



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 02:30 pm BST

PDB ID : 1BR1  
Title : SMOOTH MUSCLE MYOSIN MOTOR DOMAIN-ESSENTIAL LIGHT CHAIN COMPLEX WITH MGADP.ALF4 BOUND AT THE ACTIVE SITE  
Authors : Dominguez, R.; Trybus, K.M.; Cohen, C.  
Deposited on : 1998-08-26  
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

<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  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

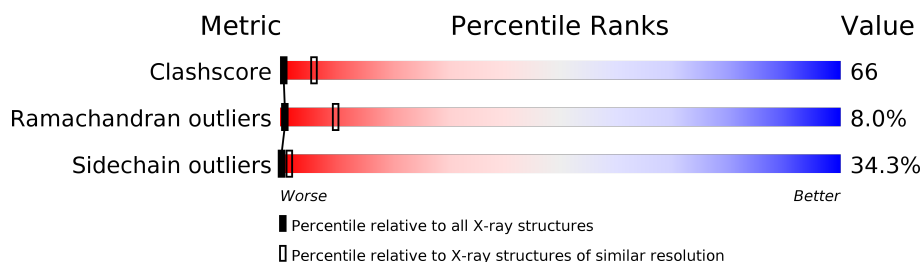
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	820	
1	C	820	
1	E	820	
1	G	820	
2	B	150	
2	D	150	
2	F	150	
2	H	150	

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 30132 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 MYOSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	787	Total	C	N	O	S	0	0	0
			6337	4036	1089	1183	29			
1	C	787	Total	C	N	O	S	0	0	0
			6337	4036	1089	1183	29			
1	E	787	Total	C	N	O	S	0	0	0
			6337	4036	1089	1183	29			
1	G	787	Total	C	N	O	S	0	0	0
			6337	4036	1089	1183	29			

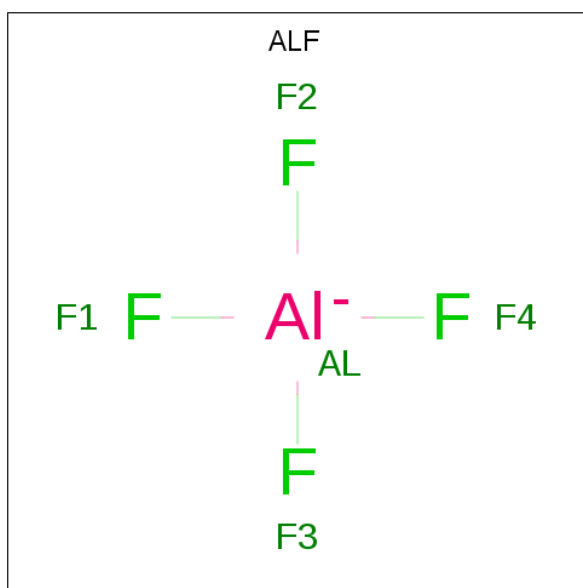
- Molecule 2 is a protein called MYOSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	148	Total	C	N	O	S	0	0	0
			1161	722	193	235	11			
2	D	148	Total	C	N	O	S	0	0	0
			1161	722	193	235	11			
2	F	148	Total	C	N	O	S	0	0	0
			1161	722	193	235	11			
2	H	148	Total	C	N	O	S	0	0	0
			1161	722	193	235	11			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		

- Molecule 4 is TETRAFLUOROALUMINATE ION (three-letter code: ALF) (formula:  $\text{AlF}_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Al	F	0	0
			5	1	4		
4	C	1	Total	Al	F	0	0
			5	1	4		
4	E	1	Total	Al	F	0	0
			5	1	4		
4	G	1	Total	Al	F	0	0
			5	1	4		

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$ ).



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

- Molecule 6 is water.

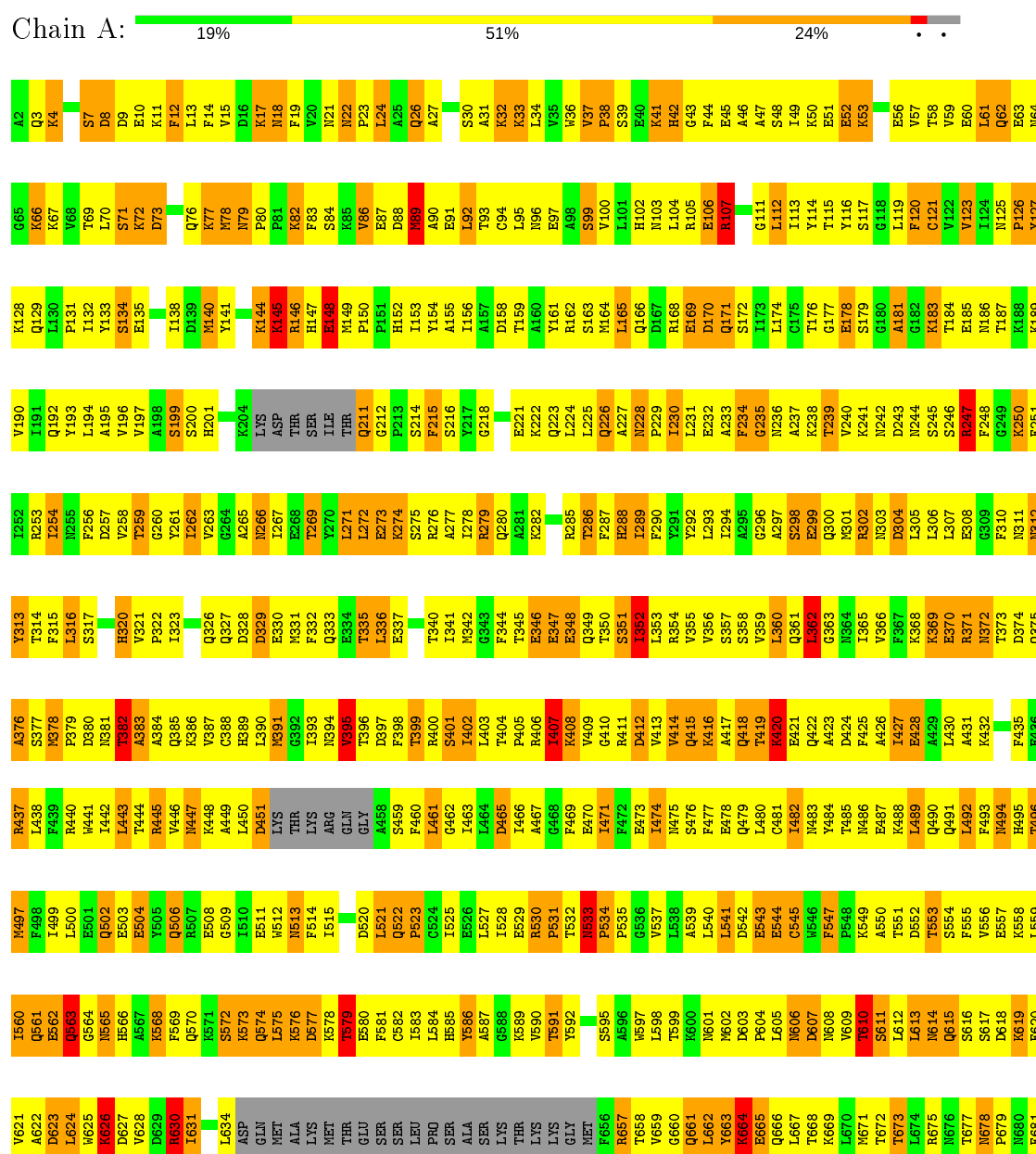
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	O	0	0
			2	2		
6	C	2	Total	O	0	0
			2	2		
6	E	2	Total	O	0	0
			2	2		
6	G	2	Total	O	0	0
			2	2		

### 3 Residue-property plots

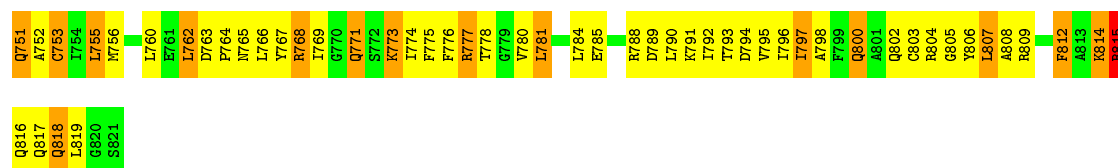
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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: MYOSIN

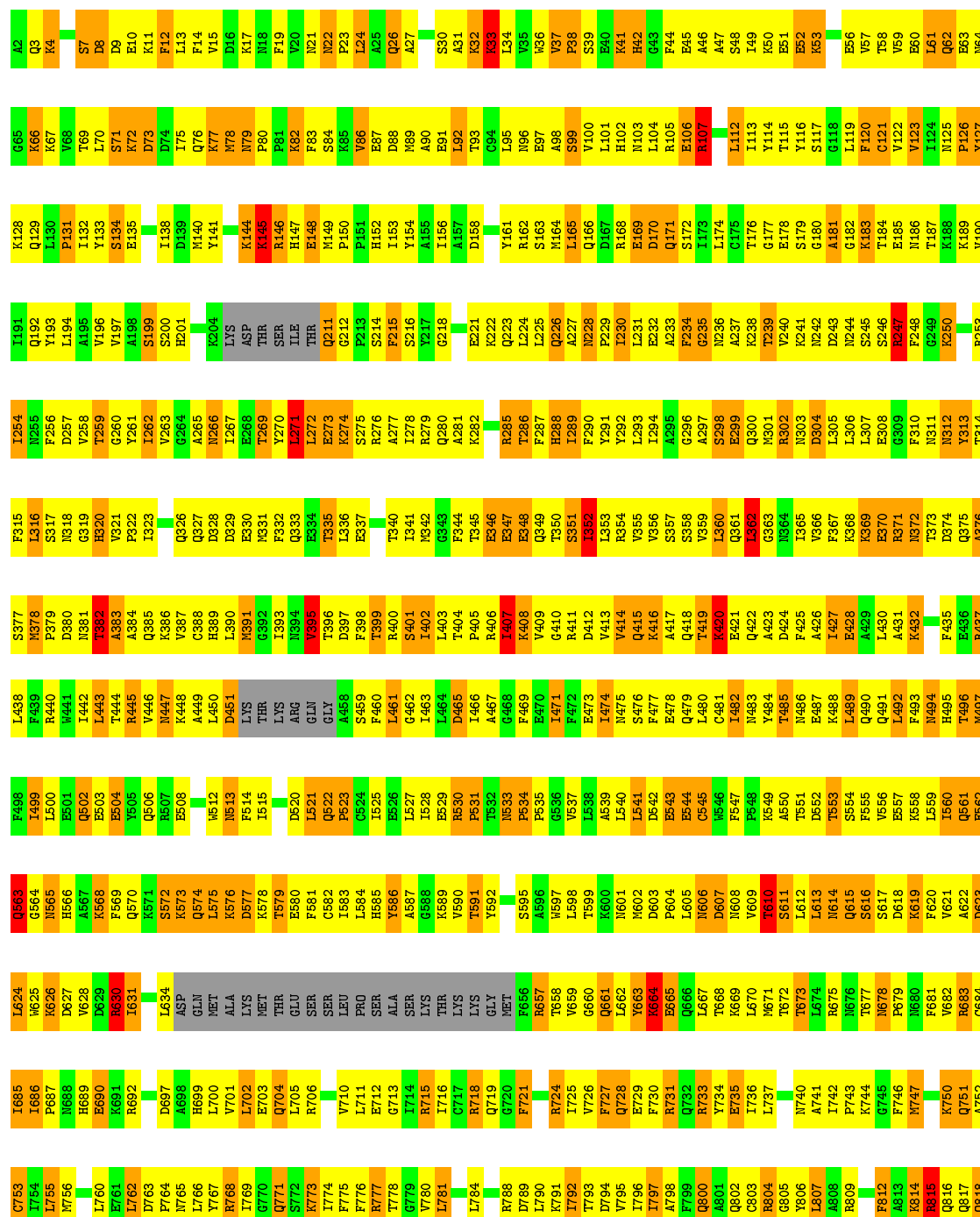






# • Molecule 1: MYOSIN

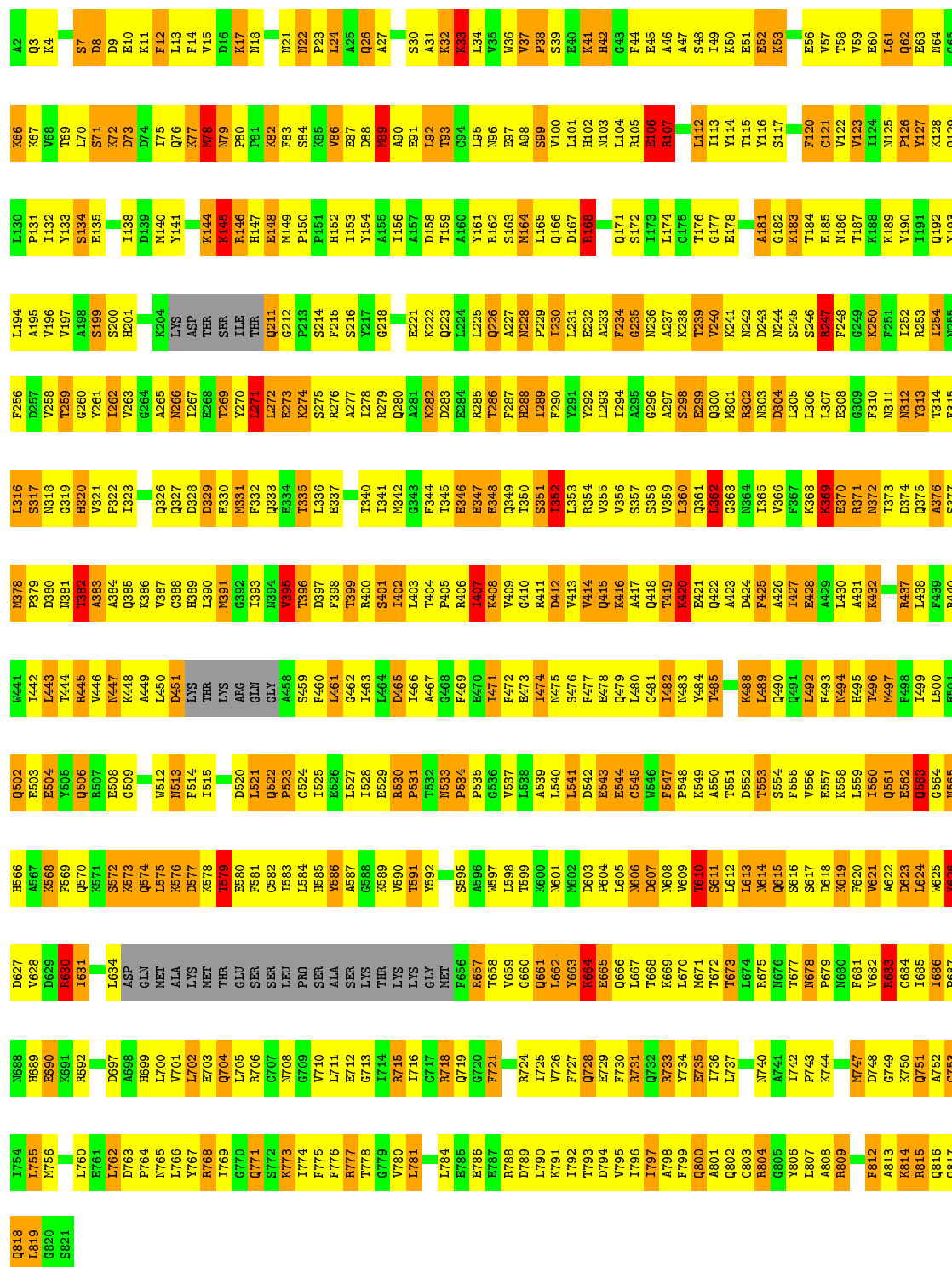
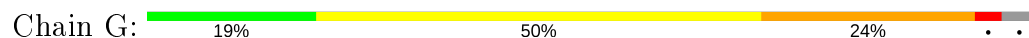
Chain E: 19% 51% 24%






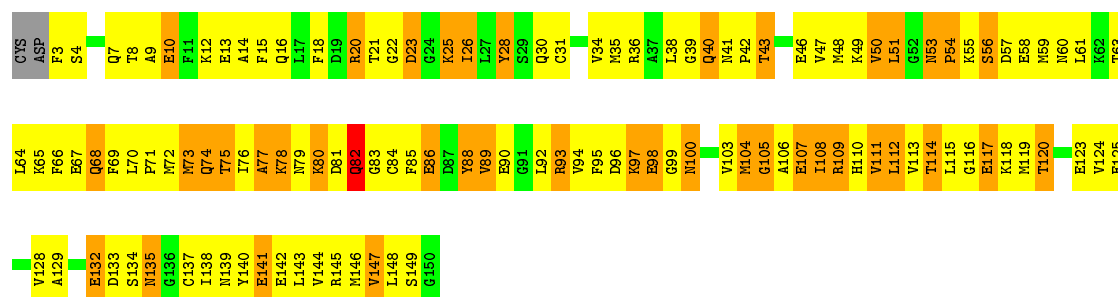


- Molecule 1: MYOSIN




- Molecule 2: MYOSIN

Chain B: 




• Molecule 2: MYOSIN

Chain D: 




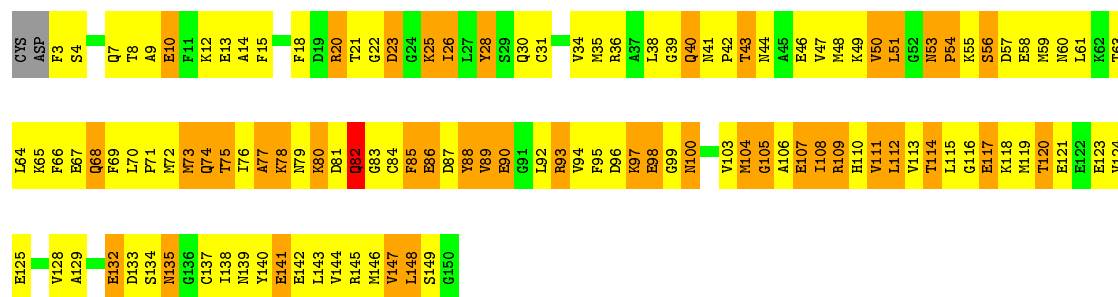
• Molecule 2: MYOSIN

Chain F: 



• Molecule 2: MYOSIN

Chain H: 



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	95.32Å 144.66Å 147.29Å 111.21° 106.10° 92.58°	Depositor
Resolution (Å)	10.00 – 3.50	Depositor
% Data completeness (in resolution range)	91.5 (10.00-3.50)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.227 , 0.305	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	30132	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	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: ALF, MG, ADP

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	0.57	0/6456	0.74	9/8700 (0.1%)
1	C	0.57	0/6456	0.74	8/8700 (0.1%)
1	E	0.57	0/6456	0.74	8/8700 (0.1%)
1	G	0.57	0/6456	0.74	9/8700 (0.1%)
2	B	0.46	0/1176	0.60	0/1575
2	D	0.46	0/1176	0.62	1/1575 (0.1%)
2	F	0.49	0/1176	0.66	2/1575 (0.1%)
2	H	0.57	0/1176	0.65	0/1575
All	All	0.56	0/30528	0.73	37/41100 (0.1%)

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	630	ARG	NE-CZ-NH2	7.60	124.10	120.30
1	G	630	ARG	NE-CZ-NH2	7.58	124.09	120.30
1	A	285	ARG	NE-CZ-NH2	7.56	124.08	120.30
1	A	247	ARG	NE-CZ-NH2	7.54	124.07	120.30
1	E	285	ARG	NE-CZ-NH2	7.51	124.05	120.30
1	A	630	ARG	NE-CZ-NH2	7.50	124.05	120.30
1	C	247	ARG	NE-CZ-NH2	7.46	124.03	120.30
1	E	630	ARG	NE-CZ-NH2	7.44	124.02	120.30
1	G	285	ARG	NE-CZ-NH2	7.42	124.01	120.30
1	A	279	ARG	NE-CZ-NH2	7.37	123.98	120.30
1	C	285	ARG	NE-CZ-NH2	7.36	123.98	120.30
1	G	247	ARG	NE-CZ-NH2	7.35	123.98	120.30
1	G	168	ARG	NE-CZ-NH2	7.33	123.97	120.30
1	E	247	ARG	NE-CZ-NH2	7.27	123.93	120.30
2	F	85	PHE	CA-C-N	-7.16	101.44	117.20
1	G	715	ARG	NE-CZ-NH2	6.71	123.65	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	715	ARG	NE-CZ-NH2	6.70	123.65	120.30
1	C	815	ARG	NE-CZ-NH2	6.68	123.64	120.30
1	E	107	ARG	NE-CZ-NH2	6.60	123.60	120.30
1	A	715	ARG	NE-CZ-NH2	6.58	123.59	120.30
2	F	22	GLY	N-CA-C	6.56	129.50	113.10
1	C	715	ARG	NE-CZ-NH2	6.54	123.57	120.30
1	E	815	ARG	NE-CZ-NH2	6.48	123.54	120.30
1	A	107	ARG	NE-CZ-NH2	6.47	123.54	120.30
1	C	107	ARG	NE-CZ-NH2	6.46	123.53	120.30
1	G	107	ARG	NE-CZ-NH2	6.44	123.52	120.30
1	G	78	MET	CG-SD-CE	6.14	110.03	100.20
1	E	78	MET	CG-SD-CE	6.13	110.01	100.20
1	C	78	MET	CG-SD-CE	6.13	110.00	100.20
1	G	164	MET	CG-SD-CE	6.12	110.00	100.20
1	A	78	MET	CG-SD-CE	6.12	109.99	100.20
1	A	140	MET	CG-SD-CE	5.89	109.62	100.20
1	G	747	MET	CG-SD-CE	5.64	109.22	100.20
1	C	747	MET	CG-SD-CE	5.63	109.21	100.20
1	A	747	MET	CG-SD-CE	5.60	109.16	100.20
1	E	747	MET	CG-SD-CE	5.57	109.11	100.20
2	D	85	PHE	CA-C-N	-5.21	105.75	117.20

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6337	0	6346	865	5
1	C	6337	0	6346	858	0
1	E	6337	0	6346	841	4
1	G	6337	0	6346	860	12
2	B	1161	0	1126	146	0
2	D	1161	0	1126	151	8
2	F	1161	0	1126	152	5
2	H	1161	0	1126	163	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
4	A	5	0	0	1	0
4	C	5	0	0	1	0
4	E	5	0	0	1	0
4	G	5	0	0	1	0
5	A	27	0	12	1	0
5	C	27	0	12	4	0
5	E	27	0	12	4	0
5	G	27	0	12	3	0
6	A	2	0	0	0	0
6	C	2	0	0	0	0
6	E	2	0	0	0	0
6	G	2	0	0	0	0
All	All	30132	0	29936	3959	17

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 66.

