H:70:HIS:O	2:H:71:LEU:C	2.57	0.42
1:A:9:ILE:HG23	1:A:73:LEU:HD21	2.02	0.42
2:M:85:ASP:HB3	2:M:88:LEU:HB2	2.02	0.42
1:C:442:PHE:HB3	2:I:83:ARG:HH12	1.84	0.42
2:M:153:LEU:HB3	2:M:167:PHE:CZ	2.55	0.42
2:H:37:LEU:HD21	2:H:57:PHE:CE2	2.55	0.42
2:H:44:ALA:HB2	2:H:97:VAL:HG12	2.00	0.42
1:A:443:ILE:HG12	2:G:112:VAL:HG23	2.01	0.42
2:L:67:HIS:CG	2:L:73:LYS:HE2	2.54	0.42
1:A:38:MET:HA	1:A:45:ARG:HG3	2.02	0.42
2:H:7:ARG:HB3	2:H:119:GLN:CB	2.50	0.42
2:H:82:TRP:CD1	2:H:88:LEU:HB3	2.54	0.42
1:C:250:GLN:NE2	1:C:250:GLN:CA	2.80	0.42
1:B:84:THR:C	1:B:86:PHE:N	2.72	0.42
2:H:56:LEU:HD13	2:H:56:LEU:C	2.40	0.42
1:C:329:ILE:C	1:C:330:ARG:HG2	2.39	0.42
2:H:136:ALA:C	2:H:138:VAL:N	2.72	0.42
2:N:53:ALA:HA	2:N:56:LEU:HB2	2.02	0.42
2:N:164:ASN:OD1	2:N:166:ASN:N	2.52	0.42
2:L:44:ALA:HB1	2:L:96:ILE:O	2.19	0.42
2:G:89:ARG:HG2	2:G:89:ARG:NH1	2.30	0.42
2:M:28:LYS:CG	2:M:29:GLY:N	2.82	0.42
1:A:53:ILE:HG22	1:A:54:LEU:N	2.34	0.42
2:G:5:SER:HB2	2:G:14:VAL:HG13	2.01	0.42
1:C:262:ILE:HA	1:C:275:ARG:HB3	2.02	0.42
2:G:7:ARG:NH2	2:G:12:VAL:HG21	2.35	0.42
1:B:384:VAL:O	1:B:385:ASN:C	2.58	0.42
1:A:434:VAL:HG12	1:A:435:GLU:N	2.34	0.42
2:I:17:ASP:OD2	2:I:33:LYS:NZ	2.51	0.42
2:M:104:LEU:HD12	2:M:104:LEU:N	2.35	0.42
2:H:134:ALA:O	2:H:138:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:L:141:THR:HG22	2:L:142:GLU:N	2.34	0.42
2:L:136:ALA:O	2:L:139:GLU:HB2	2.20	0.42
1:A:61:VAL:HG11	1:A:335:ALA:HA	2.01	0.42
1:A:414:MET:O	1:A:417:GLN:HG3	2.20	0.42
1:C:374:VAL:O	1:C:377:ILE:N	2.53	0.42
1:C:17:ILE:HG21	1:C:66:ILE:CD1	2.50	0.42
2:L:82:TRP:CE2	2:L:108:GLY:HA2	2.55	0.42
2:H:1:THR:HB	6:H:0:LVS:H1'3	2.01	0.42
1:B:345:LEU:CD2	1:B:378:ALA:HB2	2.50	0.42
1:C:260:ASP:HB3	1:C:311:PHE:CZ	2.55	0.42
1:B:22:ASP:OD2	1:B:22:ASP:N	2.49	0.42
2:G:153:LEU:HB2	2:G:167:PHE:CE1	2.55	0.42
2:I:67:HIS:CD2	2:I:73:LYS:HG2	2.52	0.42
1:C:48:VAL:O	1:C:48:VAL:HG22	2.19	0.42
2:M:106:ILE:N	2:M:106:ILE:CD1	2.78	0.42
1:A:79:ILE:HD12	1:A:80:LYS:N	2.35	0.42
1:B:293:THR:C	1:B:295:HIS:H	2.22	0.42
1:C:259:ILE:O	1:C:262:ILE:HG12	2.20	0.42
2:N:92:GLU:O	2:N:93:ALA:HB2	2.19	0.42
2:H:99:ASP:O	2:H:100:GLU:C	2.58	0.41
1:A:394:ARG:O	1:A:397:HIS:HB2	2.20	0.41
1:A:65:GLU:CG	3:A:450:ADP:H2'	2.50	0.41
1:A:383:ARG:HA	1:A:383:ARG:HD2	1.95	0.41
1:A:101:ARG:O	1:A:105:ASP:OD1	2.38	0.41
2:N:45:GLY:N	2:N:96:ILE:O	2.53	0.41
2:G:69:GLY:O	2:G:71:LEU:N	2.53	0.41
2:L:56:LEU:HD11	2:L:82:TRP:CZ2	2.55	0.41
2:I:115:PRO:HG3	2:I:121:LEU:CD1	2.50	0.41
2:N:82:TRP:HB3	2:N:83:ARG:H	1.65	0.41
2:I:129:TYR:O	2:I:130:ALA:C	2.58	0.41
2:L:129:TYR:O	2:L:132:SER:HB2	2.20	0.41
2:M:6:VAL:CG2	2:M:149:VAL:HG22	2.51	0.41
2:G:165:THR:HA	2:G:167:PHE:CE2	2.55	0.41
2:G:154:ARG:HA	2:G:167:PHE:HZ	1.85	0.41
2:M:157:GLY:HA2	2:M:163:THR:HB	2.02	0.41
1:A:3:GLU:OE1	1:A:4:MET:SD	2.78	0.41
2:N:108:GLY:C	2:N:110:GLY:N	2.71	0.41
1:C:283:LEU:C	1:C:285:LEU:N	2.74	0.41
2:I:4:VAL:HG12	2:I:153:LEU:HD21	2.01	0.41
1:A:351:SER:N	1:A:354:GLU:HB2	2.35	0.41
2:M:165:THR:HA	2:M:167:PHE:CE2	2.56	0.41
2:H:24:ASN:O	2:M:161:VAL:HG22	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:141:THR:CG2	2:H:143:LEU:H	2.18	0.41
1:C:403:LEU:HD23	1:C:404:MET:CA	2.50	0.41
1:A:278:VAL:O	1:A:279:GLN:C	2.58	0.41
2:G:131:LEU:HD11	2:G:135:ARG:HH11	1.77	0.41
2:H:117:GLU:C	2:H:119:GLN:H	2.23	0.41
2:G:89:ARG:CG	2:G:89:ARG:NH1	2.83	0.41
2:L:135:ARG:O	2:L:136:ALA:C	2.57	0.41
1:C:29:ILE:O	1:C:30:ALA:C	2.58	0.41
2:M:18:GLY:O	2:M:29:GLY:HA2	2.20	0.41
1:A:25:ARG:HG2	1:A:25:ARG:HH11	1.85	0.41
2:G:63:LYS:HD2	2:G:63:LYS:HA	1.70	0.41
2:M:144:SER:C	2:M:146:HIS:N	2.72	0.41
2:I:42:VAL:HG23	2:I:42:VAL:O	2.20	0.41
1:C:374:VAL:O	1:C:375:LYS:C	2.58	0.41
2:G:118:ASP:OD2	2:G:135:ARG:HD3	2.20	0.41
2:H:136:ALA:HB2	2:N:155:ILE:HD11	1.97	0.41
2:M:42:VAL:HG12	2:M:42:VAL:O	2.20	0.41
2:I:76:VAL:O	2:I:80:LYS:HG2	2.21	0.41
2:L:80:LYS:HB3	2:L:80:LYS:HZ2	1.83	0.41
1:A:34:ARG:CZ	1:A:251:ASN:HB2	2.51	0.41
2:L:43:LEU:HD23	2:L:98:ALA:O	2.20	0.41
1:A:341:PHE:O	1:A:342:GLU:C	2.58	0.41
1:A:55:MET:HE3	1:A:306:ILE:HG21	2.02	0.41
2:M:3:ILE:O	2:M:122:ALA:HA	2.19	0.41
2:G:125:SER:HG	2:G:160:CYS:HG	1.69	0.41
1:A:4:MET:SD	1:A:4:MET:N	2.93	0.41
2:N:19:GLN:HA	2:N:28:LYS:O	2.20	0.41
1:C:22:ASP:O	1:C:25:ARG:N	2.54	0.41
2:I:89:ARG:HB3	2:I:90:LYS:H	1.69	0.41
1:B:352:LEU:HD23	1:B:352:LEU:HA	1.60	0.41
2:I:34:VAL:HG13	2:I:44:ALA:O	2.20	0.41
1:C:394:ARG:O	1:C:397:HIS:HB2	2.21	0.41
1:A:315:ARG:HE	1:A:316:PRO:CD	2.34	0.41
1:A:351:SER:O	1:A:352:LEU:C	2.59	0.41
1:C:263:CYS:SG	1:C:319:LEU:HD23	2.61	0.41
1:C:351:SER:O	1:C:355:GLN:HB2	2.20	0.41
1:B:412:SER:OG	1:C:5:THR:HB	2.21	0.41
2:H:2:THR:OG1	2:H:126:GLY:HA3	2.21	0.41
1:B:23:ALA:O	1:B:27:VAL:HG22	2.21	0.41
1:A:3:GLU:HA	1:A:3:GLU:OE1	2.21	0.41
1:C:371:THR:HG23	1:C:375:LYS:HE2	2.01	0.41
2:G:38:TYR:CD1	2:G:69:GLY:HA3	2.55	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:L:133:ALA:HB2	2:L:155:ILE:HG21	2.03	0.41