All (3959) 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)
2:F:89:VAL:HG12	2:F:144:VAL:HG21	1.29	1.14
1:C:8:ASP:HA	1:C:11:LYS:HD2	1.31	1.11
2:D:89:VAL:HG12	2:D:144:VAL:HG21	1.29	1.10
1:A:8:ASP:HA	1:A:11:LYS:HD2	1.32	1.09
1:G:8:ASP:HA	1:G:11:LYS:HD2	1.28	1.08
1:C:628:VAL:HG13	1:C:631:ILE:HG13	1.33	1.07
1:E:8:ASP:HA	1:E:11:LYS:HD2	1.31	1.06
1:E:82:LYS:O	1:E:82:LYS:HG2	1.50	1.06
1:C:628:VAL:HG13	1:C:631:ILE:CG1	1.85	1.05
1:E:49:ILE:HA	1:E:59:VAL:HG22	1.36	1.05
1:A:49:ILE:HA	1:A:59:VAL:HG22	1.40	1.04
1:A:751:GLN:HG3	1:G:809:ARG:HB2	1.39	1.03
1:G:82:LYS:HG2	1:G:82:LYS:O	1.58	1.03
1:G:49:ILE:HA	1:G:59:VAL:HG22	1.41	1.03
1:C:49:ILE:HA	1:C:59:VAL:HG22	1.37	1.02
1:A:743:PRO:HG2	1:G:816:GLN:HB3	1.42	1.01
1:C:610:THR:HG21	1:C:631:ILE:HG13	1.42	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:628:VAL:O	1:E:631:ILE:HG12	1.61	1.01
1:E:79:ASN:HD22	1:E:80:PRO:HD2	1.21	1.01
2:B:89:VAL:HG12	2:B:144:VAL:HG21	1.43	1.00
1:A:805:GLY:HA2	2:B:36:ARG:HG2	1.42	1.00
1:A:541:LEU:HD23	1:A:601:ASN:HD22	1.25	1.00
1:A:610:THR:HG21	1:A:631:ILE:HG13	1.42	0.99
1:G:541:LEU:HD23	1:G:601:ASN:HD22	1.27	0.99
1:G:419:THR:H	1:G:422:GLN:HE21	1.07	0.99
1:C:805:GLY:HA2	2:D:36:ARG:HG2	1.42	0.99
1:A:628:VAL:HG13	1:A:631:ILE:HG13	1.45	0.99
1:E:541:LEU:HD23	1:E:601:ASN:HD22	1.23	0.98
2:F:84:CYS:SG	2:F:86:GLU:HB2	2.04	0.97
1:E:419:THR:H	1:E:422:GLN:HE21	1.04	0.97
1:E:269:THR:HG21	1:E:443:LEU:HD13	1.44	0.97
1:G:628:VAL:CG1	1:G:628:VAL:O	2.11	0.97
1:C:269:THR:HG21	1:C:443:LEU:HD13	1.46	0.97
1:C:541:LEU:HD23	1:C:601:ASN:HD22	1.28	0.97
1:G:628:VAL:HG13	1:G:631:ILE:HG13	1.47	0.97
1:G:269:THR:HG21	1:G:443:LEU:HD13	1.45	0.97
1:G:678:ASN:HD22	1:G:679:PRO:HD2	1.26	0.96
1:C:13:LEU:HD11	1:C:132:ILE:HB	1.44	0.96
1:G:610:THR:HG21	1:G:631:ILE:HG13	1.48	0.96
1:C:527:LEU:O	1:C:527:LEU:HD23	1.66	0.96
1:C:678:ASN:HD22	1:C:679:PRO:HD2	1.28	0.96
1:C:419:THR:H	1:C:422:GLN:HE21	1.09	0.96
1:A:79:ASN:HD22	1:A:80:PRO:HD2	1.29	0.95
1:C:628:VAL:O	1:C:628:VAL:CG1	2.14	0.95
1:A:419:THR:H	1:A:422:GLN:HE21	1.06	0.95
1:A:628:VAL:HG13	1:A:631:ILE:CG1	1.95	0.95
1:C:82:LYS:HG2	1:C:82:LYS:O	1.64	0.95
1:A:82:LYS:O	1:A:82:LYS:HG2	1.62	0.95
2:F:84:CYS:O	2:F:87:ASP:N	1.99	0.95
1:E:610:THR:HG21	1:E:631:ILE:HG13	1.47	0.94
1:A:13:LEU:HD11	1:A:132:ILE:HB	1.49	0.94
1:C:36:TRP:NE1	1:C:78:MET:HG3	1.82	0.94
1:A:678:ASN:HD22	1:A:679:PRO:HD2	1.32	0.94
1:G:527:LEU:HD23	1:G:527:LEU:O	1.68	0.94
1:G:36:TRP:NE1	1:G:78:MET:HG3	1.83	0.93
1:A:269:THR:HG21	1:A:443:LEU:HD13	1.46	0.93
1:E:678:ASN:HD22	1:E:679:PRO:HD2	1.30	0.93
2:H:84:CYS:O	2:H:88:TYR:CD2	2.22	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:628:VAL:HG13	1:G:631:ILE:CG1	1.99	0.93
2:H:89:VAL:HG12	2:H:144:VAL:HG21	1.51	0.93
1:A:527:LEU:HD23	1:A:527:LEU:O	1.68	0.92
1:G:628:VAL:HG12	1:G:628:VAL:O	1.70	0.92
1:E:471:ILE:HG12	1:E:471:ILE:O	1.70	0.91
1:A:471:ILE:O	1:A:471:ILE:HG12	1.70	0.91
1:A:628:VAL:O	1:A:631:ILE:HG12	1.71	0.91
1:E:805:GLY:HA2	2:F:36:ARG:HG2	1.53	0.90
1:G:471:ILE:HG12	1:G:471:ILE:O	1.67	0.90
1:E:36:TRP:NE1	1:E:78:MET:HG3	1.86	0.90
1:E:527:LEU:HD23	1:E:527:LEU:O	1.71	0.90
1:C:345:THR:HB	1:C:348:GLU:HB2	1.54	0.90
1:C:576:LYS:HA	1:C:579:THR:HA	1.53	0.90
1:G:576:LYS:HA	1:G:579:THR:HA	1.53	0.90
1:A:135:GLU:HB2	1:A:212:GLY:O	1.71	0.90
1:C:79:ASN:HD22	1:C:80:PRO:HD2	1.37	0.90
1:E:250:LYS:HE2	1:E:465:ASP:OD2	1.70	0.90
1:A:345:THR:HB	1:A:348:GLU:HB2	1.53	0.90
1:G:401:SER:HB3	1:G:608:ASN:HB3	1.54	0.89
1:C:401:SER:HB3	1:C:608:ASN:HB3	1.54	0.89
1:E:607:ASP:HA	1:E:610:THR:HB	1.54	0.89
1:G:345:THR:HB	1:G:348:GLU:HB2	1.55	0.89
1:A:36:TRP:NE1	1:A:78:MET:HG3	1.86	0.89
1:E:401:SER:HB3	1:E:608:ASN:HB3	1.53	0.89
1:A:576:LYS:HA	1:A:579:THR:HA	1.54	0.89
1:G:377:SER:O	1:G:379:PRO:HD3	1.73	0.89
1:E:419:THR:N	1:E:422:GLN:HE21	1.71	0.88
1:G:236:ASN:ND2	1:G:246:SER:HA	1.87	0.88
1:G:79:ASN:HD22	1:G:80:PRO:HD2	1.37	0.88
2:H:26:ILE:HG23	2:H:30:GLN:HB2	1.54	0.88
2:D:26:ILE:HG23	2:D:30:GLN:HB2	1.54	0.88
1:A:401:SER:HB3	1:A:608:ASN:HB3	1.53	0.88
2:B:26:ILE:HG23	2:B:30:GLN:HB2	1.54	0.88
1:C:13:LEU:CD1	1:C:132:ILE:HB	2.03	0.88
1:E:135:GLU:HB2	1:E:212:GLY:O	1.72	0.88
1:C:471:ILE:HG12	1:C:471:ILE:O	1.70	0.88
1:G:230:ILE:HG22	1:G:231:LEU:HD23	1.56	0.87
1:G:806:TYR:CD2	2:H:147:VAL:HA	2.10	0.87
2:F:26:ILE:HG23	2:F:30:GLN:HB2	1.54	0.87
1:C:250:LYS:HE2	1:C:465:ASP:OD2	1.74	0.87
1:C:607:ASP:HA	1:C:610:THR:HB	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:607:ASP:HA	1:A:610:THR:HB	1.55	0.87
1:C:376:ALA:HB2	1:C:420:LYS:HB2	1.54	0.87
1:E:659:VAL:HG12	1:E:660:GLY:N	1.90	0.87
1:A:187:THR:HG23	1:A:463:ILE:HG21	1.56	0.87
1:G:135:GLU:HB2	1:G:212:GLY:O	1.74	0.87
1:E:236:ASN:ND2	1:E:246:SER:HA	1.91	0.86
1:A:419:THR:N	1:A:422:GLN:HE21	1.73	0.86
1:C:135:GLU:HB2	1:C:212:GLY:O	1.75	0.85
1:C:377:SER:O	1:C:379:PRO:HD3	1.77	0.85
1:C:331:MET:O	1:C:335:THR:HG23	1.76	0.85
1:E:806:TYR:CD2	2:F:147:VAL:HA	2.12	0.85
1:E:576:LYS:HA	1:E:579:THR:HA	1.56	0.85
1:A:625:TRP:O	1:A:627:ASP:N	2.10	0.85
1:A:230:ILE:HG22	1:A:231:LEU:HD23	1.58	0.84
1:G:187:THR:HG23	1:G:463:ILE:HG21	1.57	0.84
1:E:814:LYS:HE3	1:E:818:GLN:HE22	1.42	0.84
1:A:236:ASN:ND2	1:A:246:SER:HA	1.93	0.84
1:E:345:THR:HB	1:E:348:GLU:HB2	1.57	0.84
1:E:79:ASN:HD22	1:E:80:PRO:CD	1.90	0.84
1:G:814:LYS:HE3	1:G:818:GLN:HE22	1.42	0.84
1:G:250:LYS:HE2	1:G:465:ASP:OD2	1.77	0.83
1:G:814:LYS:O	1:G:817:GLN:HG2	1.78	0.83
1:E:331:MET:O	1:E:335:THR:HG23	1.78	0.83
1:E:377:SER:O	1:E:379:PRO:HD3	1.77	0.83
1:A:747:MET:HG3	1:G:812:PHE:CE2	2.13	0.83
1:C:232:GLU:HA	1:C:236:ASN:OD1	1.78	0.83
1:C:806:TYR:CD2	2:D:147:VAL:HA	2.13	0.83
1:G:471:ILE:O	1:G:471:ILE:CG1	2.26	0.83
1:C:814:LYS:HE3	1:C:818:GLN:HE22	1.43	0.83
1:E:582:CYS:SG	1:E:591:THR:HG23	2.18	0.83
1:E:804:ARG:HH11	1:E:804:ARG:HG2	1.41	0.83
1:A:232:GLU:HA	1:A:236:ASN:OD1	1.79	0.83
1:E:576:LYS:O	1:E:579:THR:HG23	1.79	0.83
1:A:471:ILE:O	1:A:471:ILE:CG1	2.26	0.83
1:G:607:ASP:HA	1:G:610:THR:HB	1.57	0.83
1:C:628:VAL:O	1:C:628:VAL:HG12	1.78	0.83
1:E:62:GLN:HG3	1:E:62:GLN:O	1.78	0.83
1:C:814:LYS:O	1:C:817:GLN:HG2	1.78	0.82
1:A:576:LYS:O	1:A:579:THR:HG23	1.78	0.82
1:C:419:THR:N	1:C:422:GLN:HE21	1.76	0.82
1:A:377:SER:O	1:A:379:PRO:HD3	1.79	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:VAL:HG12	1:A:38:PRO:HD2	1.61	0.82
1:C:37:VAL:HG12	1:C:38:PRO:HD2	1.61	0.82
1:C:62:GLN:O	1:C:62:GLN:HG3	1.79	0.82
1:E:232:GLU:HA	1:E:236:ASN:OD1	1.77	0.82
1:E:493:PHE:O	1:E:497:MET:HB2	1.79	0.82
1:G:419:THR:N	1:G:422:GLN:HE21	1.76	0.82
2:H:83:GLY:HA3	2:H:88:TYR:OH	1.79	0.82
1:C:471:ILE:CG1	1:C:471:ILE:O	2.28	0.81
1:C:792:ILE:O	1:C:796:ILE:HG12	1.80	0.81
1:E:424:ASP:HA	1:E:427:ILE:HG22	1.62	0.81
1:A:751:GLN:OE1	1:G:813:ALA:CB	2.28	0.81
1:C:236:ASN:ND2	1:C:246:SER:HA	1.95	0.81
1:E:471:ILE:CG1	1:E:471:ILE:O	2.28	0.81
1:C:493:PHE:O	1:C:497:MET:HB2	1.80	0.81
1:G:747:MET:HE3	1:G:752:ALA:HA	1.61	0.81
1:C:230:ILE:HG22	1:C:231:LEU:HD23	1.63	0.81
1:A:743:PRO:CG	1:G:816:GLN:HB3	2.09	0.81
1:G:493:PHE:O	1:G:497:MET:HB2	1.80	0.81
1:A:405:PRO:HB2	1:A:407:ILE:CG2	2.11	0.81
1:E:418:GLN:HB3	1:E:422:GLN:HB2	1.63	0.81
1:G:424:ASP:HA	1:G:427:ILE:HG22	1.61	0.81
1:A:62:GLN:O	1:A:62:GLN:HG3	1.79	0.81
2:D:58:GLU:HA	2:D:61:LEU:HD12	1.62	0.81
2:B:58:GLU:HA	2:B:61:LEU:HD12	1.63	0.81
2:F:58:GLU:HA	2:F:61:LEU:HD12	1.63	0.81
1:G:232:GLU:HA	1:G:236:ASN:OD1	1.81	0.81
2:H:58:GLU:HA	2:H:61:LEU:HD12	1.63	0.80
1:A:540:LEU:HD12	1:A:559:LEU:HD12	1.63	0.80
1:E:352:ILE:HG21	1:E:442:ILE:HD11	1.63	0.80
1:G:37:VAL:HG12	1:G:38:PRO:HD2	1.61	0.80
1:G:418:GLN:HB3	1:G:422:GLN:HB2	1.62	0.80
1:E:814:LYS:O	1:E:817:GLN:HG2	1.81	0.80
1:A:437:ARG:HE	1:A:625:TRP:HA	1.47	0.80
1:E:230:ILE:HG22	1:E:231:LEU:HD23	1.62	0.80
1:G:161:TYR:O	1:G:165:LEU:HD12	1.81	0.80
1:G:376:ALA:HB2	1:G:420:LYS:HB2	1.63	0.80
1:A:628:VAL:CG1	1:A:628:VAL:O	2.30	0.80
1:C:582:CYS:SG	1:C:591:THR:HG23	2.21	0.80
1:G:62:GLN:HG3	1:G:62:GLN:O	1.80	0.80
1:A:806:TYR:CD2	2:B:147:VAL:HA	2.16	0.80
1:C:424:ASP:HA	1:C:427:ILE:HG22	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:331:MET:O	1:G:335:THR:HG23	1.81	0.80
2:H:85:PHE:CE1	2:H:145:ARG:HG2	2.15	0.80
1:A:420:LYS:O	1:A:423:ALA:HB3	1.82	0.80
1:E:792:ILE:O	1:E:796:ILE:HG12	1.82	0.80
1:E:405:PRO:HB2	1:E:407:ILE:CG2	2.12	0.79
1:A:424:ASP:HA	1:A:427:ILE:HG22	1.64	0.79
1:A:259:THR:HB	1:A:261:TYR:CE1	2.18	0.79
1:E:323:ILE:HG23	1:E:326:GLN:HB3	1.63	0.79
1:A:331:MET:O	1:A:335:THR:HG23	1.82	0.79
1:A:804:ARG:HH11	1:A:804:ARG:HG2	1.48	0.79
1:G:576:LYS:O	1:G:579:THR:HG23	1.82	0.79
1:A:493:PHE:O	1:A:497:MET:HB2	1.82	0.79
1:E:37:VAL:HG12	1:E:38:PRO:HD2	1.62	0.79
1:G:420:LYS:O	1:G:423:ALA:HB3	1.83	0.79
1:C:187:THR:HG23	1:C:463:ILE:HG21	1.65	0.79
1:G:502:GLN:HG2	1:G:512:TRP:HE1	1.47	0.79
1:A:751:GLN:OE1	1:G:813:ALA:HB2	1.81	0.79
1:A:352:ILE:HG21	1:A:442:ILE:HD11	1.65	0.79
1:A:558:LYS:O	1:A:561:GLN:HB3	1.82	0.79
1:G:405:PRO:HB2	1:G:407:ILE:CG2	2.12	0.79
1:G:437:ARG:HE	1:G:625:TRP:HA	1.47	0.79
1:A:148:GLU:O	1:A:149:MET:HG2	1.83	0.78
1:A:582:CYS:SG	1:A:591:THR:HG23	2.23	0.78
2:B:65:LYS:HD2	2:B:68:GLN:HE21	1.48	0.78
1:C:558:LYS:O	1:C:561:GLN:HB3	1.83	0.78
1:E:502:GLN:HG2	1:E:512:TRP:HE1	1.47	0.78
1:E:690:GLU:HB3	1:E:692:ARG:HG3	1.65	0.78
1:E:407:ILE:HG13	1:E:414:VAL:O	1.84	0.78
2:F:65:LYS:HD2	2:F:68:GLN:HE21	1.49	0.78
1:A:244:ASN:ND2	1:A:244:ASN:O	2.17	0.78
1:C:747:MET:HE3	1:C:752:ALA:HA	1.64	0.78
1:E:376:ALA:HB2	1:E:420:LYS:HB2	1.65	0.78
1:A:376:ALA:HB2	1:A:420:LYS:HB2	1.65	0.78
1:G:558:LYS:O	1:G:561:GLN:HB3	1.82	0.78
1:C:610:THR:CG2	1:C:628:VAL:HG11	2.14	0.78
1:C:690:GLU:HB3	1:C:692:ARG:HG3	1.63	0.78
2:F:84:CYS:SG	2:F:87:ASP:OD2	2.42	0.78
1:A:323:ILE:HG23	1:A:326:GLN:HB3	1.65	0.78
2:D:10:GLU:HA	2:D:13:GLU:HG3	1.66	0.78
1:G:352:ILE:HG21	1:G:442:ILE:HD11	1.64	0.78
1:G:33:LYS:HB3	1:G:49:ILE:HB	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:582:CYS:SG	1:G:591:THR:HG23	2.24	0.78
1:A:83:PHE:HB3	1:A:92:LEU:HD23	1.64	0.77
1:C:418:GLN:HB3	1:C:422:GLN:HB2	1.65	0.77
1:C:33:LYS:HB3	1:C:49:ILE:HB	1.66	0.77
1:C:502:GLN:HG2	1:C:512:TRP:HE1	1.49	0.77
1:G:148:GLU:O	1:G:149:MET:HG2	1.84	0.77
1:A:418:GLN:HB3	1:A:422:GLN:HB2	1.65	0.77
1:C:814:LYS:HG3	1:C:815:ARG:N	1.97	0.77
1:A:610:THR:HG22	1:A:611:SER:N	2.00	0.77
1:E:259:THR:HB	1:E:261:TYR:CE1	2.19	0.77
1:G:659:VAL:HG12	1:G:660:GLY:N	1.98	0.77
1:G:804:ARG:HH11	1:G:804:ARG:HG2	1.48	0.77
1:C:437:ARG:HE	1:C:625:TRP:HA	1.49	0.77
1:E:187:THR:HG23	1:E:463:ILE:HG21	1.64	0.77
1:A:502:GLN:HG2	1:A:512:TRP:HE1	1.49	0.77
1:A:747:MET:HE3	1:A:752:ALA:HA	1.65	0.77
1:C:405:PRO:HB2	1:C:407:ILE:CG2	2.14	0.77
1:E:663:TYR:O	1:E:665:GLU:N	2.17	0.77
1:C:259:THR:HB	1:C:261:TYR:CE1	2.19	0.77
2:D:65:LYS:HD2	2:D:68:GLN:HE21	1.48	0.77
1:C:628:VAL:HG13	1:C:631:ILE:HG12	1.67	0.77
2:H:65:LYS:HD2	2:H:68:GLN:HE21	1.48	0.77
1:C:148:GLU:O	1:C:149:MET:HG2	1.85	0.77
1:E:558:LYS:O	1:E:561:GLN:HB3	1.84	0.77
1:G:259:THR:HB	1:G:261:TYR:CE1	2.20	0.77
1:A:690:GLU:HB3	1:A:692:ARG:HG3	1.65	0.76
1:C:663:TYR:O	1:C:665:GLU:N	2.18	0.76
1:C:659:VAL:HG12	1:C:660:GLY:N	1.98	0.76
1:A:659:VAL:HG12	1:A:660:GLY:N	2.00	0.76
1:C:352:ILE:HG21	1:C:442:ILE:HD11	1.66	0.76
1:C:540:LEU:HD12	1:C:559:LEU:HD12	1.67	0.76
1:C:79:ASN:OD1	1:C:92:LEU:HB3	1.84	0.76
1:G:323:ILE:HG23	1:G:326:GLN:HB3	1.68	0.76
1:A:814:LYS:HE3	1:A:818:GLN:HE22	1.47	0.76
1:C:804:ARG:HG2	1:C:804:ARG:HH11	1.50	0.76
2:F:85:PHE:HA	2:F:89:VAL:HG13	1.65	0.76
1:G:625:TRP:O	1:G:627:ASP:N	2.19	0.76
2:D:141:GLU:O	2:D:145:ARG:HG3	1.85	0.76
1:C:747:MET:HB3	1:C:752:ALA:HB2	1.67	0.76
1:E:13:LEU:HD11	1:E:152:HIS:CD2	2.21	0.76
1:C:576:LYS:O	1:C:579:THR:HG23	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:690:GLU:HB3	1:G:692:ARG:HG3	1.65	0.76
2:H:10:GLU:HA	2:H:13:GLU:HG3	1.67	0.76
2:B:10:GLU:HA	2:B:13:GLU:HG3	1.66	0.75
1:E:420:LYS:O	1:E:423:ALA:HB3	1.85	0.75
1:E:80:PRO:HG2	1:E:83:PHE:CE2	2.20	0.75
1:E:44:PHE:CE2	1:E:702:LEU:HD21	2.21	0.75
1:E:747:MET:HB3	1:E:752:ALA:HB2	1.65	0.75
1:G:663:TYR:O	1:G:665:GLU:N	2.19	0.75
1:A:814:LYS:O	1:A:817:GLN:HG2	1.85	0.75
1:E:743:PRO:HD2	1:E:747:MET:HE1	1.68	0.75
1:C:610:THR:HG22	1:C:611:SER:N	2.01	0.75
1:G:540:LEU:HD12	1:G:559:LEU:HD12	1.67	0.75
1:C:114:TYR:CE2	1:C:153:ILE:HB	2.21	0.75
1:C:420:LYS:O	1:C:423:ALA:HB3	1.87	0.75
2:H:114:THR:C	2:H:115:LEU:HD12	2.07	0.75
1:A:114:TYR:CE2	1:A:153:ILE:HB	2.21	0.75
2:D:114:THR:C	2:D:115:LEU:HD12	2.07	0.75
1:E:540:LEU:HD12	1:E:559:LEU:HD12	1.67	0.75
1:G:747:MET:HB3	1:G:752:ALA:HB2	1.68	0.75
2:F:10:GLU:HA	2:F:13:GLU:HG3	1.66	0.75
1:G:114:TYR:CE2	1:G:153:ILE:HB	2.22	0.75
1:E:552:ASP:O	1:E:556:VAL:HG23	1.87	0.74
1:E:568:LYS:HD3	1:E:584:LEU:HB2	1.69	0.74
1:G:79:ASN:HD22	1:G:80:PRO:CD	1.99	0.74
1:E:148:GLU:O	1:E:149:MET:HG2	1.86	0.74
1:C:541:LEU:HD21	1:C:597:TRP:HB3	1.69	0.74
1:E:134:SER:HB2	1:E:212:GLY:HA2	1.68	0.74
1:E:244:ASN:O	1:E:244:ASN:ND2	2.20	0.74
1:G:244:ASN:O	1:G:244:ASN:ND2	2.20	0.74
1:E:619:LYS:O	1:E:622:ALA:HB3	1.87	0.74
1:G:134:SER:HB2	1:G:212:GLY:HA2	1.69	0.74
1:C:494:ASN:H	1:C:494:ASN:HD22	1.34	0.74
1:A:79:ASN:HD22	1:A:80:PRO:CD	1.99	0.74
1:C:628:VAL:HG22	1:C:631:ILE:HD11	1.70	0.74
1:E:520:ASP:C	1:E:521:LEU:HD23	2.08	0.74
1:G:520:ASP:C	1:G:521:LEU:HD23	2.08	0.74
1:A:407:ILE:HG13	1:A:414:VAL:O	1.88	0.73
1:C:272:LEU:C	1:C:272:LEU:HD12	2.08	0.73
1:E:33:LYS:HB3	1:E:49:ILE:HB	1.67	0.73
1:G:10:GLU:O	1:G:14:PHE:HB2	1.88	0.73
1:G:610:THR:HG22	1:G:611:SER:N	2.01	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:678:ASN:ND2	1:G:679:PRO:HD2	2.03	0.73
1:C:527:LEU:O	1:C:537:VAL:HG23	1.88	0.73
1:C:715:ARG:O	1:C:719:GLN:HG2	1.86	0.73
1:A:33:LYS:HB3	1:A:49:ILE:HB	1.70	0.73
1:A:663:TYR:O	1:A:665:GLU:N	2.20	0.73
1:C:323:ILE:HG23	1:C:326:GLN:HB3	1.69	0.73
1:A:22:ASN:OD1	1:A:24:LEU:HB2	1.88	0.73
2:B:141:GLU:O	2:B:145:ARG:HG3	1.88	0.73
1:C:721:PHE:N	1:C:721:PHE:CD1	2.56	0.73
1:C:234:PHE:HD1	1:C:289:ILE:HG21	1.51	0.73
1:C:700:LEU:HD23	1:C:704:GLN:HE22	1.53	0.73
1:E:272:LEU:C	1:E:272:LEU:HD12	2.08	0.73
1:G:407:ILE:HG13	1:G:414:VAL:O	1.87	0.73
2:H:85:PHE:HB3	2:H:86:GLU:OE1	1.88	0.73
1:A:792:ILE:O	1:A:796:ILE:HG12	1.89	0.73
1:E:302:ARG:O	1:E:307:LEU:HD12	1.89	0.73
1:G:89:MET:HE2	1:G:104:LEU:HD21	1.70	0.73
1:E:114:TYR:CE2	1:E:153:ILE:HB	2.24	0.73
1:E:715:ARG:O	1:E:719:GLN:HG2	1.89	0.73
1:G:272:LEU:HD12	1:G:272:LEU:C	2.09	0.73
1:G:365:ILE:HD13	1:G:427:ILE:HD11	1.70	0.73
1:A:715:ARG:O	1:A:719:GLN:HG2	1.89	0.73
1:G:792:ILE:O	1:G:796:ILE:HG12	1.89	0.73
1:G:814:LYS:HG3	1:G:815:ARG:N	2.04	0.72
1:A:18:ASN:O	1:A:19:PHE:CD1	2.42	0.72
1:C:313:TYR:HB2	1:C:316:LEU:CD1	2.20	0.72
1:E:10:GLU:O	1:E:14:PHE:HB2	1.88	0.72
1:C:628:VAL:O	1:C:631:ILE:HG12	1.89	0.72
1:C:736:ILE:HG23	1:C:737:LEU:HD23	1.70	0.72
1:A:302:ARG:O	1:A:307:LEU:HD12	1.89	0.72
1:C:568:LYS:HD3	1:C:584:LEU:HB2	1.70	0.72
1:E:243:ASP:HB3	1:E:323:ILE:HD11	1.71	0.72
1:E:610:THR:HG22	1:E:611:SER:N	2.03	0.72
2:D:65:LYS:O	2:D:68:GLN:HG3	1.90	0.72
1:A:50:LYS:HE3	1:A:60:GLU:HB3	1.72	0.72
1:A:568:LYS:HD3	1:A:584:LEU:HB2	1.72	0.72
1:C:407:ILE:HD12	1:C:408:LYS:N	2.05	0.72
2:F:114:THR:C	2:F:115:LEU:HD12	2.10	0.72
1:A:10:GLU:O	1:A:14:PHE:HB2	1.90	0.72
1:A:700:LEU:HD23	1:A:704:GLN:HE22	1.54	0.72
1:A:13:LEU:CD1	1:A:132:ILE:HB	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:520:ASP:C	1:C:521:LEU:HD23	2.09	0.72
1:C:79:ASN:HD22	1:C:80:PRO:CD	2.03	0.72
1:E:161:TYR:O	1:E:165:LEU:HD12	1.89	0.72
1:G:700:LEU:HD23	1:G:704:GLN:HE22	1.54	0.72
1:A:407:ILE:HD12	1:A:408:LYS:N	2.04	0.72
1:C:161:TYR:O	1:C:165:LEU:HD12	1.88	0.72
2:H:141:GLU:O	2:H:145:ARG:HG3	1.88	0.72
1:C:244:ASN:ND2	1:C:244:ASN:O	2.23	0.71
2:F:65:LYS:O	2:F:68:GLN:HG3	1.89	0.71
2:H:65:LYS:O	2:H:68:GLN:HG3	1.90	0.71
2:B:65:LYS:O	2:B:68:GLN:HG3	1.90	0.71
1:C:678:ASN:HD22	1:C:679:PRO:CD	2.02	0.71
1:E:399:THR:HG22	1:E:403:LEU:HD11	1.71	0.71
1:E:79:ASN:ND2	1:E:80:PRO:HD2	2.02	0.71
1:G:552:ASP:O	1:G:556:VAL:HG23	1.89	0.71
1:E:135:GLU:CD	1:E:215:PHE:HB2	2.11	0.71
1:E:541:LEU:HD23	1:E:601:ASN:ND2	2.03	0.71
1:G:302:ARG:O	1:G:307:LEU:HD12	1.90	0.71
2:B:4:SER:N	2:B:7:GLN:HE21	1.89	0.71
1:C:10:GLU:O	1:C:14:PHE:HB2	1.89	0.71
1:C:376:ALA:HB3	1:C:420:LYS:HA	1.72	0.71
1:C:407:ILE:HD12	1:C:409:VAL:N	2.05	0.71
1:C:771:GLN:HE21	1:C:771:GLN:C	1.94	0.71
1:C:796:ILE:HG22	1:C:800:GLN:OE1	1.90	0.71
1:G:568:LYS:HD3	1:G:584:LEU:HB2	1.72	0.71
1:A:135:GLU:CD	1:A:215:PHE:HB2	2.11	0.71
2:B:114:THR:C	2:B:115:LEU:HD12	2.11	0.71
1:A:736:ILE:HG23	1:A:737:LEU:HD23	1.72	0.71
1:C:134:SER:HB2	1:C:212:GLY:HA2	1.71	0.71
1:C:302:ARG:O	1:C:307:LEU:HD12	1.89	0.71
1:E:407:ILE:HD11	1:E:414:VAL:HB	1.73	0.71
1:E:407:ILE:HD12	1:E:408:LYS:N	2.05	0.71
1:E:269:THR:CG2	1:E:443:LEU:HD13	2.19	0.71
1:A:399:THR:HG22	1:A:403:LEU:HD11	1.73	0.71
1:C:535:PRO:HB2	1:C:540:LEU:HD21	1.73	0.71
1:E:409:VAL:HG22	1:E:634:LEU:HD12	1.73	0.71
1:G:313:TYR:HB2	1:G:316:LEU:CD1	2.21	0.71
1:G:715:ARG:O	1:G:719:GLN:HG2	1.91	0.71
1:A:520:ASP:C	1:A:521:LEU:HD23	2.11	0.71
1:C:50:LYS:HE3	1:C:60:GLU:HB3	1.73	0.71
1:C:678:ASN:ND2	1:C:679:PRO:HD2	2.04	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:50:LYS:HE3	1:E:60:GLU:HB3	1.72	0.71
1:G:243:ASP:HB3	1:G:323:ILE:HD11	1.73	0.71
1:C:306:LEU:HD12	1:C:390:LEU:HD21	1.72	0.71
1:E:721:PHE:N	1:E:721:PHE:CD1	2.58	0.71
1:G:234:PHE:HD1	1:G:289:ILE:HG21	1.55	0.71
1:G:686:ILE:HD13	1:G:687:PRO:HD2	1.72	0.71
1:C:365:ILE:HD13	1:C:427:ILE:HD11	1.73	0.71
2:D:4:SER:N	2:D:7:GLN:HE21	1.89	0.71
1:E:13:LEU:HD11	1:E:152:HIS:HD2	1.56	0.71
1:E:481:CYS:O	1:E:484:TYR:HB3	1.91	0.71
1:G:376:ALA:HB3	1:G:420:LYS:HA	1.71	0.71
1:G:407:ILE:HD12	1:G:408:LYS:N	2.05	0.71
1:G:721:PHE:N	1:G:721:PHE:CD1	2.58	0.71
1:A:293:LEU:HD22	1:A:353:LEU:HD23	1.73	0.70
1:A:619:LYS:O	1:A:622:ALA:HB3	1.91	0.70
2:F:4:SER:N	2:F:7:GLN:HE21	1.88	0.70
1:E:30:SER:C	1:E:32:LYS:H	1.94	0.70
1:G:8:ASP:CA	1:G:11:LYS:HD2	2.16	0.70
1:G:399:THR:HG22	1:G:403:LEU:HD11	1.73	0.70
1:G:481:CYS:O	1:G:484:TYR:HB3	1.90	0.70
1:G:50:LYS:HE3	1:G:60:GLU:HB3	1.71	0.70
1:A:745:GLY:N	1:G:819:LEU:HD21	2.06	0.70
1:E:199:SER:HB2	1:E:221:GLU:HG2	1.73	0.70
1:E:242:ASN:OD1	1:E:244:ASN:N	2.23	0.70
1:E:533:ASN:HB3	1:E:534:PRO:HD2	1.74	0.70
1:E:627:ASP:OD1	1:E:627:ASP:O	2.08	0.70
1:G:753:CYS:O	1:G:756:MET:HG3	1.91	0.70
1:C:552:ASP:O	1:C:556:VAL:HG23	1.91	0.70
1:E:313:TYR:HB2	1:E:316:LEU:CD1	2.21	0.70
1:G:302:ARG:HH21	1:G:307:LEU:N	1.89	0.70
1:A:721:PHE:CD1	1:A:721:PHE:N	2.57	0.70
1:A:747:MET:HB3	1:A:752:ALA:HB2	1.73	0.70
1:C:169:GLU:HG2	1:C:169:GLU:O	1.91	0.70
1:C:689:HIS:CE1	1:C:700:LEU:HD11	2.27	0.70
1:G:135:GLU:CD	1:G:215:PHE:HB2	2.12	0.70
1:G:269:THR:CG2	1:G:443:LEU:HD13	2.22	0.70
1:A:306:LEU:HD12	1:A:390:LEU:HD21	1.74	0.70
1:C:302:ARG:HH21	1:C:307:LEU:N	1.90	0.70
1:E:302:ARG:HH21	1:E:307:LEU:N	1.88	0.70
1:E:496:THR:HA	1:E:500:LEU:HD12	1.71	0.70
1:A:746:PHE:O	1:G:816:GLN:NE2	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:MET:HB3	1:A:149:MET:HE3	1.73	0.70
1:A:771:GLN:C	1:A:771:GLN:HE21	1.95	0.70
1:G:199:SER:HB2	1:G:221:GLU:HG2	1.73	0.70
2:B:83:GLY:HA3	2:B:88:TYR:CZ	2.27	0.69
1:C:33:LYS:HD3	1:C:49:ILE:HD12	1.74	0.69
1:C:399:THR:HG22	1:C:403:LEU:HD11	1.73	0.69
1:C:407:ILE:HD11	1:C:414:VAL:HB	1.74	0.69
1:C:271:LEU:HD21	1:C:663:TYR:CE1	2.26	0.69
1:E:469:PHE:CE2	1:E:587:ALA:HB3	2.26	0.69
2:F:141:GLU:O	2:F:145:ARG:HG3	1.91	0.69
2:F:85:PHE:O	2:F:86:GLU:C	2.28	0.69
1:G:271:LEU:HD21	1:G:663:TYR:CE1	2.27	0.69
1:G:30:SER:C	1:G:32:LYS:H	1.94	0.69
2:H:4:SER:N	2:H:7:GLN:HE21	1.89	0.69
1:A:269:THR:CG2	1:A:443:LEU:HD13	2.21	0.69
1:A:30:SER:C	1:A:32:LYS:H	1.94	0.69
1:A:365:ILE:HD13	1:A:427:ILE:HD11	1.72	0.69
1:C:320:HIS:C	1:C:320:HIS:HD1	1.96	0.69
1:C:407:ILE:HG13	1:C:414:VAL:O	1.92	0.69
1:C:494:ASN:HD22	1:C:494:ASN:N	1.90	0.69
1:A:242:ASN:OD1	1:A:244:ASN:N	2.24	0.69
1:A:814:LYS:HG3	1:A:815:ARG:N	2.06	0.69
1:C:120:PHE:H	1:C:120:PHE:HD1	1.39	0.69
1:C:199:SER:HB2	1:C:221:GLU:HG2	1.75	0.69
1:C:243:ASP:HB3	1:C:323:ILE:HD11	1.74	0.69
1:G:83:PHE:HB3	1:G:92:LEU:HD23	1.72	0.69
1:A:272:LEU:HD12	1:A:272:LEU:C	2.12	0.69
1:A:552:ASP:O	1:A:556:VAL:HG23	1.92	0.69
1:C:481:CYS:O	1:C:484:TYR:HB3	1.92	0.69
2:D:4:SER:O	2:D:7:GLN:HG2	1.92	0.69
1:E:814:LYS:HG3	1:E:815:ARG:N	2.07	0.69
1:E:182:GLY:HA2	5:E:998:ADP:PA	2.32	0.69
1:A:344:PHE:CE1	1:A:445:ARG:HB3	2.27	0.69
1:A:494:ASN:H	1:A:494:ASN:HD22	1.39	0.69
1:A:541:LEU:HD23	1:A:601:ASN:ND2	2.05	0.69
1:C:135:GLU:CD	1:C:215:PHE:HB2	2.11	0.69
1:C:407:ILE:CD1	1:C:409:VAL:HG23	2.22	0.69
2:D:43:THR:O	2:D:47:VAL:HG23	1.93	0.69
1:E:250:LYS:CE	1:E:465:ASP:OD2	2.40	0.69
1:E:80:PRO:HD2	1:E:83:PHE:CD2	2.27	0.69
2:F:4:SER:O	2:F:7:GLN:HG2	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:527:LEU:O	1:G:537:VAL:HG23	1.92	0.69
1:A:678:ASN:HD22	1:A:679:PRO:CD	2.05	0.69
1:C:407:ILE:HD13	1:C:409:VAL:HG23	1.74	0.69
1:E:13:LEU:HD21	1:E:132:ILE:HD12	1.73	0.69
1:G:44:PHE:CE2	1:G:702:LEU:HD21	2.28	0.69
2:H:43:THR:O	2:H:47:VAL:HG23	1.93	0.69
1:A:134:SER:HB2	1:A:212:GLY:HA2	1.74	0.69
1:A:243:ASP:HB3	1:A:323:ILE:HD11	1.73	0.69
1:A:628:VAL:HG13	1:A:631:ILE:HG12	1.74	0.69
2:D:140:TYR:HD1	2:D:141:GLU:H	1.40	0.69
1:E:419:THR:H	1:E:422:GLN:NE2	1.85	0.69
1:C:89:MET:HE3	1:C:100:VAL:HG13	1.74	0.69
1:E:320:HIS:C	1:E:320:HIS:HD1	1.96	0.69
2:F:25:LYS:HB3	2:F:63:THR:HB	1.74	0.69
2:F:93:ARG:O	2:F:93:ARG:HG3	1.92	0.69
2:H:4:SER:O	2:H:7:GLN:HG2	1.92	0.69
1:E:736:ILE:HG23	1:E:737:LEU:HD23	1.75	0.69
1:G:377:SER:C	1:G:379:PRO:HD3	2.13	0.69
2:H:25:LYS:HB3	2:H:63:THR:HB	1.74	0.69
1:A:161:TYR:O	1:A:165:LEU:HD12	1.93	0.69
2:B:36:ARG:HA	2:B:40:GLN:O	1.93	0.69
2:B:25:LYS:HB3	2:B:63:THR:HB	1.74	0.69
1:C:344:PHE:CE1	1:C:445:ARG:HB3	2.27	0.69
1:C:700:LEU:CD2	1:C:704:GLN:HE22	2.06	0.69
1:E:120:PHE:HD1	1:E:120:PHE:H	1.41	0.69
1:E:700:LEU:HD23	1:E:704:GLN:HE22	1.57	0.69
1:A:407:ILE:HD12	1:A:409:VAL:N	2.09	0.69
1:E:313:TYR:HB2	1:E:316:LEU:HD11	1.75	0.69
1:E:678:ASN:ND2	1:E:679:PRO:HD2	2.07	0.69
1:E:97:GLU:OE2	1:E:702:LEU:HG	1.93	0.69
1:C:700:LEU:HD23	1:C:704:GLN:NE2	2.07	0.68
2:F:43:THR:O	2:F:47:VAL:HG23	1.93	0.68
1:G:678:ASN:HD22	1:G:679:PRO:CD	2.02	0.68
1:A:199:SER:HB2	1:A:221:GLU:HG2	1.75	0.68
1:A:301:MET:HA	1:A:304:ASP:HB2	1.75	0.68
1:A:302:ARG:HH21	1:A:307:LEU:N	1.90	0.68
1:A:450:LEU:N	1:A:450:LEU:HD23	2.09	0.68
1:C:313:TYR:HB2	1:C:316:LEU:HD11	1.75	0.68
1:C:377:SER:C	1:C:379:PRO:HD3	2.14	0.68
1:C:527:LEU:HD12	1:C:566:HIS:CG	2.27	0.68
1:E:306:LEU:HD12	1:E:390:LEU:HD21	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:LYS:HD3	1:A:49:ILE:HD12	1.75	0.68
2:B:113:VAL:HG13	2:B:119:MET:O	1.93	0.68
1:E:407:ILE:HD12	1:E:409:VAL:N	2.08	0.68
1:E:535:PRO:HB2	1:E:540:LEU:HD21	1.75	0.68
1:C:301:MET:HA	1:C:304:ASP:HB2	1.76	0.68
2:D:25:LYS:HB3	2:D:63:THR:HB	1.74	0.68
1:E:301:MET:HA	1:E:304:ASP:HB2	1.76	0.68
1:E:437:ARG:HE	1:E:625:TRP:HA	1.57	0.68
1:G:140:MET:HB3	1:G:149:MET:HE3	1.76	0.68
1:G:230:ILE:HG22	1:G:231:LEU:N	2.07	0.68
1:A:313:TYR:HB2	1:A:316:LEU:CD1	2.23	0.68
1:C:189:LYS:HD3	1:C:192:GLN:OE1	1.93	0.68
1:C:30:SER:C	1:C:32:LYS:H	1.95	0.68
1:C:293:LEU:HD22	1:C:353:LEU:HD23	1.75	0.68
1:C:450:LEU:N	1:C:450:LEU:HD23	2.08	0.68
1:C:628:VAL:HG13	1:C:628:VAL:O	1.94	0.68
2:F:36:ARG:HA	2:F:40:GLN:O	1.93	0.68
1:G:689:HIS:CE1	1:G:700:LEU:HD11	2.28	0.68
1:G:736:ILE:HG23	1:G:737:LEU:HD23	1.73	0.68
1:G:36:TRP:HE1	1:G:78:MET:HG3	1.58	0.68
1:G:293:LEU:HD22	1:G:353:LEU:HD23	1.76	0.68
1:G:490:GLN:O	1:G:494:ASN:ND2	2.26	0.68
1:A:407:ILE:HD11	1:A:414:VAL:HB	1.75	0.68
1:A:419:THR:H	1:A:422:GLN:NE2	1.87	0.68
1:E:376:ALA:HB3	1:E:420:LYS:HA	1.75	0.68
1:E:490:GLN:O	1:E:494:ASN:ND2	2.27	0.68
1:E:89:MET:HE1	1:E:104:LEU:HG	1.76	0.68
1:G:306:LEU:HD12	1:G:390:LEU:HD21	1.74	0.68
1:G:400:ARG:HG2	1:G:404:THR:OG1	1.93	0.68
1:G:619:LYS:O	1:G:622:ALA:HB3	1.94	0.68
2:H:85:PHE:CZ	2:H:145:ARG:HG2	2.28	0.68
2:B:4:SER:O	2:B:7:GLN:HG2	1.92	0.68
1:A:13:LEU:HD21	1:A:132:ILE:CD1	2.24	0.68
1:A:376:ALA:HB3	1:A:420:LYS:HA	1.75	0.68
1:A:47:ALA:HA	1:A:62:GLN:H	1.59	0.68
1:G:189:LYS:HD3	1:G:192:GLN:OE1	1.94	0.68
1:G:313:TYR:HB2	1:G:316:LEU:HD11	1.76	0.68
1:C:13:LEU:HD21	1:C:132:ILE:CD1	2.24	0.68
1:C:469:PHE:CE2	1:C:587:ALA:HB3	2.29	0.68
1:C:48:SER:C	1:C:59:VAL:HG13	2.15	0.68
1:C:555:PHE:CZ	1:C:559:LEU:HD13	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:610:THR:HG23	1:C:628:VAL:HG21	1.76	0.68
2:F:113:VAL:HG13	2:F:119:MET:O	1.94	0.68
1:G:796:ILE:HG22	1:G:800:GLN:OE1	1.94	0.68
1:A:145:LYS:HG3	1:A:146:ARG:HE	1.59	0.67
1:A:57:VAL:O	1:A:69:THR:HG23	1.94	0.67
2:B:43:THR:O	2:B:47:VAL:HG23	1.93	0.67
1:C:13:LEU:HD21	1:C:132:ILE:HD12	1.75	0.67
1:E:555:PHE:CZ	1:E:559:LEU:HD13	2.29	0.67
1:E:7:SER:HB3	1:E:10:GLU:OE1	1.95	0.67
1:G:407:ILE:HD11	1:G:414:VAL:HB	1.74	0.67
1:G:61:LEU:C	1:G:63:GLU:H	1.96	0.67
1:C:496:THR:HA	1:C:500:LEU:HD12	1.76	0.67
1:C:533:ASN:HB3	1:C:534:PRO:HD2	1.75	0.67
1:C:61:LEU:C	1:C:63:GLU:H	1.98	0.67
1:C:686:ILE:HD13	1:C:687:PRO:HD2	1.76	0.67
2:H:36:ARG:HA	2:H:40:GLN:O	1.93	0.67
1:A:533:ASN:HB3	1:A:534:PRO:HD2	1.75	0.67
1:C:490:GLN:O	1:C:494:ASN:ND2	2.27	0.67
1:C:619:LYS:O	1:C:622:ALA:HB3	1.93	0.67
2:D:85:PHE:O	2:D:86:GLU:C	2.32	0.67
2:D:93:ARG:O	2:D:93:ARG:HG3	1.94	0.67
1:E:125:ASN:OD1	1:E:126:PRO:HD2	1.95	0.67
1:E:527:LEU:HD12	1:E:566:HIS:CG	2.30	0.67
1:E:12:PHE:CD2	1:E:131:PRO:CD	2.78	0.67
1:E:659:VAL:CG1	1:E:660:GLY:N	2.57	0.67
1:G:362:LEU:HD22	1:G:431:ALA:HB2	1.77	0.67
1:G:344:PHE:CE1	1:G:445:ARG:HB3	2.30	0.67
1:A:689:HIS:CE1	1:A:700:LEU:HD11	2.29	0.67
1:A:747:MET:SD	1:G:816:GLN:OE1	2.53	0.67
1:G:33:LYS:HD3	1:G:49:ILE:HD12	1.75	0.67
1:G:409:VAL:HG22	1:G:634:LEU:HD12	1.76	0.67
1:G:44:PHE:HE2	1:G:702:LEU:HD21	1.58	0.67
1:A:61:LEU:C	1:A:63:GLU:H	1.96	0.67
1:C:362:LEU:HD23	1:C:427:ILE:HG13	1.76	0.67
1:C:552:ASP:O	1:C:555:PHE:HB3	1.94	0.67
1:C:480:LEU:HD22	1:C:597:TRP:CH2	2.30	0.67
1:C:661:GLN:O	1:C:665:GLU:HB2	1.95	0.67
1:E:169:GLU:HG2	1:E:169:GLU:O	1.94	0.67
1:E:400:ARG:HG2	1:E:404:THR:OG1	1.94	0.67
1:E:678:ASN:HD22	1:E:679:PRO:CD	2.05	0.67
1:G:301:MET:HA	1:G:304:ASP:HB2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:LEU:HD23	1:A:427:ILE:HG13	1.76	0.67
1:A:407:ILE:HD13	1:A:409:VAL:HG23	1.76	0.67
1:C:242:ASN:OD1	1:C:244:ASN:N	2.23	0.67
1:E:8:ASP:CA	1:E:11:LYS:HD2	2.19	0.67
1:E:753:CYS:O	1:E:756:MET:HG3	1.95	0.67
1:G:89:MET:HE2	1:G:104:LEU:CD2	2.23	0.67
1:A:234:PHE:HD1	1:A:289:ILE:HG21	1.59	0.67
1:A:556:VAL:HG12	1:A:560:ILE:HD11	1.77	0.67
1:E:61:LEU:C	1:E:63:GLU:H	1.96	0.67
1:G:419:THR:H	1:G:422:GLN:NE2	1.89	0.67
1:G:533:ASN:HB3	1:G:534:PRO:HD2	1.75	0.67
1:G:628:VAL:HG13	1:G:631:ILE:HG12	1.76	0.67
2:H:25:LYS:HA	2:H:64:LEU:O	1.95	0.67
1:C:391:MET:HG2	1:C:613:LEU:CD2	2.25	0.67
1:E:377:SER:C	1:E:379:PRO:HD3	2.14	0.67
1:E:613:LEU:O	1:E:615:GLN:N	2.28	0.67
2:F:128:VAL:HB	2:F:138:ILE:HD11	1.76	0.67
1:G:555:PHE:CZ	1:G:559:LEU:HD13	2.29	0.67
1:G:556:VAL:HG12	1:G:560:ILE:HD11	1.76	0.67
2:B:31:CYS:O	2:B:35:MET:HG3	1.95	0.66
2:B:86:GLU:CD	2:B:86:GLU:H	1.98	0.66
1:E:796:ILE:HG22	1:E:800:GLN:OE1	1.95	0.66
1:A:527:LEU:HD12	1:A:566:HIS:CG	2.30	0.66
1:A:48:SER:C	1:A:59:VAL:HG13	2.15	0.66
1:A:700:LEU:HD23	1:A:704:GLN:NE2	2.10	0.66
2:D:36:ARG:HA	2:D:40:GLN:O	1.94	0.66
1:A:169:GLU:O	1:A:169:GLU:HG2	1.93	0.66
1:C:76:GLN:HB3	1:C:96:ASN:ND2	2.11	0.66
2:D:31:CYS:O	2:D:35:MET:HG3	1.95	0.66
1:E:47:ALA:HA	1:E:62:GLN:H	1.60	0.66
1:E:271:LEU:HD21	1:E:663:TYR:CE1	2.31	0.66
2:H:31:CYS:O	2:H:35:MET:HG3	1.94	0.66
1:A:496:THR:HA	1:A:500:LEU:HD12	1.76	0.66
2:B:25:LYS:HA	2:B:64:LEU:O	1.95	0.66
1:E:230:ILE:HG22	1:E:231:LEU:N	2.11	0.66
1:G:480:LEU:HD22	1:G:597:TRP:CH2	2.31	0.66
1:G:700:LEU:HD23	1:G:704:GLN:NE2	2.09	0.66
1:A:259:THR:HB	1:A:261:TYR:HE1	1.61	0.66
1:A:377:SER:C	1:A:379:PRO:HD3	2.14	0.66
1:C:89:MET:HE1	1:C:104:LEU:HG	1.77	0.66
1:C:97:GLU:OE2	1:C:702:LEU:HG	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:279:ARG:NH2	1:E:428:GLU:HG3	2.11	0.66
1:E:365:ILE:HD13	1:E:427:ILE:HD11	1.76	0.66
1:E:362:LEU:HD22	1:E:431:ALA:HB2	1.77	0.66
1:G:771:GLN:HE21	1:G:771:GLN:C	1.99	0.66
1:G:7:SER:HB3	1:G:10:GLU:OE1	1.96	0.66
1:C:556:VAL:HG12	1:C:560:ILE:HD11	1.76	0.66
1:C:753:CYS:O	1:C:756:MET:HG3	1.95	0.66
1:G:47:ALA:HA	1:G:62:GLN:H	1.60	0.66
2:H:113:VAL:HG13	2:H:119:MET:O	1.95	0.66
1:A:494:ASN:N	1:A:494:ASN:HD22	1.92	0.66
1:C:362:LEU:HD22	1:C:431:ALA:HB2	1.78	0.66
1:E:689:HIS:CE1	1:E:700:LEU:HD11	2.31	0.66
1:G:527:LEU:HD12	1:G:566:HIS:CG	2.30	0.66
1:A:407:ILE:CD1	1:A:409:VAL:HG23	2.24	0.66
1:A:747:MET:HB2	1:G:816:GLN:HE22	1.61	0.66
1:C:269:THR:CG2	1:C:443:LEU:HD13	2.22	0.66
1:C:728:GLN:CA	1:C:728:GLN:HE21	2.08	0.66
1:G:57:VAL:O	1:G:69:THR:HG23	1.96	0.66
1:A:527:LEU:O	1:A:537:VAL:HG23	1.95	0.66
1:C:181:ALA:O	1:C:684:CYS:HB3	1.96	0.66
1:E:607:ASP:CA	1:E:610:THR:HB	2.26	0.66
2:F:31:CYS:O	2:F:35:MET:HG3	1.95	0.66
1:G:407:ILE:HD13	1:G:409:VAL:HG23	1.78	0.66
1:E:302:ARG:NH2	1:E:303:ASN:HA	2.11	0.66
1:E:586:TYR:HD1	1:E:586:TYR:H	1.44	0.66
1:G:187:THR:HG23	1:G:463:ILE:CG2	2.26	0.66
1:G:320:HIS:C	1:G:320:HIS:HD1	1.97	0.66
2:B:93:ARG:O	2:B:93:ARG:HG3	1.94	0.65
1:E:293:LEU:HD22	1:E:353:LEU:HD23	1.77	0.65
1:E:494:ASN:HD22	1:E:494:ASN:H	1.43	0.65
1:E:33:LYS:HD3	1:E:49:ILE:HD12	1.76	0.65
2:F:25:LYS:HA	2:F:64:LEU:O	1.95	0.65
1:G:407:ILE:CD1	1:G:409:VAL:HG23	2.26	0.65
1:A:120:PHE:HD1	1:A:120:PHE:H	1.43	0.65
1:A:230:ILE:HG22	1:A:231:LEU:N	2.12	0.65
1:A:678:ASN:ND2	1:A:679:PRO:HD2	2.10	0.65
1:A:686:ILE:HD13	1:A:687:PRO:HD2	1.77	0.65
1:C:613:LEU:O	1:C:615:GLN:N	2.28	0.65
1:E:804:ARG:NH1	1:E:804:ARG:HG2	2.11	0.65
1:E:89:MET:HE3	1:E:100:VAL:HG13	1.78	0.65
1:G:407:ILE:HD12	1:G:409:VAL:N	2.10	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:496:THR:HA	1:G:500:LEU:HD12	1.79	0.65
1:G:586:TYR:HD1	1:G:586:TYR:H	1.44	0.65
1:G:613:LEU:O	1:G:615:GLN:N	2.28	0.65
1:A:522:GLN:N	1:A:523:PRO:HD2	2.11	0.65
1:A:700:LEU:CD2	1:A:704:GLN:HE22	2.10	0.65
1:G:247:ARG:HA	1:G:247:ARG:HH11	1.59	0.65
2:H:93:ARG:HG3	2:H:93:ARG:O	1.97	0.65
1:E:399:THR:HG22	1:E:403:LEU:CD1	2.26	0.65
1:E:344:PHE:CE1	1:E:445:ARG:HB3	2.30	0.65
1:E:250:LYS:HG2	1:E:465:ASP:HB3	1.78	0.65
1:E:89:MET:C	1:E:91:GLU:H	1.98	0.65
1:G:120:PHE:HD1	1:G:120:PHE:H	1.43	0.65
1:A:189:LYS:HD3	1:A:192:GLN:OE1	1.95	0.65
1:A:400:ARG:HG2	1:A:404:THR:OG1	1.97	0.65
1:A:751:GLN:HG3	1:G:809:ARG:CB	2.22	0.65
1:C:419:THR:H	1:C:422:GLN:NE2	1.90	0.65
1:C:502:GLN:HG2	1:C:512:TRP:NE1	2.11	0.65
1:E:247:ARG:HA	1:E:247:ARG:HH11	1.62	0.65
1:E:48:SER:C	1:E:59:VAL:HG13	2.16	0.65
1:E:628:VAL:HG13	1:E:631:ILE:HG13	1.78	0.65
1:E:747:MET:HE3	1:E:752:ALA:HA	1.76	0.65
2:H:85:PHE:HE1	2:H:145:ARG:HG2	1.61	0.65
1:A:279:ARG:NH2	1:A:428:GLU:HG3	2.11	0.65
1:A:728:GLN:CA	1:A:728:GLN:HE21	2.08	0.65
2:D:25:LYS:HA	2:D:64:LEU:O	1.96	0.65
1:E:323:ILE:CG2	1:E:326:GLN:HB3	2.27	0.65
1:E:673:THR:O	1:E:677:THR:HG23	1.96	0.65
1:G:535:PRO:HB2	1:G:540:LEU:HD21	1.77	0.65
2:H:55:LYS:HB2	2:H:58:GLU:OE2	1.96	0.65
1:A:552:ASP:O	1:A:555:PHE:HB3	1.97	0.65
1:C:400:ARG:HG2	1:C:404:THR:OG1	1.97	0.65
1:C:527:LEU:HD23	1:C:537:VAL:HG23	1.79	0.65
1:E:480:LEU:HD22	1:E:597:TRP:CH2	2.32	0.65
1:E:609:VAL:O	1:E:612:LEU:HB3	1.97	0.65
1:E:700:LEU:HD23	1:E:704:GLN:NE2	2.12	0.65
1:G:313:TYR:HD2	1:G:360:LEU:HB3	1.61	0.65
1:G:628:VAL:HG13	1:G:628:VAL:O	1.97	0.65
1:G:56:GLU:HG3	1:G:71:SER:HA	1.79	0.65
1:A:313:TYR:HB2	1:A:316:LEU:HD11	1.78	0.65
1:C:47:ALA:HA	1:C:62:GLN:H	1.61	0.65
1:C:7:SER:HB3	1:C:10:GLU:OE1	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:407:ILE:CD1	1:E:409:VAL:HG23	2.26	0.65
1:E:79:ASN:OD1	1:E:92:LEU:HB3	1.97	0.65
1:G:552:ASP:O	1:G:555:PHE:HB3	1.97	0.65
1:G:673:THR:O	1:G:677:THR:HG23	1.97	0.65
1:A:89:MET:HE1	1:A:104:LEU:HG	1.79	0.65
1:A:370:GLU:O	1:A:374:ASP:N	2.29	0.65
2:B:55:LYS:HB2	2:B:58:GLU:OE2	1.97	0.65
1:C:405:PRO:HB2	1:C:407:ILE:HG23	1.79	0.65
1:E:320:HIS:C	1:E:320:HIS:ND1	2.51	0.65
1:E:771:GLN:C	1:E:771:GLN:HE21	2.00	0.65
1:A:630:ARG:HH22	1:A:657:ARG:CB	2.10	0.65
1:C:250:LYS:CE	1:C:465:ASP:OD2	2.44	0.65
2:D:113:VAL:HG13	2:D:119:MET:O	1.97	0.65
2:D:55:LYS:HB2	2:D:58:GLU:OE2	1.97	0.65
1:E:671:MET:O	1:E:675:ARG:HD2	1.97	0.65
1:G:469:PHE:CE2	1:G:587:ALA:HB3	2.32	0.65
1:G:48:SER:C	1:G:59:VAL:HG13	2.16	0.65
1:A:535:PRO:HB2	1:A:540:LEU:HD21	1.78	0.64
1:C:60:GLU:HG3	1:C:66:LYS:O	1.97	0.64
1:E:407:ILE:HD13	1:E:409:VAL:HG23	1.79	0.64
1:G:158:ASP:HB2	1:G:193:TYR:OH	1.98	0.64
1:G:502:GLN:HG2	1:G:512:TRP:NE1	2.12	0.64
1:G:630:ARG:HH22	1:G:657:ARG:CB	2.10	0.64
1:G:661:GLN:O	1:G:665:GLU:HB2	1.95	0.64
1:A:606:ASN:OD1	1:A:609:VAL:HG12	1.98	0.64
1:A:181:ALA:O	1:A:684:CYS:HB3	1.98	0.64
1:C:586:TYR:H	1:C:586:TYR:HD1	1.44	0.64
2:D:3:PHE:HA	2:D:7:GLN:HE21	1.63	0.64
1:E:527:LEU:O	1:E:537:VAL:HG23	1.96	0.64
1:E:552:ASP:O	1:E:555:PHE:HB3	1.97	0.64
1:E:391:MET:HG2	1:E:613:LEU:CD2	2.27	0.64
2:F:3:PHE:HA	2:F:7:GLN:HE21	1.63	0.64
1:G:33:LYS:HB3	1:G:49:ILE:CB	2.27	0.64
1:A:345:THR:HB	1:A:348:GLU:CB	2.27	0.64
1:A:361:GLN:C	1:A:363:GLY:H	1.99	0.64
1:A:661:GLN:O	1:A:665:GLU:HB2	1.97	0.64
1:A:79:ASN:ND2	1:A:80:PRO:HD2	2.09	0.64
1:A:97:GLU:OE2	1:A:702:LEU:HG	1.96	0.64
1:E:502:GLN:HG2	1:E:512:TRP:NE1	2.11	0.64
1:E:527:LEU:HG	1:E:563:GLN:HG3	1.79	0.64
2:F:55:LYS:HB2	2:F:58:GLU:OE2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:HIS:HD1	1:A:320:HIS:C	1.99	0.64
1:A:530:ARG:HG2	1:A:534:PRO:O	1.98	0.64
1:A:586:TYR:H	1:A:586:TYR:HD1	1.45	0.64
1:C:140:MET:HB3	1:C:149:MET:HE3	1.80	0.64
2:D:83:GLY:HA3	2:D:88:TYR:CZ	2.33	0.64
2:D:89:VAL:HG12	2:D:144:VAL:CG2	2.19	0.64
2:F:89:VAL:HG12	2:F:144:VAL:CG2	2.19	0.64
1:C:370:GLU:O	1:C:374:ASP:N	2.30	0.64
1:G:812:PHE:C	1:G:814:LYS:H	1.99	0.64
1:A:613:LEU:O	1:A:615:GLN:N	2.31	0.64
1:A:627:ASP:OD1	1:A:627:ASP:O	2.15	0.64
1:C:320:HIS:C	1:C:320:HIS:ND1	2.50	0.64
1:C:606:ASN:OD1	1:C:609:VAL:HG12	1.98	0.64
1:C:609:VAL:O	1:C:612:LEU:HB3	1.97	0.64
1:E:405:PRO:HB2	1:E:407:ILE:HG23	1.78	0.64
1:G:320:HIS:C	1:G:320:HIS:ND1	2.51	0.64
1:G:370:GLU:O	1:G:374:ASP:N	2.31	0.64
1:G:667:LEU:HG	1:G:667:LEU:O	1.97	0.64
1:A:187:THR:HG23	1:A:463:ILE:CG2	2.26	0.64
1:C:409:VAL:HG22	1:C:634:LEU:HD12	1.79	0.64
1:G:391:MET:HG2	1:G:613:LEU:CD2	2.28	0.64
1:G:97:GLU:OE2	1:G:702:LEU:HG	1.97	0.64
1:A:405:PRO:HB2	1:A:407:ILE:HG23	1.79	0.64
1:C:8:ASP:CA	1:C:11:LYS:HD2	2.17	0.64
2:D:140:TYR:CD1	2:D:141:GLU:HG2	2.32	0.64
2:B:3:PHE:HA	2:B:7:GLN:HE21	1.63	0.64
1:E:235:GLY:O	1:E:247:ARG:HB2	1.97	0.64
1:E:234:PHE:HD1	1:E:289:ILE:HG21	1.63	0.64
1:G:181:ALA:O	1:G:684:CYS:HB3	1.97	0.64
1:G:627:ASP:O	1:G:627:ASP:CG	2.37	0.64
1:G:700:LEU:CD2	1:G:704:GLN:HE22	2.10	0.64
1:A:502:GLN:HG2	1:A:512:TRP:NE1	2.12	0.63
1:C:235:GLY:O	1:C:247:ARG:HB2	1.97	0.63
1:E:181:ALA:O	1:E:684:CYS:HB3	1.98	0.63
2:F:112:LEU:HD13	2:F:119:MET:HE2	1.80	0.63
1:G:797:ILE:HG13	2:H:117:GLU:H	1.63	0.63
1:A:481:CYS:O	1:A:484:TYR:HB3	1.97	0.63
1:E:164:MET:HE3	1:E:461:LEU:HD12	1.81	0.63
1:G:399:THR:HG22	1:G:403:LEU:CD1	2.28	0.63
1:A:362:LEU:HD22	1:A:431:ALA:HB2	1.79	0.63
1:A:409:VAL:HG22	1:A:634:LEU:HD12	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:671:MET:O	1:A:675:ARG:HD2	1.99	0.63
1:C:247:ARG:HA	1:C:247:ARG:HH11	1.64	0.63
1:C:663:TYR:OH	1:C:667:LEU:HD13	1.97	0.63
1:E:494:ASN:N	1:E:494:ASN:HD22	1.96	0.63
1:E:700:LEU:CD2	1:E:704:GLN:HE22	2.12	0.63
2:H:55:LYS:O	2:H:58:GLU:HG2	1.98	0.63
1:A:555:PHE:CZ	1:A:559:LEU:HD13	2.32	0.63
1:A:673:THR:O	1:A:677:THR:HG23	1.98	0.63
1:C:56:GLU:HG3	1:C:71:SER:HA	1.80	0.63
2:D:35:MET:O	2:D:40:GLN:HB2	1.98	0.63
1:E:328:ASP:HA	1:E:331:MET:HB2	1.78	0.63
1:E:661:GLN:O	1:E:665:GLU:HB2	1.99	0.63
1:G:235:GLY:O	1:G:247:ARG:HB2	1.97	0.63
1:G:361:GLN:C	1:G:363:GLY:H	2.02	0.63
1:A:158:ASP:HB2	1:A:193:TYR:OH	1.99	0.63
1:A:399:THR:HG22	1:A:403:LEU:CD1	2.28	0.63
1:A:44:PHE:CE2	1:A:702:LEU:HD21	2.33	0.63
1:A:743:PRO:CB	1:G:816:GLN:HB3	2.29	0.63
1:E:189:LYS:HD3	1:E:192:GLN:OE1	1.98	0.63
1:E:193:TYR:CE1	1:E:197:VAL:HG21	2.33	0.63
1:E:259:THR:HB	1:E:261:TYR:HE1	1.64	0.63
1:E:60:GLU:HG3	1:E:66:LYS:O	1.99	0.63
1:G:541:LEU:HD23	1:G:601:ASN:ND2	2.07	0.63
1:C:437:ARG:HB3	1:C:624:LEU:HD23	1.81	0.63
1:C:610:THR:CG2	1:C:628:VAL:CG1	2.77	0.63
2:D:84:CYS:O	2:D:88:TYR:N	2.25	0.63
1:E:728:GLN:HE21	1:E:728:GLN:CA	2.10	0.63
1:G:405:PRO:HB2	1:G:407:ILE:HG23	1.80	0.63
1:A:747:MET:HG3	1:G:812:PHE:HE2	1.62	0.63
1:A:628:VAL:O	1:A:628:VAL:HG12	1.99	0.63
2:B:35:MET:O	2:B:40:GLN:HB2	1.98	0.63
1:C:361:GLN:C	1:C:363:GLY:H	2.02	0.63
2:D:128:VAL:HB	2:D:138:ILE:HD11	1.79	0.63
1:C:13:LEU:HG	1:C:132:ILE:HG21	1.81	0.63
1:C:382:THR:O	1:C:385:GLN:HB3	1.99	0.63
1:C:541:LEU:HD23	1:C:601:ASN:ND2	2.08	0.63
1:G:345:THR:HB	1:G:348:GLU:CB	2.29	0.63
1:G:362:LEU:HD23	1:G:427:ILE:HG13	1.80	0.63
1:A:267:ILE:HD11	1:A:450:LEU:HD12	1.81	0.63
1:A:753:CYS:O	1:A:756:MET:HG3	1.99	0.63
1:A:788:ARG:HG2	1:A:788:ARG:HH11	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:328:ASP:HA	1:C:331:MET:HB2	1.81	0.63
1:C:279:ARG:NH2	1:C:428:GLU:HG3	2.13	0.63
1:C:57:VAL:O	1:C:69:THR:HG23	1.98	0.63
2:F:70:LEU:N	2:F:71:PRO:HD2	2.14	0.63
1:C:345:THR:HB	1:C:348:GLU:CB	2.28	0.62
1:E:242:ASN:OD1	1:E:242:ASN:C	2.37	0.62
1:E:667:LEU:HG	1:E:667:LEU:O	1.99	0.62
2:F:43:THR:HG23	2:F:46:GLU:CD	2.20	0.62
2:F:72:MET:HA	2:F:75:THR:OG1	1.99	0.62
1:A:89:MET:HE3	1:A:100:VAL:HG13	1.80	0.62
1:A:305:LEU:HD22	1:A:354:ARG:HB3	1.81	0.62
1:A:609:VAL:O	1:A:612:LEU:HB3	1.99	0.62
1:A:686:ILE:HG22	1:A:700:LEU:HD21	1.80	0.62
1:C:36:TRP:HE1	1:C:78:MET:HG3	1.59	0.62
1:E:13:LEU:HD11	1:E:132:ILE:HB	1.81	0.62
1:C:33:LYS:HB3	1:C:49:ILE:CB	2.29	0.62
1:C:673:THR:O	1:C:677:THR:HG23	1.98	0.62
2:F:84:CYS:O	2:F:88:TYR:N	2.32	0.62
1:G:418:GLN:HB3	1:G:422:GLN:CB	2.28	0.62
1:G:609:VAL:O	1:G:612:LEU:HB3	1.98	0.62
1:C:313:TYR:HD2	1:C:360:LEU:HB3	1.63	0.62
1:C:522:GLN:N	1:C:523:PRO:HD2	2.15	0.62
1:C:527:LEU:HG	1:C:563:GLN:HG3	1.80	0.62
1:C:607:ASP:CA	1:C:610:THR:HB	2.29	0.62
1:E:313:TYR:HD2	1:E:360:LEU:HB3	1.65	0.62
1:E:370:GLU:O	1:E:374:ASP:N	2.32	0.62
1:E:482:ILE:HG22	1:E:483:ASN:N	2.15	0.62
1:G:278:ILE:HA	1:G:315:PHE:CD1	2.35	0.62
1:G:450:LEU:HD23	1:G:450:LEU:N	2.13	0.62
1:G:522:GLN:N	1:G:523:PRO:HD2	2.14	0.62
1:G:606:ASN:OD1	1:G:609:VAL:HG12	2.00	0.62
1:G:611:SER:O	1:G:615:GLN:NE2	2.32	0.62
1:A:320:HIS:ND1	1:A:320:HIS:C	2.52	0.62
2:D:70:LEU:N	2:D:71:PRO:HD2	2.14	0.62
1:E:57:VAL:O	1:E:69:THR:HG23	1.98	0.62
1:G:267:ILE:HD11	1:G:450:LEU:HD12	1.82	0.62
1:G:60:GLU:HG3	1:G:66:LYS:O	1.99	0.62
1:A:302:ARG:NH2	1:A:303:ASN:HA	2.14	0.62
1:A:418:GLN:HB3	1:A:422:GLN:CB	2.28	0.62
1:A:266:ASN:HA	1:A:447:ASN:OD1	2.00	0.62
1:C:250:LYS:HG2	1:C:465:ASP:HB3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:35:MET:O	2:H:40:GLN:HB2	1.98	0.62
2:H:3:PHE:HA	2:H:7:GLN:HE21	1.63	0.62
1:A:409:VAL:HB	1:A:414:VAL:HG21	1.82	0.62
1:A:561:GLN:OE1	1:A:562:GLU:HG2	1.99	0.62
2:B:43:THR:HG23	2:B:46:GLU:CD	2.20	0.62
1:C:302:ARG:NH2	1:C:303:ASN:HA	2.13	0.62
1:C:812:PHE:C	1:C:814:LYS:H	2.03	0.62
2:D:43:THR:HG23	2:D:46:GLU:CD	2.20	0.62
1:E:382:THR:O	1:E:385:GLN:HB3	1.99	0.62
2:B:72:MET:HA	2:B:75:THR:OG1	2.00	0.62
1:C:399:THR:HG22	1:C:403:LEU:CD1	2.29	0.62
1:C:418:GLN:HB3	1:C:422:GLN:CB	2.30	0.62
1:E:278:ILE:HA	1:E:315:PHE:CD1	2.35	0.62
1:E:527:LEU:HD11	1:E:569:PHE:HB2	1.81	0.62
1:E:561:GLN:OE1	1:E:562:GLU:HG2	1.99	0.62
1:E:56:GLU:HG3	1:E:71:SER:HA	1.81	0.62
2:F:35:MET:O	2:F:40:GLN:HB2	1.98	0.62
1:G:382:THR:O	1:G:385:GLN:HB3	2.00	0.62
1:A:469:PHE:CE2	1:A:587:ALA:HB3	2.34	0.62
1:C:553:THR:O	1:C:557:GLU:HG2	2.00	0.62
1:C:671:MET:O	1:C:675:ARG:HD2	1.99	0.62
1:E:469:PHE:CZ	1:E:587:ALA:HB3	2.35	0.62
1:G:250:LYS:CE	1:G:465:ASP:OD2	2.47	0.62
1:G:477:PHE:O	1:G:480:LEU:HB3	2.00	0.62
1:G:490:GLN:NE2	1:G:494:ASN:HD21	1.97	0.62
1:C:158:ASP:HB2	1:C:193:TYR:OH	2.00	0.62
2:D:4:SER:H	2:D:7:GLN:HE21	1.48	0.62
1:A:323:ILE:CG2	1:A:326:GLN:HB3	2.29	0.61
1:A:480:LEU:HD22	1:A:597:TRP:CH2	2.34	0.61
2:B:70:LEU:N	2:B:71:PRO:HD2	2.14	0.61
2:D:85:PHE:CD1	2:D:144:VAL:HG11	2.35	0.61
1:E:158:ASP:HB2	1:E:193:TYR:OH	2.00	0.61
1:A:60:GLU:HG3	1:A:66:LYS:O	2.00	0.61
1:E:267:ILE:HD11	1:E:450:LEU:HD12	1.81	0.61
1:E:310:PHE:CD2	1:E:320:HIS:HB2	2.35	0.61
1:E:489:LEU:O	1:E:492:LEU:HB3	1.99	0.61
1:E:568:LYS:CD	1:E:584:LEU:HB2	2.29	0.61
1:G:305:LEU:HD22	1:G:354:ARG:HB3	1.81	0.61
1:G:766:LEU:HB3	1:G:780:VAL:HG21	1.82	0.61
2:D:125:GLU:O	2:D:129:ALA:HB2	2.00	0.61
1:G:302:ARG:NH2	1:G:303:ASN:HA	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:302:ARG:HH21	1:G:307:LEU:H	1.48	0.61
1:A:747:MET:HG3	1:G:812:PHE:CZ	2.36	0.61
2:H:70:LEU:N	2:H:71:PRO:HD2	2.15	0.61
1:A:271:LEU:HD21	1:A:663:TYR:CE1	2.34	0.61
1:C:362:LEU:HD21	1:C:430:LEU:HD23	1.81	0.61
1:C:527:LEU:HD11	1:C:569:PHE:HB2	1.81	0.61
1:C:627:ASP:O	1:C:627:ASP:CG	2.37	0.61
1:C:705:LEU:HD22	1:C:710:VAL:HG21	1.82	0.61
2:D:65:LYS:HD2	2:D:68:GLN:NE2	2.15	0.61
1:E:52:GLU:HA	1:E:57:VAL:HG13	1.82	0.61
1:E:686:ILE:HD13	1:E:687:PRO:HD2	1.82	0.61
1:G:490:GLN:HE21	1:G:494:ASN:HD21	1.47	0.61
1:G:50:LYS:HE3	1:G:60:GLU:CB	2.30	0.61
1:G:541:LEU:HD21	1:G:597:TRP:HB3	1.82	0.61
1:G:627:ASP:OD1	1:G:627:ASP:O	2.18	0.61
1:G:686:ILE:HG22	1:G:700:LEU:HD21	1.80	0.61
2:H:43:THR:HG23	2:H:46:GLU:CD	2.20	0.61
1:A:313:TYR:HD2	1:A:360:LEU:HB3	1.65	0.61
1:C:561:GLN:OE1	1:C:562:GLU:HG2	2.00	0.61
1:E:33:LYS:HB3	1:E:49:ILE:CB	2.31	0.61
1:E:50:LYS:HE3	1:E:60:GLU:CB	2.30	0.61
1:G:242:ASN:OD1	1:G:244:ASN:N	2.29	0.61
1:A:527:LEU:HD23	1:A:537:VAL:HG23	1.82	0.61
2:B:55:LYS:O	2:B:58:GLU:HG2	2.01	0.61
1:E:243:ASP:HB3	1:E:323:ILE:CD1	2.30	0.61
1:E:305:LEU:HD22	1:E:354:ARG:HB3	1.83	0.61
1:E:399:THR:O	1:E:403:LEU:HD12	2.00	0.61
1:E:530:ARG:HG2	1:E:534:PRO:O	2.01	0.61
1:G:227:ALA:C	1:G:229:PRO:HD2	2.20	0.61
1:A:227:ALA:C	1:A:229:PRO:HD2	2.20	0.61
1:A:243:ASP:HB3	1:A:323:ILE:CD1	2.31	0.61
2:D:84:CYS:SG	2:D:87:ASP:OD2	2.59	0.61
1:E:23:PRO:HA	1:E:26:GLN:HB3	1.82	0.61
1:E:362:LEU:HD23	1:E:427:ILE:HG13	1.82	0.61
2:F:44:ASN:HB2	2:F:117:GLU:CD	2.21	0.61
1:A:242:ASN:OD1	1:A:242:ASN:C	2.38	0.61
1:C:107:ARG:HH11	1:C:115:THR:HG23	1.66	0.61
1:C:497:MET:HA	1:C:497:MET:HE3	1.83	0.61
1:C:530:ARG:HG2	1:C:534:PRO:O	2.01	0.61
2:D:140:TYR:CD1	2:D:141:GLU:N	2.68	0.61
2:D:140:TYR:HD1	2:D:141:GLU:N	1.97	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:250:LYS:HG2	1:G:465:ASP:HB3	1.82	0.61
1:G:57:VAL:C	1:G:69:THR:HG23	2.21	0.61
1:G:815:ARG:HA	1:G:818:GLN:CD	2.21	0.61
2:H:72:MET:HA	2:H:75:THR:OG1	2.00	0.61
1:A:541:LEU:HD21	1:A:597:TRP:HB3	1.83	0.61
1:A:607:ASP:CA	1:A:610:THR:HB	2.28	0.61
1:A:728:GLN:HA	1:A:728:GLN:HE21	1.66	0.61
1:C:52:GLU:HA	1:C:57:VAL:HG13	1.81	0.61
1:C:610:THR:HG22	1:C:628:VAL:HG11	1.82	0.61
1:E:556:VAL:HG12	1:E:560:ILE:HD11	1.82	0.61
1:G:273:GLU:O	1:G:273:GLU:HG2	2.01	0.61
1:G:328:ASP:HA	1:G:331:MET:HB2	1.81	0.61
1:G:551:THR:N	1:G:554:SER:OG	2.32	0.61
1:G:553:THR:O	1:G:557:GLU:HG2	2.01	0.61
1:G:728:GLN:CA	1:G:728:GLN:HE21	2.12	0.61
1:G:89:MET:C	1:G:91:GLU:H	2.02	0.61
1:A:328:ASP:HA	1:A:331:MET:HB2	1.82	0.61
1:A:551:THR:N	1:A:554:SER:OG	2.30	0.61
2:B:4:SER:H	2:B:7:GLN:HE21	1.48	0.61
1:C:57:VAL:C	1:C:69:THR:HG23	2.21	0.61
1:E:450:LEU:N	1:E:450:LEU:HD23	2.15	0.61
1:E:553:THR:CG2	1:E:579:THR:HG21	2.31	0.61
1:G:527:LEU:HD23	1:G:537:VAL:HG23	1.83	0.61
1:A:405:PRO:HD2	1:A:417:ALA:HA	1.83	0.60
1:A:57:VAL:C	1:A:69:THR:HG23	2.21	0.60
1:C:747:MET:CG	1:C:751:GLN:HE22	2.14	0.60
1:E:134:SER:CB	1:E:212:GLY:HA2	2.29	0.60
2:F:4:SER:H	2:F:7:GLN:HE21	1.48	0.60
1:G:279:ARG:NH2	1:G:428:GLU:HG3	2.16	0.60
2:H:65:LYS:HD2	2:H:68:GLN:NE2	2.15	0.60
1:A:145:LYS:CG	1:A:146:ARG:H	2.12	0.60
1:A:362:LEU:HD21	1:A:430:LEU:HD23	1.83	0.60
1:C:125:ASN:OD1	1:C:126:PRO:HD2	2.02	0.60
1:C:267:ILE:HD11	1:C:450:LEU:HD12	1.83	0.60
2:D:55:LYS:O	2:D:58:GLU:HG2	2.00	0.60
2:D:84:CYS:O	2:D:87:ASP:N	2.33	0.60
1:E:418:GLN:HB3	1:E:422:GLN:CB	2.29	0.60
1:E:478:GLU:N	1:E:478:GLU:OE1	2.21	0.60
1:G:323:ILE:CG2	1:G:326:GLN:HB3	2.31	0.60
1:G:52:GLU:HA	1:G:57:VAL:HG13	1.84	0.60
1:G:104:LEU:HD12	1:G:705:LEU:HD11	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:746:PHE:CE2	2:H:13:GLU:OE1	2.54	0.60
1:A:382:THR:O	1:A:385:GLN:HB3	2.01	0.60
1:A:627:ASP:O	1:A:627:ASP:CG	2.38	0.60
2:B:65:LYS:HD2	2:B:68:GLN:NE2	2.15	0.60
1:C:230:ILE:HG22	1:C:231:LEU:N	2.15	0.60
1:C:477:PHE:O	1:C:480:LEU:HB3	2.01	0.60
1:C:89:MET:C	1:C:91:GLU:H	2.05	0.60
2:D:72:MET:HA	2:D:75:THR:OG1	2.00	0.60
1:E:145:LYS:HG3	1:E:146:ARG:HE	1.66	0.60
1:E:812:PHE:C	1:E:814:LYS:H	2.03	0.60
1:G:807:LEU:O	1:G:807:LEU:HD23	2.01	0.60
1:A:527:LEU:HD11	1:A:569:PHE:HB2	1.82	0.60
1:A:721:PHE:N	1:A:721:PHE:HD1	1.99	0.60
1:C:145:LYS:HG3	1:C:146:ARG:HE	1.66	0.60
1:C:302:ARG:HH21	1:C:307:LEU:H	1.49	0.60
1:C:568:LYS:CD	1:C:584:LEU:HB2	2.31	0.60
1:E:302:ARG:HH21	1:E:307:LEU:H	1.47	0.60
2:F:125:GLU:O	2:F:129:ALA:HB2	2.01	0.60
2:F:84:CYS:O	2:F:85:PHE:C	2.40	0.60
1:G:480:LEU:HD11	1:G:528:ILE:HD12	1.83	0.60
1:G:630:ARG:HH22	1:G:657:ARG:HB3	1.66	0.60
1:A:164:MET:HE3	1:A:461:LEU:HD12	1.83	0.60
2:B:140:TYR:CD1	2:B:141:GLU:HG2	2.37	0.60
1:C:721:PHE:HD1	1:C:721:PHE:N	1.99	0.60
1:E:533:ASN:CB	1:E:534:PRO:HD2	2.31	0.60
1:E:663:TYR:OH	1:E:667:LEU:HD13	2.01	0.60
1:G:530:ARG:HG2	1:G:534:PRO:O	2.01	0.60
1:A:667:LEU:O	1:A:667:LEU:HG	2.01	0.60
1:A:731:ARG:HG2	1:A:731:ARG:HH11	1.66	0.60
1:C:259:THR:HB	1:C:261:TYR:HE1	1.63	0.60
1:C:50:LYS:HE3	1:C:60:GLU:CB	2.31	0.60
1:E:480:LEU:HD11	1:E:528:ILE:HD12	1.83	0.60
1:G:145:LYS:HG3	1:G:146:ARG:HE	1.65	0.60
1:G:242:ASN:OD1	1:G:242:ASN:C	2.37	0.60
1:A:391:MET:HG2	1:A:613:LEU:CD2	2.31	0.60
1:A:36:TRP:HE1	1:A:78:MET:HG3	1.65	0.60
1:E:606:ASN:OD1	1:E:609:VAL:HG12	2.01	0.60
1:E:57:VAL:C	1:E:69:THR:HG23	2.22	0.60
1:E:711:LEU:HD22	1:E:711:LEU:N	2.17	0.60
2:F:55:LYS:O	2:F:58:GLU:HG2	2.01	0.60
1:G:23:PRO:HA	1:G:26:GLN:HB3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:482:ILE:HG22	1:G:483:ASN:N	2.15	0.60
1:A:103:ASN:O	1:A:107:ARG:HG3	2.02	0.60
1:A:568:LYS:CD	1:A:584:LEU:HB2	2.32	0.60
1:A:804:ARG:HG2	1:A:804:ARG:NH1	2.15	0.60
1:C:352:ILE:CG2	1:C:442:ILE:HD11	2.32	0.60
1:C:469:PHE:CZ	1:C:587:ALA:HB3	2.37	0.60
1:C:728:GLN:HA	1:C:728:GLN:HE21	1.67	0.60
1:E:490:GLN:NE2	1:E:494:ASN:HD21	1.99	0.60
1:G:494:ASN:H	1:G:494:ASN:HD22	1.49	0.60
1:G:561:GLN:OE1	1:G:562:GLU:HG2	2.01	0.60
2:H:84:CYS:O	2:H:88:TYR:CG	2.54	0.60
1:A:186:ASN:O	1:A:190:VAL:HG23	2.01	0.60
1:A:50:LYS:HE3	1:A:60:GLU:CB	2.32	0.60
1:C:568:LYS:HA	1:C:568:LYS:HE3	1.84	0.60
1:G:382:THR:HA	1:G:385:GLN:OE1	2.01	0.60
2:H:4:SER:H	2:H:7:GLN:HE21	1.49	0.60
1:A:7:SER:HB3	1:A:10:GLU:OE1	2.00	0.60
2:B:140:TYR:CD1	2:B:141:GLU:N	2.70	0.60
1:G:259:THR:HB	1:G:261:TYR:HE1	1.64	0.60
1:G:416:LYS:HE2	1:G:417:ALA:H	1.66	0.60
1:G:489:LEU:O	1:G:492:LEU:HB3	2.02	0.60
1:A:527:LEU:HG	1:A:563:GLN:HG3	1.83	0.59
1:A:663:TYR:OH	1:A:667:LEU:HD13	2.02	0.59
1:C:419:THR:O	1:C:420:LYS:C	2.41	0.59
1:G:186:ASN:O	1:G:190:VAL:HG23	2.02	0.59
1:A:745:GLY:CA	1:G:819:LEU:HD21	2.31	0.59
1:A:419:THR:O	1:A:420:LYS:C	2.40	0.59
1:C:405:PRO:HD2	1:C:417:ALA:HA	1.84	0.59
1:C:703:GLU:O	1:C:706:ARG:HB2	2.02	0.59
1:C:797:ILE:HG13	2:D:117:GLU:H	1.65	0.59
1:E:12:PHE:CD2	1:E:131:PRO:HD2	2.37	0.59
2:F:97:LYS:C	2:F:98:GLU:HG3	2.21	0.59
1:G:218:GLY:HA3	1:G:221:GLU:OE1	2.03	0.59
2:B:85:PHE:CZ	2:B:145:ARG:CZ	2.85	0.59
1:C:305:LEU:HD22	1:C:354:ARG:HB3	1.82	0.59
1:E:176:THR:O	1:E:183:LYS:CD	2.50	0.59
2:F:44:ASN:HD22	2:F:117:GLU:HB3	1.67	0.59
1:G:13:LEU:HD11	1:G:132:ILE:HB	1.84	0.59
1:G:254:ILE:O	1:G:460:PHE:HA	2.03	0.59
1:G:527:LEU:HG	1:G:563:GLN:HG3	1.83	0.59
1:A:705:LEU:HD22	1:A:710:VAL:HG21	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:145:LYS:CG	1:C:146:ARG:H	2.15	0.59
1:C:278:ILE:HA	1:C:315:PHE:CD1	2.37	0.59
1:C:533:ASN:CB	1:C:534:PRO:HD2	2.32	0.59
1:C:271:LEU:HD21	1:C:663:TYR:CD1	2.36	0.59
1:E:553:THR:HG23	1:E:579:THR:HG21	1.84	0.59
1:E:686:ILE:HG22	1:E:700:LEU:HD21	1.84	0.59
1:E:719:GLN:HA	1:E:719:GLN:NE2	2.17	0.59
1:A:399:THR:O	1:A:403:LEU:HD12	2.03	0.59
1:A:56:GLU:HG3	1:A:71:SER:HA	1.83	0.59
1:C:242:ASN:C	1:C:242:ASN:OD1	2.40	0.59
1:C:489:LEU:O	1:C:492:LEU:HB3	2.03	0.59
1:C:630:ARG:HH22	1:C:657:ARG:CB	2.15	0.59
1:C:667:LEU:O	1:C:667:LEU:HG	2.02	0.59
1:C:36:TRP:CE2	1:C:78:MET:HG3	2.37	0.59
1:G:13:LEU:HD11	1:G:152:HIS:HD2	1.68	0.59
1:G:568:LYS:HA	1:G:568:LYS:HE3	1.84	0.59
1:G:671:MET:O	1:G:675:ARG:HD2	2.01	0.59
1:G:703:GLU:O	1:G:706:ARG:HB2	2.03	0.59
1:G:804:ARG:NH2	2:H:44:ASN:HD21	2.01	0.59
1:G:79:ASN:ND2	1:G:80:PRO:HD2	2.11	0.59
1:C:7:SER:O	1:C:11:LYS:HG3	2.03	0.59
1:C:310:PHE:CD2	1:C:320:HIS:HB2	2.38	0.59
2:D:85:PHE:O	2:D:87:ASP:N	2.36	0.59
1:E:227:ALA:C	1:E:229:PRO:HD2	2.23	0.59
1:E:273:GLU:O	1:E:273:GLU:HG2	2.02	0.59
1:E:735:GLU:HA	1:E:756:MET:HE1	1.85	0.59
1:E:747:MET:HE3	1:E:755:LEU:HD22	1.82	0.59
2:F:65:LYS:HD2	2:F:68:GLN:NE2	2.15	0.59
1:G:731:ARG:HG2	1:G:731:ARG:HH11	1.68	0.59
1:G:788:ARG:HG2	1:G:788:ARG:HH11	1.66	0.59
1:A:100:VAL:O	1:A:104:LEU:HG	2.03	0.59
1:C:13:LEU:HG	1:C:132:ILE:CG2	2.32	0.59
2:D:140:TYR:O	2:D:141:GLU:C	2.40	0.59
1:E:527:LEU:HD23	1:E:537:VAL:HG23	1.83	0.59
1:E:703:GLU:O	1:E:706:ARG:HB2	2.02	0.59
1:E:788:ARG:HH11	1:E:788:ARG:HG2	1.68	0.59
2:F:40:GLN:HB3	2:F:42:PRO:HD3	1.85	0.59
2:F:80:LYS:HD2	2:F:80:LYS:H	1.67	0.59
1:G:437:ARG:HB3	1:G:624:LEU:HD23	1.85	0.59
1:A:380:ASP:OD1	1:A:382:THR:HG23	2.02	0.59
1:A:104:LEU:HD12	1:A:705:LEU:HD11	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:581:PHE:HZ	1:C:597:TRP:CH2	2.21	0.59
1:C:88:ASP:HB3	1:C:91:GLU:OE1	2.03	0.59
1:E:145:LYS:CG	1:E:146:ARG:H	2.15	0.59
1:E:522:GLN:N	1:E:523:PRO:HD2	2.16	0.59
1:G:469:PHE:CZ	1:G:587:ALA:HB3	2.38	0.59
1:G:607:ASP:CA	1:G:610:THR:HB	2.31	0.59
1:G:804:ARG:NH1	1:G:804:ARG:HG2	2.17	0.59
2:B:125:GLU:O	2:B:129:ALA:HB2	2.03	0.59
1:C:659:VAL:CG1	1:C:660:GLY:N	2.65	0.59
1:E:123:VAL:HG12	1:E:123:VAL:O	2.03	0.59
1:E:437:ARG:HB3	1:E:624:LEU:HD23	1.85	0.59
1:E:477:PHE:O	1:E:480:LEU:HB3	2.03	0.59
1:A:23:PRO:HA	1:A:26:GLN:HB3	1.84	0.59
1:A:702:LEU:O	1:A:706:ARG:HG3	2.02	0.59
1:C:293:LEU:HD11	1:C:301:MET:CE	2.33	0.59
1:C:482:ILE:HG22	1:C:483:ASN:N	2.18	0.59
1:C:815:ARG:HA	1:C:818:GLN:CD	2.23	0.59
1:E:193:TYR:CZ	1:E:197:VAL:HG21	2.38	0.59
1:E:568:LYS:CE	1:E:584:LEU:HB2	2.33	0.59
1:A:490:GLN:O	1:A:494:ASN:ND2	2.36	0.58
1:A:533:ASN:CB	1:A:534:PRO:HD2	2.33	0.58
1:A:52:GLU:HA	1:A:57:VAL:HG13	1.84	0.58
2:D:40:GLN:HB3	2:D:42:PRO:HD3	1.85	0.58
1:G:242:ASN:ND2	1:G:245:SER:HA	2.18	0.58
1:G:659:VAL:CG1	1:G:660:GLY:N	2.65	0.58
2:H:86:GLU:N	2:H:86:GLU:OE1	2.34	0.58
1:A:443:LEU:O	1:A:447:ASN:HB2	2.03	0.58
1:A:33:LYS:HB3	1:A:49:ILE:CB	2.32	0.58
1:A:607:ASP:HA	1:A:610:THR:CB	2.32	0.58
1:A:630:ARG:HH22	1:A:657:ARG:HB3	1.67	0.58
1:A:750:LYS:NZ	1:G:809:ARG:HH22	2.01	0.58
1:A:763:ASP:HB3	1:A:766:LEU:HD11	1.85	0.58
2:B:85:PHE:CE1	2:B:145:ARG:HG2	2.38	0.58
2:B:97:LYS:C	2:B:98:GLU:HG3	2.22	0.58
1:E:218:GLY:HA3	1:E:221:GLU:OE1	2.03	0.58
1:E:22:ASN:OD1	1:E:24:LEU:HB2	2.01	0.58
1:E:382:THR:HA	1:E:385:GLN:OE1	2.02	0.58
1:E:405:PRO:HD2	1:E:417:ALA:HA	1.85	0.58
1:E:551:THR:N	1:E:554:SER:OG	2.33	0.58
1:E:553:THR:O	1:E:557:GLU:HG2	2.02	0.58
1:G:310:PHE:CD2	1:G:320:HIS:HB2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:40:GLN:HB3	2:B:42:PRO:HD3	1.85	0.58
1:E:138:ILE:HD13	1:E:154:TYR:CE2	2.38	0.58
1:E:413:VAL:HG12	1:E:413:VAL:O	2.03	0.58
1:E:570:GLN:OE1	1:E:589:LYS:HE2	2.04	0.58
1:G:721:PHE:CZ	1:G:768:ARG:HG2	2.37	0.58
1:C:243:ASP:HB3	1:C:323:ILE:CD1	2.32	0.58
1:G:103:ASN:ND2	1:G:107:ARG:HD2	2.18	0.58
1:G:123:VAL:O	1:G:123:VAL:HG12	2.03	0.58
1:G:362:LEU:HD21	1:G:430:LEU:HD23	1.84	0.58
1:G:271:LEU:HD21	1:G:663:TYR:CD1	2.38	0.58
1:G:83:PHE:CE1	1:G:92:LEU:HA	2.38	0.58
1:A:8:ASP:CA	1:A:11:LYS:HD2	2.20	0.58
1:A:310:PHE:CD2	1:A:320:HIS:HB2	2.39	0.58
1:A:437:ARG:HB3	1:A:624:LEU:HD23	1.85	0.58
1:A:812:PHE:C	1:A:814:LYS:H	2.06	0.58
1:C:242:ASN:ND2	1:C:245:SER:HA	2.18	0.58
1:C:8:ASP:HA	1:C:11:LYS:CD	2.21	0.58
1:E:731:ARG:HH11	1:E:731:ARG:HG2	1.67	0.58
1:E:797:ILE:HG13	2:F:117:GLU:H	1.69	0.58
1:G:22:ASN:OD1	1:G:24:LEU:HB2	2.04	0.58
1:G:243:ASP:HB3	1:G:323:ILE:CD1	2.32	0.58
1:G:533:ASN:CB	1:G:534:PRO:HD2	2.33	0.58
1:G:712:GLU:OE1	1:G:712:GLU:N	2.35	0.58
1:G:804:ARG:NH2	2:H:44:ASN:ND2	2.51	0.58
1:C:165:LEU:HD21	1:C:260:GLY:HA2	1.85	0.58
1:C:164:MET:HE3	1:C:461:LEU:HD12	1.86	0.58
1:C:788:ARG:HG2	1:C:788:ARG:HH11	1.67	0.58
2:D:64:LEU:HD23	2:D:68:GLN:OE1	2.03	0.58
1:G:416:LYS:HE2	1:G:417:ALA:N	2.18	0.58
1:G:419:THR:O	1:G:420:LYS:C	2.41	0.58
1:G:369:LYS:HZ2	1:G:420:LYS:HB3	1.68	0.58
1:A:361:GLN:O	1:A:363:GLY:N	2.36	0.58
1:C:686:ILE:HG22	1:C:700:LEU:HD21	1.86	0.58
1:E:419:THR:O	1:E:420:LYS:C	2.42	0.58
1:E:711:LEU:H	1:E:711:LEU:CD2	2.17	0.58
2:F:140:TYR:CD1	2:F:141:GLU:N	2.72	0.58
1:G:568:LYS:CD	1:G:584:LEU:HB2	2.32	0.58
2:H:125:GLU:O	2:H:129:ALA:HB2	2.03	0.58
1:A:125:ASN:OD1	1:A:126:PRO:HD2	2.04	0.58
1:A:302:ARG:HH21	1:A:307:LEU:H	1.49	0.58
1:A:610:THR:HG23	1:A:628:VAL:CG2	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:85:PHE:HE1	2:B:145:ARG:HG2	1.67	0.58
1:C:227:ALA:C	1:C:229:PRO:HD2	2.24	0.58
1:E:165:LEU:HD21	1:E:260:GLY:HA2	1.85	0.58
1:E:293:LEU:HA	1:E:332:PHE:CE1	2.39	0.58
1:G:292:TYR:CE2	1:G:331:MET:HB3	2.39	0.58
1:G:409:VAL:HB	1:G:414:VAL:HG21	1.85	0.58
1:G:527:LEU:HD11	1:G:569:PHE:HB2	1.86	0.58
2:H:40:GLN:HB3	2:H:42:PRO:HD3	1.85	0.58
1:A:796:ILE:HG22	1:A:800:GLN:OE1	2.04	0.58
1:C:265:ALA:HB3	1:C:450:LEU:HB3	1.86	0.58
1:C:266:ASN:HA	1:C:447:ASN:OD1	2.04	0.58
1:C:731:ARG:HH11	1:C:731:ARG:HG2	1.69	0.58
1:C:735:GLU:HA	1:C:756:MET:HE1	1.85	0.58
1:E:140:MET:HB3	1:E:149:MET:HE3	1.84	0.58
1:E:362:LEU:HD21	1:E:430:LEU:HD23	1.85	0.58
1:E:254:ILE:O	1:E:460:PHE:HA	2.03	0.58
1:E:611:SER:O	1:E:615:GLN:NE2	2.35	0.58
1:G:37:VAL:CG1	1:G:38:PRO:HD2	2.34	0.58
1:G:265:ALA:HB3	1:G:450:LEU:HB3	1.86	0.58
2:H:64:LEU:HD23	2:H:68:GLN:OE1	2.04	0.58
2:D:80:LYS:HD2	2:D:80:LYS:H	1.68	0.58
1:E:345:THR:HB	1:E:348:GLU:CB	2.29	0.58
1:G:705:LEU:HD22	1:G:710:VAL:HG21	1.84	0.58
1:G:797:ILE:HG12	2:H:117:GLU:HG2	1.84	0.58
2:H:14:ALA:CB	2:H:38:LEU:HD21	2.34	0.58
1:A:293:LEU:HD11	1:A:301:MET:CE	2.34	0.57
1:A:703:GLU:O	1:A:706:ARG:HB2	2.02	0.57
1:C:123:VAL:HG12	1:C:123:VAL:O	2.03	0.57
1:C:273:GLU:O	1:C:273:GLU:HG2	2.03	0.57
1:C:413:VAL:O	1:C:413:VAL:HG12	2.03	0.57
1:E:265:ALA:HB3	1:E:450:LEU:HB3	1.86	0.57
1:G:134:SER:CB	1:G:212:GLY:HA2	2.32	0.57
2:B:140:TYR:HD1	2:B:141:GLU:N	2.02	0.57
1:C:100:VAL:O	1:C:104:LEU:HG	2.03	0.57
1:C:743:PRO:HD2	1:C:747:MET:HE1	1.87	0.57
1:E:51:GLU:HG2	1:E:53:LYS:HE3	1.84	0.57
1:G:161:TYR:CZ	1:G:165:LEU:HD11	2.39	0.57
1:G:380:ASP:OD1	1:G:382:THR:HG23	2.04	0.57
1:G:266:ASN:HA	1:G:447:ASN:OD1	2.05	0.57
1:G:50:LYS:HG3	1:G:67:LYS:HE3	1.86	0.57
1:A:13:LEU:HD21	1:A:132:ILE:HD13	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:568:LYS:HA	1:A:568:LYS:HE3	1.85	0.57
1:C:187:THR:HG23	1:C:463:ILE:CG2	2.34	0.57
1:C:134:SER:CB	1:C:212:GLY:HA2	2.35	0.57
1:C:267:ILE:HB	1:C:447:ASN:ND2	2.19	0.57
1:C:323:ILE:CG2	1:C:326:GLN:HB3	2.33	0.57
1:C:763:ASP:HB3	1:C:766:LEU:HD11	1.85	0.57
1:C:803:CYS:O	1:C:807:LEU:HB2	2.05	0.57
1:E:607:ASP:HA	1:E:610:THR:CB	2.31	0.57
1:E:807:LEU:HD23	1:E:807:LEU:O	2.04	0.57
1:G:125:ASN:OD1	1:G:126:PRO:HD2	2.03	0.57
1:G:769:ILE:HD13	1:G:774:ILE:HG12	1.85	0.57
1:A:247:ARG:HH11	1:A:247:ARG:HA	1.68	0.57
1:C:176:THR:O	1:C:183:LYS:CD	2.52	0.57
2:D:97:LYS:C	2:D:98:GLU:HG3	2.23	0.57
1:E:369:LYS:NZ	1:E:420:LYS:HB3	2.19	0.57
2:F:14:ALA:CB	2:F:38:LEU:HD21	2.35	0.57
2:F:64:LEU:HD23	2:F:68:GLN:OE1	2.04	0.57
1:G:405:PRO:HD2	1:G:417:ALA:HA	1.85	0.57
1:G:413:VAL:O	1:G:413:VAL:HG12	2.04	0.57
1:G:721:PHE:N	1:G:721:PHE:HD1	2.01	0.57
1:G:769:ILE:CD1	1:G:774:ILE:HG12	2.35	0.57
1:A:13:LEU:HD21	1:A:132:ILE:HD12	1.86	0.57
1:A:138:ILE:HD13	1:A:154:TYR:CE2	2.39	0.57
1:A:477:PHE:O	1:A:480:LEU:HB3	2.04	0.57
1:A:659:VAL:CG1	1:A:660:GLY:N	2.67	0.57
1:C:48:SER:O	1:C:59:VAL:HG13	2.04	0.57
1:C:797:ILE:HG22	1:C:798:ALA:N	2.19	0.57
1:C:79:ASN:ND2	1:C:80:PRO:HD2	2.15	0.57
1:E:298:SER:O	1:E:302:ARG:HB2	2.03	0.57
1:E:815:ARG:HA	1:E:818:GLN:CD	2.24	0.57
1:E:88:ASP:HB3	1:E:91:GLU:OE1	2.05	0.57
1:G:165:LEU:HD21	1:G:260:GLY:HA2	1.87	0.57
1:G:669:LYS:O	1:G:672:THR:HB	2.04	0.57
1:G:814:LYS:HD2	1:G:818:GLN:OE1	2.04	0.57
1:G:96:ASN:HB2	1:G:99:SER:OG	2.04	0.57
1:A:469:PHE:CZ	1:A:587:ALA:HB3	2.38	0.57
1:A:711:LEU:H	1:A:711:LEU:CD2	2.18	0.57
1:E:541:LEU:HD21	1:E:597:TRP:HB3	1.86	0.57
1:E:581:PHE:HZ	1:E:597:TRP:CH2	2.23	0.57
1:E:763:ASP:HB3	1:E:766:LEU:HD11	1.87	0.57
1:G:275:SER:O	1:G:277:ALA:N	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:352:ILE:CG2	1:G:442:ILE:HD11	2.34	0.57
2:H:84:CYS:C	2:H:88:TYR:CD2	2.77	0.57
1:A:568:LYS:CE	1:A:584:LEU:HB2	2.35	0.57
1:A:747:MET:CE	1:A:755:LEU:HD22	2.35	0.57
1:A:815:ARG:HA	1:A:818:GLN:CD	2.25	0.57
1:A:88:ASP:HB3	1:A:91:GLU:OE1	2.03	0.57
2:B:64:LEU:HD23	2:B:68:GLN:OE1	2.04	0.57
1:C:382:THR:HA	1:C:385:GLN:OE1	2.05	0.57
1:E:702:LEU:O	1:E:706:ARG:HG3	2.03	0.57
1:E:36:TRP:HE1	1:E:78:MET:HG3	1.65	0.57
1:G:33:LYS:CB	1:G:49:ILE:HB	2.34	0.57
1:G:51:GLU:HG2	1:G:53:LYS:HE3	1.85	0.57
1:G:79:ASN:OD1	1:G:92:LEU:HB3	2.04	0.57
1:A:766:LEU:HB3	1:A:780:VAL:HG21	1.85	0.57
1:A:771:GLN:CA	1:A:771:GLN:HE21	2.17	0.57
1:C:308:GLU:N	1:C:313:TYR:OH	2.38	0.57
1:C:804:ARG:NH1	1:C:804:ARG:HG2	2.18	0.57
1:E:104:LEU:HD12	1:E:705:LEU:HD11	1.86	0.57