2:N:38:TYR:CE1	2:N:64:LEU:HD13	2.56	0.41
1:B:426:VAL:HG12	1:B:427:ALA:N	2.36	0.41
1:A:60:GLY:HA2	3:A:450:ADP:O3A	2.20	0.41
2:N:4:VAL:HG12	2:N:153:LEU:CD2	2.50	0.41
1:B:324:GLN:O	1:B:326:ARG:N	2.54	0.41
2:M:3:ILE:HG22	2:M:96:ILE:HD12	2.03	0.41
1:C:371:THR:O	1:C:375:LYS:HG3	2.21	0.41
1:A:421:ILE:HA	1:A:425:TYR:HD2	1.86	0.41
2:L:54:PHE:C	2:L:56:LEU:N	2.74	0.41
2:H:27:MET:HE2	2:H:27:MET:O	2.21	0.41
2:M:63:LYS:HZ1	2:M:77:GLU:HB3	1.84	0.41
1:B:407:ILE:HD11	1:B:425:TYR:CE1	2.50	0.41
2:I:134:ALA:HA	2:I:148:ILE:HG23	2.03	0.41
2:N:169:ILE:HG22	2:N:170:GLU:N	2.36	0.41
1:B:349:HIS:O	1:B:350:ALA:HB3	2.21	0.41
1:B:382:PHE:C	1:B:382:PHE:CD2	2.94	0.41
2:L:156:ALA:O	2:L:159:ILE:N	2.51	0.41
2:H:71:LEU:HD11	2:H:97:VAL:CG2	2.51	0.40
1:C:330:ARG:CB	1:C:330:ARG:NH1	2.80	0.40
2:H:120:ILE:HD11	2:H:138:VAL:HG21	2.02	0.40
1:A:347:GLU:HB2	1:A:348:PRO:HD3	2.03	0.40
2:L:12:VAL:HG11	2:L:172:LEU:HD13	2.03	0.40
1:C:45:ARG:O	1:C:45:ARG:HG3	2.21	0.40
2:L:72:LEU:HB2	2:L:102:GLU:OE1	2.21	0.40
2:I:28:LYS:CE	2:I:30:ASN:OD1	2.69	0.40
2:M:62:ARG:HH11	2:M:62:ARG:HG2	1.86	0.40
1:C:293:THR:C	1:C:295:HIS:N	2.73	0.40
2:I:43:LEU:HD21	2:I:172:LEU:HG	2.03	0.40
2:I:38:TYR:C	2:I:40:GLY:N	2.72	0.40
1:C:34:ARG:NH2	1:C:251:ASN:CA	2.84	0.40
1:A:249:GLU:HG2	1:A:299:LYS:O	2.21	0.40
1:A:33:ASN:HA	1:A:36:ARG:HB2	2.03	0.40
2:N:3:ILE:HB	2:N:123:ILE:CG1	2.46	0.40
2:I:111:ASP:OD2	2:I:111:ASP:O	2.38	0.40
1:A:260:ASP:HB3	1:A:311:PHE:CD2	2.57	0.40
1:B:264:LYS:O	1:B:265:LYS:HB3	2.22	0.40
1:C:353:THR:O	1:C:354:GLU:C	2.60	0.40
2:G:38:TYR:C	2:G:40:GLY:N	2.75	0.40
2:H:131:LEU:HD21	2:H:135:ARG:CZ	2.51	0.40
1:C:20:GLN:O	1:C:24:LYS:HG3	2.21	0.40
2:H:50:THR:O	2:H:51:ALA:C	2.60	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:347:GLU:N	1:B:348:PRO:HD2	2.37	0.40
1:B:98:SER:O	1:B:101:ARG:N	2.54	0.40
2:N:78:LEU:HD12	2:N:78:LEU:O	2.21	0.40
1:A:340:ASP:O	1:A:343:ARG:HB2	2.21	0.40
2:L:149:VAL:O	2:L:150:GLU:C	2.58	0.40
1:A:41:GLN:HA	1:A:41:GLN:NE2	2.37	0.40
2:M:82:TRP:O	2:M:89:ARG:HG2	2.20	0.40
1:A:336:LEU:HD12	1:A:336:LEU:HA	1.78	0.40
1:C:323:LEU:O	1:C:324:GLN:C	2.59	0.40
2:N:148:ILE:C	2:N:150:GLU:N	2.74	0.40
2:N:172:LEU:HB2	2:N:173:PRO:HD3	2.03	0.40
2:N:95:LEU:HB2	2:N:106:ILE:HB	2.02	0.40
2:L:70:HIS:CB	2:L:73:LYS:HD3	2.47	0.40
1:B:347:GLU:N	1:B:348:PRO:CD	2.84	0.40
2:H:9:ASN:O	2:H:11:GLN:HG2	2.22	0.40
2:M:165:THR:HA	2:M:167:PHE:HE2	1.86	0.40