2:F:84:CYS:C	2:F:86:GLU:N	2.51	0.57
1:G:182:GLY:HA2	5:G:998:ADP:PA	2.45	0.57
1:G:259:THR:HB	1:G:261:TYR:CD1	2.40	0.57
1:G:443:LEU:O	1:G:447:ASN:HB2	2.05	0.57
2:H:110:HIS:O	2:H:113:VAL:N	2.26	0.57
1:A:611:SER:O	1:A:615:GLN:NE2	2.37	0.57
1:C:293:LEU:HA	1:C:332:PHE:CE1	2.40	0.57
1:C:527:LEU:HB2	1:C:566:HIS:NE2	2.20	0.57
1:C:610:THR:HG23	1:C:628:VAL:CG2	2.34	0.57
1:C:721:PHE:CZ	1:C:768:ARG:HG2	2.40	0.57
1:E:271:LEU:HD21	1:E:663:TYR:CD1	2.39	0.57
1:G:702:LEU:O	1:G:706:ARG:HG3	2.05	0.57
2:H:112:LEU:HD13	2:H:119:MET:HE3	1.87	0.57
1:A:272:LEU:O	1:A:274:LYS:N	2.38	0.57
1:A:570:GLN:OE1	1:A:589:LYS:HE2	2.04	0.57
2:B:14:ALA:CB	2:B:38:LEU:HD21	2.35	0.57
1:C:186:ASN:O	1:C:190:VAL:HG23	2.05	0.57
1:E:187:THR:HG23	1:E:463:ILE:CG2	2.32	0.57
1:E:44:PHE:HE2	1:E:702:LEU:HD21	1.70	0.57
1:G:132:ILE:HD12	1:G:152:HIS:CD2	2.40	0.57
1:G:145:LYS:CG	1:G:146:ARG:H	2.18	0.57
1:A:161:TYR:CZ	1:A:165:LEU:HD11	2.40	0.56
1:A:273:GLU:HG2	1:A:273:GLU:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:GLN:C	1:A:363:GLY:N	2.58	0.56
1:C:409:VAL:HB	1:C:414:VAL:HG21	1.87	0.56
1:C:814:LYS:HD2	1:C:818:GLN:OE1	2.06	0.56
1:G:164:MET:CE	1:G:256:PHE:CE2	2.87	0.56
1:G:312:ASN:HD22	1:G:312:ASN:N	2.03	0.56
1:A:435:PHE:O	1:A:438:LEU:N	2.32	0.56
1:A:553:THR:O	1:A:557:GLU:HG2	2.04	0.56
1:A:797:ILE:HG22	1:A:798:ALA:N	2.19	0.56
2:B:140:TYR:HD1	2:B:141:GLU:H	1.51	0.56
2:D:14:ALA:CB	2:D:38:LEU:HD21	2.35	0.56
1:E:37:VAL:CG1	1:E:38:PRO:HD2	2.35	0.56
1:E:731:ARG:NH1	1:E:731:ARG:HG2	2.21	0.56
1:G:542:ASP:O	1:G:545:CYS:HB3	2.05	0.56
1:G:728:GLN:HE21	1:G:728:GLN:HA	1.70	0.56
1:G:721:PHE:HB3	1:G:776:PHE:O	2.05	0.56
1:A:267:ILE:HB	1:A:447:ASN:ND2	2.20	0.56
2:B:112:LEU:HD13	2:B:119:MET:HE2	1.86	0.56
1:C:570:GLN:OE1	1:C:589:LYS:HE2	2.05	0.56
1:E:36:TRP:CE2	1:E:78:MET:HG3	2.40	0.56
1:E:541:LEU:CD2	1:E:601:ASN:HD22	2.09	0.56
1:G:36:TRP:CE2	1:G:78:MET:HG3	2.39	0.56
1:A:308:GLU:N	1:A:313:TYR:OH	2.38	0.56
1:C:22:ASN:OD1	1:C:24:LEU:HB2	2.05	0.56
1:C:265:ALA:N	1:C:450:LEU:O	2.39	0.56
1:C:807:LEU:HD23	1:C:807:LEU:O	2.06	0.56
1:E:13:LEU:CD1	1:E:132:ILE:HB	2.35	0.56
1:E:83:PHE:HB3	1:E:92:LEU:HD23	1.87	0.56
1:G:278:ILE:HG13	1:G:279:ARG:N	2.20	0.56
1:G:568:LYS:CE	1:G:584:LEU:HB2	2.35	0.56
1:G:66:LYS:HD3	1:G:67:LYS:H	1.70	0.56
1:A:293:LEU:HA	1:A:332:PHE:CE1	2.40	0.56
1:A:788:ARG:HG2	1:A:788:ARG:NH1	2.20	0.56
2:B:80:LYS:H	2:B:80:LYS:HD2	1.70	0.56
2:B:84:CYS:O	2:B:85:PHE:C	2.43	0.56
1:E:107:ARG:HA	1:E:112:LEU:HD12	1.88	0.56
1:E:527:LEU:HB2	1:E:566:HIS:NE2	2.21	0.56
2:F:144:VAL:HG12	2:F:145:ARG:N	2.18	0.56
1:G:103:ASN:O	1:G:107:ARG:HG3	2.04	0.56
1:G:308:GLU:N	1:G:313:TYR:OH	2.39	0.56
1:G:361:GLN:C	1:G:363:GLY:N	2.59	0.56
1:A:478:GLU:OE1	1:A:478:GLU:N	2.24	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:628:VAL:HG13	1:A:628:VAL:O	2.04	0.56
1:C:480:LEU:HD11	1:C:528:ILE:HD12	1.87	0.56
1:C:551:THR:N	1:C:554:SER:OG	2.32	0.56
2:D:112:LEU:HD13	2:D:119:MET:HE2	1.88	0.56
1:E:409:VAL:HB	1:E:414:VAL:HG21	1.85	0.56
1:G:228:ASN:N	1:G:229:PRO:HD2	2.21	0.56
1:G:797:ILE:HG22	1:G:798:ALA:N	2.21	0.56
2:H:95:PHE:O	2:H:103:VAL:HG13	2.06	0.56
1:A:242:ASN:ND2	1:A:245:SER:HA	2.21	0.56
1:A:278:ILE:HA	1:A:315:PHE:CD1	2.40	0.56
1:A:743:PRO:HD2	1:A:747:MET:HE1	1.88	0.56
1:C:259:THR:HB	1:C:261:TYR:CD1	2.41	0.56
1:C:278:ILE:HG13	1:C:279:ARG:N	2.20	0.56
1:C:409:VAL:HG13	1:C:634:LEU:CD1	2.35	0.56
2:D:84:CYS:O	2:D:85:PHE:C	2.43	0.56
1:E:186:ASN:O	1:E:190:VAL:HG23	2.05	0.56
1:E:572:SER:CB	1:E:580:GLU:HG3	2.35	0.56
1:E:669:LYS:O	1:E:672:THR:HB	2.05	0.56
2:F:28:TYR:CD2	2:F:51:LEU:HD13	2.41	0.56
1:G:293:LEU:HA	1:G:332:PHE:CE1	2.40	0.56
1:G:369:LYS:NZ	1:G:420:LYS:HB3	2.20	0.56
1:G:623:ASP:HA	1:G:626:LYS:HB3	1.87	0.56
1:A:226:GLN:O	1:A:229:PRO:HG2	2.06	0.56
1:A:36:TRP:CE2	1:A:78:MET:HG3	2.40	0.56
1:C:443:LEU:O	1:C:447:ASN:HB2	2.06	0.56
1:C:490:GLN:NE2	1:C:494:ASN:HD21	2.03	0.56
1:C:719:GLN:HA	1:C:719:GLN:NE2	2.21	0.56
1:E:103:ASN:ND2	1:E:107:ARG:HD2	2.21	0.56
1:E:145:LYS:HB3	1:E:148:GLU:HG3	1.88	0.56
1:E:361:GLN:C	1:E:363:GLY:H	2.07	0.56
1:E:703:GLU:O	1:E:706:ARG:N	2.38	0.56
1:E:742:ILE:HD11	1:E:756:MET:HG2	1.87	0.56
1:G:525:ILE:O	1:G:529:GLU:N	2.38	0.56
1:A:480:LEU:HD11	1:A:528:ILE:HD12	1.86	0.56
1:A:50:LYS:HG3	1:A:67:LYS:HE3	1.87	0.56
1:A:769:ILE:HD13	1:A:774:ILE:HG23	1.87	0.56
1:A:89:MET:C	1:A:91:GLU:H	2.09	0.56
2:B:85:PHE:HE1	2:B:145:ARG:CG	2.18	0.56
1:C:164:MET:SD	1:C:256:PHE:CD2	2.99	0.56
1:C:477:PHE:O	1:C:480:LEU:N	2.37	0.56
1:E:308:GLU:N	1:E:313:TYR:OH	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:478:GLU:N	1:G:478:GLU:OE1	2.23	0.56
1:A:369:LYS:NZ	1:A:420:LYS:HB3	2.20	0.56
1:A:711:LEU:N	1:A:711:LEU:HD22	2.20	0.56
1:A:742:ILE:HD11	1:A:756:MET:HG2	1.86	0.56
1:C:145:LYS:HB3	1:C:148:GLU:HG3	1.88	0.56
1:C:161:TYR:CZ	1:C:165:LEU:HD11	2.41	0.56
1:C:305:LEU:HD12	1:C:307:LEU:HD11	1.87	0.56
1:C:380:ASP:OD1	1:C:382:THR:HG23	2.06	0.56
1:E:182:GLY:HA2	5:E:998:ADP:O1A	2.05	0.56
1:E:490:GLN:HE21	1:E:494:ASN:HD21	1.51	0.56
1:E:568:LYS:HE3	1:E:568:LYS:HA	1.87	0.56
1:G:107:ARG:HH11	1:G:115:THR:HG23	1.69	0.56
1:G:145:LYS:HB3	1:G:148:GLU:HG3	1.87	0.56
1:G:13:LEU:HD11	1:G:152:HIS:CD2	2.40	0.56
1:G:553:THR:CG2	1:G:579:THR:HG21	2.36	0.56
1:G:747:MET:CG	1:G:751:GLN:HE22	2.18	0.56
1:G:788:ARG:HG2	1:G:788:ARG:NH1	2.21	0.56
2:H:28:TYR:CD2	2:H:51:LEU:HD13	2.41	0.56
1:A:572:SER:HB3	1:A:580:GLU:O	2.06	0.56
1:A:750:LYS:HZ1	1:G:809:ARG:HH22	1.53	0.56
2:B:48:MET:HG3	2:B:53:ASN:HA	1.88	0.56
1:E:416:LYS:HE2	1:E:417:ALA:N	2.21	0.56
1:E:80:PRO:HG2	1:E:83:PHE:HE2	1.68	0.56
1:G:145:LYS:HB3	1:G:148:GLU:CG	2.35	0.56
1:G:164:MET:SD	1:G:256:PHE:CD2	2.99	0.56
1:G:521:LEU:O	1:G:525:ILE:HG13	2.06	0.56
1:G:763:ASP:HB3	1:G:766:LEU:HD11	1.88	0.56
2:H:80:LYS:H	2:H:80:LYS:HD2	1.70	0.56
1:A:275:SER:O	1:A:277:ALA:N	2.39	0.55
1:A:382:THR:HA	1:A:385:GLN:OE1	2.06	0.55
1:A:44:PHE:HE2	1:A:702:LEU:HD21	1.69	0.55
1:A:51:GLU:HG2	1:A:53:LYS:HE3	1.87	0.55
1:A:807:LEU:HD23	1:A:807:LEU:O	2.07	0.55
1:A:815:ARG:O	1:A:818:GLN:HG2	2.06	0.55
1:C:298:SER:O	1:C:302:ARG:HB2	2.06	0.55
1:C:525:ILE:O	1:C:529:GLU:N	2.38	0.55
1:C:771:GLN:HE21	1:C:771:GLN:CA	2.19	0.55
1:C:815:ARG:NE	1:C:818:GLN:HE21	2.05	0.55
1:E:416:LYS:HE2	1:E:417:ALA:H	1.72	0.55
1:E:728:GLN:HE21	1:E:728:GLN:HA	1.69	0.55
1:E:747:MET:CG	1:E:751:GLN:HE22	2.19	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:721:PHE:HB3	1:E:776:PHE:O	2.06	0.55
2:F:48:MET:HG3	2:F:53:ASN:HA	1.88	0.55
1:G:803:CYS:O	1:G:807:LEU:HB2	2.06	0.55
1:A:37:VAL:CG1	1:A:38:PRO:HD2	2.35	0.55
1:A:533:ASN:O	1:A:534:PRO:C	2.45	0.55
1:C:193:TYR:CE1	1:C:197:VAL:HG21	2.42	0.55
1:E:164:MET:SD	1:E:256:PHE:CD2	3.00	0.55
1:G:7:SER:O	1:G:11:LYS:HG3	2.06	0.55
1:G:529:GLU:O	1:G:664:LYS:NZ	2.39	0.55
1:A:48:SER:O	1:A:59:VAL:HG13	2.06	0.55
1:C:23:PRO:HA	1:C:26:GLN:HB3	1.87	0.55
1:C:33:LYS:CB	1:C:49:ILE:HB	2.36	0.55
2:D:23:ASP:HB2	2:D:25:LYS:HD3	1.89	0.55
1:E:256:PHE:CE1	1:E:262:ILE:HG13	2.42	0.55
1:E:352:ILE:CG2	1:E:442:ILE:HD11	2.34	0.55
1:G:298:SER:O	1:G:302:ARG:HB2	2.06	0.55
1:G:539:ALA:O	1:G:542:ASP:HB2	2.06	0.55
1:G:658:THR:HG23	1:G:661:GLN:HB3	1.89	0.55
1:G:88:ASP:HB3	1:G:91:GLU:OE1	2.05	0.55
2:H:140:TYR:CD1	2:H:141:GLU:HG2	2.41	0.55
1:A:489:LEU:O	1:A:492:LEU:HB3	2.07	0.55
1:A:731:ARG:HG2	1:A:731:ARG:NH1	2.21	0.55
1:C:126:PRO:O	1:C:127:TYR:HB2	2.07	0.55
1:C:153:ILE:HG23	1:C:154:TYR:N	2.21	0.55
1:C:702:LEU:O	1:C:706:ARG:HG3	2.06	0.55
2:D:28:TYR:CD2	2:D:51:LEU:HD13	2.41	0.55
1:E:312:ASN:N	1:E:312:ASN:HD22	2.04	0.55
1:E:663:TYR:C	1:E:665:GLU:H	2.10	0.55
1:E:788:ARG:NH1	1:E:788:ARG:HG2	2.22	0.55
2:F:89:VAL:CG1	2:F:144:VAL:HG21	2.20	0.55
1:A:352:ILE:CG2	1:A:442:ILE:HD11	2.35	0.55
1:A:541:LEU:CD2	1:A:601:ASN:HD22	2.11	0.55
2:B:28:TYR:CD2	2:B:51:LEU:HD13	2.41	0.55
1:C:669:LYS:O	1:C:672:THR:HB	2.06	0.55
1:E:145:LYS:HB3	1:E:148:GLU:CG	2.36	0.55
1:E:259:THR:HB	1:E:261:TYR:CD1	2.41	0.55
1:E:293:LEU:HD13	1:E:353:LEU:HD22	1.89	0.55
1:E:293:LEU:HD11	1:E:301:MET:CE	2.36	0.55
1:E:418:GLN:CB	1:E:422:GLN:HB2	2.35	0.55
1:E:443:LEU:O	1:E:447:ASN:HB2	2.06	0.55
1:E:711:LEU:HD22	1:E:711:LEU:H	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:152:HIS:CE1	1:G:154:TYR:CD2	2.95	0.55
1:G:663:TYR:OH	1:G:667:LEU:HD13	2.06	0.55
1:G:731:ARG:NH1	1:G:731:ARG:HG2	2.22	0.55
2:H:116:GLY:O	2:H:118:LYS:N	2.40	0.55
2:H:140:TYR:CD1	2:H:141:GLU:N	2.73	0.55
1:G:802:GLN:HG3	2:H:88:TYR:OH	2.07	0.55
1:A:623:ASP:HA	1:A:626:LYS:HB3	1.88	0.55
1:C:607:ASP:HA	1:C:610:THR:CB	2.34	0.55
1:G:293:LEU:HD13	1:G:353:LEU:HD22	1.88	0.55
1:G:361:GLN:O	1:G:363:GLY:N	2.39	0.55
1:G:409:VAL:HG13	1:G:634:LEU:CD1	2.37	0.55
2:H:48:MET:HG3	2:H:53:ASN:HA	1.89	0.55
2:H:76:ILE:O	2:H:79:ASN:ND2	2.40	0.55
1:A:107:ARG:CA	1:A:112:LEU:HD12	2.37	0.55
1:A:18:ASN:O	1:A:19:PHE:HD1	1.88	0.55
1:A:418:GLN:CB	1:A:422:GLN:HB2	2.35	0.55
1:A:669:LYS:O	1:A:672:THR:HB	2.07	0.55
1:C:369:LYS:NZ	1:C:420:LYS:HB3	2.21	0.55
1:C:627:ASP:O	1:C:627:ASP:OD1	2.25	0.55
1:E:380:ASP:OD1	1:E:382:THR:HG23	2.06	0.55
1:E:721:PHE:N	1:E:721:PHE:HD1	2.02	0.55
1:E:803:CYS:O	1:E:807:LEU:HB2	2.06	0.55
1:E:814:LYS:HD2	1:E:818:GLN:OE1	2.07	0.55
1:A:743:PRO:HB3	1:G:816:GLN:O	2.07	0.55
1:A:123:VAL:HG12	1:A:123:VAL:O	2.04	0.55
1:A:165:LEU:HD21	1:A:260:GLY:HA2	1.88	0.55
1:A:312:ASN:HD22	1:A:312:ASN:N	2.05	0.55
1:A:803:CYS:O	1:A:807:LEU:HB2	2.06	0.55
2:D:3:PHE:HA	2:D:7:GLN:NE2	2.22	0.55
1:E:435:PHE:O	1:E:438:LEU:N	2.34	0.55
1:E:529:GLU:O	1:E:664:LYS:NZ	2.40	0.55
1:E:409:VAL:HG13	1:E:634:LEU:CD1	2.36	0.55
1:E:66:LYS:HD3	1:E:67:LYS:H	1.72	0.55
1:G:663:TYR:C	1:G:665:GLU:H	2.10	0.55
1:A:250:LYS:HG2	1:A:465:ASP:OD2	2.07	0.55
1:A:797:ILE:HG13	2:B:117:GLU:H	1.72	0.55
1:C:144:LYS:HG3	1:C:148:GLU:HB2	1.89	0.55
1:C:407:ILE:HD12	1:C:409:VAL:H	1.72	0.55
1:C:568:LYS:CE	1:C:584:LEU:HB2	2.36	0.55
1:E:226:GLN:O	1:E:229:PRO:HG2	2.07	0.55
1:E:369:LYS:HZ2	1:E:420:LYS:HB3	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:4:SER:H	2:F:7:GLN:NE2	2.04	0.55
1:A:259:THR:HB	1:A:261:TYR:CD1	2.41	0.55
1:A:278:ILE:HG13	1:A:279:ARG:N	2.21	0.55
1:A:347:GLU:C	1:A:349:GLN:H	2.11	0.55
1:A:265:ALA:HB3	1:A:450:LEU:HB3	1.88	0.55
1:A:540:LEU:O	1:A:542:ASP:N	2.40	0.55
1:C:815:ARG:O	1:C:818:GLN:HG2	2.07	0.55
1:G:293:LEU:HD11	1:G:301:MET:CE	2.37	0.55
2:H:3:PHE:HA	2:H:7:GLN:NE2	2.22	0.55
1:A:347:GLU:O	1:A:349:GLN:N	2.40	0.54
1:A:66:LYS:HD3	1:A:67:LYS:H	1.71	0.54
2:B:3:PHE:HA	2:B:7:GLN:NE2	2.22	0.54
1:C:226:GLN:O	1:C:229:PRO:HG2	2.07	0.54
1:C:61:LEU:HD12	1:C:64:ASN:HB3	1.89	0.54
1:C:663:TYR:C	1:C:665:GLU:H	2.11	0.54
1:E:61:LEU:HD12	1:E:64:ASN:HB3	1.88	0.54
1:G:359:VAL:O	1:G:359:VAL:HG12	2.07	0.54
1:G:494:ASN:HD22	1:G:494:ASN:N	2.04	0.54
1:G:719:GLN:HA	1:G:719:GLN:NE2	2.22	0.54
1:G:747:MET:CE	1:G:755:LEU:HD22	2.37	0.54
1:C:323:ILE:HG21	1:C:326:GLN:NE2	2.22	0.54
1:C:405:PRO:HD2	1:C:416:LYS:O	2.06	0.54
1:C:376:ALA:CB	1:C:420:LYS:HB2	2.32	0.54
1:C:556:VAL:HG21	1:C:579:THR:HB	1.89	0.54
1:E:13:LEU:HD21	1:E:132:ILE:CD1	2.37	0.54
1:E:533:ASN:O	1:E:534:PRO:C	2.44	0.54
1:E:797:ILE:HG22	1:E:798:ALA:N	2.21	0.54
1:G:100:VAL:O	1:G:104:LEU:HG	2.08	0.54
1:G:138:ILE:HD13	1:G:154:TYR:CE2	2.41	0.54
1:G:399:THR:O	1:G:403:LEU:HD12	2.06	0.54
1:A:103:ASN:ND2	1:A:107:ARG:HD2	2.22	0.54
1:A:107:ARG:HA	1:A:112:LEU:HD12	1.89	0.54
1:A:134:SER:CB	1:A:212:GLY:HA2	2.37	0.54
1:A:218:GLY:HA3	1:A:221:GLU:OE1	2.08	0.54
1:A:292:TYR:CE2	1:A:331:MET:HB3	2.42	0.54
1:A:416:LYS:HE2	1:A:417:ALA:H	1.72	0.54
1:A:539:ALA:O	1:A:542:ASP:HB2	2.07	0.54
1:A:527:LEU:HB2	1:A:566:HIS:NE2	2.23	0.54
1:A:61:LEU:HD12	1:A:64:ASN:HB3	1.88	0.54
1:C:529:GLU:O	1:C:664:LYS:NZ	2.40	0.54
1:E:103:ASN:O	1:E:107:ARG:HG3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:290:PHE:CD1	1:E:360:LEU:HD11	2.43	0.54
1:G:176:THR:O	1:G:183:LYS:CD	2.55	0.54
1:C:107:ARG:CA	1:C:112:LEU:HD12	2.37	0.54
1:C:312:ASN:N	1:C:312:ASN:HD22	2.05	0.54
1:C:369:LYS:HG3	1:C:370:GLU:N	2.22	0.54
1:C:478:GLU:HB2	1:C:479:GLN:OE1	2.07	0.54
1:C:658:THR:HG23	1:C:661:GLN:HB3	1.89	0.54
1:C:797:ILE:HG12	2:D:117:GLU:HG2	1.90	0.54
1:E:100:VAL:O	1:E:104:LEU:HG	2.08	0.54
1:E:199:SER:HB2	1:E:221:GLU:CG	2.37	0.54
1:E:288:HIS:HB3	1:E:292:TYR:CE1	2.43	0.54
1:E:630:ARG:HH22	1:E:657:ARG:HB3	1.73	0.54
1:E:719:GLN:HA	1:E:719:GLN:HE21	1.72	0.54
1:G:226:GLN:O	1:G:229:PRO:HG2	2.08	0.54
1:G:420:LYS:HD2	1:G:421:GLU:CD	2.28	0.54
2:H:83:GLY:HA3	2:H:88:TYR:CZ	2.42	0.54
2:H:97:LYS:C	2:H:98:GLU:HG3	2.28	0.54
1:A:529:GLU:O	1:A:664:LYS:NZ	2.39	0.54
1:A:766:LEU:O	1:A:777:ARG:HB2	2.08	0.54
1:C:269:THR:HG23	1:C:440:ARG:NH1	2.21	0.54
1:C:278:ILE:O	1:C:279:ARG:HG3	2.07	0.54
1:C:267:ILE:HB	1:C:447:ASN:HD21	1.73	0.54
1:C:44:PHE:CE2	1:C:702:LEU:HD21	2.43	0.54
1:E:495:HIS:ND1	1:E:499:ILE:HD12	2.23	0.54
1:E:572:SER:HB3	1:E:580:GLU:O	2.08	0.54
1:G:199:SER:HB2	1:G:221:GLU:CG	2.37	0.54
1:G:267:ILE:H	1:G:447:ASN:HD21	1.55	0.54
1:A:33:LYS:HB3	1:A:49:ILE:N	2.22	0.54
1:A:663:TYR:C	1:A:665:GLU:H	2.11	0.54
1:C:107:ARG:HA	1:C:112:LEU:HD12	1.88	0.54
1:C:269:THR:HG21	1:C:443:LEU:CD1	2.30	0.54
1:C:50:LYS:HG3	1:C:67:LYS:HE3	1.89	0.54
1:E:269:THR:HG23	1:E:440:ARG:NH1	2.23	0.54
1:E:420:LYS:HD2	1:E:421:GLU:CD	2.27	0.54
1:E:766:LEU:O	1:E:777:ARG:HB2	2.08	0.54
1:G:313:TYR:CD2	1:G:360:LEU:HB3	2.42	0.54
1:G:370:GLU:O	1:G:374:ASP:HA	2.08	0.54
1:G:514:PHE:CD1	1:G:515:ILE:N	2.76	0.54
1:G:570:GLN:OE1	1:G:589:LYS:HE2	2.07	0.54
2:H:4:SER:H	2:H:7:GLN:NE2	2.05	0.54
1:A:482:ILE:HG22	1:A:483:ASN:N	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:553:THR:CG2	1:A:579:THR:HG21	2.38	0.54
1:C:103:ASN:ND2	1:C:107:ARG:HD2	2.23	0.54
1:C:145:LYS:HB3	1:C:148:GLU:CG	2.37	0.54
1:C:290:PHE:CD1	1:C:360:LEU:HD11	2.42	0.54
1:C:400:ARG:O	1:C:404:THR:N	2.40	0.54
1:C:104:LEU:HD12	1:C:705:LEU:HD11	1.88	0.54
2:F:3:PHE:HA	2:F:7:GLN:NE2	2.22	0.54
1:G:144:LYS:HG3	1:G:148:GLU:HB2	1.90	0.54
1:G:48:SER:O	1:G:59:VAL:HG13	2.08	0.54
1:A:126:PRO:O	1:A:127:TYR:HB2	2.07	0.54
2:D:89:VAL:CG1	2:D:144:VAL:HG21	2.20	0.54
2:D:48:MET:HG3	2:D:53:ASN:HA	1.88	0.54
1:E:628:VAL:CG1	1:E:628:VAL:O	2.56	0.54
1:E:50:LYS:HG3	1:E:67:LYS:HE3	1.89	0.54
1:G:298:SER:O	1:G:302:ARG:N	2.41	0.54
1:G:3:GLN:O	1:G:18:ASN:ND2	2.40	0.54
1:G:527:LEU:HB2	1:G:566:HIS:NE2	2.21	0.54
1:G:762:LEU:HD13	1:G:766:LEU:CD1	2.38	0.54
1:A:490:GLN:NE2	1:A:494:ASN:HD21	2.06	0.54
1:A:96:ASN:HB2	1:A:99:SER:OG	2.07	0.54
1:C:86:VAL:HG12	1:C:103:ASN:ND2	2.23	0.54
2:D:144:VAL:HG12	2:D:145:ARG:N	2.23	0.54
1:E:153:ILE:HG23	1:E:154:TYR:N	2.23	0.54
1:E:370:GLU:O	1:E:374:ASP:HA	2.07	0.54
1:E:721:PHE:CZ	1:E:768:ARG:HG2	2.42	0.54
2:F:140:TYR:HD1	2:F:141:GLU:N	2.06	0.54
1:G:815:ARG:O	1:G:818:GLN:HG2	2.08	0.54
1:A:347:GLU:C	1:A:349:GLN:N	2.60	0.54
1:A:610:THR:HG23	1:A:628:VAL:HG21	1.90	0.54
2:B:144:VAL:HG12	2:B:145:ARG:N	2.22	0.54
2:B:4:SER:H	2:B:7:GLN:NE2	2.05	0.54
2:D:4:SER:H	2:D:7:GLN:NE2	2.05	0.54
1:C:802:GLN:NE2	2:D:88:TYR:OH	2.38	0.54
1:E:275:SER:O	1:E:277:ALA:N	2.41	0.54
1:E:266:ASN:HA	1:E:447:ASN:OD1	2.08	0.54
1:E:586:TYR:CD1	1:E:587:ALA:N	2.76	0.54
1:E:658:THR:HG23	1:E:661:GLN:HB3	1.90	0.54
1:G:33:LYS:HB3	1:G:49:ILE:N	2.23	0.54
1:A:405:PRO:HD2	1:A:416:LYS:O	2.07	0.53
1:A:369:LYS:HZ2	1:A:420:LYS:HB3	1.72	0.53
1:A:745:GLY:H	1:G:819:LEU:HD21	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:104:MET:C	2:B:106:ALA:H	2.11	0.53
1:C:66:LYS:HD3	1:C:67:LYS:H	1.74	0.53
1:C:747:MET:CE	1:C:755:LEU:HD22	2.39	0.53
1:G:145:LYS:CB	1:G:148:GLU:HG3	2.38	0.53
1:G:359:VAL:CG1	1:G:359:VAL:O	2.56	0.53
1:G:572:SER:HB3	1:G:580:GLU:O	2.08	0.53
1:G:711:LEU:HD22	1:G:711:LEU:N	2.23	0.53
2:H:98:GLU:O	2:H:100:ASN:N	2.41	0.53
1:A:145:LYS:HB3	1:A:148:GLU:HG3	1.90	0.53
1:A:228:ASN:N	1:A:229:PRO:HD2	2.23	0.53
1:A:254:ILE:O	1:A:460:PHE:HA	2.08	0.53
1:A:521:LEU:O	1:A:525:ILE:HG13	2.07	0.53
1:C:271:LEU:HD21	1:C:663:TYR:CZ	2.44	0.53
1:E:132:ILE:HD12	1:E:152:HIS:CD2	2.42	0.53
1:E:712:GLU:CD	1:E:712:GLU:H	2.11	0.53
1:E:80:PRO:HD2	1:E:83:PHE:HD2	1.71	0.53
1:G:418:GLN:CB	1:G:422:GLN:HB2	2.35	0.53
1:G:437:ARG:NH2	1:G:625:TRP:HE3	2.06	0.53
1:G:61:LEU:HD12	1:G:64:ASN:HB3	1.90	0.53
2:H:92:LEU:HD13	2:H:108:ILE:HD11	1.90	0.53
2:H:140:TYR:O	2:H:141:GLU:C	2.47	0.53
2:B:140:TYR:O	2:B:141:GLU:C	2.45	0.53
1:C:199:SER:HB2	1:C:221:GLU:CG	2.38	0.53
1:C:514:PHE:CD1	1:C:515:ILE:N	2.76	0.53
2:D:98:GLU:O	2:D:100:ASN:N	2.41	0.53
1:E:292:TYR:CE2	1:E:331:MET:HB3	2.43	0.53
1:E:556:VAL:O	1:E:559:LEU:HB3	2.09	0.53
2:F:23:ASP:HB2	2:F:25:LYS:HD3	1.90	0.53
1:A:267:ILE:HB	1:A:447:ASN:HD21	1.72	0.53
1:A:305:LEU:HD12	1:A:307:LEU:HD11	1.90	0.53
1:A:437:ARG:NH2	1:A:625:TRP:HE3	2.07	0.53
1:A:610:THR:CG2	1:A:611:SER:N	2.70	0.53
1:C:132:ILE:HD12	1:C:152:HIS:CD2	2.43	0.53
1:C:292:TYR:CE2	1:C:331:MET:HB3	2.43	0.53
1:C:361:GLN:O	1:C:363:GLY:N	2.41	0.53
1:C:399:THR:O	1:C:403:LEU:HD12	2.08	0.53
1:C:416:LYS:HE2	1:C:417:ALA:N	2.22	0.53
1:C:556:VAL:O	1:C:559:LEU:HB3	2.09	0.53
1:E:242:ASN:ND2	1:E:245:SER:HA	2.22	0.53
1:E:743:PRO:CD	1:E:747:MET:HE1	2.37	0.53
1:E:797:ILE:HG12	2:F:117:GLU:HG2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:107:ARG:HA	1:G:112:LEU:HD12	1.90	0.53
1:G:153:ILE:HG23	1:G:154:TYR:N	2.24	0.53
1:G:628:VAL:O	1:G:631:ILE:HG12	2.09	0.53
2:H:128:VAL:HB	2:H:138:ILE:HD11	1.89	0.53
1:A:418:GLN:HA	1:A:422:GLN:NE2	2.23	0.53
1:A:344:PHE:HE1	1:A:445:ARG:HB3	1.72	0.53
1:A:86:VAL:HG12	1:A:103:ASN:ND2	2.23	0.53
1:C:361:GLN:C	1:C:363:GLY:N	2.61	0.53
1:C:572:SER:HB3	1:C:580:GLU:O	2.09	0.53
1:C:731:ARG:NH1	1:C:731:ARG:HG2	2.23	0.53
1:C:766:LEU:O	1:C:777:ARG:HB2	2.08	0.53
1:E:13:LEU:CD1	1:E:152:HIS:CD2	2.90	0.53
1:E:428:GLU:C	1:E:430:LEU:H	2.12	0.53
1:G:581:PHE:HZ	1:G:597:TRP:CH2	2.25	0.53
1:A:107:ARG:HB3	1:A:112:LEU:HD12	1.89	0.53
1:A:298:SER:O	1:A:302:ARG:N	2.40	0.53
1:A:370:GLU:O	1:A:374:ASP:HA	2.07	0.53
1:C:407:ILE:CD1	1:C:409:VAL:H	2.22	0.53
1:C:51:GLU:HG2	1:C:53:LYS:HE3	1.89	0.53
1:E:733:ARG:HG2	1:E:734:TYR:CE1	2.44	0.53
2:F:140:TYR:O	2:F:141:GLU:C	2.46	0.53
1:G:630:ARG:HH12	1:G:657:ARG:HB3	1.73	0.53
1:A:369:LYS:HG3	1:A:370:GLU:N	2.24	0.53
1:A:416:LYS:HE2	1:A:417:ALA:N	2.23	0.53
1:A:712:GLU:OE1	1:A:712:GLU:N	2.35	0.53
1:A:36:TRP:HB2	1:A:76:GLN:HB2	1.91	0.53
1:C:138:ILE:HD13	1:C:154:TYR:CE2	2.43	0.53
1:C:275:SER:O	1:C:277:ALA:N	2.41	0.53
1:C:293:LEU:HD13	1:C:353:LEU:HD22	1.90	0.53
1:E:33:LYS:CB	1:E:49:ILE:HB	2.38	0.53
1:G:32:LYS:C	1:G:34:LEU:H	2.12	0.53
1:G:497:MET:HE3	1:G:497:MET:HA	1.91	0.53
1:G:553:THR:HG23	1:G:579:THR:HG21	1.90	0.53
1:A:298:SER:O	1:A:302:ARG:HB2	2.08	0.53
1:A:388:CYS:SG	1:A:393:ILE:HD11	2.49	0.53
1:A:271:LEU:HD21	1:A:663:TYR:CD1	2.44	0.53
1:A:721:PHE:CZ	1:A:768:ARG:HG2	2.44	0.53
2:B:116:GLY:O	2:B:118:LYS:N	2.41	0.53
1:C:193:TYR:CZ	1:C:197:VAL:HG21	2.43	0.53
1:C:36:TRP:HE1	1:C:78:MET:HA	1.74	0.53
1:C:254:ILE:O	1:C:460:PHE:HA	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:525:ILE:O	1:E:529:GLU:N	2.39	0.53
1:G:437:ARG:NH2	1:G:625:TRP:CE3	2.77	0.53
2:H:94:VAL:O	2:H:94:VAL:HG12	2.07	0.53
1:A:293:LEU:HD11	1:A:301:MET:HE1	1.90	0.53
2:B:76:ILE:O	2:B:79:ASN:ND2	2.42	0.53
1:C:490:GLN:HE21	1:C:494:ASN:HD21	1.55	0.53
1:C:552:ASP:CG	1:C:596:ALA:H	2.12	0.53
1:C:788:ARG:NH1	1:C:788:ARG:HG2	2.24	0.53
1:E:305:LEU:HD12	1:E:307:LEU:HD11	1.91	0.53
1:E:96:ASN:HB2	1:E:99:SER:OG	2.09	0.53
1:G:87:GLU:OE1	1:G:107:ARG:NH2	2.42	0.53
1:G:107:ARG:CA	1:G:112:LEU:HD12	2.39	0.53
1:G:164:MET:CE	1:G:256:PHE:HE2	2.21	0.53
1:G:267:ILE:N	1:G:447:ASN:HD21	2.07	0.53
1:G:351:SER:O	1:G:354:ARG:HG2	2.09	0.53
1:G:572:SER:CB	1:G:580:GLU:HG3	2.39	0.53
1:G:766:LEU:O	1:G:777:ARG:HB2	2.09	0.53
1:G:812:PHE:C	1:G:814:LYS:N	2.62	0.53
2:H:23:ASP:HB2	2:H:25:LYS:HD3	1.91	0.53
1:C:313:TYR:HB2	1:C:316:LEU:HD12	1.90	0.53
1:C:347:GLU:O	1:C:349:GLN:N	2.42	0.53
1:C:33:LYS:HB3	1:C:49:ILE:N	2.24	0.53
1:C:742:ILE:HD11	1:C:756:MET:HG2	1.91	0.53
1:C:88:ASP:O	1:C:91:GLU:N	2.42	0.53
1:E:480:LEU:HD11	1:E:528:ILE:CD1	2.38	0.53
1:E:627:ASP:CG	1:E:627:ASP:O	2.48	0.53
1:E:89:MET:C	1:E:91:GLU:N	2.62	0.53
2:F:92:LEU:HD13	2:F:108:ILE:HD11	1.91	0.53
2:F:140:TYR:CD1	2:F:141:GLU:HG2	2.44	0.53
2:F:76:ILE:O	2:F:79:ASN:ND2	2.42	0.53
1:G:313:TYR:HB2	1:G:316:LEU:HD12	1.91	0.53
1:A:33:LYS:CB	1:A:49:ILE:HB	2.37	0.52
1:A:267:ILE:N	1:A:447:ASN:HD21	2.07	0.52
1:A:542:ASP:O	1:A:545:CYS:HB3	2.09	0.52
1:A:711:LEU:H	1:A:711:LEU:HD22	1.73	0.52
1:C:369:LYS:HZ2	1:C:420:LYS:HB3	1.74	0.52
1:C:630:ARG:HH22	1:C:657:ARG:HB3	1.73	0.52
1:E:71:SER:C	1:E:73:ASP:H	2.12	0.52
1:G:290:PHE:CD1	1:G:360:LEU:HD11	2.45	0.52
1:G:361:GLN:HB3	1:G:387:VAL:HG22	1.90	0.52
1:G:743:PRO:HD2	1:G:747:MET:HE1	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:36:TRP:HE1	1:G:78:MET:HA	1.75	0.52
1:A:176:THR:O	1:A:183:LYS:CD	2.58	0.52
1:A:290:PHE:CD1	1:A:360:LEU:HD11	2.44	0.52
1:A:400:ARG:O	1:A:404:THR:N	2.40	0.52
1:A:622:ALA:O	1:A:626:LYS:N	2.40	0.52
1:A:658:THR:HG23	1:A:661:GLN:HB3	1.91	0.52
1:C:228:ASN:N	1:C:229:PRO:HD2	2.25	0.52
1:C:286:THR:HB	1:C:290:PHE:HD2	1.75	0.52
1:C:437:ARG:NH2	1:C:625:TRP:HE3	2.07	0.52
1:C:64:ASN:C	1:C:66:LYS:H	2.13	0.52
1:G:286:THR:HB	1:G:290:PHE:HD2	1.74	0.52
1:G:533:ASN:O	1:G:534:PRO:C	2.43	0.52
1:A:351:SER:O	1:A:354:ARG:HG2	2.09	0.52
1:A:553:THR:HG23	1:A:579:THR:HG21	1.91	0.52
2:B:23:ASP:HB2	2:B:25:LYS:HD3	1.90	0.52
1:C:218:GLY:HA3	1:C:221:GLU:OE1	2.09	0.52
1:C:572:SER:CB	1:C:580:GLU:HG3	2.39	0.52
1:E:161:TYR:CZ	1:E:165:LEU:HD11	2.45	0.52
1:E:521:LEU:O	1:E:525:ILE:HG13	2.09	0.52
1:E:705:LEU:HD22	1:E:710:VAL:HG21	1.90	0.52
2:F:95:PHE:O	2:F:103:VAL:HG13	2.10	0.52
1:G:540:LEU:O	1:G:542:ASP:N	2.43	0.52
2:H:105:GLY:O	2:H:109:ARG:NH1	2.42	0.52
1:A:164:MET:SD	1:A:256:PHE:CD2	3.03	0.52
1:A:525:ILE:O	1:A:529:GLU:N	2.40	0.52
1:A:604:PRO:O	1:A:605:LEU:HB2	2.09	0.52
1:A:610:THR:CG2	1:A:628:VAL:HG11	2.39	0.52
1:C:419:THR:O	1:C:421:GLU:N	2.42	0.52
1:C:33:LYS:HB2	1:C:48:SER:OG	2.08	0.52
2:D:108:ILE:HG22	2:D:109:ARG:N	2.23	0.52
1:E:145:LYS:CB	1:E:148:GLU:HG3	2.40	0.52
1:G:199:SER:CB	1:G:221:GLU:HG2	2.39	0.52
1:G:288:HIS:HB3	1:G:292:TYR:CE1	2.44	0.52
1:G:428:GLU:C	1:G:430:LEU:H	2.12	0.52
1:G:563:GLN:O	1:G:565:ASN:N	2.42	0.52
2:H:144:VAL:HG12	2:H:145:ARG:N	2.24	0.52
1:A:7:SER:O	1:A:11:LYS:HG3	2.09	0.52
1:A:132:ILE:HD12	1:A:152:HIS:CD2	2.43	0.52
1:A:278:ILE:O	1:A:279:ARG:HG3	2.09	0.52
1:C:405:PRO:HG2	1:C:416:LYS:HG3	1.92	0.52
1:C:521:LEU:O	1:C:525:ILE:HG13	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:298:SER:O	1:E:302:ARG:N	2.41	0.52
1:E:400:ARG:O	1:E:404:THR:N	2.38	0.52
1:E:542:ASP:O	1:E:545:CYS:HB3	2.10	0.52
1:G:267:ILE:HB	1:G:447:ASN:ND2	2.24	0.52
1:G:269:THR:HG23	1:G:440:ARG:NH1	2.24	0.52
1:A:144:LYS:HG3	1:A:148:GLU:HB2	1.90	0.52
1:A:413:VAL:HG12	1:A:413:VAL:O	2.08	0.52
1:A:437:ARG:NH2	1:A:625:TRP:CE3	2.78	0.52
1:A:495:HIS:ND1	1:A:499:ILE:HD12	2.25	0.52
1:C:32:LYS:C	1:C:34:LEU:H	2.13	0.52
1:C:267:ILE:N	1:C:447:ASN:HD21	2.08	0.52
1:E:269:THR:CG2	1:E:443:LEU:CD1	2.87	0.52
1:E:313:TYR:CD2	1:E:360:LEU:HB3	2.44	0.52
1:E:337:GLU:O	1:E:340:THR:OG1	2.27	0.52
2:F:44:ASN:HB2	2:F:117:GLU:OE2	2.10	0.52
1:G:305:LEU:HD12	1:G:307:LEU:HD11	1.92	0.52
1:G:369:LYS:HG3	1:G:370:GLU:N	2.25	0.52
2:H:40:GLN:C	2:H:42:PRO:HD3	2.30	0.52
1:A:114:TYR:HE2	1:A:153:ILE:HB	1.70	0.52
1:A:513:ASN:C	1:A:513:ASN:HD22	2.13	0.52
1:A:551:THR:H	1:A:554:SER:CB	2.23	0.52
1:A:586:TYR:CD1	1:A:587:ALA:N	2.78	0.52
1:C:226:GLN:C	1:C:229:PRO:HD2	2.30	0.52
1:C:347:GLU:C	1:C:349:GLN:N	2.62	0.52
1:C:521:LEU:N	1:C:521:LEU:HD23	2.24	0.52
1:C:71:SER:C	1:C:73:ASP:H	2.13	0.52
1:C:721:PHE:CE2	1:C:768:ARG:HG2	2.45	0.52
1:E:815:ARG:O	1:E:818:GLN:HG2	2.10	0.52
1:A:119:LEU:HD13	1:A:497:MET:HE1	1.91	0.52
1:A:235:GLY:O	1:A:247:ARG:HB2	2.10	0.52
1:A:814:LYS:HD2	1:A:818:GLN:OE1	2.09	0.52
1:C:152:HIS:CE1	1:C:154:TYR:CD2	2.98	0.52
1:C:424:ASP:C	1:C:426:ALA:N	2.62	0.52
1:E:521:LEU:HD23	1:E:521:LEU:N	2.25	0.52
1:E:539:ALA:O	1:E:542:ASP:HB2	2.10	0.52
1:E:747:MET:CE	1:E:755:LEU:HD22	2.38	0.52
1:G:307:LEU:HA	1:G:313:TYR:OH	2.10	0.52
1:A:269:THR:HG23	1:A:440:ARG:NH1	2.24	0.52
1:C:607:ASP:OD1	1:C:607:ASP:N	2.31	0.52
1:C:815:ARG:NE	1:C:818:GLN:NE2	2.58	0.52
2:D:66:PHE:CE1	2:D:70:LEU:HB2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:405:PRO:HD2	1:E:416:LYS:O	2.10	0.52
2:F:15:PHE:O	2:F:18:PHE:HB2	2.10	0.52
1:E:805:GLY:CA	2:F:36:ARG:HG2	2.32	0.52
1:G:604:PRO:O	1:G:605:LEU:HB2	2.10	0.52
1:G:271:LEU:HD21	1:G:663:TYR:CZ	2.45	0.52
1:G:815:ARG:NE	1:G:818:GLN:HE21	2.08	0.52
2:H:85:PHE:HD1	2:H:148:LEU:CD2	2.23	0.52
1:A:226:GLN:C	1:A:229:PRO:HD2	2.30	0.52
1:A:248:PHE:O	1:A:248:PHE:CD1	2.62	0.52
1:A:572:SER:CB	1:A:580:GLU:HG3	2.40	0.52
1:A:71:SER:C	1:A:73:ASP:H	2.13	0.52
1:C:562:GLU:OE1	1:C:562:GLU:HA	2.10	0.52
1:E:89:MET:O	1:E:91:GLU:N	2.43	0.52
1:G:226:GLN:C	1:G:229:PRO:HD2	2.30	0.52
1:G:405:PRO:C	1:G:407:ILE:H	2.13	0.52
1:G:480:LEU:HD11	1:G:528:ILE:CD1	2.40	0.52
1:G:657:ARG:HH11	1:G:657:ARG:HB2	1.75	0.52
1:G:89:MET:C	1:G:91:GLU:N	2.63	0.52
1:A:193:TYR:CE1	1:A:197:VAL:HG21	2.44	0.51
1:C:267:ILE:H	1:C:447:ASN:HD21	1.58	0.51
1:C:37:VAL:CG1	1:C:38:PRO:HD2	2.34	0.51
1:C:610:THR:CG2	1:C:631:ILE:HG13	2.29	0.51
1:C:703:GLU:O	1:C:706:ARG:N	2.39	0.51
2:D:15:PHE:O	2:D:18:PHE:HB2	2.10	0.51
1:E:224:LEU:O	1:E:224:LEU:HD12	2.09	0.51
1:E:228:ASN:N	1:E:229:PRO:HD2	2.24	0.51
1:E:33:LYS:HB2	1:E:48:SER:OG	2.10	0.51
1:E:369:LYS:HG3	1:E:370:GLU:N	2.25	0.51
1:E:418:GLN:HA	1:E:422:GLN:NE2	2.24	0.51
1:E:630:ARG:HH22	1:E:657:ARG:CB	2.24	0.51
2:F:116:GLY:O	2:F:118:LYS:N	2.44	0.51
1:G:521:LEU:HD23	1:G:521:LEU:N	2.25	0.51
2:H:15:PHE:O	2:H:18:PHE:HB2	2.10	0.51
1:A:293:LEU:HD13	1:A:353:LEU:HD22	1.92	0.51
1:A:33:LYS:HB2	1:A:48:SER:OG	2.10	0.51
1:A:428:GLU:C	1:A:430:LEU:H	2.11	0.51
1:A:514:PHE:CD1	1:A:515:ILE:N	2.78	0.51
1:A:721:PHE:HB3	1:A:776:PHE:O	2.10	0.51
2:B:94:VAL:O	2:B:94:VAL:HG12	2.10	0.51
1:C:114:TYR:HE2	1:C:153:ILE:HB	1.74	0.51
1:C:352:ILE:HG21	1:C:442:ILE:CD1	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:HIS:C	1:C:44:PHE:H	2.14	0.51
1:E:278:ILE:HG13	1:E:279:ARG:N	2.26	0.51
1:E:351:SER:O	1:E:353:LEU:N	2.43	0.51
1:E:430:LEU:HB2	1:E:605:LEU:HD11	1.91	0.51
1:E:514:PHE:CD1	1:E:515:ILE:N	2.79	0.51
1:E:712:GLU:OE1	1:E:712:GLU:N	2.38	0.51
1:G:269:THR:CG2	1:G:443:LEU:CD1	2.88	0.51
1:G:42:HIS:C	1:G:44:PHE:H	2.14	0.51
1:G:541:LEU:CD2	1:G:601:ASN:HD22	2.12	0.51
1:A:361:GLN:HB3	1:A:387:VAL:HG22	1.92	0.51
1:A:562:GLU:HA	1:A:562:GLU:OE1	2.09	0.51
1:A:100:VAL:HG21	1:A:711:LEU:CD1	2.40	0.51
1:A:815:ARG:NE	1:A:818:GLN:NE2	2.58	0.51
2:B:66:PHE:CE1	2:B:70:LEU:HB2	2.45	0.51
1:C:145:LYS:CB	1:C:148:GLU:HG3	2.40	0.51
1:C:170:ASP:C	1:C:171:GLN:HG2	2.30	0.51
1:C:428:GLU:C	1:C:430:LEU:H	2.14	0.51
1:C:756:MET:O	1:C:760:LEU:HG	2.10	0.51
2:D:55:LYS:HB2	2:D:58:GLU:CD	2.31	0.51
1:E:232:GLU:O	1:E:236:ASN:HB2	2.10	0.51
1:E:361:GLN:HB3	1:E:387:VAL:HG22	1.93	0.51
1:E:36:TRP:HE1	1:E:78:MET:HA	1.76	0.51
2:F:40:GLN:C	2:F:42:PRO:HD3	2.31	0.51
1:G:495:HIS:ND1	1:G:499:ILE:HD12	2.24	0.51
1:G:495:HIS:CD2	1:G:500:LEU:HG	2.45	0.51
1:G:556:VAL:HG21	1:G:579:THR:HB	1.93	0.51
1:A:152:HIS:CE1	1:A:154:TYR:CD2	2.99	0.51
1:A:327:GLN:HG2	1:A:330:GLU:HG2	1.93	0.51
1:A:359:VAL:HG12	1:A:359:VAL:O	2.10	0.51
1:C:256:PHE:CE1	1:C:262:ILE:HG13	2.46	0.51
1:C:416:LYS:HE2	1:C:417:ALA:H	1.74	0.51
2:D:8:THR:O	2:D:12:LYS:HG3	2.10	0.51
1:E:107:ARG:CA	1:E:112:LEU:HD12	2.41	0.51
1:E:272:LEU:O	1:E:274:LYS:N	2.42	0.51
1:E:628:VAL:HG13	1:E:631:ILE:CG1	2.40	0.51
2:F:98:GLU:O	2:F:100:ASN:N	2.44	0.51
2:F:94:VAL:O	2:F:94:VAL:HG12	2.10	0.51
1:G:320:HIS:ND1	1:G:320:HIS:O	2.42	0.51
2:H:85:PHE:HD1	2:H:148:LEU:HD23	1.75	0.51
2:H:87:ASP:O	2:H:90:GLU:HB3	2.11	0.51
1:A:145:LYS:HB3	1:A:148:GLU:CG	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:TYR:CZ	1:A:197:VAL:HG21	2.46	0.51
1:A:307:LEU:HA	1:A:313:TYR:OH	2.10	0.51
1:A:495:HIS:CD2	1:A:500:LEU:HG	2.46	0.51
1:A:556:VAL:O	1:A:559:LEU:HB3	2.11	0.51
1:C:370:GLU:O	1:C:374:ASP:HA	2.11	0.51
1:C:586:TYR:CD1	1:C:587:ALA:N	2.79	0.51
1:C:628:VAL:CG1	1:C:631:ILE:HG13	2.23	0.51
1:C:762:LEU:HD13	1:C:766:LEU:CD1	2.41	0.51
1:C:80:PRO:HD2	1:C:83:PHE:CD2	2.45	0.51
1:E:508:GLU:HG3	1:E:775:PHE:HE1	1.76	0.51
1:E:766:LEU:HB3	1:E:780:VAL:HG21	1.93	0.51
1:E:815:ARG:NE	1:E:818:GLN:HE21	2.09	0.51
2:F:3:PHE:CA	2:F:7:GLN:HE21	2.23	0.51
1:G:107:ARG:HB3	1:G:112:LEU:HD12	1.92	0.51
1:G:77:LYS:HD2	1:G:77:LYS:H	1.75	0.51
1:A:199:SER:HB2	1:A:221:GLU:CG	2.40	0.51
1:A:61:LEU:C	1:A:63:GLU:N	2.64	0.51
1:A:657:ARG:HB2	1:A:657:ARG:HH11	1.76	0.51
1:C:120:PHE:N	1:C:120:PHE:CD1	2.74	0.51
1:C:420:LYS:HD2	1:C:421:GLU:CD	2.31	0.51
1:C:700:LEU:HD23	1:C:700:LEU:C	2.31	0.51
2:D:104:MET:C	2:D:106:ALA:H	2.14	0.51
1:E:361:GLN:C	1:E:363:GLY:N	2.64	0.51
1:E:405:PRO:C	1:E:407:ILE:H	2.14	0.51
1:E:477:PHE:O	1:E:480:LEU:N	2.41	0.51
1:E:36:TRP:HB2	1:E:76:GLN:HB2	1.92	0.51
2:F:108:ILE:HG22	2:F:109:ARG:N	2.26	0.51
1:G:610:THR:HG23	1:G:628:VAL:HG21	1.93	0.51
1:G:711:LEU:H	1:G:711:LEU:CD2	2.24	0.51
2:H:55:LYS:HB2	2:H:58:GLU:CD	2.31	0.51
1:A:584:LEU:N	1:A:584:LEU:HD23	2.25	0.51
1:A:64:ASN:C	1:A:66:LYS:H	2.14	0.51
2:B:55:LYS:HB2	2:B:58:GLU:CD	2.31	0.51
1:C:176:THR:O	1:C:183:LYS:HD2	2.10	0.51
2:D:40:GLN:C	2:D:42:PRO:HD3	2.31	0.51
1:E:166:GLN:HE22	2:F:107:GLU:HG2	1.75	0.51
1:E:313:TYR:HB2	1:E:316:LEU:HD12	1.92	0.51
1:E:562:GLU:OE1	1:E:562:GLU:HA	2.10	0.51
1:E:771:GLN:CA	1:E:771:GLN:HE21	2.24	0.51
1:G:232:GLU:O	1:G:236:ASN:HB2	2.11	0.51
1:G:400:ARG:O	1:G:404:THR:N	2.38	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:401:SER:O	1:G:606:ASN:ND2	2.43	0.51
1:G:442:ILE:O	1:G:445:ARG:N	2.38	0.51
1:G:71:SER:C	1:G:73:ASP:H	2.14	0.51
1:G:88:ASP:O	1:G:91:GLU:N	2.44	0.51
1:G:806:TYR:CB	2:H:147:VAL:HG12	2.41	0.51
1:G:802:GLN:NE2	2:H:88:TYR:OH	2.40	0.51
1:A:153:ILE:HG23	1:A:154:TYR:N	2.25	0.51
1:A:359:VAL:O	1:A:359:VAL:CG1	2.59	0.51
1:A:405:PRO:C	1:A:407:ILE:H	2.13	0.51
1:A:420:LYS:HD2	1:A:421:GLU:CD	2.30	0.51
1:A:521:LEU:HD23	1:A:521:LEU:N	2.26	0.51
1:A:735:GLU:HA	1:A:756:MET:HE1	1.91	0.51
1:A:747:MET:CG	1:A:751:GLN:HE22	2.22	0.51
1:C:107:ARG:HB3	1:C:112:LEU:HD12	1.92	0.51
1:C:298:SER:O	1:C:302:ARG:N	2.42	0.51
1:C:533:ASN:O	1:C:534:PRO:C	2.45	0.51
1:C:542:ASP:O	1:C:545:CYS:HB3	2.11	0.51
1:E:121:CYS:SG	1:E:156:ILE:HD11	2.50	0.51
1:E:22:ASN:O	1:E:22:ASN:ND2	2.44	0.51
1:E:424:ASP:C	1:E:426:ALA:N	2.63	0.51
1:G:797:ILE:CG1	2:H:117:GLU:HG2	2.41	0.51
1:A:409:VAL:HG13	1:A:634:LEU:CD1	2.40	0.51
1:A:551:THR:H	1:A:554:SER:HG	1.56	0.51
1:C:103:ASN:O	1:C:107:ARG:HG3	2.11	0.51
1:C:313:TYR:CD2	1:C:360:LEU:HB3	2.44	0.51
1:C:407:ILE:CD1	1:C:409:VAL:N	2.72	0.51
1:E:152:HIS:CE1	1:E:153:ILE:HG22	2.46	0.51
1:E:31:ALA:O	1:E:33:LYS:N	2.44	0.51
1:E:347:GLU:C	1:E:349:GLN:N	2.64	0.51
1:E:540:LEU:O	1:E:542:ASP:N	2.44	0.51
1:E:76:GLN:HB3	1:E:96:ASN:ND2	2.26	0.51
1:G:282:LYS:O	1:G:283:ASP:HB2	2.10	0.51
1:G:405:PRO:HD2	1:G:416:LYS:O	2.11	0.51
1:G:424:ASP:C	1:G:426:ALA:N	2.62	0.51
1:G:721:PHE:CE2	1:G:768:ARG:HG2	2.45	0.51
2:H:3:PHE:CA	2:H:7:GLN:HE21	2.24	0.51
1:A:743:PRO:HB2	1:G:816:GLN:HG2	1.93	0.51
1:C:306:LEU:HD22	1:C:386:LYS:HD3	1.93	0.51
1:C:553:THR:O	1:C:554:SER:C	2.48	0.51
1:E:296:GLY:HA3	1:E:332:PHE:CG	2.46	0.51
2:F:66:PHE:CE1	2:F:70:LEU:HB2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:256:PHE:CE1	1:G:262:ILE:HG13	2.46	0.51
1:G:543:GLU:C	1:G:545:CYS:H	2.14	0.51
1:G:725:ILE:HD13	1:G:730:PHE:HB2	1.93	0.51
1:A:250:LYS:HG2	1:A:465:ASP:HB3	1.93	0.50
1:A:581:PHE:HZ	1:A:597:TRP:CH2	2.30	0.50
1:A:610:THR:CG2	1:A:631:ILE:HG13	2.28	0.50
1:A:815:ARG:NE	1:A:818:GLN:HE21	2.09	0.50
1:A:166:GLN:HE22	2:B:107:GLU:HG2	1.76	0.50
1:C:288:HIS:HB3	1:C:292:TYR:CE1	2.46	0.50
1:C:437:ARG:NH2	1:C:628:VAL:HG23	2.26	0.50
1:E:286:THR:HB	1:E:290:PHE:HD2	1.76	0.50
1:E:657:ARG:HB2	1:E:657:ARG:HH11	1.75	0.50
2:F:8:THR:O	2:F:12:LYS:HG3	2.10	0.50
1:G:405:PRO:O	1:G:407:ILE:HG23	2.11	0.50
1:A:170:ASP:C	1:A:171:GLN:HG2	2.31	0.50
1:A:337:GLU:O	1:A:340:THR:OG1	2.28	0.50
1:A:480:LEU:HD11	1:A:528:ILE:CD1	2.40	0.50
1:A:733:ARG:HG2	1:A:734:TYR:CE1	2.47	0.50
2:B:128:VAL:HB	2:B:138:ILE:HD11	1.92	0.50
1:C:239:THR:C	1:C:241:LYS:H	2.14	0.50
1:C:539:ALA:O	1:C:542:ASP:HB2	2.11	0.50
2:D:95:PHE:O	2:D:103:VAL:HG13	2.10	0.50
1:E:100:VAL:HG21	1:E:711:LEU:CD1	2.41	0.50
1:E:144:LYS:HG3	1:E:148:GLU:HB2	1.92	0.50
1:E:812:PHE:C	1:E:814:LYS:N	2.64	0.50
1:G:265:ALA:N	1:G:450:LEU:O	2.45	0.50
1:G:771:GLN:CA	1:G:771:GLN:HE21	2.20	0.50
2:H:105:GLY:O	2:H:109:ARG:HB2	2.10	0.50
2:H:8:THR:O	2:H:12:LYS:HG3	2.10	0.50
2:H:139:ASN:HD21	2:H:141:GLU:HG3	1.76	0.50
1:A:42:HIS:C	1:A:44:PHE:H	2.13	0.50
2:B:15:PHE:O	2:B:18:PHE:HB2	2.10	0.50
1:C:311:ASN:N	1:C:311:ASN:HD22	2.10	0.50
1:C:31:ALA:O	1:C:33:LYS:N	2.44	0.50
1:C:404:THR:OG1	1:C:404:THR:O	2.28	0.50
1:C:657:ARG:HB2	1:C:657:ARG:HH11	1.75	0.50
1:C:766:LEU:HB3	1:C:780:VAL:HG21	1.94	0.50
2:D:3:PHE:CA	2:D:7:GLN:HE21	2.24	0.50
1:E:126:PRO:O	1:E:127:TYR:HB2	2.09	0.50
1:E:161:TYR:CG	1:E:161:TYR:O	2.64	0.50
1:E:267:ILE:HB	1:E:447:ASN:ND2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:442:ILE:O	1:E:445:ARG:N	2.39	0.50
2:F:55:LYS:HB2	2:F:58:GLU:CD	2.31	0.50
1:G:30:SER:C	1:G:32:LYS:N	2.64	0.50
1:G:430:LEU:HB2	1:G:605:LEU:HD11	1.92	0.50
1:G:630:ARG:HH22	1:G:657:ARG:HB2	1.76	0.50
2:H:66:PHE:CE1	2:H:70:LEU:HB2	2.45	0.50
1:A:719:GLN:HA	1:A:719:GLN:NE2	2.26	0.50
1:A:763:ASP:HB3	1:A:766:LEU:CD1	2.42	0.50
2:B:40:GLN:C	2:B:42:PRO:HD3	2.31	0.50
2:B:3:PHE:CA	2:B:7:GLN:HE21	2.23	0.50
1:C:269:THR:CG2	1:C:443:LEU:CD1	2.88	0.50
1:C:320:HIS:ND1	1:C:320:HIS:O	2.40	0.50
1:C:540:LEU:O	1:C:542:ASP:N	2.45	0.50
1:C:83:PHE:HB3	1:C:92:LEU:HD23	1.94	0.50
2:D:35:MET:SD	2:D:76:ILE:HD12	2.51	0.50
2:D:55:LYS:H	2:D:58:GLU:CG	2.25	0.50
2:D:94:VAL:HG12	2:D:94:VAL:O	2.12	0.50
1:E:32:LYS:C	1:E:34:LEU:H	2.15	0.50
1:E:42:HIS:C	1:E:44:PHE:H	2.14	0.50
1:E:563:GLN:O	1:E:565:ASN:N	2.44	0.50
1:E:401:SER:O	1:E:606:ASN:ND2	2.45	0.50
1:A:269:THR:CG2	1:A:443:LEU:CD1	2.88	0.50
1:A:30:SER:C	1:A:32:LYS:N	2.64	0.50
1:A:553:THR:O	1:A:554:SER:C	2.49	0.50
1:C:351:SER:O	1:C:354:ARG:HG2	2.11	0.50
1:C:405:PRO:C	1:C:407:ILE:H	2.15	0.50
1:C:409:VAL:HG13	1:C:634:LEU:HD11	1.94	0.50
2:D:139:ASN:HD21	2:D:141:GLU:HG3	1.77	0.50
1:E:64:ASN:C	1:E:66:LYS:H	2.13	0.50
2:F:104:MET:C	2:F:106:ALA:H	2.13	0.50
1:G:236:ASN:ND2	1:G:246:SER:CA	2.70	0.50
1:G:269:THR:HG21	1:G:443:LEU:CD1	2.30	0.50
1:G:31:ALA:O	1:G:33:LYS:N	2.45	0.50
1:G:513:ASN:C	1:G:513:ASN:HD22	2.15	0.50
1:G:36:TRP:HB2	1:G:76:GLN:HB2	1.92	0.50
2:H:35:MET:SD	2:H:76:ILE:HD12	2.51	0.50
1:A:478:GLU:HB2	1:A:479:GLN:OE1	2.12	0.50
2:B:135:ASN:HB2	2:B:137:CYS:SG	2.52	0.50
1:C:102:HIS:O	1:C:105:ARG:N	2.45	0.50
1:E:267:ILE:HB	1:E:447:ASN:HD21	1.77	0.50
1:E:58:THR:HA	1:E:69:THR:OG1	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:35:MET:SD	2:F:76:ILE:HD12	2.51	0.50
1:G:533:ASN:O	1:G:535:PRO:N	2.45	0.50
1:A:145:LYS:HG3	1:A:146:ARG:NE	2.26	0.50
1:A:253:ARG:O	1:A:265:ALA:HA	2.11	0.50
1:A:313:TYR:CD2	1:A:360:LEU:HB3	2.45	0.50
1:A:32:LYS:C	1:A:34:LEU:H	2.14	0.50
1:A:543:GLU:C	1:A:545:CYS:H	2.15	0.50
1:A:544:GLU:OE1	1:A:550:ALA:HB1	2.11	0.50
2:B:68:GLN:O	2:B:71:PRO:HG2	2.12	0.50
1:C:199:SER:CB	1:C:221:GLU:HG2	2.40	0.50
2:D:36:ARG:O	2:D:39:GLY:N	2.44	0.50
2:D:76:ILE:O	2:D:79:ASN:ND2	2.44	0.50
1:E:265:ALA:N	1:E:450:LEU:O	2.44	0.50
1:E:351:SER:O	1:E:354:ARG:HG2	2.12	0.50
1:E:33:LYS:HB3	1:E:49:ILE:N	2.27	0.50
1:E:7:SER:O	1:E:11:LYS:HG3	2.11	0.50
1:G:347:GLU:C	1:G:349:GLN:N	2.64	0.50
1:G:622:ALA:O	1:G:626:LYS:N	2.44	0.50
1:A:145:LYS:CB	1:A:148:GLU:HG3	2.41	0.50
1:A:293:LEU:O	1:A:297:ALA:HB2	2.12	0.50
1:A:533:ASN:O	1:A:535:PRO:N	2.45	0.50
2:B:35:MET:SD	2:B:76:ILE:HD12	2.51	0.50
1:C:152:HIS:CE1	1:C:153:ILE:HG22	2.46	0.50
1:C:232:GLU:O	1:C:236:ASN:HB2	2.11	0.50
1:C:442:ILE:O	1:C:445:ARG:N	2.38	0.50
1:C:569:PHE:CD2	1:C:570:GLN:N	2.80	0.50
1:E:107:ARG:HH11	1:E:115:THR:HG23	1.77	0.50
1:E:44:PHE:HD2	1:E:101:LEU:HD23	1.77	0.50
1:E:728:GLN:O	1:E:728:GLN:NE2	2.44	0.50
1:E:800:GLN:HA	2:F:119:MET:HE1	1.94	0.50
1:G:278:ILE:O	1:G:279:ARG:HG3	2.11	0.50
1:G:351:SER:O	1:G:353:LEU:N	2.45	0.50
1:G:586:TYR:CD1	1:G:587:ALA:N	2.79	0.50
1:G:703:GLU:O	1:G:706:ARG:N	2.39	0.50
1:G:733:ARG:HG2	1:G:734:TYR:CE1	2.46	0.50
1:G:815:ARG:NE	1:G:818:GLN:NE2	2.60	0.50
1:G:806:TYR:HB3	2:H:147:VAL:HG12	1.93	0.50
1:A:174:LEU:HD12	1:A:681:PHE:CE1	2.47	0.50
1:A:313:TYR:HB2	1:A:316:LEU:HD12	1.93	0.50
1:A:267:ILE:H	1:A:447:ASN:HD21	1.60	0.50
1:A:630:ARG:HH22	1:A:657:ARG:HB2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:LEU:HD11	1:C:152:HIS:HD2	1.77	0.50
1:C:30:SER:C	1:C:32:LYS:N	2.65	0.50
1:C:347:GLU:C	1:C:349:GLN:H	2.15	0.50
1:C:553:THR:CG2	1:C:579:THR:HG21	2.41	0.50
1:C:437:ARG:NH2	1:C:625:TRP:CE3	2.80	0.50
1:C:96:ASN:HB2	1:C:99:SER:OG	2.12	0.50
1:C:166:GLN:HE22	2:D:107:GLU:HG2	1.77	0.50
1:E:145:LYS:HG3	1:E:146:ARG:H	1.76	0.50
1:E:359:VAL:HG12	1:E:359:VAL:O	2.11	0.50
1:E:407:ILE:HD12	1:E:409:VAL:H	1.76	0.50
1:G:584:LEU:HD23	1:G:584:LEU:N	2.26	0.50
1:G:735:GLU:HA	1:G:756:MET:HE1	1.93	0.50
2:H:96:ASP:O	2:H:98:GLU:N	2.45	0.50
1:A:404:THR:O	1:A:404:THR:OG1	2.31	0.49
1:A:405:PRO:O	1:A:407:ILE:HG23	2.12	0.49
1:A:504:GLU:OE2	1:A:508:GLU:HG2	2.12	0.49
2:B:36:ARG:O	2:B:39:GLY:N	2.44	0.49
1:C:495:HIS:CD2	1:C:500:LEU:HG	2.46	0.49
1:C:814:LYS:O	1:C:818:GLN:OE1	2.30	0.49
2:D:68:GLN:O	2:D:71:PRO:HG2	2.12	0.49
1:E:333:GLN:O	1:E:337:GLU:HG3	2.12	0.49
1:E:522:GLN:OE1	1:E:525:ILE:HD12	2.12	0.49
1:E:533:ASN:O	1:E:535:PRO:N	2.45	0.49
1:G:446:VAL:HG12	1:G:447:ASN:N	2.26	0.49
1:A:224:LEU:O	1:A:224:LEU:HD12	2.12	0.49
1:A:320:HIS:ND1	1:A:320:HIS:O	2.39	0.49
1:A:419:THR:O	1:A:421:GLU:N	2.44	0.49
2:B:64:LEU:HD21	2:B:72:MET:CE	2.42	0.49
1:C:141:TYR:CE1	1:C:149:MET:HB3	2.47	0.49
1:C:544:GLU:OE1	1:C:550:ALA:HB1	2.12	0.49
1:C:719:GLN:HA	1:C:719:GLN:HE21	1.75	0.49
2:D:64:LEU:HD21	2:D:72:MET:CE	2.42	0.49
2:F:76:ILE:O	2:F:78:LYS:N	2.46	0.49
2:F:97:LYS:HG2	2:F:98:GLU:HG3	1.94	0.49
1:G:299:GLU:O	1:G:302:ARG:CB	2.60	0.49
1:G:607:ASP:N	1:G:607:ASP:OD1	2.31	0.49
1:G:83:PHE:HE2	1:G:93:THR:HG1	1.57	0.49
1:G:76:GLN:OE1	1:G:98:ALA:HB2	2.11	0.49
1:G:166:GLN:HE22	2:H:107:GLU:HG2	1.76	0.49
2:H:68:GLN:O	2:H:71:PRO:HG2	2.12	0.49
1:A:351:SER:O	1:A:353:LEU:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:8:THR:O	2:B:12:LYS:HG3	2.10	0.49
1:C:224:LEU:HD12	1:C:224:LEU:O	2.12	0.49
1:C:344:PHE:HE1	1:C:445:ARG:HB3	1.72	0.49
1:C:697:ASP:C	1:C:697:ASP:OD1	2.50	0.49
1:G:424:ASP:O	1:G:426:ALA:N	2.46	0.49
1:G:58:THR:HA	1:G:69:THR:OG1	2.12	0.49
1:A:232:GLU:O	1:A:236:ASN:HB2	2.12	0.49
1:C:293:LEU:O	1:C:297:ALA:HB2	2.12	0.49
1:C:293:LEU:HD11	1:C:301:MET:HE1	1.92	0.49
1:C:418:GLN:HA	1:C:422:GLN:NE2	2.26	0.49
1:C:721:PHE:HB3	1:C:776:PHE:O	2.11	0.49
1:E:176:THR:O	1:E:183:LYS:HD2	2.13	0.49
1:E:199:SER:CB	1:E:221:GLU:HG2	2.39	0.49
1:G:128:LYS:HG2	1:G:129:GLN:N	2.27	0.49
1:G:145:LYS:HG3	1:G:146:ARG:H	1.77	0.49
1:G:407:ILE:CG1	1:G:414:VAL:O	2.60	0.49
1:G:477:PHE:O	1:G:480:LEU:N	2.43	0.49
1:G:610:THR:HG23	1:G:628:VAL:CG2	2.42	0.49
2:H:104:MET:C	2:H:106:ALA:H	2.16	0.49
2:H:36:ARG:O	2:H:39:GLY:N	2.44	0.49
2:H:64:LEU:HD21	2:H:72:MET:CE	2.42	0.49
1:A:610:THR:CG2	1:A:628:VAL:CG1	2.90	0.49
1:C:747:MET:HG2	1:C:751:GLN:NE2	2.27	0.49
1:C:747:MET:CG	1:C:751:GLN:NE2	2.75	0.49
2:D:92:LEU:HD13	2:D:108:ILE:HD11	1.93	0.49
1:E:327:GLN:HG2	1:E:330:GLU:HG2	1.94	0.49
1:E:359:VAL:CG1	1:E:359:VAL:O	2.59	0.49
1:E:478:GLU:HB2	1:E:479:GLN:OE1	2.12	0.49
1:G:310:PHE:O	1:G:311:ASN:HB2	2.13	0.49
1:G:551:THR:H	1:G:554:SER:CB	2.25	0.49
1:A:313:TYR:CD1	1:A:313:TYR:N	2.81	0.49
1:A:80:PRO:HD2	1:A:83:PHE:CD2	2.48	0.49
2:B:104:MET:O	2:B:106:ALA:N	2.46	0.49
1:C:261:TYR:CD1	1:C:261:TYR:N	2.80	0.49
1:C:307:LEU:HA	1:C:313:TYR:OH	2.11	0.49
1:C:418:GLN:CB	1:C:422:GLN:HB2	2.36	0.49
1:E:495:HIS:CD2	1:E:500:LEU:HG	2.47	0.49
1:E:572:SER:HB2	1:E:580:GLU:HG3	1.94	0.49
1:E:610:THR:CG2	1:E:611:SER:N	2.72	0.49
1:G:237:ALA:HA	1:G:288:HIS:CD2	2.48	0.49
1:G:556:VAL:O	1:G:559:LEU:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:100:VAL:HG21	1:G:711:LEU:CD1	2.42	0.49
1:G:742:ILE:HD11	1:G:756:MET:HG2	1.94	0.49
1:A:430:LEU:HB2	1:A:605:LEU:HD11	1.95	0.49
1:A:250:LYS:HE2	1:A:465:ASP:OD2	2.11	0.49
1:A:545:CYS:HA	1:A:598:LEU:HD22	1.94	0.49
1:A:563:GLN:O	1:A:565:ASN:N	2.46	0.49
1:A:767:TYR:O	1:A:768:ARG:HD3	2.12	0.49
2:B:143:LEU:O	2:B:147:VAL:HG22	2.13	0.49
1:C:257:ASP:C	1:C:257:ASP:OD1	2.50	0.49
1:C:351:SER:O	1:C:353:LEU:N	2.45	0.49
1:C:435:PHE:O	1:C:438:LEU:N	2.37	0.49
1:C:630:ARG:HH22	1:C:657:ARG:HB2	1.78	0.49
2:D:55:LYS:O	2:D:56:SER:C	2.51	0.49
1:E:556:VAL:HG21	1:E:579:THR:HB	1.93	0.49
1:G:103:ASN:HD21	1:G:107:ARG:HD2	1.77	0.49
1:G:280:GLN:N	1:G:280:GLN:NE2	2.61	0.49
1:G:329:ASP:OD1	1:G:329:ASP:N	2.42	0.49
1:G:354:ARG:HG3	1:G:355:VAL:N	2.28	0.49
1:G:418:GLN:HA	1:G:422:GLN:NE2	2.27	0.49
2:H:55:LYS:H	2:H:58:GLU:CG	2.26	0.49
2:H:85:PHE:O	2:H:88:TYR:HB2	2.13	0.49
1:A:128:LYS:HG2	1:A:129:GLN:N	2.27	0.49
1:C:128:LYS:HG2	1:C:129:GLN:N	2.28	0.49
1:C:13:LEU:HD11	1:C:152:HIS:CD2	2.48	0.49
1:C:313:TYR:N	1:C:313:TYR:CD1	2.81	0.49
1:C:401:SER:O	1:C:606:ASN:ND2	2.45	0.49
1:C:563:GLN:O	1:C:565:ASN:N	2.46	0.49
2:D:54:PRO:HB2	2:D:59:MET:HG2	1.95	0.49
1:E:226:GLN:C	1:E:229:PRO:HD2	2.32	0.49
1:E:347:GLU:O	1:E:349:GLN:N	2.44	0.49
1:E:405:PRO:HG2	1:E:416:LYS:HG3	1.95	0.49
1:E:543:GLU:C	1:E:545:CYS:H	2.16	0.49
1:E:551:THR:H	1:E:554:SER:CB	2.26	0.49
1:E:553:THR:O	1:E:554:SER:C	2.49	0.49
1:E:174:LEU:HD12	1:E:681:PHE:CE1	2.48	0.49
1:E:88:ASP:O	1:E:91:GLU:N	2.45	0.49
2:F:68:GLN:O	2:F:71:PRO:HG2	2.12	0.49
1:G:311:ASN:N	1:G:311:ASN:HD22	2.11	0.49
2:H:54:PRO:HB2	2:H:59:MET:HG2	1.95	0.49
1:A:401:SER:O	1:A:606:ASN:ND2	2.46	0.49
1:A:703:GLU:O	1:A:706:ARG:N	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:83:GLY:HA3	2:B:88:TYR:CE2	2.47	0.49
1:C:36:TRP:NE1	1:C:78:MET:HA	2.27	0.49
1:C:382:THR:C	1:C:385:GLN:HB3	2.33	0.49
1:C:361:GLN:HB3	1:C:387:VAL:HG22	1.94	0.49
1:C:543:GLU:C	1:C:545:CYS:H	2.16	0.49
1:C:725:ILE:HD13	1:C:730:PHE:HB2	1.95	0.49
1:C:812:PHE:C	1:C:814:LYS:N	2.64	0.49
1:E:345:THR:HG22	1:E:346:GLU:HG2	1.94	0.49
1:G:351:SER:C	1:G:353:LEU:N	2.66	0.49
1:G:520:ASP:OD1	1:G:523:PRO:HD2	2.12	0.49
1:G:61:LEU:C	1:G:63:GLU:N	2.64	0.49
1:G:712:GLU:H	1:G:712:GLU:CD	2.07	0.49
2:H:135:ASN:HB2	2:H:137:CYS:SG	2.52	0.49
1:A:553:THR:HG22	1:A:557:GLU:OE2	2.13	0.49
1:A:556:VAL:O	1:A:560:ILE:HG12	2.13	0.49
2:B:95:PHE:O	2:B:103:VAL:HG13	2.13	0.49
2:B:124:VAL:O	2:B:128:VAL:HG22	2.13	0.49
1:C:299:GLU:O	1:C:302:ARG:CB	2.61	0.49
1:C:89:MET:C	1:C:91:GLU:N	2.66	0.49
2:D:105:GLY:O	2:D:109:ARG:NH1	2.46	0.49
2:D:76:ILE:O	2:D:78:LYS:N	2.45	0.49
1:E:513:ASN:C	1:E:513:ASN:HD22	2.15	0.49
1:E:48:SER:O	1:E:59:VAL:HG13	2.12	0.49
1:E:618:ASP:HB3	1:E:621:VAL:HG23	1.95	0.49
2:F:139:ASN:HD21	2:F:141:GLU:HG3	1.77	0.49
1:G:425:PHE:CD1	1:G:425:PHE:O	2.66	0.49
1:G:478:GLU:HB2	1:G:479:GLN:OE1	2.12	0.49
1:G:562:GLU:HA	1:G:562:GLU:OE1	2.12	0.49
1:G:475:ASN:HB2	1:G:592:TYR:HA	1.95	0.49
1:A:345:THR:HG22	1:A:346:GLU:HG2	1.94	0.48
1:A:511:GLU:HG3	2:H:85:PHE:CD2	2.48	0.48
1:A:623:ASP:N	1:A:623:ASP:OD1	2.45	0.48
2:B:105:GLY:O	2:B:109:ARG:HB2	2.13	0.48
1:C:199:SER:HB2	1:C:221:GLU:OE2	2.13	0.48
1:C:430:LEU:HB2	1:C:605:LEU:HD11	1.95	0.48
1:C:36:TRP:HB2	1:C:76:GLN:HB2	1.94	0.48
1:E:145:LYS:HE3	1:E:145:LYS:HB2	1.58	0.48
1:E:237:ALA:HA	1:E:288:HIS:CD2	2.47	0.48
1:E:261:TYR:CD1	1:E:261:TYR:N	2.79	0.48
1:E:256:PHE:HE1	1:E:262:ILE:HG13	1.78	0.48
1:G:120:PHE:N	1:G:120:PHE:CD1	2.75	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:337:GLU:O	1:G:340:THR:OG1	2.28	0.48
1:G:504:GLU:OE2	1:G:508:GLU:HG2	2.12	0.48
2:H:41:ASN:N	2:H:42:PRO:HD3	2.28	0.48
2:H:55:LYS:O	2:H:56:SER:C	2.51	0.48
1:A:145:LYS:HG3	1:A:146:ARG:H	1.76	0.48
1:A:152:HIS:CE1	1:A:154:TYR:CG	3.02	0.48
1:A:286:THR:HB	1:A:290:PHE:HD2	1.77	0.48
2:B:76:ILE:O	2:B:78:LYS:N	2.46	0.48
1:E:419:THR:O	1:E:421:GLU:N	2.46	0.48
1:E:659:VAL:HG12	1:E:660:GLY:H	1.71	0.48
1:G:211:GLN:HG3	1:G:214:SER:HB2	1.95	0.48
1:G:171:GLN:HA	1:G:678:ASN:H	1.78	0.48
1:G:682:VAL:HG12	1:G:682:VAL:O	2.11	0.48
1:G:814:LYS:O	1:G:818:GLN:OE1	2.31	0.48
2:H:124:VAL:O	2:H:128:VAL:HG22	2.13	0.48
1:A:288:HIS:HB3	1:A:292:TYR:CE1	2.48	0.48
1:A:296:GLY:HA3	1:A:332:PHE:CG	2.48	0.48
1:A:36:TRP:HE1	1:A:78:MET:HA	1.77	0.48
1:A:520:ASP:OD1	1:A:523:PRO:HD2	2.14	0.48
2:B:108:ILE:HG22	2:B:109:ARG:N	2.27	0.48
2:B:55:LYS:O	2:B:56:SER:C	2.51	0.48
2:B:98:GLU:O	2:B:100:ASN:N	2.45	0.48
1:C:138:ILE:HG21	1:C:196:VAL:HG11	1.95	0.48
1:C:237:ALA:HA	1:C:288:HIS:CD2	2.49	0.48
1:C:280:GLN:NE2	1:C:315:PHE:O	2.45	0.48
1:C:533:ASN:O	1:C:535:PRO:N	2.46	0.48
1:C:527:LEU:HD12	1:C:566:HIS:CD2	2.48	0.48
1:C:584:LEU:HD23	1:C:584:LEU:N	2.27	0.48
1:C:437:ARG:NE	1:C:625:TRP:HA	2.24	0.48
2:D:97:LYS:HG2	2:D:98:GLU:HG3	1.95	0.48
1:E:307:LEU:HA	1:E:313:TYR:OH	2.13	0.48
1:E:320:HIS:O	1:E:320:HIS:ND1	2.40	0.48
1:E:361:GLN:O	1:E:363:GLY:N	2.46	0.48
1:E:700:LEU:HD23	1:E:700:LEU:C	2.34	0.48
1:E:756:MET:O	1:E:760:LEU:HG	2.14	0.48
1:E:806:TYR:CG	2:F:147:VAL:HG12	2.47	0.48
1:G:327:GLN:HG2	1:G:330:GLU:HG2	1.95	0.48
1:G:404:THR:O	1:G:404:THR:OG1	2.30	0.48
1:G:89:MET:O	1:G:91:GLU:N	2.47	0.48
1:A:31:ALA:O	1:A:33:LYS:N	2.46	0.48
1:A:490:GLN:HE21	1:A:494:ASN:HD21	1.59	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:THR:HA	1:C:69:THR:OG1	2.13	0.48
2:D:41:ASN:N	2:D:42:PRO:HD3	2.28	0.48
1:E:311:ASN:HD22	1:E:311:ASN:N	2.11	0.48
1:E:352:ILE:HG21	1:E:442:ILE:CD1	2.41	0.48
1:E:356:VAL:O	1:E:360:LEU:HD12	2.13	0.48
1:G:607:ASP:HA	1:G:610:THR:CB	2.35	0.48
1:G:756:MET:O	1:G:760:LEU:HG	2.14	0.48
1:G:803:CYS:HB2	2:H:119:MET:HE2	1.94	0.48
1:A:239:THR:C	1:A:241:LYS:H	2.16	0.48
1:A:299:GLU:O	1:A:302:ARG:CB	2.60	0.48
1:A:382:THR:OG1	1:A:383:ALA:N	2.46	0.48
1:A:405:PRO:HG2	1:A:416:LYS:HG3	1.95	0.48
1:A:556:VAL:HG21	1:A:579:THR:HB	1.95	0.48
1:A:746:PHE:CD2	2:H:13:GLU:OE1	2.67	0.48
1:A:797:ILE:HG12	2:B:117:GLU:HG2	1.94	0.48
1:C:33:LYS:O	1:C:48:SER:HA	2.12	0.48
1:C:362:LEU:HD12	1:C:387:VAL:HG13	1.96	0.48
1:C:491:GLN:OE1	1:C:521:LEU:HG	2.14	0.48
1:C:553:THR:HG23	1:C:579:THR:HG21	1.94	0.48
2:D:10:GLU:HA	2:D:13:GLU:CG	2.42	0.48
2:D:120:THR:HG23	2:D:123:GLU:CD	2.34	0.48
1:E:278:ILE:O	1:E:279:ARG:HG3	2.13	0.48
1:E:313:TYR:CD1	1:E:313:TYR:N	2.81	0.48
1:E:349:GLN:HA	1:E:352:ILE:HG13	1.94	0.48
1:E:382:THR:C	1:E:385:GLN:HB3	2.33	0.48
1:E:575:LEU:HA	1:E:577:ASP:OD2	2.13	0.48
1:E:719:GLN:HE21	1:E:719:GLN:CA	2.26	0.48
1:G:114:TYR:HE2	1:G:153:ILE:HB	1.74	0.48
1:G:449:ALA:C	1:G:451:ASP:H	2.16	0.48
1:G:64:ASN:C	1:G:66:LYS:H	2.15	0.48
1:G:776:PHE:CD2	1:G:781:LEU:HD22	2.48	0.48
1:A:199:SER:CB	1:A:221:GLU:HG2	2.42	0.48
1:A:370:GLU:O	1:A:374:ASP:CA	2.61	0.48
1:A:58:THR:HA	1:A:69:THR:OG1	2.13	0.48
1:A:743:PRO:HB3	1:G:816:GLN:C	2.33	0.48
2:B:30:GLN:O	2:B:31:CYS:C	2.52	0.48
1:C:145:LYS:HG3	1:C:146:ARG:H	1.76	0.48
1:C:333:GLN:O	1:C:337:GLU:HG3	2.13	0.48
1:E:102:HIS:O	1:E:105:ARG:N	2.47	0.48
1:E:7:SER:N	1:E:10:GLU:OE1	2.43	0.48
1:E:199:SER:HB2	1:E:221:GLU:OE2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:299:GLU:O	1:E:302:ARG:CB	2.61	0.48
1:E:584:LEU:N	1:E:584:LEU:HD23	2.29	0.48
1:E:607:ASP:O	1:E:610:THR:HB	2.13	0.48
1:E:86:VAL:HG12	1:E:103:ASN:ND2	2.28	0.48
2:F:30:GLN:O	2:F:31:CYS:C	2.52	0.48
2:F:55:LYS:O	2:F:56:SER:C	2.51	0.48
1:G:623:ASP:OD1	1:G:623:ASP:N	2.46	0.48
1:G:719:GLN:HA	1:G:719:GLN:HE21	1.78	0.48
2:H:128:VAL:HG23	2:H:129:ALA:N	2.28	0.48
1:A:161:TYR:CG	1:A:161:TYR:O	2.67	0.48
1:A:621:VAL:HG12	1:A:625:TRP:CD1	2.49	0.48
1:C:272:LEU:O	1:C:274:LYS:N	2.45	0.48
1:C:61:LEU:C	1:C:63:GLU:N	2.66	0.48
1:C:630:ARG:HH12	1:C:657:ARG:HB3	1.78	0.48
1:C:663:TYR:CZ	1:C:667:LEU:HD13	2.48	0.48
1:C:711:LEU:HD22	1:C:711:LEU:N	2.28	0.48
1:C:763:ASP:HB3	1:C:766:LEU:CD1	2.44	0.48
2:D:30:GLN:O	2:D:31:CYS:C	2.52	0.48
1:E:347:GLU:C	1:E:349:GLN:H	2.15	0.48
1:E:36:TRP:NE1	1:E:78:MET:HA	2.29	0.48
1:E:618:ASP:CG	1:E:621:VAL:HG23	2.34	0.48
1:G:182:GLY:HA2	5:G:998:ADP:O1A	2.13	0.48
1:G:344:PHE:HE1	1:G:445:ARG:HB3	1.77	0.48
1:G:544:GLU:OE1	1:G:550:ALA:HB1	2.14	0.48
1:G:566:HIS:CE1	1:G:568:LYS:HB2	2.48	0.48
1:A:280:GLN:NE2	1:A:315:PHE:O	2.43	0.48
1:A:479:GLN:OE1	1:A:479:GLN:N	2.47	0.48
2:B:41:ASN:N	2:B:42:PRO:HD3	2.28	0.48
1:C:494:ASN:N	1:C:494:ASN:ND2	2.58	0.48
1:C:495:HIS:ND1	1:C:499:ILE:HD12	2.28	0.48
1:C:520:ASP:OD1	1:C:523:PRO:HD2	2.14	0.48
1:E:13:LEU:CD1	1:E:152:HIS:HD2	2.23	0.48
1:E:180:GLY:O	1:E:182:GLY:N	2.47	0.48
1:E:199:SER:HB2	1:E:221:GLU:CD	2.34	0.48
1:E:407:ILE:CD1	1:E:409:VAL:H	2.27	0.48
1:G:141:TYR:CE1	1:G:149:MET:HB3	2.49	0.48
1:G:610:THR:CG2	1:G:628:VAL:HG11	2.44	0.48
1:G:697:ASP:C	1:G:697:ASP:OD1	2.52	0.48
2:H:120:THR:HG23	2:H:123:GLU:CD	2.34	0.48
1:A:147:HIS:C	1:A:149:MET:H	2.15	0.48
1:A:321:VAL:HG13	1:A:322:PRO:HD2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:LEU:CD2	1:A:427:ILE:HG13	2.43	0.48
1:A:494:ASN:ND2	1:A:494:ASN:N	2.61	0.48
1:A:725:ILE:HD13	1:A:730:PHE:HB2	1.94	0.48
2:B:55:LYS:H	2:B:58:GLU:CG	2.26	0.48
1:C:551:THR:H	1:C:554:SER:CB	2.26	0.48
1:C:551:THR:O	1:C:552:ASP:C	2.52	0.48
1:C:610:THR:HG21	1:C:628:VAL:CG1	2.43	0.48
1:C:806:TYR:CB	2:D:147:VAL:HG12	2.44	0.48
1:E:293:LEU:O	1:E:297:ALA:HB2	2.13	0.48
1:E:293:LEU:HD11	1:E:301:MET:HE1	1.96	0.48
1:E:432:LYS:HE2	1:E:432:LYS:HB2	1.74	0.48
1:E:762:LEU:HD13	1:E:766:LEU:CD1	2.43	0.48
1:E:77:LYS:H	1:E:77:LYS:HD2	1.79	0.48
1:E:88:ASP:O	1:E:91:GLU:HB2	2.14	0.48
1:G:152:HIS:CE1	1:G:154:TYR:CG	3.02	0.48
1:G:199:SER:HB2	1:G:221:GLU:CD	2.34	0.48
1:G:89:MET:HA	1:G:92:LEU:HD12	1.94	0.48
1:A:800:GLN:HA	2:B:119:MET:HE1	1.96	0.48
1:C:133:TYR:HB3	1:C:154:TYR:OH	2.14	0.48
1:C:351:SER:C	1:C:353:LEU:H	2.18	0.48
1:C:391:MET:HB3	1:C:393:ILE:HG12	1.95	0.48
1:C:797:ILE:CG1	2:D:117:GLU:HG2	2.44	0.48
1:E:211:GLN:HG3	1:E:214:SER:HB2	1.95	0.48
1:E:574:GLN:C	1:E:576:LYS:HE3	2.33	0.48
1:E:721:PHE:CE2	1:E:768:ARG:HG2	2.49	0.48
2:F:64:LEU:HD21	2:F:72:MET:CE	2.42	0.48
2:F:69:PHE:CZ	2:F:73:MET:HG2	2.49	0.48
1:G:333:GLN:O	1:G:337:GLU:HG3	2.14	0.48
1:G:347:GLU:O	1:G:349:GLN:N	2.47	0.48
1:G:551:THR:O	1:G:552:ASP:C	2.53	0.48
1:G:36:TRP:NE1	1:G:78:MET:HA	2.29	0.48
2:H:140:TYR:HD1	2:H:141:GLU:N	2.11	0.48
1:A:107:ARG:HH11	1:A:115:THR:HG23	1.79	0.47
1:A:630:ARG:HH12	1:A:657:ARG:HB3	1.77	0.47
1:A:712:GLU:CD	1:A:712:GLU:H	2.10	0.47
1:A:812:PHE:C	1:A:814:LYS:N	2.68	0.47
2:B:54:PRO:HB2	2:B:59:MET:HG2	1.95	0.47
2:B:69:PHE:CZ	2:B:73:MET:HG2	2.49	0.47
1:C:199:SER:HB2	1:C:221:GLU:CD	2.33	0.47
1:C:321:VAL:HG13	1:C:322:PRO:HD2	1.96	0.47
1:C:513:ASN:O	1:C:515:ILE:HD12	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:149:MET:HB3	1:E:150:PRO:HD2	1.96	0.47
1:E:189:LYS:O	1:E:192:GLN:HB3	2.14	0.47
1:E:30:SER:C	1:E:32:LYS:N	2.64	0.47
1:G:126:PRO:O	1:G:127:TYR:HB2	2.13	0.47
1:G:351:SER:C	1:G:353:LEU:H	2.18	0.47
1:G:767:TYR:O	1:G:768:ARG:HD3	2.14	0.47
2:H:35:MET:HE1	2:H:73:MET:HA	1.96	0.47
1:A:89:MET:HA	1:A:92:LEU:HD12	1.96	0.47
1:C:551:THR:O	1:C:554:SER:N	2.47	0.47
1:C:618:ASP:HB3	1:C:621:VAL:HG23	1.96	0.47
1:E:170:ASP:C	1:E:171:GLN:HG2	2.34	0.47
1:E:349:GLN:O	1:E:350:THR:C	2.53	0.47
1:E:351:SER:C	1:E:353:LEU:N	2.67	0.47
1:E:402:ILE:HG22	1:E:403:LEU:HG	1.96	0.47
1:E:508:GLU:HG3	1:E:775:PHE:CE1	2.49	0.47
1:E:776:PHE:CD2	1:E:781:LEU:HD22	2.50	0.47
2:F:41:ASN:N	2:F:42:PRO:HD3	2.28	0.47
1:G:60:GLU:OE1	1:G:67:LYS:HD2	2.14	0.47
1:G:700:LEU:C	1:G:700:LEU:HD23	2.34	0.47
2:H:10:GLU:HA	2:H:13:GLU:CG	2.43	0.47
2:H:139:ASN:OD1	2:H:142:GLU:HG2	2.14	0.47
2:H:143:LEU:O	2:H:147:VAL:HG22	2.15	0.47
1:A:424:ASP:C	1:A:426:ALA:N	2.63	0.47
1:A:746:PHE:CZ	2:H:13:GLU:OE1	2.68	0.47
1:C:44:PHE:CD2	1:C:98:ALA:HA	2.50	0.47
2:D:85:PHE:HA	2:D:89:VAL:HG13	1.95	0.47
1:E:354:ARG:HG3	1:E:355:VAL:N	2.29	0.47
1:E:391:MET:HB3	1:E:393:ILE:HG12	1.96	0.47
1:E:420:LYS:HD2	1:E:421:GLU:OE2	2.13	0.47
1:E:815:ARG:NE	1:E:818:GLN:NE2	2.62	0.47
1:G:370:GLU:O	1:G:374:ASP:CA	2.62	0.47
1:G:513:ASN:O	1:G:515:ILE:HD12	2.14	0.47
1:G:618:ASP:HB3	1:G:621:VAL:HG23	1.97	0.47
1:G:409:VAL:HG13	1:G:634:LEU:HD11	1.97	0.47
1:G:711:LEU:HD22	1:G:711:LEU:H	1.79	0.47
1:G:716:ILE:HA	1:G:719:GLN:HB2	1.96	0.47
1:A:310:PHE:O	1:A:311:ASN:HB2	2.15	0.47
1:A:362:LEU:HD12	1:A:387:VAL:HG13	1.96	0.47
1:A:513:ASN:O	1:A:515:ILE:HD12	2.14	0.47
1:C:183:LYS:HE2	5:C:998:ADP:O1B	2.14	0.47
1:C:22:ASN:HA	1:C:23:PRO:HD3	1.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:378:MET:HA	1:C:378:MET:CE	2.45	0.47
1:C:424:ASP:O	1:C:426:ALA:N	2.47	0.47
1:C:449:ALA:C	1:C:451:ASP:H	2.18	0.47
1:C:100:VAL:HG21	1:C:711:LEU:CD1	2.44	0.47
1:C:89:MET:HA	1:C:92:LEU:HD12	1.97	0.47
1:G:149:MET:HB3	1:G:150:PRO:HD2	1.95	0.47
1:G:235:GLY:HA3	1:G:248:PHE:CE1	2.50	0.47
1:G:513:ASN:ND2	1:G:513:ASN:O	2.44	0.47
1:G:556:VAL:O	1:G:560:ILE:HG12	2.15	0.47
1:G:574:GLN:C	1:G:576:LYS:HE3	2.35	0.47
2:H:30:GLN:O	2:H:31:CYS:C	2.53	0.47
1:A:13:LEU:HG	1:A:132:ILE:HG21	1.96	0.47
1:A:261:TYR:CD1	1:A:261:TYR:N	2.82	0.47
1:A:333:GLN:O	1:A:337:GLU:HG3	2.15	0.47
1:A:349:GLN:O	1:A:350:THR:C	2.53	0.47
1:A:424:ASP:O	1:A:426:ALA:N	2.48	0.47
1:A:728:GLN:NE2	1:A:728:GLN:O	2.47	0.47
2:B:105:GLY:O	2:B:109:ARG:NH1	2.47	0.47
1:C:12:PHE:CD2	1:C:131:PRO:CD	2.98	0.47
1:C:149:MET:HB3	1:C:150:PRO:HD2	1.96	0.47
1:C:574:GLN:C	1:C:576:LYS:HE3	2.35	0.47
1:C:711:LEU:CD2	1:C:711:LEU:H	2.27	0.47
2:D:140:TYR:O	2:D:142:GLU:N	2.47	0.47
1:E:370:GLU:O	1:E:374:ASP:CA	2.62	0.47
1:E:663:TYR:C	1:E:665:GLU:N	2.66	0.47
2:F:36:ARG:O	2:F:39:GLY:N	2.44	0.47
1:G:321:VAL:HG13	1:G:322:PRO:HD2	1.95	0.47
1:G:33:LYS:HB2	1:G:48:SER:OG	2.14	0.47
1:G:407:ILE:CD1	1:G:409:VAL:N	2.78	0.47
1:G:449:ALA:C	1:G:451:ASP:N	2.68	0.47
1:G:747:MET:CG	1:G:751:GLN:NE2	2.78	0.47
1:G:768:ARG:HA	1:G:768:ARG:HD3	1.61	0.47
2:H:69:PHE:CZ	2:H:73:MET:HG2	2.49	0.47
1:A:407:ILE:CD1	1:A:409:VAL:N	2.76	0.47
1:A:449:ALA:C	1:A:451:ASP:H	2.17	0.47
1:A:569:PHE:CD2	1:A:570:GLN:N	2.83	0.47
1:A:711:LEU:N	1:A:711:LEU:CD2	2.78	0.47
1:A:77:LYS:H	1:A:77:LYS:HD2	1.79	0.47
1:E:107:ARG:HB3	1:E:112:LEU:HD12	1.96	0.47
1:E:152:HIS:CE1	1:E:154:TYR:CD2	3.02	0.47
1:E:606:ASN:OD1	1:E:608:ASN:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:55:LYS:H	2:F:58:GLU:CG	2.27	0.47
1:G:193:TYR:CZ	1:G:197:VAL:HG21	2.50	0.47
1:G:382:THR:OG1	1:G:383:ALA:N	2.47	0.47
1:G:382:THR:C	1:G:385:GLN:HB3	2.34	0.47
1:G:416:LYS:NZ	1:G:417:ALA:O	2.42	0.47
1:G:174:LEU:HD12	1:G:681:PHE:CE1	2.50	0.47
1:A:79:ASN:OD1	1:A:94:CYS:HB2	2.15	0.47
1:C:345:THR:HG22	1:C:346:GLU:HG2	1.97	0.47
1:C:575:LEU:C	1:C:577:ASP:H	2.18	0.47
1:C:806:TYR:CG	2:D:147:VAL:HG12	2.50	0.47
1:E:355:VAL:HG21	1:E:620:PHE:CE2	2.49	0.47
1:E:814:LYS:O	1:E:818:GLN:OE1	2.32	0.47
1:E:806:TYR:CB	2:F:147:VAL:HG12	2.44	0.47
2:F:54:PRO:HB2	2:F:59:MET:HG2	1.96	0.47
1:E:802:GLN:NE2	2:F:88:TYR:OH	2.42	0.47
1:G:164:MET:HG2	1:G:165:LEU:N	2.29	0.47
1:G:405:PRO:HG2	1:G:416:LYS:HG3	1.96	0.47
1:G:479:GLN:N	1:G:479:GLN:OE1	2.48	0.47
2:H:95:PHE:CZ	2:H:111:VAL:HG21	2.49	0.47
1:A:271:LEU:HD21	1:A:663:TYR:CZ	2.49	0.47
1:A:700:LEU:C	1:A:700:LEU:HD23	2.35	0.47
1:A:814:LYS:O	1:A:818:GLN:OE1	2.32	0.47
1:C:9:ASP:O	1:C:12:PHE:HB2	2.15	0.47
1:C:683:ARG:H	1:C:683:ARG:HG2	1.39	0.47
1:E:287:PHE:O	1:E:288:HIS:C	2.52	0.47
1:E:226:GLN:HG2	1:E:341:ILE:HB	1.95	0.47
1:E:806:TYR:HB3	2:F:147:VAL:HG12	1.97	0.47
1:E:80:PRO:HD2	1:E:83:PHE:CE2	2.50	0.47
1:G:267:ILE:HB	1:G:447:ASN:HD21	1.80	0.47
1:A:745:GLY:HA3	1:G:819:LEU:HD21	1.96	0.47
2:H:110:HIS:O	2:H:111:VAL:C	2.53	0.47
2:H:76:ILE:O	2:H:78:LYS:N	2.47	0.47
1:A:351:SER:C	1:A:353:LEU:N	2.68	0.47
1:A:79:ASN:OD1	1:A:92:LEU:HB3	2.15	0.47
1:C:87:GLU:OE1	1:C:107:ARG:NH2	2.48	0.47
2:D:69:PHE:CZ	2:D:73:MET:HG2	2.49	0.47
1:E:306:LEU:HD22	1:E:386:LYS:HD3	1.97	0.47
1:E:308:GLU:OE1	1:E:312:ASN:HB3	2.14	0.47
1:E:382:THR:OG1	1:E:383:ALA:N	2.48	0.47
1:E:119:LEU:HD13	1:E:497:MET:HE1	1.97	0.47
1:E:89:MET:HA	1:E:92:LEU:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:105:GLY:O	2:F:109:ARG:NH1	2.47	0.47
1:G:86:VAL:HG12	1:G:103:ASN:ND2	2.29	0.47
1:G:228:ASN:N	1:G:229:PRO:CD	2.78	0.47
1:G:278:ILE:HG22	1:G:315:PHE:CE1	2.50	0.47
1:G:172:SER:HA	1:G:462:GLY:O	2.15	0.47
1:G:569:PHE:CD2	1:G:570:GLN:N	2.83	0.47
2:H:20:ARG:HB2	2:H:20:ARG:HE	1.45	0.47
1:A:184:THR:O	1:A:185:GLU:C	2.53	0.47
1:A:311:ASN:N	1:A:311:ASN:HD22	2.12	0.47
1:A:573:LYS:HD2	1:A:573:LYS:N	2.29	0.47
1:A:355:VAL:HG21	1:A:620:PHE:CE2	2.49	0.47
1:C:152:HIS:CE1	1:C:154:TYR:CG	3.03	0.47
1:C:294:ILE:HB	1:C:310:PHE:CZ	2.50	0.47
1:C:369:LYS:HG3	1:C:370:GLU:H	1.79	0.47
1:C:513:ASN:C	1:C:513:ASN:HD22	2.18	0.47
1:C:182:GLY:HA2	5:C:998:ADP:PA	2.55	0.47
1:E:253:ARG:O	1:E:265:ALA:HA	2.14	0.47
1:E:409:VAL:HG13	1:E:634:LEU:HD11	1.96	0.47
1:E:556:VAL:O	1:E:560:ILE:HG12	2.14	0.47
1:E:607:ASP:OD1	1:E:607:ASP:N	2.33	0.47
2:F:105:GLY:O	2:F:109:ARG:HB2	2.15	0.47
1:G:193:TYR:CE1	1:G:197:VAL:HG21	2.49	0.47
1:G:347:GLU:C	1:G:349:GLN:H	2.16	0.47
1:G:558:LYS:O	1:G:561:GLN:N	2.48	0.47
1:G:662:LEU:HD12	1:G:662:LEU:HA	1.73	0.47
1:A:235:GLY:HA3	1:A:248:PHE:HE2	1.79	0.47
1:A:382:THR:C	1:A:385:GLN:HB3	2.35	0.47
1:A:625:TRP:C	1:A:627:ASP:H	2.19	0.47
1:A:36:TRP:NE1	1:A:78:MET:HA	2.30	0.47
2:B:74:GLN:O	2:B:75:THR:C	2.53	0.47
1:C:189:LYS:O	1:C:192:GLN:HB3	2.15	0.47
1:C:746:PHE:O	1:C:747:MET:HB2	2.14	0.47