2:I:63:LYS:HE3	2:I:63:LYS:N	2.36	0.40
2:N:42:VAL:HG22	2:N:99:ASP:CB	2.31	0.40
2:N:120:ILE:HD12	2:N:135:ARG:HG2	2.03	0.40
1:B:323:LEU:O	1:B:324:GLN:C	2.60	0.40
1:C:64:THR:O	1:C:68:ARG:HB2	2.22	0.40
1:B:57:GLY:HA2	1:B:58:PRO:HD3	1.92	0.40
1:B:359:LEU:HD12	1:B:359:LEU:HA	1.87	0.40
2:H:117:GLU:O	2:H:119:GLN:HG2	2.21	0.40
2:L:144:SER:N	2:L:147:GLU:HB2	2.37	0.40
1:B:399:VAL:O	1:B:400:MET:C	2.60	0.40
1:B:391:ILE:O	1:B:391:ILE:HG13	2.21	0.40
2:M:134:ALA:O	2:M:137:LEU:N	2.55	0.40
1:C:71:ALA:CB	1:C:78:PHE:HB2	2.51	0.40
1:B:437:GLU:OE1	1:C:315:ARG:NH1	2.53	0.40
2:L:111:ASP:O	2:L:112:VAL:O	2.39	0.40
1:B:77:PRO:HB2	1:B:103:LEU:HD11	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	293/310 (94%)	229 (78%)	50 (17%)	14 (5%)	4	27
1	B	289/310 (93%)	217 (75%)	54 (19%)	18 (6%)	2	19
1	C	290/310 (94%)	219 (76%)	53 (18%)	18 (6%)	2	19
2	G	172/174 (99%)	128 (74%)	33 (19%)	11 (6%)	2	17
2	H	172/174 (99%)	131 (76%)	31 (18%)	10 (6%)	3	21
2	I	172/174 (99%)	128 (74%)	31 (18%)	13 (8%)	2	12
2	L	172/174 (99%)	122 (71%)	35 (20%)	15 (9%)	1	8
2	M	172/174 (99%)	109 (63%)	49 (28%)	14 (8%)	1	10
2	N	172/174 (99%)	121 (70%)	35 (20%)	16 (9%)	1	8
All	All	1904/1974 (96%)	1404 (74%)	371 (20%)	129 (7%)	2	15

All (129) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	96	VAL
1	A	435	GLU
1	B	42	GLU
1	B	85	LYS
1	C	47	GLU
1	C	338	ALA
1	C	371	THR
1	C	426	VAL
2	G	71	LEU
2	G	84	THR
2	H	90	LYS
2	H	100	GLU
2	I	30	ASN
2	I	89	ARG
2	I	90	LYS
2	I	111	ASP
2	I	119	GLN
2	L	17	ASP
2	L	70	HIS
2	L	112	VAL
2	L	134	ALA
2	M	30	ASN
2	M	82	TRP

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Mol	Chain	Res	Type
2	M	147	GLU
2	N	12	VAL
2	N	82	TRP
2	N	115	PRO
2	N	127	GLY
1	A	93	GLY
1	A	383	ARG
1	A	431	GLY
1	A	432	GLU
1	B	26	ALA
1	B	27	VAL
1	B	411	ALA
1	C	85	LYS
1	C	288	GLY
1	C	294	LYS
1	C	425	TYR
1	C	431	GLY
1	C	432	GLU
2	G	17	ASP
2	G	70	HIS
2	G	89	ARG
2	G	116	GLU
2	G	137	LEU
2	G	141	THR
2	H	38	TYR
2	H	137	LEU
2	I	92	GLU
2	I	133	ALA
2	I	135	ARG
2	L	110	GLY
2	L	127	GLY
2	M	117	GLU
2	M	139	GLU
2	M	156	ALA
2	N	93	ALA
2	N	117	GLU
2	N	143	LEU
1	C	342	GLU
1	C	405	ASP
2	G	68	GLN
2	G	127	GLY
2	H	50	THR

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Mol	Chain	Res	Type
2	H	62	ARG
2	H	131	LEU
2	I	68	GLN
2	L	135	ARG
2	L	150	GLU
2	M	39	ASN
2	M	53	ALA
2	M	69	GLY
2	M	172	LEU
2	N	19	GLN
2	N	59	LEU
2	N	69	GLY
2	N	109	ILE
1	A	246	ASP
1	A	405	ASP
1	A	441	ARG
1	B	16	HIS
1	B	427	ALA
1	C	348	PRO
2	H	39	ASN
2	H	115	PRO
2	H	133	ALA
2	I	100	GLU
2	L	117	GLU
2	L	157	GLY
2	M	35	ARG
2	M	68	GLN
2	N	9	ASN
2	N	83	ARG
2	N	134	ALA
2	N	172	LEU
1	A	43	PRO
1	A	77	PRO
1	B	43	PRO
1	B	349	HIS
1	B	350	ALA
1	B	375	LYS
1	B	404	MET
1	B	405	ASP
1	C	30	ALA
1	C	284	PRO
2	I	17	ASP

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Mol	Chain	Res	Type
2	L	69	GLY
1	B	40	LEU
1	B	283	LEU
1	C	434	VAL
2	G	136	ALA
2	I	71	LEU
2	I	110	GLY
2	L	71	LEU
2	L	115	PRO
2	M	108	GLY
2	N	157	GLY
1	A	328	PRO
1	A	348	PRO
1	C	60	GLY
1	A	433	VAL
1	B	321	PRO
2	L	161	VAL
2	M	138	VAL
1	C	99	ILE
1	B	284	PRO
1	B	325	GLY
2	L	173	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	249/256 (97%)	216 (87%)	33 (13%)	6	27
1	B	246/256 (96%)	224 (91%)	22 (9%)	14	49
1	C	246/256 (96%)	220 (89%)	26 (11%)	10	38
2	G	139/140 (99%)	130 (94%)	9 (6%)	24	68
2	H	139/140 (99%)	128 (92%)	11 (8%)	18	58
2	I	139/140 (99%)	122 (88%)	17 (12%)	7	31
2	L	139/140 (99%)	131 (94%)	8 (6%)	28	73
2	M	139/140 (99%)	129 (93%)	10 (7%)	21	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	N	139/140 (99%)	135 (97%)	4 (3%)	55	88
All	All	1575/1608 (98%)	1435 (91%)	140 (9%)	14	49

All (140) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	MET
1	A	11	SER
1	A	12	GLU
1	A	20	GLN
1	A	34	ARG
1	A	39	GLN
1	A	43	PRO
1	A	59	THR
1	A	79	ILE
1	A	86	PHE
1	A	105	ASP
1	A	259	ILE
1	A	264	LYS
1	A	279	GLN
1	A	281	ASP
1	A	291	VAL
1	A	293	THR
1	A	301	ASP
1	A	330	ARG
1	A	336	LEU
1	A	345	LEU
1	A	359	LEU
1	A	367	ILE
1	A	370	THR
1	A	372	ASP
1	A	379	GLU
1	A	384	VAL
1	A	394	ARG
1	A	403	LEU
1	A	413	ASP
1	A	428	ASP
1	A	435	GLU
1	A	441	ARG
1	B	4	MET
1	B	11	SER
1	B	20	GLN

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Mol	Chain	Res	Type
1	B	22	ASP
1	B	39	GLN
1	B	46	HIS
1	B	70	LEU
1	B	97	ASP
1	B	298	VAL
1	B	303	ILE
1	B	321	PRO
1	B	336	LEU
1	B	345	LEU
1	B	359	LEU
1	B	367	ILE
1	B	375	LYS
1	B	384	VAL
1	B	394	ARG
1	B	413	ASP
1	B	418	THR
1	B	428	ASP
1	B	441	ARG
1	C	6	PRO
1	C	12	GLU
1	C	34	ARG
1	C	38	MET
1	C	39	GLN
1	C	48	VAL
1	C	68	ARG
1	C	86	PHE
1	C	104	THR
1	C	251	ASN
1	C	281	ASP
1	C	286	VAL
1	C	330	ARG
1	C	331	VAL
1	C	336	LEU
1	C	349	HIS
1	C	355	GLN
1	C	359	LEU
1	C	362	THR
1	C	383	ARG
1	C	384	VAL
1	C	403	LEU
1	C	408	SER

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Mol	Chain	Res	Type
1	C	425	TYR
1	C	428	ASP
1	C	441	ARG
2	G	26	VAL
2	G	46	PHE
2	G	55	THR
2	G	56	LEU
2	G	63	LYS
2	G	71	LEU