2:F:104:MET:O	2:F:106:ALA:N	2.48	0.47
1:G:199:SER:HB2	1:G:221:GLU:OE2	2.14	0.47
1:G:239:THR:C	1:G:241:LYS:H	2.18	0.47
1:A:354:ARG:HG3	1:A:355:VAL:N	2.30	0.46
1:A:416:LYS:NZ	1:A:417:ALA:O	2.40	0.46
1:A:747:MET:HE3	1:A:755:LEU:HD22	1.96	0.46
1:A:769:ILE:CD1	1:A:774:ILE:HG12	2.45	0.46
2:B:64:LEU:HD21	2:B:72:MET:HE1	1.96	0.46
1:C:183:LYS:HB2	1:C:183:LYS:HE2	1.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:597:TRP:O	1:C:601:ASN:HB2	2.15	0.46
1:C:618:ASP:CG	1:C:621:VAL:HG23	2.35	0.46
1:E:87:GLU:OE1	1:E:107:ARG:NH2	2.48	0.46
1:E:272:LEU:CD1	1:E:272:LEU:C	2.80	0.46
2:F:135:ASN:HB2	2:F:137:CYS:SG	2.56	0.46
1:G:250:LYS:HD2	1:G:252:ILE:HD11	1.96	0.46
1:A:446:VAL:HG12	1:A:447:ASN:N	2.29	0.46
1:A:721:PHE:CE2	1:A:768:ARG:HG2	2.50	0.46
1:A:726:VAL:HA	1:A:773:LYS:HA	1.97	0.46
1:A:756:MET:O	1:A:760:LEU:HG	2.15	0.46
2:B:139:ASN:HD21	2:B:141:GLU:HG3	1.79	0.46
1:C:733:ARG:HG2	1:C:734:TYR:CE1	2.50	0.46
1:E:351:SER:C	1:E:353:LEU:H	2.17	0.46
1:E:769:ILE:HD13	1:E:774:ILE:HG12	1.96	0.46
1:G:196:VAL:CG1	1:G:197:VAL:N	2.78	0.46
1:G:726:VAL:HA	1:G:773:LYS:HA	1.96	0.46
2:H:97:LYS:HG2	2:H:98:GLU:HG3	1.97	0.46
1:A:211:GLN:HG3	1:A:214:SER:HB2	1.97	0.46
1:A:199:SER:HB2	1:A:221:GLU:OE2	2.15	0.46
1:A:607:ASP:O	1:A:610:THR:HB	2.16	0.46
1:C:184:THR:O	1:C:185:GLU:C	2.54	0.46
1:C:235:GLY:HA3	1:C:248:PHE:HE1	1.80	0.46
1:C:351:SER:C	1:C:353:LEU:N	2.67	0.46
2:D:104:MET:O	2:D:106:ALA:N	2.48	0.46
2:D:140:TYR:CE1	2:D:141:GLU:HG2	2.50	0.46
1:E:133:TYR:HB3	1:E:154:TYR:OH	2.16	0.46
1:E:378:MET:CE	1:E:378:MET:HA	2.45	0.46
1:E:545:CYS:HA	1:E:598:LEU:HD22	1.97	0.46
2:F:120:THR:HG23	2:F:123:GLU:CD	2.36	0.46
1:G:9:ASP:O	1:G:12:PHE:HB2	2.15	0.46
1:G:189:LYS:O	1:G:192:GLN:HB3	2.15	0.46
1:G:293:LEU:HD11	1:G:301:MET:HE2	1.97	0.46
1:G:313:TYR:N	1:G:313:TYR:CD1	2.83	0.46
1:G:575:LEU:C	1:G:577:ASP:H	2.19	0.46
1:G:508:GLU:HG3	1:G:775:PHE:HE1	1.80	0.46
1:A:237:ALA:HA	1:A:288:HIS:CD2	2.50	0.46
1:A:294:ILE:HB	1:A:310:PHE:CZ	2.50	0.46
1:A:420:LYS:HD2	1:A:421:GLU:OE2	2.15	0.46
1:A:474:ILE:H	1:A:474:ILE:HG13	1.48	0.46
1:A:100:VAL:HG21	1:A:711:LEU:HD11	1.96	0.46
1:A:768:ARG:HA	1:A:768:ARG:HD3	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:177:GLY:O	1:C:183:LYS:NZ	2.44	0.46
1:C:280:GLN:OE1	1:C:316:LEU:HA	2.15	0.46
1:C:327:GLN:HG2	1:C:330:GLU:HG2	1.96	0.46
1:C:425:PHE:O	1:C:425:PHE:CD1	2.68	0.46
1:C:508:GLU:HG3	1:C:775:PHE:HE1	1.80	0.46
1:C:541:LEU:CD2	1:C:601:ASN:HD22	2.14	0.46
1:E:416:LYS:NZ	1:E:417:ALA:O	2.41	0.46
1:E:437:ARG:HD2	1:E:624:LEU:O	2.14	0.46
1:E:747:MET:HG2	1:E:751:GLN:NE2	2.30	0.46
1:E:763:ASP:HB3	1:E:766:LEU:CD1	2.44	0.46
1:G:253:ARG:O	1:G:265:ALA:HA	2.14	0.46
1:G:402:ILE:HG22	1:G:403:LEU:HG	1.96	0.46
1:G:553:THR:O	1:G:554:SER:C	2.54	0.46
1:G:763:ASP:N	1:G:766:LEU:HD12	2.31	0.46
1:A:751:GLN:CD	1:G:813:ALA:HB2	2.36	0.46
2:H:108:ILE:HG22	2:H:109:ARG:N	2.31	0.46
1:A:280:GLN:OE1	1:A:316:LEU:HA	2.15	0.46
1:A:718:ARG:HG3	1:A:719:GLN:N	2.30	0.46
1:A:80:PRO:HD2	1:A:83:PHE:HD2	1.81	0.46
1:C:296:GLY:HA3	1:C:332:PHE:CG	2.50	0.46
1:C:522:GLN:OE1	1:C:525:ILE:HD12	2.15	0.46
1:C:545:CYS:HA	1:C:598:LEU:HD22	1.96	0.46
2:D:70:LEU:HG	2:D:74:GLN:HE21	1.81	0.46
1:E:544:GLU:OE1	1:E:550:ALA:HB1	2.14	0.46
2:F:4:SER:N	2:F:7:GLN:NE2	2.61	0.46
1:G:13:LEU:HD21	1:G:132:ILE:HD12	1.97	0.46
2:H:74:GLN:O	2:H:75:THR:C	2.53	0.46
1:A:806:TYR:CB	2:B:147:VAL:HG12	2.45	0.46
1:C:226:GLN:HG2	1:C:341:ILE:HB	1.98	0.46
1:C:234:PHE:HD1	1:C:289:ILE:CG2	2.25	0.46
1:C:308:GLU:OE1	1:C:312:ASN:HB3	2.15	0.46
1:C:337:GLU:O	1:C:340:THR:OG1	2.28	0.46
1:C:416:LYS:NZ	1:C:417:ALA:O	2.41	0.46
1:C:60:GLU:OE1	1:C:67:LYS:HD2	2.16	0.46
1:C:89:MET:HE2	1:C:104:LEU:HD21	1.97	0.46
2:D:116:GLY:O	2:D:118:LYS:N	2.47	0.46
2:D:143:LEU:O	2:D:147:VAL:HG22	2.15	0.46
1:E:235:GLY:HA3	1:E:248:PHE:HE1	1.81	0.46
1:E:293:LEU:HA	1:E:332:PHE:HE1	1.79	0.46
1:E:520:ASP:OD1	1:E:523:PRO:HD2	2.15	0.46
1:E:271:LEU:HD21	1:E:663:TYR:CZ	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:697:ASP:C	1:E:697:ASP:OD1	2.51	0.46
1:E:763:ASP:N	1:E:766:LEU:HD12	2.31	0.46
1:G:147:HIS:C	1:G:149:MET:H	2.19	0.46
1:G:231:LEU:N	1:G:231:LEU:HD23	2.30	0.46
1:G:308:GLU:OE1	1:G:312:ASN:HB3	2.16	0.46
1:G:349:GLN:O	1:G:350:THR:C	2.54	0.46
1:G:361:GLN:CG	1:G:387:VAL:HG23	2.45	0.46
1:A:551:THR:O	1:A:554:SER:N	2.48	0.46
1:A:763:ASP:OD1	1:A:765:ASN:N	2.48	0.46
1:C:306:LEU:HD22	1:C:386:LYS:CD	2.46	0.46
1:C:480:LEU:HD11	1:C:528:ILE:CD1	2.46	0.46
1:C:712:GLU:OE1	1:C:712:GLU:N	2.38	0.46
2:D:124:VAL:HG23	2:D:125:GLU:N	2.31	0.46
2:D:74:GLN:O	2:D:75:THR:C	2.53	0.46
2:D:74:GLN:O	2:D:78:LYS:HD2	2.16	0.46
1:E:479:GLN:N	1:E:479:GLN:OE1	2.49	0.46
1:E:487:GLU:OE1	1:E:585:HIS:HA	2.16	0.46
2:F:43:THR:HG23	2:F:46:GLU:OE1	2.16	0.46
2:F:70:LEU:HG	2:F:74:GLN:HE21	1.81	0.46
1:G:280:GLN:OE1	1:G:316:LEU:HA	2.16	0.46
1:G:551:THR:O	1:G:554:SER:N	2.49	0.46
1:A:141:TYR:CE1	1:A:149:MET:HB3	2.51	0.46
1:A:378:MET:CE	1:A:378:MET:HA	2.45	0.46
1:A:267:ILE:CD1	1:A:450:LEU:HD12	2.45	0.46
1:A:469:PHE:N	1:A:486:ASN:OD1	2.46	0.46
1:A:543:GLU:C	1:A:545:CYS:N	2.69	0.46
1:A:574:GLN:C	1:A:576:LYS:HE3	2.37	0.46
2:B:43:THR:HG23	2:B:46:GLU:OE1	2.16	0.46
1:C:235:GLY:HA3	1:C:248:PHE:CE1	2.51	0.46
1:C:370:GLU:O	1:C:374:ASP:CA	2.64	0.46
1:C:381:ASN:O	1:C:382:THR:C	2.54	0.46
1:C:663:TYR:C	1:C:665:GLU:N	2.66	0.46
1:C:699:HIS:HA	1:C:702:LEU:HB2	1.96	0.46
1:E:172:SER:HA	1:E:462:GLY:O	2.15	0.46
1:E:310:PHE:O	1:E:311:ASN:HB2	2.16	0.46
1:E:39:SER:OG	1:E:42:HIS:HB2	2.16	0.46
1:E:513:ASN:O	1:E:515:ILE:HD12	2.15	0.46
1:E:553:THR:HA	1:E:579:THR:HG21	1.97	0.46
1:E:100:VAL:HG21	1:E:711:LEU:HD11	1.98	0.46
1:G:104:LEU:CD1	1:G:705:LEU:HD11	2.45	0.46
1:G:256:PHE:HE1	1:G:262:ILE:HG13	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:381:ASN:O	1:G:382:THR:C	2.54	0.46
1:G:408:LYS:HG2	1:G:412:ASP:O	2.16	0.46
1:G:543:GLU:C	1:G:545:CYS:N	2.69	0.46
1:G:804:ARG:O	1:G:808:ALA:HB2	2.15	0.46
2:H:70:LEU:HG	2:H:74:GLN:HE21	1.80	0.46
1:A:226:GLN:HG2	1:A:341:ILE:HB	1.97	0.46
1:A:504:GLU:HG3	1:A:504:GLU:O	2.15	0.46
1:A:697:ASP:OD1	1:A:697:ASP:C	2.55	0.46
2:B:74:GLN:O	2:B:78:LYS:HD2	2.16	0.46
1:C:382:THR:OG1	1:C:383:ALA:N	2.49	0.46
1:C:475:ASN:HB2	1:C:592:TYR:HA	1.98	0.46
1:C:619:LYS:HA	1:C:622:ALA:HB3	1.97	0.46
1:C:726:VAL:HA	1:C:773:LYS:HA	1.98	0.46
1:C:77:LYS:HD2	1:C:77:LYS:H	1.80	0.46
2:D:111:VAL:HG12	2:D:112:LEU:HD23	1.97	0.46
1:C:800:GLN:HA	2:D:119:MET:HE1	1.97	0.46
1:E:267:ILE:CD1	1:E:450:LEU:HD12	2.46	0.46
1:E:604:PRO:O	1:E:605:LEU:HB2	2.16	0.46
1:G:161:TYR:CE1	1:G:165:LEU:HD11	2.51	0.46
1:G:22:ASN:O	1:G:22:ASN:ND2	2.49	0.46
1:G:235:GLY:HA3	1:G:248:PHE:HE1	1.81	0.46
1:G:407:ILE:HD12	1:G:409:VAL:H	1.80	0.46
1:G:527:LEU:HD12	1:G:566:HIS:CD2	2.50	0.46
1:G:611:SER:HA	1:G:614:ASN:HB2	1.97	0.46
1:G:355:VAL:HG21	1:G:620:PHE:CE2	2.51	0.46
1:G:699:HIS:HA	1:G:702:LEU:HB2	1.98	0.46
1:G:763:ASP:HB3	1:G:766:LEU:CD1	2.46	0.46
1:A:13:LEU:HD11	1:A:132:ILE:CB	2.35	0.46
1:A:306:LEU:HD22	1:A:386:LYS:HD3	1.98	0.46
1:A:663:TYR:C	1:A:665:GLU:N	2.69	0.46
2:B:120:THR:HG23	2:B:123:GLU:CD	2.35	0.46
1:C:438:LEU:HA	1:C:438:LEU:HD12	1.77	0.46
1:C:682:VAL:HG12	1:C:682:VAL:O	2.15	0.46
1:C:712:GLU:CD	1:C:712:GLU:H	2.12	0.46
1:C:724:ARG:HB3	1:C:724:ARG:HE	1.62	0.46
1:C:803:CYS:HB2	2:D:119:MET:HE1	1.96	0.46
1:E:280:GLN:OE1	1:E:316:LEU:HA	2.15	0.46
1:E:425:PHE:CD1	1:E:425:PHE:O	2.69	0.46
1:E:682:VAL:O	1:E:682:VAL:HG12	2.16	0.46
1:E:711:LEU:N	1:E:711:LEU:CD2	2.76	0.46
2:F:74:GLN:O	2:F:75:THR:C	2.53	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:345:THR:HG22	1:G:346:GLU:HG2	1.97	0.46
1:G:573:LYS:HD2	1:G:573:LYS:N	2.31	0.46
2:H:135:ASN:N	2:H:135:ASN:ND2	2.64	0.46
1:A:133:TYR:HB3	1:A:154:TYR:OH	2.15	0.45
1:A:381:ASN:O	1:A:382:THR:C	2.55	0.45
1:A:449:ALA:C	1:A:451:ASP:N	2.69	0.45
1:A:621:VAL:HG12	1:A:625:TRP:HD1	1.80	0.45
2:B:133:ASP:OD1	2:B:135:ASN:N	2.49	0.45
1:C:513:ASN:ND2	1:C:513:ASN:O	2.46	0.45
1:C:581:PHE:CZ	1:C:597:TRP:CH2	3.03	0.45
1:C:623:ASP:OD1	1:C:623:ASP:N	2.49	0.45
1:C:716:ILE:HA	1:C:719:GLN:HB2	1.98	0.45
2:D:43:THR:HG23	2:D:46:GLU:OE1	2.16	0.45
1:E:275:SER:O	1:E:278:ILE:HG12	2.16	0.45
1:E:424:ASP:O	1:E:426:ALA:N	2.49	0.45
2:F:74:GLN:O	2:F:78:LYS:HD2	2.16	0.45
1:G:164:MET:HE1	1:G:256:PHE:HE2	1.80	0.45
1:G:747:MET:HG2	1:G:751:GLN:NE2	2.31	0.45
2:H:111:VAL:HA	2:H:115:LEU:HD13	1.98	0.45
1:A:132:ILE:HD12	1:A:152:HIS:HD2	1.82	0.45
1:A:287:PHE:O	1:A:288:HIS:C	2.54	0.45
1:A:566:HIS:CE1	1:A:568:LYS:HB2	2.50	0.45
1:A:508:GLU:HG3	1:A:775:PHE:HE1	1.80	0.45
2:B:97:LYS:HG2	2:B:98:GLU:HG3	1.97	0.45
1:C:250:LYS:HD2	1:C:252:ILE:HD11	1.98	0.45
1:C:362:LEU:CD2	1:C:427:ILE:HG13	2.45	0.45
1:C:575:LEU:HD23	1:C:577:ASP:OD1	2.17	0.45
1:E:293:LEU:HD11	1:E:301:MET:HE2	1.97	0.45
1:E:278:ILE:HG22	1:E:315:PHE:CE1	2.51	0.45
1:E:407:ILE:CD1	1:E:409:VAL:N	2.76	0.45
1:E:446:VAL:HG12	1:E:447:ASN:N	2.31	0.45
1:E:475:ASN:HB2	1:E:592:TYR:HA	1.98	0.45
1:E:530:ARG:HG3	1:E:531:PRO:N	2.31	0.45
1:E:581:PHE:CZ	1:E:597:TRP:CH2	3.05	0.45
1:E:61:LEU:C	1:E:63:GLU:N	2.65	0.45
1:E:623:ASP:OD1	1:E:623:ASP:N	2.48	0.45
1:E:9:ASP:O	1:E:12:PHE:HB2	2.16	0.45
1:G:100:VAL:HG21	1:G:711:LEU:HD11	1.97	0.45
1:G:145:LYS:HE3	1:G:145:LYS:HB2	1.57	0.45
1:G:161:TYR:O	1:G:161:TYR:CG	2.68	0.45
1:G:530:ARG:HA	1:G:531:PRO:HD3	1.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:683:ARG:HG2	1:G:683:ARG:H	1.35	0.45
1:G:769:ILE:HD13	1:G:774:ILE:HG23	1.98	0.45
2:H:74:GLN:O	2:H:78:LYS:HD2	2.16	0.45
1:A:527:LEU:HD12	1:A:566:HIS:CD2	2.51	0.45
1:A:747:MET:CG	1:A:751:GLN:NE2	2.79	0.45
2:D:35:MET:CE	2:D:73:MET:HA	2.47	0.45
1:E:164:MET:HG2	1:E:165:LEU:N	2.31	0.45
1:E:33:LYS:O	1:E:48:SER:HA	2.16	0.45
1:E:449:ALA:C	1:E:451:ASP:N	2.69	0.45
1:E:53:LYS:HD2	1:E:58:THR:HG23	1.98	0.45
1:E:763:ASP:OD1	1:E:765:ASN:N	2.49	0.45
1:E:769:ILE:CD1	1:E:774:ILE:HG12	2.47	0.45
2:F:85:PHE:CA	2:F:89:VAL:HG13	2.40	0.45
1:G:164:MET:HE1	1:G:256:PHE:CE2	2.51	0.45
1:G:294:ILE:HB	1:G:310:PHE:CZ	2.50	0.45
1:G:391:MET:HB3	1:G:393:ILE:HG12	1.98	0.45
1:G:420:LYS:HD2	1:G:421:GLU:OE2	2.16	0.45
1:G:432:LYS:HE2	1:G:432:LYS:HB2	1.80	0.45
1:G:508:GLU:HG3	1:G:775:PHE:CE1	2.52	0.45
2:H:43:THR:HG23	2:H:46:GLU:OE1	2.16	0.45
1:A:134:SER:O	1:A:135:GLU:C	2.55	0.45
1:A:682:VAL:O	1:A:682:VAL:HG12	2.16	0.45
1:A:763:ASP:N	1:A:766:LEU:HD12	2.32	0.45
1:C:13:LEU:HD21	1:C:132:ILE:HD13	1.97	0.45
1:C:153:ILE:CG2	1:C:154:TYR:N	2.79	0.45
1:C:293:LEU:HA	1:C:332:PHE:HE1	1.80	0.45
1:C:449:ALA:C	1:C:451:ASP:N	2.70	0.45
1:C:474:ILE:HG13	1:C:474:ILE:H	1.48	0.45
1:C:611:SER:O	1:C:615:GLN:NE2	2.49	0.45
1:C:767:TYR:CD1	1:C:767:TYR:C	2.90	0.45
1:C:776:PHE:CD2	1:C:781:LEU:HD22	2.51	0.45
1:C:806:TYR:HB3	2:D:147:VAL:HG12	1.97	0.45
1:E:184:THR:O	1:E:185:GLU:C	2.55	0.45
2:F:44:ASN:ND2	2:F:117:GLU:HB3	2.29	0.45
1:G:293:LEU:HA	1:G:332:PHE:HE1	1.81	0.45
1:G:352:ILE:HG21	1:G:442:ILE:CD1	2.41	0.45
1:A:508:GLU:HG3	1:A:775:PHE:CE1	2.51	0.45
1:A:662:LEU:HD12	1:A:662:LEU:HA	1.74	0.45
2:B:70:LEU:HG	2:B:74:GLN:HE21	1.81	0.45
1:C:164:MET:HB2	1:C:164:MET:HE2	1.90	0.45
1:C:475:ASN:ND2	1:C:590:VAL:CG1	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:607:ASP:O	1:C:610:THR:HB	2.17	0.45
2:D:26:ILE:O	2:D:26:ILE:HG22	2.16	0.45
1:E:147:HIS:C	1:E:149:MET:H	2.18	0.45
1:E:551:THR:O	1:E:552:ASP:C	2.55	0.45
1:E:611:SER:HA	1:E:614:ASN:HB2	1.99	0.45
1:E:699:HIS:HA	1:E:702:LEU:HB2	1.98	0.45
1:E:746:PHE:O	1:E:747:MET:HB2	2.17	0.45
1:G:145:LYS:HG3	1:G:146:ARG:NE	2.32	0.45
1:G:39:SER:OG	1:G:42:HIS:HB2	2.17	0.45
1:A:226:GLN:O	1:A:230:ILE:HD12	2.17	0.45
1:A:43:GLY:HA2	1:A:699:HIS:CE1	2.51	0.45
1:A:719:GLN:HA	1:A:719:GLN:HE21	1.81	0.45
1:C:116:TYR:HD1	1:C:121:CYS:HB2	1.80	0.45
1:C:196:VAL:CG1	1:C:197:VAL:N	2.79	0.45
1:C:282:LYS:O	1:C:283:ASP:HB2	2.17	0.45
1:C:420:LYS:HD2	1:C:421:GLU:OE2	2.17	0.45
1:C:89:MET:O	1:C:91:GLU:N	2.49	0.45
1:E:797:ILE:CG1	2:F:117:GLU:HG2	2.46	0.45
1:G:362:LEU:HD12	1:G:387:VAL:HG13	1.97	0.45
1:G:8:ASP:HA	1:G:11:LYS:CD	2.21	0.45
2:H:71:PRO:HA	2:H:74:GLN:NE2	2.32	0.45
1:A:17:LYS:HB3	1:A:17:LYS:HE2	1.66	0.45
1:A:272:LEU:CD1	1:A:272:LEU:C	2.83	0.45
1:A:699:HIS:HA	1:A:702:LEU:HB2	1.98	0.45
1:A:806:TYR:CG	2:B:147:VAL:HG12	2.52	0.45
2:B:140:TYR:CE1	2:B:141:GLU:HG2	2.51	0.45
2:B:140:TYR:O	2:B:142:GLU:N	2.50	0.45
2:B:85:PHE:CD1	2:B:144:VAL:HG11	2.52	0.45
2:B:35:MET:CE	2:B:73:MET:HA	2.47	0.45
2:B:71:PRO:HA	2:B:74:GLN:NE2	2.32	0.45
1:C:147:HIS:C	1:C:149:MET:H	2.20	0.45
1:C:132:ILE:HD12	1:C:152:HIS:HD2	1.82	0.45
1:C:236:ASN:ND2	1:C:246:SER:CA	2.76	0.45
1:C:348:GLU:O	1:C:352:ILE:HG13	2.16	0.45
1:C:504:GLU:HG3	1:C:504:GLU:O	2.15	0.45
1:C:557:GLU:O	1:C:560:ILE:HG12	2.16	0.45
1:C:728:GLN:O	1:C:728:GLN:NE2	2.50	0.45
1:E:352:ILE:O	1:E:356:VAL:HG23	2.16	0.45
1:E:344:PHE:HE1	1:E:445:ARG:HB3	1.78	0.45
1:E:543:GLU:HG2	1:E:544:GLU:N	2.31	0.45
1:E:575:LEU:HD23	1:E:577:ASP:OD1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:747:MET:CG	1:E:751:GLN:NE2	2.80	0.45
1:G:267:ILE:CD1	1:G:450:LEU:HD12	2.45	0.45
1:G:522:GLN:OE1	1:G:525:ILE:HD12	2.17	0.45
2:H:132:GLU:HG2	2:H:132:GLU:H	1.49	0.45
1:A:308:GLU:OE1	1:A:312:ASN:HB3	2.16	0.45
1:A:351:SER:C	1:A:353:LEU:H	2.19	0.45
1:A:409:VAL:HB	1:A:414:VAL:CG2	2.46	0.45
1:A:265:ALA:N	1:A:450:LEU:O	2.49	0.45
1:A:776:PHE:CD2	1:A:781:LEU:HD22	2.51	0.45
1:C:145:LYS:HB2	1:C:145:LYS:HE3	1.57	0.45
1:C:293:LEU:HD11	1:C:301:MET:HE2	1.98	0.45
1:C:566:HIS:CE1	1:C:568:LYS:HB2	2.52	0.45
2:D:95:PHE:CZ	2:D:111:VAL:HG21	2.50	0.45
2:D:114:THR:O	2:D:115:LEU:HD12	2.16	0.45
1:E:14:PHE:HE2	1:E:140:MET:HE1	1.81	0.45
1:E:267:ILE:N	1:E:447:ASN:HD21	2.15	0.45
4:E:999:ALF:F4	5:E:998:ADP:PB	2.65	0.45
2:F:35:MET:CE	2:F:73:MET:HA	2.47	0.45
1:G:762:LEU:HD13	1:G:766:LEU:HD13	1.98	0.45
2:H:26:ILE:O	2:H:26:ILE:HG22	2.17	0.45
1:A:149:MET:HB3	1:A:150:PRO:HD2	1.99	0.45
1:A:425:PHE:CD1	1:A:425:PHE:O	2.69	0.45
1:A:611:SER:HA	1:A:614:ASN:HB2	1.98	0.45
1:A:762:LEU:HD13	1:A:766:LEU:CD1	2.47	0.45
4:A:999:ALF:F4	5:A:998:ADP:PB	2.64	0.45
2:B:85:PHE:O	2:B:86:GLU:C	2.54	0.45
2:B:92:LEU:HD13	2:B:108:ILE:HD11	1.98	0.45
1:C:522:GLN:O	1:C:525:ILE:HG13	2.16	0.45
4:C:999:ALF:F4	5:C:998:ADP:PB	2.65	0.45
1:C:802:GLN:HG3	2:D:88:TYR:OH	2.17	0.45
1:E:267:ILE:H	1:E:447:ASN:HD21	1.64	0.45
1:E:449:ALA:C	1:E:451:ASP:H	2.18	0.45
1:E:437:ARG:NH2	1:E:625:TRP:CE3	2.85	0.45
1:E:183:LYS:HE2	5:E:998:ADP:O1B	2.17	0.45
2:F:80:LYS:H	2:F:80:LYS:CD	2.29	0.45
2:F:92:LEU:C	2:F:94:VAL:H	2.20	0.45
1:G:376:ALA:CB	1:G:420:LYS:HB2	2.42	0.45
1:G:53:LYS:HD2	1:G:58:THR:HG23	1.98	0.45
2:H:133:ASP:OD1	2:H:135:ASN:N	2.50	0.45
1:A:177:GLY:O	1:A:183:LYS:NZ	2.49	0.45
1:A:199:SER:HB2	1:A:221:GLU:CD	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:LYS:HD2	1:A:58:THR:HG23	1.99	0.45
1:C:146:ARG:NH1	1:C:159:THR:HG23	2.32	0.45
1:C:211:GLN:HG3	1:C:214:SER:HB2	1.97	0.45
1:C:256:PHE:HE1	1:C:262:ILE:HG13	1.81	0.45
1:C:582:CYS:HG	1:C:591:THR:HG23	1.78	0.45
1:C:765:ASN:O	1:C:777:ARG:NH2	2.47	0.45
1:C:80:PRO:HD2	1:C:83:PHE:HD2	1.81	0.45
2:D:105:GLY:O	2:D:109:ARG:HB2	2.16	0.45
1:E:239:THR:C	1:E:241:LYS:H	2.19	0.45
1:G:344:PHE:N	1:G:344:PHE:CD1	2.83	0.45
1:G:683:ARG:HE	1:G:683:ARG:HB3	1.53	0.45
1:G:806:TYR:CG	2:H:147:VAL:HG12	2.51	0.45
1:A:228:ASN:N	1:A:229:PRO:CD	2.80	0.44
1:A:551:THR:O	1:A:552:ASP:C	2.55	0.44
1:A:575:LEU:C	1:A:577:ASP:H	2.19	0.44
1:A:663:TYR:CZ	1:A:667:LEU:HD13	2.52	0.44
1:A:88:ASP:O	1:A:91:GLU:N	2.50	0.44
1:C:352:ILE:O	1:C:356:VAL:HG23	2.17	0.44
1:C:375:GLN:HG3	1:C:418:GLN:O	2.18	0.44
1:C:419:THR:O	1:C:422:GLN:N	2.51	0.44
1:C:504:GLU:OE2	1:C:508:GLU:HG2	2.17	0.44
1:C:535:PRO:CB	1:C:540:LEU:HD21	2.46	0.44
1:C:747:MET:HE3	1:C:755:LEU:HD22	1.99	0.44
2:D:144:VAL:O	2:D:147:VAL:HG23	2.17	0.44
1:E:153:ILE:CG2	1:E:154:TYR:N	2.80	0.44
1:E:381:ASN:O	1:E:382:THR:C	2.55	0.44
1:E:522:GLN:O	1:E:525:ILE:HG13	2.17	0.44
1:E:569:PHE:CD2	1:E:570:GLN:N	2.84	0.44
1:E:573:LYS:HD2	1:E:573:LYS:N	2.31	0.44
1:E:719:GLN:NE2	1:E:719:GLN:CA	2.78	0.44
1:E:89:MET:HE2	1:E:104:LEU:HD21	1.99	0.44
1:G:480:LEU:HA	1:G:592:TYR:CE1	2.52	0.44
1:G:46:ALA:HB1	1:G:62:GLN:HG2	1.99	0.44
1:A:402:ILE:HG22	1:A:403:LEU:HG	1.99	0.44
1:A:525:ILE:O	1:A:529:GLU:HB3	2.18	0.44
1:A:619:LYS:HA	1:A:622:ALA:HB3	1.99	0.44
2:B:26:ILE:O	2:B:26:ILE:HG22	2.17	0.44
1:C:152:HIS:ND1	1:C:154:TYR:N	2.62	0.44
1:C:310:PHE:O	1:C:311:ASN:HB2	2.17	0.44
1:C:355:VAL:HG21	1:C:620:PHE:CE2	2.52	0.44
1:C:437:ARG:HD2	1:C:624:LEU:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:719:GLN:CA	1:C:719:GLN:HE21	2.30	0.44
1:C:508:GLU:HG3	1:C:775:PHE:CE1	2.53	0.44
2:D:135:ASN:HB2	2:D:137:CYS:SG	2.57	0.44
1:E:103:ASN:HD21	1:E:107:ARG:HD2	1.81	0.44
1:E:120:PHE:N	1:E:120:PHE:CD1	2.73	0.44
1:E:365:ILE:HD11	1:E:384:ALA:HB2	1.98	0.44
1:E:726:VAL:HA	1:E:773:LYS:HA	1.98	0.44
1:G:102:HIS:O	1:G:105:ARG:N	2.50	0.44
1:G:132:ILE:HD12	1:G:152:HIS:HD2	1.80	0.44
1:G:164:MET:HE3	1:G:461:LEU:HD12	1.99	0.44
1:G:225:LEU:HD12	1:G:225:LEU:HA	1.86	0.44
1:G:296:GLY:HA3	1:G:332:PHE:CG	2.52	0.44
1:G:553:THR:HG22	1:G:557:GLU:OE2	2.17	0.44
1:A:145:LYS:HB2	1:A:145:LYS:HE3	1.56	0.44
1:A:152:HIS:CE1	1:A:153:ILE:HG22	2.53	0.44
1:A:266:ASN:HD22	1:A:267:ILE:H	1.65	0.44
2:B:9:ALA:HA	2:B:12:LYS:CE	2.48	0.44
1:C:7:SER:N	1:C:10:GLU:OE1	2.45	0.44
1:C:575:LEU:C	1:C:577:ASP:N	2.70	0.44
1:C:763:ASP:N	1:C:766:LEU:HD12	2.32	0.44
1:E:306:LEU:HD22	1:E:386:LYS:CD	2.47	0.44
1:E:321:VAL:HG13	1:E:322:PRO:HD2	1.98	0.44
1:E:369:LYS:HG3	1:E:370:GLU:H	1.82	0.44
1:E:541:LEU:HD11	1:E:597:TRP:HB3	2.00	0.44
1:E:527:LEU:HD12	1:E:566:HIS:CD2	2.52	0.44
1:E:718:ARG:HG3	1:E:719:GLN:N	2.33	0.44
1:G:256:PHE:HA	1:G:261:TYR:O	2.18	0.44
1:G:272:LEU:O	1:G:274:LYS:N	2.47	0.44
1:G:33:LYS:O	1:G:48:SER:HA	2.17	0.44
4:G:999:ALF:F4	5:G:998:ADP:PB	2.64	0.44
1:A:103:ASN:HD21	1:A:107:ARG:HD2	1.82	0.44
1:A:145:LYS:CG	1:A:146:ARG:N	2.78	0.44
1:A:189:LYS:O	1:A:192:GLN:HB3	2.17	0.44
1:A:491:GLN:OE1	1:A:521:LEU:HG	2.16	0.44
1:A:575:LEU:C	1:A:577:ASP:N	2.71	0.44
1:A:575:LEU:HD23	1:A:577:ASP:OD1	2.17	0.44
1:A:663:TYR:HH	1:A:667:LEU:HD13	1.82	0.44
1:A:745:GLY:H	1:G:819:LEU:CD2	2.31	0.44
1:C:395:VAL:O	1:C:398:PHE:N	2.50	0.44
1:C:543:GLU:C	1:C:545:CYS:N	2.70	0.44
1:C:700:LEU:O	1:C:700:LEU:HD23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:145:LYS:HG3	1:E:146:ARG:NE	2.32	0.44
1:E:38:PRO:HG2	1:E:70:LEU:HD13	1.99	0.44
1:E:409:VAL:HB	1:E:414:VAL:CG2	2.48	0.44
1:E:489:LEU:C	1:E:489:LEU:HD12	2.38	0.44
1:E:3:GLN:O	1:E:4:LYS:O	2.36	0.44
1:E:553:THR:HG22	1:E:557:GLU:OE2	2.18	0.44
1:E:663:TYR:CZ	1:E:667:LEU:HD13	2.52	0.44
1:E:716:ILE:HA	1:E:719:GLN:HB2	1.98	0.44
2:F:104:MET:H	2:F:104:MET:HG3	1.51	0.44
2:F:71:PRO:HA	2:F:74:GLN:NE2	2.32	0.44
1:G:197:VAL:HG12	1:G:197:VAL:O	2.17	0.44
1:G:618:ASP:CG	1:G:621:VAL:HG23	2.38	0.44
1:G:437:ARG:NE	1:G:625:TRP:HA	2.26	0.44
1:A:146:ARG:NH1	1:A:159:THR:HG23	2.31	0.44
1:A:22:ASN:O	1:A:22:ASN:ND2	2.51	0.44
1:A:234:PHE:CE1	1:A:289:ILE:HG12	2.53	0.44
1:A:391:MET:HB3	1:A:393:ILE:HG12	2.00	0.44
1:A:466:ILE:HD12	1:A:467:ALA:O	2.16	0.44
1:A:171:GLN:HA	1:A:678:ASN:H	1.83	0.44
1:C:145:LYS:HG3	1:C:146:ARG:NE	2.33	0.44
1:C:402:ILE:HG22	1:C:403:LEU:HG	1.99	0.44
1:C:53:LYS:HD2	1:C:58:THR:HG23	1.99	0.44
1:C:556:VAL:O	1:C:560:ILE:HG12	2.17	0.44
1:C:769:ILE:HD13	1:C:774:ILE:HG23	2.00	0.44
2:D:71:PRO:HA	2:D:74:GLN:NE2	2.32	0.44
2:F:84:CYS:O	2:F:86:GLU:N	2.50	0.44
1:G:184:THR:O	1:G:185:GLU:C	2.55	0.44
1:G:424:ASP:C	1:G:426:ALA:H	2.20	0.44
1:G:610:THR:CG2	1:G:631:ILE:HG13	2.34	0.44
2:H:140:TYR:O	2:H:142:GLU:N	2.50	0.44
2:H:4:SER:N	2:H:7:GLN:NE2	2.61	0.44
2:H:85:PHE:CE1	2:H:144:VAL:HG12	2.52	0.44
1:A:12:PHE:CD1	1:A:111:GLY:HA3	2.53	0.44
1:A:152:HIS:ND1	1:A:154:TYR:N	2.62	0.44
1:A:172:SER:OG	1:A:679:PRO:HA	2.18	0.44
1:A:23:PRO:O	1:A:27:ALA:CB	2.66	0.44
1:A:369:LYS:HG3	1:A:370:GLU:H	1.81	0.44
1:A:408:LYS:HG2	1:A:412:ASP:O	2.17	0.44
1:A:477:PHE:O	1:A:480:LEU:N	2.46	0.44
2:B:55:LYS:H	2:B:58:GLU:HG2	1.83	0.44
1:C:13:LEU:HD11	1:C:132:ILE:CB	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:228:ASN:N	1:C:229:PRO:CD	2.81	0.44
1:C:253:ARG:O	1:C:265:ALA:HA	2.18	0.44
1:C:38:PRO:HG2	1:C:70:LEU:HD13	1.99	0.44
1:E:361:GLN:CG	1:E:387:VAL:HG23	2.47	0.44
2:F:26:ILE:O	2:F:26:ILE:HG22	2.17	0.44
1:G:116:TYR:HD1	1:G:121:CYS:HB2	1.82	0.44
1:G:582:CYS:HA	1:G:590:VAL:O	2.18	0.44
1:G:270:TYR:OH	1:G:670:LEU:HD22	2.17	0.44
1:A:475:ASN:HB2	1:A:592:TYR:HA	1.99	0.44
2:B:20:ARG:HB2	2:B:20:ARG:HE	1.47	0.44
1:C:305:LEU:HB2	1:C:307:LEU:HG	1.98	0.44
1:C:359:VAL:CG1	1:C:359:VAL:O	2.66	0.44
1:C:604:PRO:O	1:C:605:LEU:HB2	2.17	0.44
1:C:613:LEU:C	1:C:615:GLN:N	2.71	0.44
2:D:9:ALA:HA	2:D:12:LYS:CE	2.47	0.44
2:D:50:VAL:O	2:D:51:LEU:HD23	2.18	0.44
1:E:141:TYR:CE1	1:E:149:MET:HB3	2.53	0.44
1:E:397:ASP:O	1:E:398:PHE:C	2.56	0.44
1:E:419:THR:O	1:E:422:GLN:N	2.51	0.44
1:E:44:PHE:CD2	1:E:98:ALA:HA	2.53	0.44
1:E:543:GLU:C	1:E:545:CYS:N	2.71	0.44
1:E:610:THR:CG2	1:E:631:ILE:HG13	2.33	0.44
2:F:128:VAL:HG23	2:F:129:ALA:N	2.33	0.44
2:F:25:LYS:HE3	2:F:65:LYS:HE2	2.00	0.44
1:G:153:ILE:CG2	1:G:154:TYR:N	2.81	0.44
1:G:261:TYR:CD1	1:G:261:TYR:N	2.86	0.44
1:G:293:LEU:HD11	1:G:301:MET:HE1	1.99	0.44
1:G:37:VAL:CB	1:G:38:PRO:HD2	2.47	0.44
1:G:407:ILE:CD1	1:G:409:VAL:H	2.30	0.44
1:G:375:GLN:HG3	1:G:418:GLN:O	2.18	0.44
1:G:51:GLU:HB3	1:G:53:LYS:HD2	2.00	0.44
1:G:575:LEU:HD23	1:G:577:ASP:OD1	2.18	0.44
2:H:98:GLU:O	2:H:100:ASN:OD1	2.36	0.44
1:A:116:TYR:HD1	1:A:121:CYS:HB2	1.82	0.44
2:B:98:GLU:O	2:B:100:ASN:OD1	2.36	0.44
1:C:280:GLN:NE2	1:C:280:GLN:N	2.66	0.44
1:C:354:ARG:HG3	1:C:355:VAL:N	2.32	0.44
1:C:267:ILE:CD1	1:C:450:LEU:HD12	2.48	0.44
1:C:183:LYS:HZ1	1:C:468:GLY:HA3	1.83	0.44
1:C:88:ASP:O	1:C:91:GLU:HB2	2.18	0.44
2:D:14:ALA:HB3	2:D:38:LEU:HD21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:35:MET:HE1	2:D:73:MET:HA	2.00	0.44
1:E:566:HIS:CE1	1:E:568:LYS:HB2	2.52	0.44
1:E:767:TYR:O	1:E:768:ARG:HD3	2.18	0.44
2:F:125:GLU:O	2:F:129:ALA:CB	2.66	0.44
2:F:9:ALA:HA	2:F:12:LYS:CE	2.47	0.44
1:G:138:ILE:HG21	1:G:196:VAL:HG11	1.99	0.44
1:G:226:GLN:HG2	1:G:341:ILE:HB	1.99	0.44
1:G:365:ILE:HD11	1:G:384:ALA:HB2	2.00	0.44
1:G:395:VAL:O	1:G:398:PHE:N	2.51	0.44
2:H:120:THR:HG23	2:H:123:GLU:CG	2.48	0.44
2:H:35:MET:CE	2:H:73:MET:HA	2.47	0.44
1:C:275:SER:O	1:C:278:ILE:HG12	2.18	0.44
1:C:370:GLU:OE1	1:C:372:ASN:HB2	2.18	0.44
1:C:388:CYS:SG	1:C:393:ILE:HD11	2.57	0.44
1:C:45:GLU:OE2	1:C:61:LEU:HB3	2.18	0.44
1:C:64:ASN:C	1:C:66:LYS:N	2.71	0.44
1:E:128:LYS:HG2	1:E:129:GLN:N	2.32	0.44
1:E:285:ARG:HG2	1:E:291:TYR:CZ	2.52	0.44
1:E:294:ILE:HB	1:E:310:PHE:CZ	2.53	0.44
1:E:51:GLU:HB3	1:E:53:LYS:HD2	2.00	0.44
1:E:578:LYS:C	1:E:579:THR:OG1	2.56	0.44
1:E:619:LYS:O	1:E:622:ALA:CB	2.63	0.44
1:G:33:LYS:O	1:G:49:ILE:HG13	2.18	0.44
1:G:352:ILE:HG22	1:G:438:LEU:HD21	2.00	0.44
1:G:369:LYS:HG3	1:G:370:GLU:H	1.82	0.44
1:G:306:LEU:HD22	1:G:386:LYS:HD3	1.99	0.44
1:G:409:VAL:HB	1:G:414:VAL:CG2	2.48	0.44
1:G:606:ASN:OD1	1:G:608:ASN:HB2	2.17	0.44
1:G:728:GLN:NE2	1:G:728:GLN:O	2.51	0.44
2:H:9:ALA:HA	2:H:12:LYS:CE	2.48	0.44
1:A:87:GLU:OE1	1:A:107:ARG:NH2	2.51	0.43
1:A:251:PHE:CD1	1:A:251:PHE:O	2.71	0.43
1:A:33:LYS:CG	1:A:49:ILE:HB	2.48	0.43
1:A:39:SER:C	1:A:41:LYS:H	2.22	0.43
1:A:3:GLN:O	1:A:4:LYS:O	2.36	0.43
1:A:172:SER:HA	1:A:462:GLY:O	2.17	0.43
1:A:610:THR:HG22	1:A:628:VAL:HG11	2.00	0.43
1:C:172:SER:HA	1:C:462:GLY:O	2.18	0.43
1:C:367:PHE:CE1	1:C:378:MET:SD	3.11	0.43
1:C:575:LEU:HA	1:C:577:ASP:OD2	2.17	0.43
1:C:771:GLN:O	1:C:771:GLN:NE2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:138:ILE:HG21	1:E:196:VAL:HG11	2.00	0.43
1:E:362:LEU:HD12	1:E:387:VAL:HG13	2.00	0.43
1:E:389:HIS:C	1:E:389:HIS:HD1	2.21	0.43
1:E:620:PHE:O	1:E:624:LEU:HB2	2.18	0.43
1:G:176:THR:O	1:G:183:LYS:HD2	2.18	0.43
1:G:485:THR:HA	1:G:488:LYS:HB2	2.00	0.43
1:G:545:CYS:HA	1:G:598:LEU:HD22	2.01	0.43
1:G:621:VAL:HG12	1:G:625:TRP:CD1	2.53	0.43
1:A:743:PRO:HB2	1:G:816:GLN:CG	2.47	0.43
2:H:140:TYR:CE1	2:H:141:GLU:HG2	2.53	0.43
2:H:144:VAL:O	2:H:147:VAL:HG23	2.18	0.43
2:H:50:VAL:O	2:H:51:LEU:HD23	2.18	0.43
2:H:64:LEU:HD21	2:H:72:MET:HE1	2.00	0.43
1:A:121:CYS:SG	1:A:156:ILE:HD11	2.58	0.43
1:A:256:PHE:HA	1:A:261:TYR:O	2.19	0.43
1:A:256:PHE:CE1	1:A:262:ILE:HG13	2.52	0.43
1:A:442:ILE:O	1:A:445:ARG:N	2.43	0.43
1:A:487:GLU:OE1	1:A:585:HIS:HA	2.18	0.43
1:A:728:GLN:CA	1:A:728:GLN:NE2	2.80	0.43
1:C:424:ASP:C	1:C:426:ALA:H	2.21	0.43
2:D:128:VAL:HG23	2:D:129:ALA:N	2.33	0.43
1:E:257:ASP:C	1:E:257:ASP:OD1	2.54	0.43
1:E:362:LEU:CD2	1:E:427:ILE:HG13	2.48	0.43
1:E:98:ALA:O	1:E:101:LEU:HB3	2.18	0.43
2:F:111:VAL:HA	2:F:115:LEU:HD13	1.99	0.43
2:F:143:LEU:O	2:F:147:VAL:HG22	2.18	0.43
2:F:76:ILE:O	2:F:77:ALA:C	2.57	0.43
1:G:158:ASP:HB2	1:G:193:TYR:CZ	2.54	0.43
1:G:167:ASP:O	1:G:168:ARG:C	2.56	0.43
1:G:565:ASN:O	1:G:565:ASN:CG	2.56	0.43
1:G:762:LEU:HD13	1:G:766:LEU:HD12	2.00	0.43
2:H:84:CYS:N	2:H:88:TYR:CE2	2.86	0.43
1:A:407:ILE:CG1	1:A:414:VAL:O	2.63	0.43
1:A:45:GLU:OE2	1:A:61:LEU:HB3	2.19	0.43
1:A:606:ASN:OD1	1:A:608:ASN:HB2	2.18	0.43
1:A:625:TRP:C	1:A:627:ASP:N	2.68	0.43
1:C:405:PRO:O	1:C:407:ILE:HG23	2.19	0.43
1:C:265:ALA:O	1:C:450:LEU:HB2	2.18	0.43
1:C:33:LYS:O	1:C:49:ILE:HG13	2.18	0.43
1:C:573:LYS:N	1:C:573:LYS:HD2	2.32	0.43
1:C:610:THR:HG21	1:C:628:VAL:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:18:PHE:CD2	2:D:34:VAL:HG22	2.53	0.43
2:D:76:ILE:O	2:D:77:ALA:C	2.56	0.43
1:E:45:GLU:OE2	1:E:61:LEU:HB3	2.18	0.43
1:G:388:CYS:SG	1:G:393:ILE:HD11	2.58	0.43
1:G:613:LEU:C	1:G:615:GLN:N	2.72	0.43
1:G:270:TYR:CZ	1:G:670:LEU:HD22	2.53	0.43
1:A:9:ASP:O	1:A:12:PHE:HB2	2.18	0.43
1:A:323:ILE:O	1:A:323:ILE:HG23	2.18	0.43
1:A:344:PHE:N	1:A:344:PHE:CD1	2.86	0.43
1:A:373:THR:O	1:A:374:ASP:HB2	2.19	0.43
1:A:413:VAL:O	1:A:415:GLN:N	2.51	0.43
1:A:419:THR:O	1:A:422:GLN:N	2.51	0.43
1:A:618:ASP:CG	1:A:621:VAL:HG23	2.38	0.43
1:A:771:GLN:CA	1:A:771:GLN:NE2	2.81	0.43
2:B:85:PHE:CZ	2:B:145:ARG:NH1	2.86	0.43
2:B:96:ASP:O	2:B:98:GLU:N	2.52	0.43
1:C:395:VAL:O	1:C:396:THR:C	2.56	0.43
1:C:405:PRO:CD	1:C:416:LYS:O	2.66	0.43
1:E:302:ARG:CZ	1:E:303:ASN:HA	2.49	0.43
1:E:31:ALA:C	1:E:33:LYS:N	2.72	0.43
1:E:437:ARG:NH2	1:E:625:TRP:HE3	2.16	0.43
2:F:111:VAL:HG12	2:F:112:LEU:HD23	2.00	0.43
1:G:428:GLU:C	1:G:430:LEU:N	2.72	0.43
1:G:83:PHE:CZ	1:G:92:LEU:HA	2.54	0.43
2:H:104:MET:H	2:H:104:MET:HG3	1.48	0.43
2:H:109:ARG:NH2	2:H:132:GLU:OE2	2.50	0.43
1:A:33:LYS:O	1:A:49:ILE:HG13	2.18	0.43
1:A:46:ALA:HB1	1:A:62:GLN:HG2	2.00	0.43
1:A:607:ASP:N	1:A:607:ASP:OD1	2.34	0.43
1:A:60:GLU:OE1	1:A:67:LYS:HD2	2.17	0.43
1:A:743:PRO:CD	1:A:747:MET:HE1	2.48	0.43
1:A:814:LYS:C	1:A:816:GLN:N	2.72	0.43
2:B:124:VAL:HG23	2:B:125:GLU:N	2.33	0.43
1:C:347:GLU:H	1:C:347:GLU:HG3	1.55	0.43
1:C:365:ILE:HD13	1:C:427:ILE:CD1	2.47	0.43
1:C:558:LYS:O	1:C:561:GLN:N	2.51	0.43
1:C:606:ASN:OD1	1:C:608:ASN:HB2	2.17	0.43
1:C:104:LEU:CD1	1:C:705:LEU:HD11	2.48	0.43
1:C:87:GLU:HA	1:C:87:GLU:OE1	2.18	0.43
2:D:92:LEU:C	2:D:94:VAL:H	2.22	0.43
1:E:132:ILE:HD12	1:E:152:HIS:HD2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:504:GLU:OE2	1:E:508:GLU:HG2	2.18	0.43
1:E:553:THR:HG23	1:E:579:THR:CG2	2.49	0.43
1:E:409:VAL:HG13	1:E:634:LEU:HD12	2.00	0.43
1:E:64:ASN:C	1:E:66:LYS:N	2.71	0.43
1:E:80:PRO:CD	1:E:83:PHE:CD2	2.99	0.43
1:G:349:GLN:HA	1:G:352:ILE:HG13	2.00	0.43
1:G:504:GLU:O	1:G:504:GLU:HG3	2.19	0.43
1:A:247:ARG:HH22	1:A:470:GLU:CD	2.22	0.43
1:A:164:MET:CE	1:A:256:PHE:CE2	3.02	0.43
1:A:349:GLN:HA	1:A:352:ILE:HG13	2.01	0.43
1:A:375:GLN:HG3	1:A:418:GLN:O	2.18	0.43
1:A:613:LEU:C	1:A:615:GLN:N	2.72	0.43
1:A:686:ILE:O	1:A:686:ILE:HG22	2.17	0.43
1:C:329:ASP:OD1	1:C:329:ASP:N	2.42	0.43
1:C:39:SER:OG	1:C:42:HIS:HB2	2.19	0.43
1:C:446:VAL:HG12	1:C:447:ASN:N	2.33	0.43
1:C:814:LYS:CE	1:C:818:GLN:HE22	2.22	0.43
1:E:152:HIS:ND1	1:E:154:TYR:N	2.63	0.43
1:E:323:ILE:HG23	1:E:323:ILE:O	2.19	0.43
1:E:37:VAL:CB	1:E:38:PRO:HD2	2.48	0.43
1:E:582:CYS:HA	1:E:590:VAL:O	2.19	0.43
1:E:619:LYS:HA	1:E:622:ALA:CB	2.48	0.43
1:G:223:GLN:C	1:G:225:LEU:N	2.71	0.43
1:G:514:PHE:CG	1:G:515:ILE:N	2.86	0.43
2:H:114:THR:O	2:H:115:LEU:HD12	2.18	0.43
2:H:14:ALA:HB3	2:H:38:LEU:HD21	2.00	0.43
2:H:25:LYS:HE3	2:H:65:LYS:HE2	2.00	0.43
1:A:102:HIS:O	1:A:105:ARG:N	2.52	0.43
1:A:376:ALA:CB	1:A:420:LYS:HB2	2.44	0.43
1:A:492:LEU:O	1:A:496:THR:OG1	2.37	0.43
1:A:530:ARG:HA	1:A:531:PRO:HD3	1.79	0.43
1:A:89:MET:C	1:A:91:GLU:N	2.70	0.43
2:B:111:VAL:HA	2:B:115:LEU:HD13	2.00	0.43
1:A:797:ILE:CG1	2:B:117:GLU:HG2	2.49	0.43
2:B:50:VAL:O	2:B:51:LEU:HD23	2.18	0.43
1:C:373:THR:O	1:C:374:ASP:HB2	2.19	0.43
1:C:382:THR:CA	1:C:385:GLN:HB3	2.49	0.43
1:C:361:GLN:CG	1:C:387:VAL:HG23	2.48	0.43
1:C:394:ASN:OD1	1:C:397:ASP:OD2	2.37	0.43
1:C:407:ILE:HD12	1:C:408:LYS:CA	2.48	0.43
1:C:619:LYS:HA	1:C:622:ALA:CB	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:182:GLY:HA2	5:C:998:ADP:O1A	2.19	0.43
1:E:145:LYS:CG	1:E:146:ARG:N	2.81	0.43
1:E:231:LEU:HD23	1:E:231:LEU:N	2.33	0.43
1:E:565:ASN:O	1:E:565:ASN:CG	2.56	0.43
1:G:293:LEU:O	1:G:297:ALA:HB2	2.19	0.43
1:G:318:ASN:O	1:G:319:GLY:C	2.57	0.43
1:G:474:ILE:H	1:G:474:ILE:HG13	1.47	0.43
1:G:525:ILE:O	1:G:529:GLU:HB3	2.18	0.43
1:G:575:LEU:C	1:G:577:ASP:N	2.71	0.43
1:G:711:LEU:N	1:G:711:LEU:CD2	2.81	0.43
2:H:76:ILE:O	2:H:77:ALA:C	2.57	0.43
1:A:389:HIS:C	1:A:389:HIS:HD1	2.22	0.43
1:A:395:VAL:O	1:A:398:PHE:N	2.52	0.43
1:A:428:GLU:C	1:A:430:LEU:N	2.72	0.43
1:A:250:LYS:CE	1:A:465:ASP:OD2	2.66	0.43
1:A:522:GLN:OE1	1:A:525:ILE:HD12	2.19	0.43
1:A:582:CYS:HA	1:A:590:VAL:O	2.19	0.43
1:A:409:VAL:HG13	1:A:634:LEU:HD11	1.99	0.43
1:A:64:ASN:C	1:A:66:LYS:N	2.72	0.43
2:B:25:LYS:HE3	2:B:65:LYS:HE2	2.00	0.43
1:C:195:ALA:O	1:C:199:SER:HB3	2.18	0.43
1:C:389:HIS:C	1:C:389:HIS:HD1	2.21	0.43
1:C:543:GLU:HG2	1:C:544:GLU:N	2.30	0.43
1:C:551:THR:H	1:C:554:SER:HG	1.59	0.43
1:C:572:SER:HB2	1:C:580:GLU:HG3	2.01	0.43
1:C:582:CYS:HA	1:C:590:VAL:O	2.19	0.43
1:C:541:LEU:HD22	1:C:597:TRP:HE3	1.84	0.43
2:D:55:LYS:H	2:D:58:GLU:HG2	1.82	0.43
1:E:235:GLY:HA3	1:E:248:PHE:CE1	2.54	0.43
1:E:280:GLN:NE2	1:E:280:GLN:N	2.67	0.43
1:E:280:GLN:NE2	1:E:315:PHE:O	2.46	0.43
1:E:327:GLN:HB3	1:E:330:GLU:CG	2.49	0.43
1:E:344:PHE:CD1	1:E:344:PHE:N	2.85	0.43
1:E:415:GLN:OE1	1:E:416:LYS:N	2.51	0.43
2:F:139:ASN:OD1	2:F:142:GLU:HG2	2.18	0.43
1:G:134:SER:O	1:G:135:GLU:C	2.56	0.43
1:G:195:ALA:O	1:G:199:SER:HB3	2.18	0.43
1:G:743:PRO:CD	1:G:747:MET:HE1	2.48	0.43
1:G:747:MET:HE1	1:G:755:LEU:CD2	2.49	0.43
2:H:104:MET:O	2:H:106:ALA:N	2.51	0.43
1:A:806:TYR:HB3	2:B:147:VAL:HG12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:GLN:HA	1:C:678:ASN:H	1.84	0.43
2:D:111:VAL:HA	2:D:115:LEU:HD13	2.00	0.43
2:D:41:ASN:N	2:D:42:PRO:CD	2.82	0.43
1:E:39:SER:C	1:E:41:LYS:H	2.22	0.43
1:E:404:THR:O	1:E:404:THR:OG1	2.30	0.43
1:E:817:GLN:HG2	1:E:818:GLN:OE1	2.19	0.43
1:G:323:ILE:HG23	1:G:323:ILE:O	2.18	0.43
1:G:389:HIS:HD1	1:G:389:HIS:C	2.21	0.43
1:G:397:ASP:O	1:G:398:PHE:C	2.57	0.43
1:G:88:ASP:O	1:G:91:GLU:HB2	2.19	0.43
1:A:330:GLU:O	1:A:331:MET:C	2.57	0.43
1:A:361:GLN:CG	1:A:387:VAL:HG23	2.49	0.43
1:A:480:LEU:HA	1:A:592:TYR:CE1	2.54	0.43
1:C:134:SER:O	1:C:135:GLU:C	2.57	0.43
1:C:161:TYR:O	1:C:161:TYR:CG	2.71	0.43
1:C:164:MET:CE	1:C:256:PHE:CE2	3.02	0.43
1:C:467:ALA:O	1:C:486:ASN:ND2	2.44	0.43
1:C:514:PHE:CG	1:C:515:ILE:N	2.86	0.43
1:C:409:VAL:HG13	1:C:634:LEU:HD12	1.99	0.43
1:C:76:GLN:OE1	1:C:96:ASN:HB3	2.18	0.43
2:D:98:GLU:O	2:D:100:ASN:OD1	2.37	0.43
1:E:134:SER:O	1:E:135:GLU:C	2.55	0.43
1:E:180:GLY:C	1:E:182:GLY:H	2.21	0.43
1:E:371:ARG:HG3	1:E:371:ARG:H	1.42	0.43
1:E:424:ASP:C	1:E:426:ALA:H	2.22	0.43
1:E:475:ASN:ND2	1:E:590:VAL:CG1	2.82	0.43
1:E:172:SER:OG	1:E:679:PRO:HA	2.19	0.43
1:E:741:ALA:O	1:E:755:LEU:HD23	2.19	0.43
1:E:804:ARG:NH1	1:E:804:ARG:CG	2.77	0.43
2:F:50:VAL:O	2:F:51:LEU:HD23	2.18	0.43
1:G:275:SER:O	1:G:278:ILE:HG12	2.19	0.43
1:G:466:ILE:HD12	1:G:467:ALA:O	2.18	0.43
1:G:409:VAL:HG13	1:G:634:LEU:HD12	2.00	0.43
1:G:704:GLN:O	1:G:708:ASN:HB2	2.19	0.43
1:G:747:MET:HE1	1:G:755:LEU:HD22	2.00	0.43
1:A:13:LEU:HG	1:A:132:ILE:CG2	2.49	0.42
1:A:225:LEU:HA	1:A:225:LEU:HD12	1.89	0.42
1:A:356:VAL:O	1:A:360:LEU:HD12	2.19	0.42
1:A:39:SER:OG	1:A:42:HIS:HB2	2.19	0.42
1:A:407:ILE:CD1	1:A:409:VAL:H	2.30	0.42
1:A:541:LEU:HD11	1:A:597:TRP:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:769:ILE:HD13	1:A:769:ILE:HA	1.78	0.42
2:B:76:ILE:O	2:B:77:ALA:C	2.57	0.42
1:C:89:MET:HG2	1:C:116:TYR:O	2.18	0.42
1:C:174:LEU:HD12	1:C:681:PHE:CE1	2.53	0.42
1:C:762:LEU:HD13	1:C:766:LEU:HD13	2.01	0.42
1:E:183:LYS:HE2	1:E:183:LYS:HB2	1.65	0.42
1:E:375:GLN:HG3	1:E:418:GLN:O	2.19	0.42
1:E:491:GLN:OE1	1:E:521:LEU:HG	2.19	0.42
1:E:51:GLU:CG	1:E:53:LYS:HE3	2.48	0.42
1:E:619:LYS:HA	1:E:622:ALA:HB3	2.01	0.42
1:E:623:ASP:HA	1:E:626:LYS:HB3	2.01	0.42
1:E:37:VAL:HG13	1:E:75:ILE:HG22	2.01	0.42
1:E:80:PRO:CD	1:E:83:PHE:HD2	2.32	0.42
2:F:98:GLU:O	2:F:100:ASN:OD1	2.37	0.42
2:F:41:ASN:N	2:F:42:PRO:CD	2.82	0.42
1:G:146:ARG:NH1	1:G:159:THR:HG23	2.34	0.42
1:G:164:MET:SD	1:G:256:PHE:HD2	2.41	0.42
1:G:33:LYS:CG	1:G:49:ILE:HB	2.48	0.42
1:G:419:THR:O	1:G:421:GLU:N	2.51	0.42
1:G:619:LYS:HA	1:G:622:ALA:HB3	2.00	0.42
2:H:41:ASN:N	2:H:42:PRO:CD	2.82	0.42
2:H:92:LEU:C	2:H:94:VAL:H	2.23	0.42
1:A:405:PRO:HB2	1:A:407:ILE:HG22	1.98	0.42
1:A:71:SER:HB3	1:A:73:ASP:OD2	2.19	0.42
1:C:349:GLN:HA	1:C:352:ILE:HG13	2.00	0.42
1:C:359:VAL:HG12	1:C:359:VAL:O	2.19	0.42
1:C:478:GLU:N	1:C:478:GLU:OE1	2.26	0.42
2:D:135:ASN:ND2	2:D:135:ASN:N	2.67	0.42
1:E:154:TYR:OH	1:E:192:GLN:NE2	2.53	0.42
1:E:243:ASP:CB	1:E:323:ILE:HD11	2.46	0.42
1:E:545:CYS:SG	1:E:602:MET:SD	3.17	0.42
2:F:95:PHE:CZ	2:F:111:VAL:HG21	2.55	0.42
1:G:240:VAL:HG22	1:G:472:PHE:CE1	2.54	0.42
1:G:382:THR:CA	1:G:385:GLN:HB3	2.49	0.42
1:G:702:LEU:HD12	1:G:702:LEU:HA	1.82	0.42
1:G:763:ASP:H	1:G:766:LEU:CD1	2.31	0.42
1:A:178:GLU:O	1:A:183:LYS:NZ	2.53	0.42
1:A:196:VAL:CG1	1:A:197:VAL:N	2.81	0.42
1:A:275:SER:O	1:A:278:ILE:HG12	2.19	0.42
1:A:424:ASP:C	1:A:426:ALA:H	2.22	0.42
1:A:49:ILE:HG23	1:A:57:VAL:CG1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:18:PHE:CD2	2:B:34:VAL:HG22	2.54	0.42
1:C:391:MET:HE3	1:C:613:LEU:HD21	2.00	0.42
1:C:413:VAL:O	1:C:415:GLN:N	2.53	0.42
1:C:173:ILE:HD12	1:C:461:LEU:HD21	2.01	0.42
1:E:116:TYR:HD1	1:E:121:CYS:HB2	1.84	0.42
1:E:291:TYR:HD2	1:E:310:PHE:HE2	1.67	0.42
1:E:551:THR:O	1:E:554:SER:N	2.52	0.42
1:E:469:PHE:CD2	1:E:587:ALA:HB3	2.54	0.42
1:E:60:GLU:OE1	1:E:67:LYS:HD2	2.18	0.42
1:E:613:LEU:C	1:E:615:GLN:N	2.71	0.42
2:F:127:LEU:HD11	2:F:147:VAL:HG13	2.02	0.42
1:G:133:TYR:HB3	1:G:154:TYR:OH	2.19	0.42
1:G:138:ILE:HD11	1:G:154:TYR:CZ	2.54	0.42
1:G:121:CYS:SG	1:G:156:ILE:HD11	2.59	0.42
1:G:172:SER:OG	1:G:679:PRO:HA	2.20	0.42
1:G:352:ILE:O	1:G:356:VAL:HG23	2.19	0.42
1:G:37:VAL:HG13	1:G:75:ILE:HA	2.01	0.42
1:G:306:LEU:HD22	1:G:386:LYS:CD	2.49	0.42
1:G:522:GLN:N	1:G:523:PRO:CD	2.82	0.42
1:G:763:ASP:C	1:G:765:ASN:H	2.22	0.42
2:H:18:PHE:CD2	2:H:34:VAL:HG22	2.54	0.42
1:A:176:THR:O	1:A:183:LYS:HD2	2.20	0.42
1:A:24:LEU:HD23	1:A:24:LEU:N	2.34	0.42
1:A:397:ASP:O	1:A:398:PHE:C	2.57	0.42
1:C:106:GLU:O	1:C:107:ARG:C	2.57	0.42
1:C:302:ARG:CZ	1:C:303:ASN:HA	2.49	0.42
1:C:330:GLU:O	1:C:331:MET:C	2.57	0.42
1:C:565:ASN:CG	1:C:565:ASN:O	2.58	0.42
1:E:228:ASN:N	1:E:229:PRO:CD	2.82	0.42
1:E:305:LEU:HB2	1:E:307:LEU:HG	2.00	0.42
1:E:480:LEU:HA	1:E:592:TYR:CE1	2.54	0.42
1:E:535:PRO:CB	1:E:540:LEU:HD21	2.48	0.42
1:E:607:ASP:C	1:E:610:THR:HB	2.40	0.42
1:E:728:GLN:CA	1:E:728:GLN:NE2	2.81	0.42
2:F:14:ALA:HB3	2:F:38:LEU:HD21	2.00	0.42
1:G:23:PRO:O	1:G:27:ALA:CB	2.67	0.42
1:A:236:ASN:ND2	1:A:246:SER:CA	2.73	0.42
1:A:257:ASP:OD1	1:A:257:ASP:C	2.57	0.42
1:A:294:ILE:O	1:A:294:ILE:HG22	2.20	0.42
1:A:33:LYS:O	1:A:48:SER:HA	2.19	0.42
1:A:415:GLN:O	1:A:415:GLN:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:572:SER:HB2	1:A:580:GLU:HG3	2.01	0.42
1:A:683:ARG:HB3	1:A:683:ARG:HE	1.50	0.42
1:A:742:ILE:CD1	1:A:756:MET:HE3	2.50	0.42
1:A:83:PHE:CB	1:A:92:LEU:HD23	2.43	0.42
1:C:178:GLU:O	1:C:183:LYS:NZ	2.52	0.42
1:C:287:PHE:O	1:C:288:HIS:C	2.58	0.42
1:C:391:MET:CE	1:C:613:LEU:HD21	2.50	0.42
1:C:763:ASP:H	1:C:766:LEU:CD1	2.32	0.42
1:C:767:TYR:O	1:C:768:ARG:HD3	2.19	0.42
1:E:236:ASN:ND2	1:E:246:SER:CA	2.73	0.42
1:E:466:ILE:HD12	1:E:467:ALA:O	2.20	0.42
2:F:55:LYS:H	2:F:58:GLU:HG2	1.83	0.42
1:G:378:MET:CE	1:G:378:MET:HA	2.48	0.42
1:G:506:GLN:O	1:G:509:GLY:N	2.53	0.42
1:G:541:LEU:HD11	1:G:597:TRP:HB3	2.00	0.42
1:G:812:PHE:O	1:G:814:LYS:N	2.52	0.42
1:A:195:ALA:O	1:A:199:SER:HB3	2.19	0.42
1:A:43:GLY:HA2	1:A:699:HIS:NE2	2.34	0.42
1:A:513:ASN:O	1:A:513:ASN:ND2	2.41	0.42
1:A:51:GLU:CG	1:A:53:LYS:HE3	2.50	0.42
1:A:619:LYS:HA	1:A:622:ALA:CB	2.49	0.42
1:A:817:GLN:HG2	1:A:818:GLN:OE1	2.19	0.42
1:C:154:TYR:OH	1:C:192:GLN:NE2	2.53	0.42
1:C:17:LYS:HE2	1:C:17:LYS:HB3	1.67	0.42
1:C:272:LEU:HD12	1:C:273:GLU:N	2.34	0.42
1:C:344:PHE:CD1	1:C:344:PHE:N	2.88	0.42
1:C:349:GLN:O	1:C:350:THR:C	2.57	0.42
1:C:37:VAL:CB	1:C:38:PRO:HD2	2.49	0.42
1:C:485:THR:HA	1:C:488:LYS:HB2	2.01	0.42
1:C:494:ASN:H	1:C:494:ASN:ND2	2.10	0.42
1:C:97:GLU:HG2	1:C:702:LEU:HD11	2.01	0.42
1:C:89:MET:HG2	1:C:89:MET:H	1.51	0.42
1:E:685:ILE:HD11	1:E:705:LEU:HD23	2.02	0.42
2:F:10:GLU:CA	2:F:13:GLU:HG3	2.45	0.42
1:G:551:THR:H	1:G:554:SER:HG	1.60	0.42
1:G:557:GLU:O	1:G:560:ILE:HG12	2.19	0.42
1:G:572:SER:HB2	1:G:580:GLU:HG3	2.01	0.42
1:G:718:ARG:HG3	1:G:719:GLN:N	2.34	0.42
1:G:814:LYS:CE	1:G:818:GLN:HE22	2.22	0.42
1:A:106:GLU:O	1:A:107:ARG:C	2.57	0.42
1:A:244:ASN:CG	1:A:244:ASN:O	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:ILE:HG21	1:A:442:ILE:CD1	2.41	0.42
1:A:407:ILE:HD12	1:A:409:VAL:H	1.80	0.42
1:A:530:ARG:HG3	1:A:531:PRO:N	2.35	0.42
1:A:747:MET:HE1	1:A:755:LEU:CD2	2.50	0.42
2:B:14:ALA:HB3	2:B:38:LEU:HD21	2.00	0.42
2:B:41:ASN:N	2:B:42:PRO:CD	2.82	0.42
1:C:138:ILE:HG21	1:C:196:VAL:CG1	2.49	0.42
1:C:24:LEU:N	1:C:24:LEU:HD23	2.35	0.42
1:C:183:LYS:NZ	1:C:468:GLY:HA3	2.35	0.42
1:C:814:LYS:C	1:C:816:GLN:N	2.73	0.42
1:E:164:MET:CE	1:E:256:PHE:CE2	3.03	0.42
1:E:171:GLN:HA	1:E:678:ASN:H	1.85	0.42
1:E:275:SER:C	1:E:277:ALA:H	2.23	0.42
1:E:405:PRO:HB2	1:E:407:ILE:HG22	2.00	0.42
1:E:362:LEU:HD23	1:E:427:ILE:O	2.20	0.42
1:E:521:LEU:O	1:E:522:GLN:C	2.58	0.42
1:E:661:GLN:HE21	1:E:661:GLN:HB2	1.59	0.42
2:F:124:VAL:HG23	2:F:125:GLU:N	2.34	0.42
2:F:18:PHE:CD2	2:F:34:VAL:HG22	2.54	0.42
1:G:106:GLU:O	1:G:107:ARG:C	2.57	0.42
1:G:177:GLY:O	1:G:183:LYS:NZ	2.49	0.42
1:G:492:LEU:HD12	1:G:492:LEU:O	2.19	0.42
1:G:543:GLU:HG2	1:G:544:GLU:N	2.32	0.42
1:G:49:ILE:HG23	1:G:57:VAL:CG1	2.50	0.42
1:G:607:ASP:O	1:G:610:THR:HB	2.20	0.42
1:A:104:LEU:CD1	1:A:705:LEU:HD11	2.48	0.42
1:A:107:ARG:CB	1:A:112:LEU:HD12	2.48	0.42
1:A:235:GLY:HA3	1:A:248:PHE:CE2	2.54	0.42
1:A:521:LEU:O	1:A:522:GLN:C	2.58	0.42
1:A:663:TYR:O	1:A:666:GLN:N	2.53	0.42
1:A:769:ILE:HD13	1:A:774:ILE:HG12	2.00	0.42
1:A:800:GLN:O	1:A:803:CYS:HB2	2.20	0.42
2:B:71:PRO:HA	2:B:74:GLN:OE1	2.20	0.42
1:C:353:LEU:HA	1:C:356:VAL:HG23	2.02	0.42
1:C:397:ASP:O	1:C:398:PHE:C	2.57	0.42
1:C:51:GLU:HB3	1:C:53:LYS:HD2	2.02	0.42
1:C:702:LEU:HD12	1:C:702:LEU:HA	1.83	0.42
1:C:785:GLU:CD	1:C:788:ARG:HH21	2.22	0.42
1:E:318:ASN:O	1:E:319:GLY:C	2.58	0.42
1:E:365:ILE:HG13	1:E:383:ALA:HB1	2.01	0.42
1:E:494:ASN:ND2	1:E:494:ASN:N	2.64	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:49:ILE:HG23	1:E:57:VAL:CG1	2.49	0.42
1:E:104:LEU:CD1	1:E:705:LEU:HD11	2.49	0.42
1:E:725:ILE:HD13	1:E:730:PHE:HB2	2.02	0.42
1:G:120:PHE:HE1	1:G:713:GLY:O	2.03	0.42
1:G:547:PHE:HA	1:G:548:PRO:HD2	1.76	0.42
1:G:628:VAL:HG22	1:G:631:ILE:HD11	2.02	0.42
2:H:115:LEU:HD12	2:H:115:LEU:N	2.35	0.42
2:H:55:LYS:H	2:H:58:GLU:HG2	1.84	0.42
1:A:558:LYS:O	1:A:561:GLN:N	2.53	0.42
1:A:619:LYS:O	1:A:622:ALA:N	2.52	0.42
1:A:77:LYS:H	1:A:77:LYS:CD	2.33	0.42
2:B:10:GLU:HA	2:B:13:GLU:CG	2.42	0.42
2:B:140:TYR:HE1	2:B:141:GLU:OE2	2.03	0.42
1:C:239:THR:C	1:C:241:LYS:N	2.73	0.42
1:C:278:ILE:HG22	1:C:315:PHE:CE1	2.54	0.42
1:C:525:ILE:O	1:C:529:GLU:HB3	2.20	0.42
1:C:553:THR:HG22	1:C:557:GLU:OE2	2.18	0.42
1:C:683:ARG:HE	1:C:683:ARG:HB3	1.54	0.42
1:E:59:VAL:HG12	1:E:60:GLU:N	2.35	0.42
1:E:814:LYS:C	1:E:816:GLN:N	2.72	0.42
1:G:236:ASN:HD21	1:G:246:SER:HA	1.77	0.42
1:G:287:PHE:O	1:G:288:HIS:C	2.58	0.42
1:G:330:GLU:O	1:G:331:MET:C	2.58	0.42
1:G:64:ASN:C	1:G:66:LYS:N	2.73	0.42
1:G:719:GLN:CA	1:G:719:GLN:HE21	2.32	0.42
1:A:153:ILE:CG2	1:A:154:TYR:N	2.82	0.42
1:A:223:GLN:C	1:A:225:LEU:N	2.73	0.42
1:A:347:GLU:H	1:A:347:GLU:HG3	1.55	0.42
1:A:352:ILE:O	1:A:356:VAL:HG23	2.20	0.42
1:A:37:VAL:CB	1:A:38:PRO:HD2	2.50	0.42
1:A:405:PRO:CD	1:A:416:LYS:O	2.68	0.42
1:C:469:PHE:N	1:C:486:ASN:OD1	2.47	0.42
1:C:59:VAL:HG12	1:C:60:GLU:N	2.34	0.42
1:C:719:GLN:CA	1:C:719:GLN:NE2	2.82	0.42
2:D:57:ASP:OD1	2:D:57:ASP:N	2.49	0.42
2:D:96:ASP:O	2:D:98:GLU:N	2.53	0.42
1:E:177:GLY:O	1:E:183:LYS:NZ	2.48	0.42
1:E:46:ALA:HB1	1:E:62:GLN:HG2	2.01	0.42
1:E:613:LEU:O	1:E:616:SER:N	2.25	0.42
1:G:154:TYR:OH	1:G:192:GLN:NE2	2.53	0.42
1:G:33:LYS:HB3	1:G:49:ILE:CA	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:747:MET:CB	1:G:752:ALA:HB2	2.45	0.42
1:G:800:GLN:O	1:G:803:CYS:HB2	2.20	0.42
1:G:814:LYS:C	1:G:816:GLN:N	2.74	0.42
1:A:293:LEU:HA	1:A:332:PHE:HE1	1.81	0.41
1:A:33:LYS:N	1:A:33:LYS:HE2	2.35	0.41
1:A:489:LEU:HD12	1:A:489:LEU:C	2.40	0.41
1:A:38:PRO:HG2	1:A:70:LEU:HD13	2.02	0.41
2:B:128:VAL:HG23	2:B:129:ALA:N	2.35	0.41
2:B:141:GLU:HG2	2:B:141:GLU:H	1.73	0.41
1:C:103:ASN:HD21	1:C:107:ARG:HD2	1.85	0.41
1:C:121:CYS:SG	1:C:156:ILE:HD11	2.60	0.41
1:C:31:ALA:C	1:C:33:LYS:N	2.73	0.41
1:C:39:SER:C	1:C:41:LYS:H	2.24	0.41
1:C:530:ARG:HA	1:C:531:PRO:HD3	1.78	0.41
1:C:72:LYS:O	1:C:72:LYS:HG2	2.20	0.41
1:C:730:PHE:CE2	1:C:776:PHE:CZ	3.08	0.41
2:D:25:LYS:HE3	2:D:65:LYS:HE2	2.00	0.41
1:E:120:PHE:HE1	1:E:713:GLY:O	2.02	0.41
1:E:152:HIS:CE1	1:E:154:TYR:CG	3.08	0.41
1:E:270:TYR:OH	1:E:670:LEU:HD22	2.20	0.41
1:E:388:CYS:SG	1:E:393:ILE:HD11	2.60	0.41
1:E:376:ALA:CB	1:E:420:LYS:HB2	2.44	0.41
1:E:428:GLU:C	1:E:430:LEU:N	2.72	0.41
1:E:474:ILE:H	1:E:474:ILE:HG13	1.48	0.41
1:E:558:LYS:O	1:E:561:GLN:N	2.53	0.41
1:E:763:ASP:C	1:E:765:ASN:H	2.23	0.41
2:F:140:TYR:CE1	2:F:141:GLU:HG2	2.54	0.41
2:F:103:VAL:CG2	2:F:140:TYR:HD2	2.33	0.41
2:F:71:PRO:HA	2:F:74:GLN:OE1	2.20	0.41
1:G:122:VAL:C	1:G:123:VAL:HG23	2.39	0.41
1:G:161:TYR:O	1:G:165:LEU:CD1	2.62	0.41
1:G:489:LEU:C	1:G:489:LEU:HD12	2.40	0.41
1:G:658:THR:HG23	1:G:661:GLN:CB	2.50	0.41
1:G:817:GLN:HG2	1:G:818:GLN:OE1	2.20	0.41
1:A:306:LEU:HD22	1:A:386:LYS:CD	2.50	0.41
1:A:803:CYS:HB2	2:B:119:MET:HE1	2.02	0.41
2:B:46:GLU:O	2:B:50:VAL:HG23	2.20	0.41
1:C:479:GLN:OE1	1:C:479:GLN:N	2.54	0.41
1:C:43:GLY:HA2	1:C:699:HIS:NE2	2.34	0.41
1:C:751:GLN:HB3	1:C:751:GLN:HE21	1.65	0.41
1:C:768:ARG:HD3	1:C:768:ARG:HA	1.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:120:THR:HG23	2:D:123:GLU:CG	2.49	0.41
2:D:132:GLU:H	2:D:132:GLU:HG2	1.48	0.41
1:E:33:LYS:O	1:E:49:ILE:HG13	2.19	0.41
1:E:395:VAL:O	1:E:398:PHE:N	2.53	0.41
1:E:630:ARG:O	1:E:631:ILE:O	2.37	0.41
2:F:112:LEU:HA	2:F:112:LEU:HD22	1.87	0.41
1:G:138:ILE:HG21	1:G:196:VAL:CG1	2.50	0.41
1:G:275:SER:C	1:G:277:ALA:H	2.22	0.41
1:G:31:ALA:C	1:G:33:LYS:N	2.74	0.41
1:G:555:PHE:CE1	1:G:559:LEU:HD13	2.55	0.41
1:G:799:PHE:CZ	1:G:803:CYS:SG	3.13	0.41
2:H:120:THR:O	2:H:124:VAL:HG22	2.20	0.41
1:A:299:GLU:O	1:A:302:ARG:HB3	2.21	0.41
1:A:305:LEU:HB2	1:A:307:LEU:HG	2.01	0.41
1:A:514:PHE:CG	1:A:515:ILE:N	2.88	0.41
1:A:610:THR:HG21	1:A:628:VAL:HG13	2.02	0.41
1:A:156:ILE:HD13	1:A:682:VAL:HG22	2.02	0.41
2:B:104:MET:C	2:B:106:ALA:N	2.72	0.41
2:B:125:GLU:O	2:B:129:ALA:CB	2.68	0.41
1:C:179:SER:HA	1:C:183:LYS:HZ1	1.85	0.41
1:C:661:GLN:HE21	1:C:661:GLN:HB2	1.57	0.41
2:D:104:MET:C	2:D:106:ALA:N	2.74	0.41
1:E:299:GLU:O	1:E:302:ARG:HB3	2.20	0.41
1:E:33:LYS:N	1:E:33:LYS:HE2	2.36	0.41
1:E:352:ILE:HG22	1:E:438:LEU:HD21	2.02	0.41
1:E:405:PRO:O	1:E:407:ILE:HG23	2.19	0.41
1:E:525:ILE:O	1:E:529:GLU:HB3	2.20	0.41
1:E:560:ILE:HG12	1:E:560:ILE:H	1.59	0.41
2:F:120:THR:HG23	2:F:123:GLU:CG	2.50	0.41
1:G:280:GLN:OE1	1:G:317:SER:N	2.52	0.41
1:G:581:PHE:CZ	1:G:597:TRP:CH2	3.06	0.41
1:A:265:ALA:O	1:A:450:LEU:HB2	2.20	0.41
1:A:545:CYS:SG	1:A:602:MET:SD	3.19	0.41
1:A:719:GLN:CA	1:A:719:GLN:HE21	2.33	0.41
1:A:746:PHE:O	1:A:747:MET:HB2	2.20	0.41
1:A:812:PHE:CD2	1:A:813:ALA:N	2.89	0.41
2:B:104:MET:H	2:B:104:MET:HG3	1.47	0.41
1:C:22:ASN:O	1:C:22:ASN:ND2	2.54	0.41
1:C:318:ASN:O	1:C:319:GLY:C	2.57	0.41
2:D:71:PRO:HA	2:D:74:GLN:OE1	2.20	0.41
1:E:179:SER:HA	1:E:183:LYS:HZ1	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:348:GLU:O	1:E:352:ILE:HG13	2.20	0.41
1:E:382:THR:CA	1:E:385:GLN:HB3	2.50	0.41
1:E:513:ASN:O	1:E:513:ASN:ND2	2.44	0.41
1:E:80:PRO:HG2	1:E:83:PHE:CD2	2.54	0.41
1:G:122:VAL:O	1:G:123:VAL:CG2	2.69	0.41
1:G:152:HIS:CE1	1:G:153:ILE:HG22	2.55	0.41
1:G:438:LEU:HA	1:G:438:LEU:HD12	1.74	0.41
1:G:59:VAL:HG12	1:G:60:GLU:N	2.35	0.41
1:G:621:VAL:HG12	1:G:625:TRP:HD1	1.85	0.41
1:G:747:MET:HB3	1:G:752:ALA:CB	2.46	0.41
2:H:125:GLU:O	2:H:129:ALA:CB	2.68	0.41
2:H:46:GLU:O	2:H:50:VAL:HG23	2.21	0.41
1:A:275:SER:C	1:A:277:ALA:H	2.24	0.41
1:A:348:GLU:O	1:A:352:ILE:HG13	2.20	0.41
1:A:606:ASN:O	1:A:606:ASN:OD1	2.39	0.41
1:A:771:GLN:NE2	1:A:771:GLN:O	2.53	0.41
2:B:132:GLU:H	2:B:132:GLU:HG2	1.46	0.41
2:B:95:PHE:CZ	2:B:111:VAL:HG21	2.55	0.41
1:C:164:MET:HG2	1:C:165:LEU:N	2.34	0.41
1:C:280:GLN:N	1:C:280:GLN:CD	2.74	0.41
1:C:299:GLU:O	1:C:302:ARG:HB3	2.21	0.41
1:C:489:LEU:HD12	1:C:489:LEU:C	2.41	0.41
1:C:492:LEU:HD12	1:C:492:LEU:O	2.21	0.41
1:C:817:GLN:HG2	1:C:818:GLN:OE1	2.20	0.41
1:E:106:GLU:O	1:E:107:ARG:C	2.57	0.41
1:E:395:VAL:O	1:E:396:THR:C	2.58	0.41
1:E:393:ILE:HD12	1:E:612:LEU:HD21	2.01	0.41
2:F:35:MET:HE1	2:F:73:MET:HA	2.03	0.41
1:G:302:ARG:CZ	1:G:303:ASN:HA	2.50	0.41
1:G:415:GLN:OE1	1:G:416:LYS:N	2.53	0.41
1:G:419:THR:O	1:G:422:GLN:N	2.54	0.41
1:G:265:ALA:O	1:G:450:LEU:HB2	2.20	0.41
2:H:10:GLU:O	2:H:13:GLU:N	2.53	0.41
1:A:138:ILE:HG21	1:A:196:VAL:HG11	2.01	0.41
1:A:506:GLN:O	1:A:509:GLY:N	2.53	0.41
1:A:532:THR:C	1:A:533:ASN:O	2.57	0.41
1:A:87:GLU:HA	1:A:87:GLU:OE1	2.20	0.41
1:C:107:ARG:CB	1:C:112:LEU:HD12	2.51	0.41
1:C:152:HIS:CE1	1:C:154:TYR:H	2.38	0.41
1:C:33:LYS:CG	1:C:49:ILE:HB	2.50	0.41
1:C:611:SER:HA	1:C:614:ASN:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:125:GLU:O	2:D:129:ALA:CB	2.66	0.41
2:D:10:GLU:CA	2:D:13:GLU:HG3	2.44	0.41
1:C:802:GLN:NE2	2:D:88:TYR:CE2	2.88	0.41
1:E:114:TYR:HE2	1:E:153:ILE:HB	1.77	0.41
1:E:256:PHE:HA	1:E:261:TYR:O	2.20	0.41
1:E:330:GLU:O	1:E:331:MET:C	2.58	0.41
1:E:373:THR:O	1:E:374:ASP:HB2	2.21	0.41
1:E:384:ALA:HA	1:E:387:VAL:HB	2.02	0.41
1:E:413:VAL:O	1:E:415:GLN:N	2.54	0.41
1:E:514:PHE:CG	1:E:515:ILE:N	2.88	0.41
1:E:72:LYS:HG2	1:E:72:LYS:O	2.21	0.41
1:E:767:TYR:C	1:E:767:TYR:CD1	2.94	0.41
1:G:299:GLU:O	1:G:302:ARG:HB3	2.21	0.41
1:G:347:GLU:HG3	1:G:347:GLU:H	1.54	0.41
1:G:575:LEU:HA	1:G:577:ASP:OD2	2.20	0.41
1:G:751:GLN:HB3	1:G:751:GLN:HE21	1.65	0.41
2:H:124:VAL:HG23	2:H:125:GLU:N	2.36	0.41
2:H:71:PRO:HA	2:H:74:GLN:OE1	2.20	0.41
1:A:352:ILE:HG23	1:A:438:LEU:HD11	2.02	0.41
1:A:540:LEU:C	1:A:542:ASP:H	2.24	0.41
1:A:437:ARG:NE	1:A:625:TRP:HA	2.25	0.41
1:A:763:ASP:C	1:A:765:ASN:H	2.24	0.41
2:B:139:ASN:OD1	2:B:142:GLU:HG2	2.20	0.41
1:C:365:ILE:HD11	1:C:384:ALA:HB2	2.03	0.41
1:C:362:LEU:HD12	1:C:387:VAL:CG1	2.51	0.41
1:C:428:GLU:OE1	1:C:429:ALA:N	2.53	0.41
1:C:468:GLY:O	1:C:469:PHE:C	2.58	0.41
1:C:522:GLN:N	1:C:523:PRO:CD	2.82	0.41
2:D:124:VAL:O	2:D:128:VAL:HG22	2.21	0.41
1:E:31:ALA:O	1:E:34:LEU:N	2.54	0.41
1:E:418:GLN:H	1:E:418:GLN:HG3	1.73	0.41
1:E:619:LYS:O	1:E:622:ALA:N	2.54	0.41
1:E:763:ASP:H	1:E:766:LEU:CD1	2.32	0.41
1:E:765:ASN:O	1:E:777:ARG:NH2	2.47	0.41
2:F:46:GLU:O	2:F:50:VAL:HG23	2.21	0.41
1:G:243:ASP:O	1:G:323:ILE:CD1	2.68	0.41
1:G:280:GLN:N	1:G:280:GLN:CD	2.74	0.41
1:G:299:GLU:O	1:G:302:ARG:HB2	2.21	0.41
1:G:405:PRO:HB2	1:G:407:ILE:HG22	1.99	0.41
1:G:362:LEU:CD2	1:G:427:ILE:HG13	2.48	0.41
1:G:586:TYR:N	1:G:586:TYR:CD1	2.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:111:VAL:HG12	2:H:112:LEU:HD23	2.02	0.41
1:A:89:MET:HE2	1:A:104:LEU:HD21	2.03	0.41
1:A:302:ARG:CZ	1:A:303:ASN:HA	2.50	0.41
1:A:31:ALA:C	1:A:33:LYS:N	2.73	0.41
1:A:384:ALA:HA	1:A:387:VAL:HB	2.02	0.41
1:A:619:LYS:O	1:A:622:ALA:CB	2.66	0.41
1:A:72:LYS:HG2	1:A:72:LYS:O	2.20	0.41
1:A:809:ARG:HD2	2:B:36:ARG:O	2.21	0.41
2:B:81:ASP:O	2:B:82:GLN:HB2	2.20	0.41
1:C:134:SER:OG	1:C:136:LYS:HB3	2.21	0.41
1:C:31:ALA:O	1:C:34:LEU:N	2.54	0.41
1:C:487:GLU:OE1	1:C:585:HIS:HA	2.19	0.41
1:C:172:SER:OG	1:C:679:PRO:HA	2.21	0.41
1:C:804:ARG:O	1:C:808:ALA:HB2	2.21	0.41
1:E:407:ILE:CG1	1:E:414:VAL:O	2.61	0.41
1:E:469:PHE:N	1:E:486:ASN:OD1	2.52	0.41
1:E:555:PHE:CE1	1:E:559:LEU:HD13	2.56	0.41
1:E:660:GLY:O	1:E:664:LYS:HB2	2.21	0.41
1:E:724:ARG:HB3	1:E:724:ARG:HE	1.63	0.41
1:E:760:LEU:HB2	1:E:762:LEU:HD23	2.03	0.41
1:E:806:TYR:CG	2:F:147:VAL:HA	2.54	0.41
2:F:70:LEU:N	2:F:71:PRO:CD	2.83	0.41
2:F:96:ASP:O	2:F:98:GLU:N	2.54	0.41
1:G:13:LEU:CD1	1:G:132:ILE:HB	2.48	0.41
1:G:240:VAL:CG2	1:G:472:PHE:CD1	3.03	0.41
1:G:500:LEU:HD23	1:G:500:LEU:HA	1.86	0.41
1:G:522:GLN:O	1:G:525:ILE:HG13	2.20	0.41
1:A:236:ASN:HD22	1:A:245:SER:C	2.24	0.41
1:A:278:ILE:C	1:A:279:ARG:HG3	2.40	0.41
1:A:329:ASP:N	1:A:329:ASP:OD1	2.43	0.41
1:A:610:THR:HG23	1:A:628:VAL:HG22	2.02	0.41
1:A:88:ASP:HB3	1:A:91:GLU:CD	2.41	0.41
2:B:110:HIS:O	2:B:111:VAL:C	2.58	0.41
2:B:110:HIS:O	2:B:113:VAL:N	2.37	0.41
1:C:122:VAL:C	1:C:123:VAL:HG23	2.41	0.41
1:C:145:LYS:CG	1:C:146:ARG:N	2.81	0.41
1:C:337:GLU:O	1:C:341:ILE:HG12	2.20	0.41
1:C:465:ASP:CG	1:C:465:ASP:O	2.60	0.41
1:C:762:LEU:HD13	1:C:766:LEU:HD12	2.02	0.41
2:D:110:HIS:O	2:D:111:VAL:C	2.59	0.41
1:E:541:LEU:HD13	1:E:555:PHE:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:622:ALA:O	1:E:626:LYS:N	2.54	0.41
1:E:814:LYS:CE	1:E:818:GLN:HE22	2.23	0.41
2:F:12:LYS:H	2:F:12:LYS:HG3	1.58	0.41
1:G:7:SER:N	1:G:10:GLU:OE1	2.42	0.41
1:G:475:ASN:ND2	1:G:590:VAL:CG1	2.84	0.41
2:H:81:ASP:HB3	2:H:82:GLN:H	1.59	0.41
1:A:179:SER:HA	1:A:183:LYS:HZ1	1.85	0.41
1:A:22:ASN:HA	1:A:23:PRO:HD3	1.82	0.41
1:A:23:PRO:O	1:A:27:ALA:HB2	2.21	0.41
1:A:395:VAL:O	1:A:396:THR:C	2.59	0.41
1:A:520:ASP:OD1	1:A:522:GLN:N	2.49	0.41
1:A:547:PHE:C	1:A:547:PHE:CD1	2.94	0.41
2:B:10:GLU:HG3	2:B:13:GLU:CD	2.41	0.41
2:B:86:GLU:N	2:B:86:GLU:CD	2.71	0.41
1:C:240:VAL:HG22	1:C:472:PHE:CE1	2.56	0.41
1:C:275:SER:C	1:C:277:ALA:H	2.24	0.41
1:C:371:ARG:HG3	1:C:371:ARG:H	1.44	0.41
1:C:485:THR:HG23	1:C:667:LEU:HD11	2.03	0.41
1:C:52:GLU:HA	1:C:57:VAL:HG22	2.03	0.41
1:C:569:PHE:CZ	1:C:581:PHE:HB2	2.56	0.41
1:C:735:GLU:O	1:C:735:GLU:HG3	2.21	0.41
1:E:370:GLU:OE1	1:E:372:ASN:HB2	2.20	0.41
1:E:576:LYS:H	1:E:576:LYS:CD	2.32	0.41
2:F:144:VAL:O	2:F:147:VAL:HG23	2.21	0.41
1:G:183:LYS:HB2	1:G:183:LYS:HE2	1.68	0.41
1:G:32:LYS:C	1:G:34:LEU:N	2.73	0.41
1:G:370:GLU:OE1	1:G:372:ASN:HB2	2.20	0.41
1:G:541:LEU:HD13	1:G:555:PHE:CE2	2.56	0.41
1:G:553:THR:O	1:G:557:GLU:OE2	2.39	0.41
1:A:165:LEU:HD21	1:A:260:GLY:CA	2.51	0.41
1:A:183:LYS:HE2	1:A:183:LYS:HB2	1.61	0.41
1:A:32:LYS:C	1:A:34:LEU:N	2.75	0.41
1:A:465:ASP:O	1:A:465:ASP:CG	2.59	0.41
1:A:540:LEU:C	1:A:542:ASP:N	2.74	0.41
1:A:704:GLN:O	1:A:708:ASN:HB2	2.21	0.41
1:A:747:MET:HG2	1:A:751:GLN:NE2	2.36	0.41
2:B:144:VAL:O	2:B:147:VAL:HG23	2.21	0.41
1:C:269:THR:HG23	1:C:440:ARG:CZ	2.51	0.41
1:C:409:VAL:HB	1:C:414:VAL:CG2	2.49	0.41
1:C:428:GLU:C	1:C:430:LEU:N	2.73	0.41
1:C:445:ARG:HD2	1:C:445:ARG:HA	1.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:471:ILE:HG21	1:C:471:ILE:HD13	1.83	0.41
1:C:718:ARG:HG3	1:C:719:GLN:N	2.36	0.41
2:D:127:LEU:HD11	2:D:147:VAL:HG13	2.03	0.41
1:E:393:ILE:HG22	1:E:616:SER:HB2	2.03	0.41
2:F:10:GLU:HA	2:F:13:GLU:CG	2.42	0.41
1:G:17:LYS:HB3	1:G:17:LYS:HE2	1.68	0.41
1:G:196:VAL:HG13	1:G:197:VAL:N	2.36	0.41
1:G:77:LYS:H	1:G:77:LYS:CD	2.28	0.41
2:H:80:LYS:H	2:H:80:LYS:CD	2.31	0.41
2:H:92:LEU:HD23	2:H:92:LEU:N	2.35	0.41
1:A:345:THR:N	1:A:348:GLU:HB3	2.35	0.40
1:A:362:LEU:HD12	1:A:387:VAL:CG1	2.51	0.40
1:A:365:ILE:HD11	1:A:384:ALA:HB2	2.03	0.40
1:A:52:GLU:HA	1:A:57:VAL:HG22	2.03	0.40
1:C:3:GLN:O	1:C:4:LYS:O	2.39	0.40
1:C:240:VAL:CG2	1:C:472:PHE:HD1	2.34	0.40
1:C:49:ILE:HG23	1:C:57:VAL:CG1	2.51	0.40
1:C:530:ARG:HG3	1:C:531:PRO:N	2.33	0.40
1:C:769:ILE:HD13	1:C:774:ILE:HG12	2.04	0.40
1:E:223:GLN:C	1:E:225:LEU:N	2.73	0.40
1:E:23:PRO:O	1:E:27:ALA:CB	2.69	0.40
1:E:270:TYR:CZ	1:E:670:LEU:HD22	2.56	0.40
1:E:355:VAL:HG12	1:E:355:VAL:O	2.21	0.40
1:E:367:PHE:CE1	1:E:378:MET:SD	3.14	0.40
1:E:489:LEU:O	1:E:489:LEU:HD12	2.21	0.40
1:E:500:LEU:HA	1:E:500:LEU:HD23	1.88	0.40
1:G:98:ALA:O	1:G:101:LEU:HB3	2.21	0.40
1:G:305:LEU:HB2	1:G:307:LEU:HG	2.03	0.40
1:G:45:GLU:OE2	1:G:61:LEU:HB3	2.20	0.40
1:G:38:PRO:HG2	1:G:70:LEU:HD13	2.02	0.40
1:G:767:TYR:C	1:G:767:TYR:CD1	2.95	0.40
1:G:801:ALA:HA	1:G:804:ARG:HD2	2.04	0.40
1:A:299:GLU:O	1:A:302:ARG:HB2	2.22	0.40
1:A:438:LEU:O	1:A:441:TRP:HB3	2.21	0.40
1:A:581:PHE:CZ	1:A:597:TRP:CH2	3.09	0.40
1:A:8:ASP:N	1:A:8:ASP:OD1	2.53	0.40
1:C:291:TYR:HD2	1:C:310:PHE:HE2	1.69	0.40
1:C:480:LEU:HA	1:C:592:TYR:CE1	2.56	0.40
1:C:769:ILE:HA	1:C:769:ILE:HD13	1.86	0.40
2:D:120:THR:HG23	2:D:123:GLU:OE1	2.22	0.40
2:D:119:MET:HB3	2:D:123:GLU:OE1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:133:ASP:OD1	2:D:135:ASN:N	2.55	0.40
2:D:16:GLN:C	2:D:18:PHE:H	2.24	0.40
2:D:25:LYS:CE	2:D:65:LYS:HE2	2.52	0.40
1:E:89:MET:HG2	1:E:116:TYR:O	2.21	0.40
1:E:138:ILE:HG21	1:E:196:VAL:CG1	2.51	0.40
1:E:250:LYS:NZ	1:E:465:ASP:OD2	2.54	0.40
1:E:437:ARG:CD	1:E:624:LEU:O	2.70	0.40
1:E:621:VAL:HG12	1:E:625:TRP:HD1	1.87	0.40
2:F:115:LEU:HD12	2:F:115:LEU:N	2.36	0.40
2:F:120:THR:O	2:F:124:VAL:HG22	2.21	0.40
2:F:10:GLU:O	2:F:13:GLU:N	2.54	0.40
1:G:57:VAL:HG23	1:G:72:LYS:HB2	2.03	0.40
1:G:771:GLN:CA	1:G:771:GLN:NE2	2.84	0.40
1:G:77:LYS:HD2	1:G:96:ASN:HD21	1.87	0.40
1:A:445:ARG:HD2	1:A:445:ARG:HA	1.65	0.40
1:A:522:GLN:N	1:A:523:PRO:CD	2.79	0.40
1:A:685:ILE:HD11	1:A:705:LEU:HD23	2.02	0.40
1:A:716:ILE:HA	1:A:719:GLN:HB2	2.02	0.40
2:B:120:THR:O	2:B:124:VAL:HG22	2.21	0.40
1:C:153:ILE:C	1:C:155:ALA:N	2.74	0.40
1:C:272:LEU:CD1	1:C:272:LEU:C	2.79	0.40
1:C:409:VAL:O	1:C:410:GLY:C	2.60	0.40
1:C:541:LEU:CD2	1:C:597:TRP:HB3	2.45	0.40
2:D:46:GLU:O	2:D:50:VAL:HG23	2.20	0.40
1:E:13:LEU:HA	1:E:13:LEU:HD23	1.99	0.40
1:E:288:HIS:O	1:E:289:ILE:C	2.60	0.40
1:E:265:ALA:O	1:E:450:LEU:HB2	2.21	0.40
1:E:522:GLN:N	1:E:523:PRO:CD	2.84	0.40
1:E:575:LEU:C	1:E:577:ASP:N	2.74	0.40
1:E:613:LEU:C	1:E:615:GLN:H	2.24	0.40
1:E:735:GLU:HG3	1:E:735:GLU:O	2.20	0.40
1:E:727:PHE:CE2	1:E:750:LYS:HB2	2.57	0.40
1:E:762:LEU:HD13	1:E:766:LEU:HD12	2.03	0.40
1:G:22:ASN:HA	1:G:23:PRO:HD3	1.77	0.40
1:G:39:SER:C	1:G:41:LYS:H	2.25	0.40
1:G:37:VAL:O	1:G:44:PHE:HA	2.21	0.40
1:G:521:LEU:O	1:G:522:GLN:C	2.59	0.40
1:G:530:ARG:HG3	1:G:531:PRO:N	2.33	0.40
1:G:619:LYS:HA	1:G:622:ALA:CB	2.51	0.40
1:G:663:TYR:O	1:G:666:GLN:N	2.53	0.40
2:H:121:GLU:H	2:H:121:GLU:CD	2.23	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:HIS:C	1:A:149:MET:N	2.74	0.40
1:A:152:HIS:O	1:A:155:ALA:HB3	2.22	0.40
1:A:231:LEU:N	1:A:231:LEU:HD23	2.37	0.40
1:A:394:ASN:OD1	1:A:397:ASP:OD1	2.39	0.40
1:A:51:GLU:HB3	1:A:53:LYS:HD2	2.03	0.40
1:C:280:GLN:OE1	1:C:317:SER:N	2.53	0.40
1:C:32:LYS:C	1:C:34:LEU:N	2.74	0.40
1:C:240:VAL:CG2	1:C:472:PHE:CD1	3.05	0.40
1:C:605:LEU:HG	1:C:606:ASN:N	2.37	0.40
1:C:771:GLN:CA	1:C:771:GLN:NE2	2.82	0.40
1:E:294:ILE:HG22	1:E:294:ILE:O	2.21	0.40
1:E:226:GLN:HG2	1:E:341:ILE:CB	2.52	0.40
1:E:349:GLN:O	1:E:352:ILE:N	2.55	0.40
1:E:475:ASN:HB2	1:E:591:THR:O	2.21	0.40
1:G:31:ALA:O	1:G:34:LEU:N	2.54	0.40
1:G:345:THR:N	1:G:348:GLU:HB3	2.36	0.40
1:G:365:ILE:HD13	1:G:427:ILE:CD1	2.44	0.40
1:G:373:THR:O	1:G:374:ASP:HB2	2.22	0.40
1:G:395:VAL:O	1:G:396:THR:C	2.59	0.40
1:G:425:PHE:CD1	1:G:425:PHE:C	2.95	0.40
1:G:72:LYS:O	1:G:72:LYS:HG2	2.21	0.40
1:G:748:ASP:O	1:G:749:GLY:C	2.60	0.40
1:G:763:ASP:OD1	1:G:765:ASN:N	2.54	0.40
1:A:333:GLN:HA	1:A:336:LEU:HB2	2.03	0.40
1:A:370:GLU:OE1	1:A:372:ASN:HB2	2.21	0.40
1:A:382:THR:CA	1:A:385:GLN:HB3	2.51	0.40
1:A:409:VAL:HG13	1:A:634:LEU:HD12	2.03	0.40
1:A:531:PRO:O	1:A:535:PRO:HA	2.21	0.40
2:B:16:GLN:C	2:B:18:PHE:H	2.25	0.40
1:C:541:LEU:HD13	1:C:555:PHE:CE2	2.57	0.40
1:C:485:THR:CG2	1:C:667:LEU:HD11	2.52	0.40
1:C:704:GLN:O	1:C:708:ASN:HB2	2.22	0.40
1:C:748:ASP:O	1:C:749:GLY:C	2.60	0.40
1:C:77:LYS:CD	1:C:77:LYS:H	2.33	0.40
2:D:140:TYR:HE1	2:D:141:GLU:OE2	2.04	0.40
2:D:84:CYS:SG	2:D:86:GLU:HB2	2.61	0.40
1:E:257:ASP:OD1	1:E:260:GLY:N	2.55	0.40
1:E:540:LEU:H	1:E:540:LEU:HG	1.54	0.40
1:E:485:THR:HG23	1:E:667:LEU:HD11	2.04	0.40
1:E:122:VAL:CG1	1:E:685:ILE:HG13	2.52	0.40
1:E:731:ARG:HD2	1:E:731:ARG:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:104:MET:C	2:F:106:ALA:N	2.74	0.40
2:F:124:VAL:O	2:F:128:VAL:HG22	2.22	0.40
1:G:145:LYS:HB3	1:G:148:GLU:HG2	2.02	0.40
1:G:240:VAL:CG2	1:G:472:PHE:HD1	2.34	0.40
1:G:344:PHE:HA	1:G:348:GLU:OE2	2.21	0.40
2:H:42:PRO:HA	2:H:46:GLU:OE1	2.21	0.40