2	G	72	LEU
2	G	135	ARG
2	G	164	ASN
2	H	12	VAL
2	H	52	ASP
2	H	55	THR
2	H	71	LEU
2	H	72	LEU
2	H	92	GLU
2	H	95	LEU
2	H	118	ASP
2	H	135	ARG
2	H	153	LEU
2	H	164	ASN
2	I	38	TYR
2	I	43	LEU
2	I	52	ASP
2	I	55	THR
2	I	56	LEU
2	I	63	LYS
2	I	72	LEU
2	I	76	VAL
2	I	82	TRP
2	I	86	ARG
2	I	90	LYS
2	I	101	LYS
2	I	104	LEU
2	I	141	THR
2	I	150	GLU
2	I	164	ASN
2	I	167	PHE
2	L	43	LEU
2	L	54	PHE

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Mol	Chain	Res	Type
2	L	62	ARG
2	L	65	GLU
2	L	68	GLN
2	L	86	ARG
2	L	100	GLU
2	L	167	PHE
2	M	38	TYR
2	M	43	LEU
2	M	54	PHE
2	M	71	LEU
2	M	86	ARG
2	M	89	ARG
2	M	117	GLU
2	M	118	ASP
2	M	148	ILE
2	M	172	LEU
2	N	38	TYR
2	N	73	LYS
2	N	91	LEU
2	N	118	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	33	ASN
1	A	39	GLN
1	A	41	GLN
1	A	75	ASN
1	A	250	GLN
1	A	324	GLN
1	A	397	HIS
1	A	417	GLN
1	B	20	GLN
1	B	39	GLN
1	B	41	GLN
1	B	250	GLN
1	B	324	GLN
1	B	417	GLN
1	C	20	GLN
1	C	39	GLN
1	C	41	GLN

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Mol	Chain	Res	Type
1	C	52	ASN
1	C	250	GLN
1	C	312	GLN
1	C	355	GLN
2	G	19	GLN
2	G	24	ASN
2	G	68	GLN
2	G	164	ASN
2	H	19	GLN
2	H	30	ASN
2	H	68	GLN
2	H	119	GLN
2	H	164	ASN
2	I	19	GLN
2	I	24	ASN
2	I	68	GLN
2	I	164	ASN
2	L	39	ASN
2	L	166	ASN
2	M	11	GLN
2	M	68	GLN
2	N	11	GLN
2	N	19	GLN
2	N	67	HIS
2	N	119	GLN
2	N	140	ASN
2	N	166	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 21 ligands modelled in this entry, 12 are monoatomic - leaving 9 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	ADP	A	450	4	29,29,29	2.54	12 (41%)	45,45,45	2.22	4 (8%)
5	PO4	A	452	4	4,4,4	0.76	0	6,6,6	0.31	0
3	ADP	B	450	4	29,29,29	2.46	12 (41%)	45,45,45	2.22	5 (11%)
5	PO4	B	452	4	4,4,4	0.74	0	6,6,6	0.31	0
3	ADP	C	450	4	29,29,29	2.52	13 (44%)	45,45,45	2.33	7 (15%)
5	PO4	C	452	4	4,4,4	0.57	0	6,6,6	0.31	0
6	LVS	G	0	2	41,41,42	451.62	12 (29%)	53,57,59	1.73	11 (20%)
6	LVS	H	0	2	41,41,42	393.68	13 (31%)	53,57,59	1.65	10 (18%)
6	LVS	I	0	2	41,41,42	403.01	13 (31%)	53,57,59	1.76	9 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	A	450	4	-	0/16/32/32	0/1/3/3
5	PO4	A	452	4	-	0/0/0/0	0/0/0/0
3	ADP	B	450	4	-	0/16/32/32	0/1/3/3
5	PO4	B	452	4	-	0/0/0/0	0/0/0/0
3	ADP	C	450	4	-	0/16/32/32	0/1/3/3
5	PO4	C	452	4	-	0/0/0/0	0/0/0/0
6	LVS	G	0	2	-	1/46/46/46	0/1/1/1
6	LVS	H	0	2	-	1/46/46/46	0/1/1/1
6	LVS	I	0	2	-	1/46/46/46	0/1/1/1

All (75) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	0	LVS	C9-C8	2891.68	1.54	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	I	0	LVS	C9-C8	2580.34	1.52	1.39
6	H	0	LVS	C9-C8	2520.61	1.52	1.39
6	H	0	LVS	C2'-CS	16.60	1.58	1.31
6	I	0	LVS	C2'-CS	16.38	1.58	1.31
6	G	0	LVS	C2'-CS	15.38	1.56	1.31
6	I	0	LVS	O1'-S	11.77	1.58	1.44
6	I	0	LVS	O2'-S	11.33	1.58	1.44
6	G	0	LVS	O1'-S	11.30	1.58	1.44
6	I	0	LVS	C10-C5	11.24	1.50	1.39
6	H	0	LVS	O1'-S	11.14	1.58	1.44
6	G	0	LVS	C10-C5	11.05	1.50	1.39
6	H	0	LVS	O2'-S	10.53	1.57	1.44
6	H	0	LVS	C10-C5	9.79	1.48	1.39
6	G	0	LVS	O2'-S	9.59	1.56	1.44
6	G	0	LVS	O3-N4	5.51	1.32	1.23
6	I	0	LVS	O3-N4	5.39	1.32	1.23
3	B	450	ADP	C2-N1	5.30	1.44	1.33
6	I	0	LVS	C6-C7	5.21	1.50	1.39
3	C	450	ADP	C2-N1	5.01	1.43	1.33
6	H	0	LVS	O3-N4	4.93	1.31	1.23
6	H	0	LVS	C6-C7	4.86	1.50	1.39
3	C	450	ADP	PB-O1B	4.79	1.67	1.51
3	A	450	ADP	PB-O3A	4.78	1.68	1.60
3	C	450	ADP	PB-O3A	4.75	1.68	1.60
3	A	450	ADP	C2-N1	4.68	1.43	1.33
3	A	450	ADP	PB-O1B	4.60	1.66	1.51
3	C	450	ADP	C4-N3	4.58	1.42	1.35
6	G	0	LVS	C6-C7	4.58	1.49	1.39
6	H	0	LVS	C3-N1	4.52	1.43	1.34
6	G	0	LVS	CD5-CG3	-4.51	1.23	1.51
3	B	450	ADP	PB-O3A	4.46	1.68	1.60
6	H	0	LVS	CD5-CG3	-4.41	1.23	1.51
6	I	0	LVS	C3-N1	4.36	1.43	1.34
3	C	450	ADP	C8-N9	4.30	1.43	1.36
6	I	0	LVS	CD5-CG3	-4.27	1.24	1.51
6	G	0	LVS	C3-N1	4.25	1.42	1.34
3	B	450	ADP	C4-N3	4.22	1.42	1.35
3	A	450	ADP	C4-N3	4.21	1.42	1.35
3	B	450	ADP	PB-O1B	4.17	1.65	1.51
3	A	450	ADP	PA-O3A	4.14	1.67	1.59
6	I	0	LVS	C1-N2	4.07	1.43	1.34
3	A	450	ADP	C8-N9	4.03	1.42	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	450	ADP	C8-N9	3.82	1.42	1.36
3	B	450	ADP	PA-O3A	3.64	1.66	1.59
6	H	0	LVS	C2-N3	3.53	1.42	1.34
3	B	450	ADP	PB-O2B	3.53	1.67	1.54
3	A	450	ADP	PB-O2B	3.47	1.67	1.54
3	C	450	ADP	PB-O2B	3.42	1.67	1.54
6	I	0	LVS	O4-N4	3.37	1.32	1.25
6	G	0	LVS	O4-N4	3.27	1.31	1.25
3	A	450	ADP	PA-O2A	3.12	1.68	1.55
3	C	450	ADP	PA-O2A	3.09	1.68	1.55
3	B	450	ADP	PA-O2A	3.08	1.68	1.55
6	G	0	LVS	C2-N3	3.07	1.41	1.34
6	H	0	LVS	O4-N4	3.00	1.31	1.25
3	C	450	ADP	C8-N7	-2.91	1.28	1.34
3	B	450	ADP	C8-N7	-2.80	1.29	1.34
6	G	0	LVS	C1-N2	2.79	1.40	1.34
6	I	0	LVS	C2-N3	2.79	1.40	1.34
3	A	450	ADP	O4'-C1'	2.77	1.45	1.41
3	A	450	ADP	C8-N7	-2.76	1.29	1.34
6	H	0	LVS	C1-N2	2.61	1.40	1.34
3	C	450	ADP	C4-N9	2.55	1.41	1.37
3	A	450	ADP	C5-C4	-2.55	1.34	1.40
3	C	450	ADP	PA-O3A	2.48	1.64	1.59
3	C	450	ADP	C5-C4	-2.32	1.35	1.40
3	B	450	ADP	C5-C4	-2.26	1.35	1.40
3	B	450	ADP	PA-O1A	2.19	1.59	1.51