All (17) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:19:PHE:CE1	1:G:786:GLU:OE2[1_556]	1.59	0.61
1:E:19:PHE:CD1	1:G:786:GLU:OE2[1_556]	1.66	0.54
2:D:23:ASP:N	1:G:371:ARG:NH2[1_545]	1.81	0.39
2:D:22:GLY:N	1:G:371:ARG:CZ[1_545]	1.88	0.32
1:E:19:PHE:CE1	1:G:786:GLU:CD[1_556]	1.91	0.29
1:A:371:ARG:NH1	2:F:22:GLY:N[1_544]	1.91	0.29
2:D:22:GLY:CA	1:G:371:ARG:NE[1_545]	1.96	0.24
2:D:22:GLY:N	1:G:371:ARG:NH1[1_545]	1.96	0.24
2:D:22:GLY:C	1:G:371:ARG:NE[1_545]	2.07	0.13
1:A:371:ARG:NE	2:F:22:GLY:CA[1_544]	2.09	0.11
2:D:23:ASP:CG	1:G:371:ARG:NH2[1_545]	2.11	0.09
2:D:21:THR:OG1	1:G:371:ARG:NH1[1_545]	2.11	0.09
1:A:371:ARG:NE	2:F:22:GLY:C[1_544]	2.13	0.07
2:D:22:GLY:N	1:G:371:ARG:NE[1_545]	2.14	0.06
1:E:19:PHE:CD1	1:G:786:GLU:CD[1_556]	2.15	0.05
1:A:371:ARG:NE	2:F:22:GLY:O[1_544]	2.18	0.02
1:A:371:ARG:CZ	2:F:22:GLY:CA[1_544]	2.19	0.01