6	H	0	LVS	C7-N4	-2.18	1.43	1.46
3	A	450	ADP	PA-O1A	2.13	1.59	1.51
3	C	450	ADP	C6-N6	2.04	1.41	1.35
6	I	0	LVS	CB3-CA3	2.03	1.59	1.54
3	B	450	ADP	C6-N6	2.03	1.41	1.35
3	C	450	ADP	PA-O1A	2.02	1.59	1.51

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	450	ADP	N3-C2-N1	-10.06	120.30	128.71
3	C	450	ADP	N3-C2-N1	-10.03	120.32	128.71
3	B	450	ADP	N3-C2-N1	-9.74	120.56	128.71
3	C	450	ADP	PA-O3A-PB	-8.58	106.51	131.68
3	B	450	ADP	PA-O3A-PB	-7.83	108.73	131.68
3	A	450	ADP	PA-O3A-PB	-7.60	109.41	131.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	I	0	LVS	CD5-CG3-CB3	6.31	134.47	111.12
6	H	0	LVS	CD5-CG3-CB3	6.23	134.16	111.12
6	G	0	LVS	CD5-CG3-CB3	6.09	133.66	111.12
6	I	0	LVS	CB3-CA3-CS	4.17	118.11	110.94
6	I	0	LVS	CD6-CG3-CD5	-4.10	89.43	110.49
6	H	0	LVS	CD6-CG3-CD5	-4.04	89.74	110.49
6	G	0	LVS	CD6-CG3-CD5	-3.96	90.12	110.49
3	C	450	ADP	N3-C4-N9	3.60	131.92	125.43
3	A	450	ADP	N3-C4-N9	3.58	131.90	125.43
6	I	0	LVS	CA3-CS-C2'	-3.54	107.90	126.48
3	B	450	ADP	N3-C4-N9	3.30	131.40	125.43
6	G	0	LVS	CA3-CS-C2'	-3.25	109.43	126.48
6	H	0	LVS	CA3-CS-C2'	-3.11	110.15	126.48
6	G	0	LVS	C1-CA1-N1	-2.87	103.23	111.28
6	G	0	LVS	O2'-S-O1'	-2.76	107.87	117.00
6	I	0	LVS	C1'-S-C2'	2.76	112.69	105.83
3	C	450	ADP	C8-N9-C4	-2.74	104.80	106.90
6	G	0	LVS	CB3-CA3-CS	2.74	115.66	110.94
6	H	0	LVS	C1'-S-C2'	2.74	112.66	105.83
3	B	450	ADP	C8-N9-C4	-2.73	104.81	106.90
6	G	0	LVS	C8-C7-N4	2.73	124.59	120.58
6	H	0	LVS	O2'-S-O1'	-2.71	108.04	117.00
6	I	0	LVS	O2'-S-O1'	-2.70	108.08	117.00
6	I	0	LVS	CG3-CB3-CA3	2.67	120.86	114.71
6	G	0	LVS	CS-C2'-S	-2.65	116.41	123.62
6	G	0	LVS	C1'-S-C2'	2.57	112.22	105.83
3	C	450	ADP	C3'-C2'-C1'	2.54	104.88	100.91
6	H	0	LVS	CS-C2'-S	-2.35	117.22	123.62
6	H	0	LVS	CB3-CA3-CS	2.27	114.85	110.94
6	H	0	LVS	CB2-CA2-C2	2.26	116.54	110.57
3	C	450	ADP	C2-N1-C6	2.25	122.84	118.77
6	H	0	LVS	C1-CA1-N1	-2.21	105.08	111.28
6	H	0	LVS	C4-C3-N1	2.17	119.11	115.56
3	C	450	ADP	O3A-PA-O5'	2.14	112.96	103.41
6	G	0	LVS	CB1-CA1-N1	2.10	115.74	110.52
3	B	450	ADP	C2-N1-C6	2.07	122.52	118.77
6	G	0	LVS	C4-C3-N1	2.07	118.95	115.56
6	I	0	LVS	C4-C3-N1	2.06	118.94	115.56
3	A	450	ADP	C8-N9-C4	-2.04	105.34	106.90
6	I	0	LVS	C6-C7-C8	-2.01	119.00	122.31

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	H	0	LVS	CS-C2'-S-C1'
6	G	0	LVS	CS-C2'-S-C1'
6	I	0	LVS	CS-C2'-S-C1'

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.