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	779/820 (95%)	549 (70%)	172 (22%)	58 (7%)	1	11
1	C	779/820 (95%)	553 (71%)	163 (21%)	63 (8%)	1	9
1	E	779/820 (95%)	547 (70%)	173 (22%)	59 (8%)	1	10
1	G	779/820 (95%)	552 (71%)	165 (21%)	62 (8%)	1	10
2	B	146/150 (97%)	102 (70%)	30 (20%)	14 (10%)	0	8
2	D	146/150 (97%)	104 (71%)	28 (19%)	14 (10%)	0	8
2	F	146/150 (97%)	101 (69%)	33 (23%)	12 (8%)	1	9
2	H	146/150 (97%)	104 (71%)	28 (19%)	14 (10%)	0	8
All	All	3700/3880 (95%)	2612 (71%)	792 (21%)	296 (8%)	1	10

All (296) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	145	LYS
1	A	170	ASP
1	A	383	ALA
1	A	395	VAL
1	A	414	VAL
1	A	531	PRO
1	A	614	ASN
1	A	626	LYS
1	A	664	LYS
1	A	683	ARG
2	B	97	LYS
1	C	145	LYS
1	C	170	ASP
1	C	383	ALA
1	C	395	VAL
1	C	414	VAL
1	C	531	PRO
1	C	614	ASN
1	C	664	LYS
1	C	683	ARG
2	D	97	LYS
1	E	145	LYS
1	E	170	ASP
1	E	276	ARG
1	E	383	ALA
1	E	395	VAL
1	E	414	VAL

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Mol	Chain	Res	Type
1	E	531	PRO
1	E	614	ASN
1	E	631	ILE
1	E	664	LYS
1	E	683	ARG
2	F	97	LYS
1	G	145	LYS
1	G	276	ARG
1	G	383	ALA
1	G	395	VAL
1	G	414	VAL
1	G	531	PRO
1	G	614	ASN
1	G	626	LYS
1	G	664	LYS
1	G	683	ARG
2	H	97	LYS
1	A	32	LYS
1	A	38	PRO
1	A	123	VAL
1	A	181	ALA
1	A	273	GLU
1	A	276	ARG
1	A	362	LEU
1	A	376	ALA
1	A	420	LYS
1	A	541	LEU
1	A	564	GLY
1	A	572	SER
1	A	606	ASN
1	A	750	LYS
2	B	56	SER
2	B	77	ALA
2	B	99	GLY
2	B	105	GLY
2	B	117	GLU
1	C	32	LYS
1	C	38	PRO
1	C	123	VAL
1	C	181	ALA
1	C	273	GLU
1	C	276	ARG

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Mol	Chain	Res	Type
1	C	281	ALA
1	C	362	LEU
1	C	420	LYS
1	C	476	SER
1	C	564	GLY
1	C	572	SER
1	C	750	LYS
2	D	56	SER
2	D	77	ALA
2	D	99	GLY
2	D	105	GLY
2	D	117	GLU
2	D	148	LEU
1	E	32	LYS
1	E	38	PRO
1	E	90	ALA
1	E	181	ALA
1	E	273	GLU
1	E	281	ALA
1	E	304	ASP
1	E	376	ALA
1	E	420	LYS
1	E	541	LEU
1	E	564	GLY
1	E	572	SER
1	E	727	PHE
1	E	750	LYS
2	F	56	SER
2	F	77	ALA
2	F	99	GLY
2	F	105	GLY
2	F	117	GLU
2	F	148	LEU
1	G	32	LYS
1	G	38	PRO
1	G	123	VAL
1	G	168	ARG
1	G	181	ALA
1	G	273	GLU
1	G	362	LEU
1	G	420	LYS
1	G	476	SER

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Mol	Chain	Res	Type
1	G	564	GLY
1	G	572	SER
1	G	606	ASN
1	G	750	LYS
2	H	56	SER
2	H	77	ALA
2	H	99	GLY
2	H	117	GLU
2	H	148	LEU
1	A	131	PRO
1	A	288	HIS
1	A	304	ASP
1	A	348	GLU
1	A	533	ASN
1	A	562	GLU
1	A	727	PHE
2	B	82	GLN
2	B	148	LEU
1	C	90	ALA
1	C	131	PRO
1	C	288	HIS
1	C	304	ASP
1	C	348	GLU
1	C	376	ALA
1	C	533	ASN
1	C	541	LEU
1	C	562	GLU
1	C	606	ASN
1	C	727	PHE
1	C	807	LEU
2	D	22	GLY
2	D	82	GLN
2	D	86	GLU
1	E	123	VAL
1	E	131	PRO
1	E	288	HIS
1	E	362	LEU
1	E	382	THR
1	E	476	SER
1	E	533	ASN
1	E	562	GLU
1	E	606	ASN

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Mol	Chain	Res	Type
2	F	82	GLN
1	G	90	ALA
1	G	131	PRO
1	G	288	HIS
1	G	304	ASP
1	G	376	ALA
1	G	533	ASN
1	G	541	LEU
1	G	562	GLU
2	H	82	GLN
2	H	105	GLY
1	A	72	LYS
1	A	90	ALA
1	A	106	GLU
1	A	382	THR
1	A	407	ILE
1	A	476	SER
1	A	563	GLN
1	A	579	THR
1	A	610	THR
2	B	22	GLY
2	B	86	GLU
2	B	141	GLU
1	C	33	LYS
1	C	72	LYS
1	C	271	LEU
1	C	382	THR
1	C	407	ILE
1	C	425	PHE
1	C	563	GLN
1	C	579	THR
1	C	610	THR
1	C	631	ILE
2	D	141	GLU
2	D	149	SER
1	E	33	LYS
1	E	72	LYS
1	E	233	ALA
1	E	271	LEU
1	E	348	GLU
1	E	407	ILE
1	E	563	GLN

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Mol	Chain	Res	Type
1	E	610	THR
1	E	807	LEU
2	F	149	SER
1	G	33	LYS
1	G	72	LYS
1	G	233	ALA
1	G	289	ILE
1	G	348	GLU
1	G	382	THR
1	G	407	ILE
1	G	425	PHE
1	G	563	GLN
1	G	579	THR
1	G	610	THR
1	G	727	PHE
2	H	22	GLY
2	H	141	GLU
1	A	4	LYS
1	A	89	MET
1	A	168	ARG
1	A	233	ALA
1	A	300	GLN
1	A	534	PRO
1	A	631	ILE
2	B	149	SER
1	C	106	GLU
1	C	126	PRO
1	C	168	ARG
1	C	233	ALA
1	C	300	GLN
1	C	511	GLU
1	C	534	PRO
1	C	663	TYR
1	E	4	LYS
1	E	106	GLU
1	E	126	PRO
1	E	168	ARG
1	E	215	PHE
1	E	300	GLN
1	E	534	PRO
1	E	663	TYR
1	G	106	GLU

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Mol	Chain	Res	Type
1	G	271	LEU
1	G	300	GLN
1	G	524	CYS
1	G	534	PRO
1	G	585	HIS
1	G	663	TYR
2	H	85	PHE
2	H	111	VAL
2	H	149	SER
1	A	126	PRO
1	A	148	GLU
1	A	215	PHE
1	A	289	ILE
1	A	663	TYR
1	A	764	PRO
2	B	54	PRO
2	B	111	VAL
1	C	240	VAL
1	C	289	ILE
1	C	352	ILE
1	C	369	LYS
1	C	396	THR
1	C	585	HIS
1	C	764	PRO
2	D	111	VAL
1	E	289	ILE
1	E	764	PRO
2	F	54	PRO
1	G	89	MET
1	G	126	PRO
1	G	369	LYS
1	G	396	THR
1	G	764	PRO
1	A	240	VAL
1	A	352	ILE
1	C	4	LYS
1	C	410	GLY
2	D	54	PRO
1	E	352	ILE
2	F	22	GLY
1	G	352	ILE
1	G	523	PRO

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Mol	Chain	Res	Type
1	G	631	ILE
2	H	54	PRO
1	A	410	GLY
1	A	523	PRO
1	E	410	GLY
2	F	111	VAL
1	G	4	LYS
1	G	240	VAL
1	G	410	GLY
1	C	523	PRO
1	E	523	PRO
1	G	235	GLY
1	A	235	GLY
1	C	235	GLY
1	E	499	ILE
1	E	235	GLY
1	E	240	VAL

### 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	689/718 (96%)	449 (65%)	240 (35%)	0	1
1	C	689/718 (96%)	449 (65%)	240 (35%)	0	1
1	E	689/718 (96%)	452 (66%)	237 (34%)	0	1
1	G	689/718 (96%)	450 (65%)	239 (35%)	0	1
2	B	127/129 (98%)	86 (68%)	41 (32%)	0	2
2	D	127/129 (98%)	86 (68%)	41 (32%)	0	2
2	F	127/129 (98%)	87 (68%)	40 (32%)	0	2
2	H	127/129 (98%)	85 (67%)	42 (33%)	0	2
All	All	3264/3388 (96%)	2144 (66%)	1120 (34%)	0	1

All (1120) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	SER
1	A	8	ASP
1	A	12	PHE
1	A	15	VAL
1	A	17	LYS
1	A	18	ASN
1	A	21	ASN
1	A	22	ASN
1	A	24	LEU
1	A	26	GLN
1	A	33	LYS
1	A	37	VAL
1	A	41	LYS
1	A	42	HIS
1	A	52	GLU
1	A	53	LYS
1	A	61	LEU
1	A	62	GLN
1	A	66	LYS
1	A	71	SER
1	A	73	ASP
1	A	77	LYS
1	A	79	ASN
1	A	82	LYS
1	A	84	SER
1	A	86	VAL
1	A	89	MET
1	A	92	LEU
1	A	93	THR
1	A	95	LEU
1	A	99	SER
1	A	107	ARG
1	A	112	LEU
1	A	113	ILE
1	A	117	SER
1	A	120	PHE
1	A	121	CYS
1	A	127	TYR
1	A	134	SER
1	A	144	LYS
1	A	145	LYS
1	A	146	ARG
1	A	148	GLU

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Mol	Chain	Res	Type
1	A	162	ARG
1	A	163	SER
1	A	165	LEU
1	A	169	GLU
1	A	171	GLN
1	A	178	GLU
1	A	183	LYS
1	A	194	LEU
1	A	199	SER
1	A	200	SER
1	A	201	HIS
1	A	211	GLN
1	A	216	SER
1	A	222	LYS
1	A	226	GLN
1	A	228	ASN
1	A	230	ILE
1	A	234	PHE
1	A	238	LYS
1	A	239	THR
1	A	247	ARG
1	A	250	LYS
1	A	254	ILE
1	A	258	VAL
1	A	259	THR
1	A	262	ILE
1	A	263	VAL
1	A	266	ASN
1	A	269	THR
1	A	271	LEU
1	A	272	LEU
1	A	274	LYS
1	A	282	LYS
1	A	286	THR
1	A	298	SER
1	A	299	GLU
1	A	302	ARG
1	A	312	ASN
1	A	313	TYR
1	A	314	THR
1	A	316	LEU
1	A	317	SER

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Mol	Chain	Res	Type
1	A	320	HIS
1	A	329	ASP
1	A	335	THR
1	A	336	LEU
1	A	342	MET
1	A	346	GLU
1	A	347	GLU
1	A	351	SER
1	A	352	ILE
1	A	357	SER
1	A	358	SER
1	A	360	LEU
1	A	362	LEU
1	A	366	VAL
1	A	368	LYS
1	A	369	LYS
1	A	370	GLU
1	A	371	ARG
1	A	372	ASN
1	A	378	MET
1	A	382	THR
1	A	391	MET
1	A	395	VAL
1	A	399	THR
1	A	401	SER
1	A	402	ILE
1	A	406	ARG
1	A	407	ILE
1	A	408	LYS
1	A	411	ARG
1	A	412	ASP
1	A	415	GLN
1	A	416	LYS
1	A	418	GLN
1	A	419	THR
1	A	420	LYS
1	A	427	ILE
1	A	428	GLU
1	A	432	LYS
1	A	437	ARG
1	A	443	LEU
1	A	444	THR

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Mol	Chain	Res	Type
1	A	445	ARG
1	A	447	ASN
1	A	448	LYS
1	A	451	ASP
1	A	459	SER
1	A	461	LEU
1	A	465	ASP
1	A	471	ILE
1	A	473	GLU
1	A	474	ILE
1	A	482	ILE
1	A	485	THR
1	A	488	LYS
1	A	489	LEU
1	A	492	LEU
1	A	494	ASN
1	A	496	THR
1	A	497	MET
1	A	502	GLN
1	A	503	GLU
1	A	504	GLU
1	A	506	GLN
1	A	513	ASN
1	A	521	LEU
1	A	522	GLN
1	A	530	ARG
1	A	533	ASN
1	A	543	GLU
1	A	544	GLU
1	A	545	CYS
1	A	547	PHE
1	A	549	LYS
1	A	553	THR
1	A	560	ILE
1	A	561	GLN
1	A	563	GLN
1	A	565	ASN
1	A	568	LYS
1	A	573	LYS
1	A	574	GLN
1	A	575	LEU
1	A	576	LYS

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Mol	Chain	Res	Type
1	A	577	ASP
1	A	578	LYS
1	A	579	THR
1	A	583	ILE
1	A	586	TYR
1	A	591	THR
1	A	595	SER
1	A	599	THR
1	A	603	ASP
1	A	607	ASP
1	A	610	THR
1	A	611	SER
1	A	613	LEU
1	A	615	GLN
1	A	616	SER
1	A	617	SER
1	A	619	LYS
1	A	623	ASP
1	A	624	LEU
1	A	626	LYS
1	A	630	ARG
1	A	657	ARG
1	A	661	GLN
1	A	662	LEU
1	A	664	LYS
1	A	665	GLU
1	A	668	THR
1	A	673	THR
1	A	678	ASN
1	A	683	ARG
1	A	685	ILE
1	A	686	ILE
1	A	690	GLU
1	A	701	VAL
1	A	702	LEU
1	A	704	GLN
1	A	718	ARG
1	A	721	PHE
1	A	724	ARG
1	A	728	GLN
1	A	729	GLU
1	A	731	ARG

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Mol	Chain	Res	Type
1	A	733	ARG
1	A	735	GLU
1	A	740	ASN
1	A	744	LYS
1	A	751	GLN
1	A	753	CYS
1	A	755	LEU
1	A	762	LEU
1	A	768	ARG
1	A	771	GLN
1	A	773	LYS
1	A	777	ARG
1	A	778	THR
1	A	781	LEU
1	A	784	LEU
1	A	789	ASP
1	A	790	LEU
1	A	791	LYS
1	A	793	THR
1	A	794	ASP
1	A	795	VAL
1	A	797	ILE
1	A	800	GLN
1	A	809	ARG
1	A	812	PHE
1	A	814	LYS
1	A	815	ARG
1	A	818	GLN
1	A	819	LEU
2	B	10	GLU
2	B	20	ARG
2	B	21	THR
2	B	23	ASP
2	B	25	LYS
2	B	26	ILE
2	B	28	TYR
2	B	40	GLN
2	B	43	THR
2	B	49	LYS
2	B	50	VAL
2	B	51	LEU
2	B	53	ASN

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Mol	Chain	Res	Type
2	B	57	ASP
2	B	60	ASN
2	B	67	GLU
2	B	68	GLN
2	B	73	MET
2	B	74	GLN
2	B	75	THR
2	B	78	LYS
2	B	80	LYS
2	B	82	GLN
2	B	88	TYR
2	B	89	VAL
2	B	90	GLU
2	B	93	ARG
2	B	98	GLU
2	B	100	ASN
2	B	104	MET
2	B	107	GLU
2	B	108	ILE
2	B	109	ARG
2	B	112	LEU
2	B	114	THR
2	B	120	THR
2	B	132	GLU
2	B	134	SER
2	B	135	ASN
2	B	146	MET
2	B	147	VAL
1	C	7	SER
1	C	8	ASP
1	C	11	LYS
1	C	12	PHE
1	C	15	VAL
1	C	17	LYS
1	C	21	ASN
1	C	22	ASN
1	C	24	LEU
1	C	26	GLN
1	C	33	LYS
1	C	37	VAL
1	C	41	LYS
1	C	42	HIS

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Mol	Chain	Res	Type
1	C	52	GLU
1	C	53	LYS
1	C	61	LEU
1	C	62	GLN
1	C	66	LYS
1	C	71	SER
1	C	73	ASP
1	C	77	LYS
1	C	79	ASN
1	C	82	LYS
1	C	84	SER
1	C	86	VAL
1	C	89	MET
1	C	92	LEU
1	C	93	THR
1	C	95	LEU
1	C	99	SER
1	C	107	ARG
1	C	112	LEU
1	C	113	ILE
1	C	117	SER
1	C	120	PHE
1	C	121	CYS
1	C	127	TYR
1	C	134	SER
1	C	144	LYS
1	C	145	LYS
1	C	146	ARG
1	C	148	GLU
1	C	162	ARG
1	C	163	SER
1	C	165	LEU
1	C	169	GLU
1	C	171	GLN
1	C	178	GLU
1	C	183	LYS
1	C	194	LEU
1	C	200	SER
1	C	201	HIS
1	C	211	GLN
1	C	216	SER
1	C	222	LYS

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Mol	Chain	Res	Type
1	C	226	GLN
1	C	228	ASN
1	C	230	ILE
1	C	234	PHE
1	C	238	LYS
1	C	239	THR
1	C	247	ARG
1	C	250	LYS
1	C	254	ILE
1	C	258	VAL
1	C	259	THR
1	C	262	ILE
1	C	263	VAL
1	C	266	ASN
1	C	269	THR
1	C	271	LEU
1	C	272	LEU
1	C	274	LYS
1	C	282	LYS
1	C	286	THR
1	C	298	SER
1	C	299	GLU
1	C	302	ARG
1	C	312	ASN
1	C	313	TYR
1	C	314	THR
1	C	316	LEU
1	C	317	SER
1	C	320	HIS
1	C	329	ASP
1	C	335	THR
1	C	336	LEU
1	C	342	MET
1	C	346	GLU
1	C	347	GLU
1	C	351	SER
1	C	352	ILE
1	C	357	SER
1	C	358	SER
1	C	360	LEU
1	C	362	LEU
1	C	366	VAL

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Mol	Chain	Res	Type
1	C	368	LYS
1	C	369	LYS
1	C	370	GLU
1	C	371	ARG
1	C	372	ASN
1	C	378	MET
1	C	382	THR
1	C	391	MET
1	C	395	VAL
1	C	399	THR
1	C	401	SER
1	C	402	ILE
1	C	406	ARG
1	C	407	ILE
1	C	408	LYS
1	C	411	ARG
1	C	412	ASP
1	C	415	GLN
1	C	416	LYS
1	C	418	GLN
1	C	419	THR
1	C	420	LYS
1	C	427	ILE
1	C	428	GLU
1	C	432	LYS
1	C	437	ARG
1	C	443	LEU
1	C	444	THR
1	C	445	ARG
1	C	447	ASN
1	C	448	LYS
1	C	451	ASP
1	C	459	SER
1	C	461	LEU
1	C	465	ASP
1	C	471	ILE
1	C	473	GLU
1	C	474	ILE
1	C	482	ILE
1	C	485	THR
1	C	488	LYS
1	C	489	LEU

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Mol	Chain	Res	Type
1	C	492	LEU
1	C	494	ASN
1	C	496	THR
1	C	497	MET
1	C	502	GLN
1	C	503	GLU
1	C	504	GLU
1	C	506	GLN
1	C	513	ASN
1	C	521	LEU
1	C	522	GLN
1	C	530	ARG
1	C	533	ASN
1	C	543	GLU
1	C	544	GLU
1	C	545	CYS
1	C	547	PHE
1	C	549	LYS
1	C	553	THR
1	C	560	ILE
1	C	561	GLN
1	C	563	GLN
1	C	565	ASN
1	C	568	LYS
1	C	573	LYS
1	C	574	GLN
1	C	575	LEU
1	C	576	LYS
1	C	577	ASP
1	C	578	LYS
1	C	579	THR
1	C	583	ILE
1	C	586	TYR
1	C	591	THR
1	C	595	SER
1	C	599	THR
1	C	603	ASP
1	C	607	ASP
1	C	610	THR
1	C	611	SER
1	C	613	LEU
1	C	615	GLN

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Mol	Chain	Res	Type
1	C	616	SER
1	C	617	SER
1	C	619	LYS
1	C	623	ASP
1	C	624	LEU
1	C	626	LYS
1	C	628	VAL
1	C	630	ARG
1	C	657	ARG
1	C	661	GLN
1	C	662	LEU
1	C	664	LYS
1	C	665	GLU
1	C	668	THR
1	C	673	THR
1	C	678	ASN
1	C	683	ARG
1	C	685	ILE
1	C	686	ILE
1	C	690	GLU
1	C	701	VAL
1	C	702	LEU
1	C	704	GLN
1	C	718	ARG
1	C	721	PHE
1	C	724	ARG
1	C	728	GLN
1	C	729	GLU
1	C	731	ARG
1	C	733	ARG
1	C	735	GLU
1	C	740	ASN
1	C	744	LYS
1	C	751	GLN
1	C	753	CYS
1	C	755	LEU
1	C	762	LEU
1	C	768	ARG
1	C	771	GLN
1	C	773	LYS
1	C	777	ARG
1	C	778	THR

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Mol	Chain	Res	Type
1	C	781	LEU
1	C	784	LEU
1	C	789	ASP
1	C	790	LEU
1	C	791	LYS
1	C	793	THR
1	C	794	ASP
1	C	795	VAL
1	C	797	ILE
1	C	800	GLN
1	C	809	ARG
1	C	812	PHE
1	C	814	LYS
1	C	815	ARG
1	C	818	GLN
1	C	819	LEU
2	D	10	GLU
2	D	20	ARG
2	D	21	THR
2	D	23	ASP
2	D	25	LYS
2	D	26	ILE
2	D	28	TYR
2	D	40	GLN
2	D	43	THR
2	D	49	LYS
2	D	50	VAL
2	D	51	LEU
2	D	53	ASN
2	D	57	ASP
2	D	60	ASN
2	D	67	GLU
2	D	68	GLN
2	D	70	LEU
2	D	73	MET
2	D	74	GLN
2	D	75	THR
2	D	78	LYS
2	D	80	LYS
2	D	82	GLN
2	D	88	TYR
2	D	89	VAL

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Mol	Chain	Res	Type
2	D	90	GLU
2	D	98	GLU
2	D	100	ASN
2	D	104	MET
2	D	107	GLU
2	D	108	ILE
2	D	109	ARG
2	D	112	LEU
2	D	114	THR
2	D	120	THR
2	D	132	GLU
2	D	134	SER
2	D	135	ASN
2	D	146	MET
2	D	147	VAL
1	E	7	SER
1	E	8	ASP
1	E	12	PHE
1	E	15	VAL
1	E	17	LYS
1	E	21	ASN
1	E	22	ASN
1	E	24	LEU
1	E	26	GLN
1	E	33	LYS
1	E	37	VAL
1	E	41	LYS
1	E	42	HIS
1	E	52	GLU
1	E	53	LYS
1	E	61	LEU
1	E	62	GLN
1	E	66	LYS
1	E	71	SER
1	E	73	ASP
1	E	77	LYS
1	E	79	ASN
1	E	82	LYS
1	E	84	SER
1	E	86	VAL
1	E	92	LEU
1	E	93	THR

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Mol	Chain	Res	Type
1	E	95	LEU
1	E	99	SER
1	E	107	ARG
1	E	112	LEU
1	E	113	ILE
1	E	117	SER
1	E	120	PHE
1	E	121	CYS
1	E	127	TYR
1	E	134	SER
1	E	144	LYS
1	E	145	LYS
1	E	146	ARG
1	E	148	GLU
1	E	162	ARG
1	E	163	SER
1	E	165	LEU
1	E	169	GLU
1	E	171	GLN
1	E	178	GLU
1	E	183	LYS
1	E	194	LEU
1	E	199	SER
1	E	200	SER
1	E	201	HIS
1	E	211	GLN
1	E	216	SER
1	E	222	LYS
1	E	226	GLN
1	E	228	ASN
1	E	230	ILE
1	E	234	PHE
1	E	238	LYS
1	E	239	THR
1	E	247	ARG
1	E	250	LYS
1	E	254	ILE
1	E	258	VAL
1	E	259	THR
1	E	262	ILE
1	E	263	VAL
1	E	266	ASN

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Mol	Chain	Res	Type
1	E	269	THR
1	E	271	LEU
1	E	272	LEU
1	E	274	LYS
1	E	282	LYS
1	E	286	THR
1	E	298	SER
1	E	299	GLU
1	E	302	ARG
1	E	312	ASN
1	E	313	TYR
1	E	314	THR
1	E	316	LEU
1	E	317	SER
1	E	320	HIS
1	E	329	ASP
1	E	335	THR
1	E	336	LEU
1	E	342	MET
1	E	346	GLU
1	E	347	GLU
1	E	351	SER
1	E	352	ILE
1	E	357	SER
1	E	358	SER
1	E	360	LEU
1	E	362	LEU
1	E	366	VAL
1	E	368	LYS
1	E	369	LYS
1	E	370	GLU
1	E	371	ARG
1	E	372	ASN
1	E	378	MET
1	E	382	THR
1	E	391	MET
1	E	395	VAL
1	E	399	THR
1	E	401	SER
1	E	402	ILE
1	E	406	ARG
1	E	407	ILE

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Mol	Chain	Res	Type
1	E	408	LYS
1	E	411	ARG
1	E	412	ASP
1	E	415	GLN
1	E	416	LYS
1	E	419	THR
1	E	420	LYS
1	E	427	ILE
1	E	428	GLU
1	E	432	LYS
1	E	437	ARG
1	E	443	LEU
1	E	444	THR
1	E	445	ARG
1	E	447	ASN
1	E	448	LYS
1	E	451	ASP
1	E	459	SER
1	E	461	LEU
1	E	465	ASP
1	E	471	ILE
1	E	473	GLU
1	E	474	ILE
1	E	482	ILE
1	E	485	THR
1	E	488	LYS
1	E	489	LEU
1	E	492	LEU
1	E	494	ASN
1	E	496	THR
1	E	497	MET
1	E	502	GLN
1	E	503	GLU
1	E	504	GLU
1	E	506	GLN
1	E	513	ASN
1	E	521	LEU
1	E	522	GLN
1	E	530	ARG
1	E	543	GLU
1	E	544	GLU
1	E	545	CYS

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Mol	Chain	Res	Type
1	E	547	PHE
1	E	549	LYS
1	E	553	THR
1	E	560	ILE
1	E	561	GLN
1	E	563	GLN
1	E	565	ASN
1	E	568	LYS
1	E	573	LYS
1	E	574	GLN
1	E	575	LEU
1	E	576	LYS
1	E	577	ASP
1	E	579	THR
1	E	583	ILE
1	E	586	TYR
1	E	591	THR
1	E	595	SER
1	E	599	THR
1	E	603	ASP
1	E	607	ASP
1	E	610	THR
1	E	611	SER
1	E	613	LEU
1	E	615	GLN
1	E	616	SER
1	E	617	SER
1	E	619	LYS
1	E	623	ASP
1	E	624	LEU
1	E	626	LYS
1	E	630	ARG
1	E	657	ARG
1	E	661	GLN
1	E	662	LEU
1	E	664	LYS
1	E	665	GLU
1	E	668	THR
1	E	673	THR
1	E	678	ASN
1	E	683	ARG
1	E	685	ILE

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Mol	Chain	Res	Type
1	E	686	ILE
1	E	690	GLU
1	E	701	VAL
1	E	702	LEU
1	E	704	GLN
1	E	718	ARG
1	E	721	PHE
1	E	724	ARG
1	E	728	GLN
1	E	729	GLU
1	E	731	ARG
1	E	733	ARG
1	E	735	GLU
1	E	740	ASN
1	E	744	LYS
1	E	751	GLN
1	E	753	CYS
1	E	755	LEU
1	E	762	LEU
1	E	768	ARG
1	E	771	GLN
1	E	773	LYS
1	E	777	ARG
1	E	778	THR
1	E	781	LEU
1	E	784	LEU
1	E	789	ASP
1	E	790	LEU
1	E	791	LYS
1	E	792	ILE
1	E	793	THR
1	E	794	ASP
1	E	795	VAL
1	E	797	ILE
1	E	800	GLN
1	E	804	ARG
1	E	809	ARG
1	E	812	PHE
1	E	814	LYS
1	E	815	ARG
1	E	818	GLN
1	E	819	LEU

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Mol	Chain	Res	Type
2	F	10	GLU
2	F	20	ARG
2	F	21	THR
2	F	23	ASP
2	F	25	LYS
2	F	26	ILE
2	F	28	TYR
2	F	40	GLN
2	F	43	THR
2	F	49	LYS
2	F	50	VAL
2	F	51	LEU
2	F	53	ASN
2	F	57	ASP
2	F	60	ASN
2	F	67	GLU
2	F	68	GLN
2	F	73	MET
2	F	74	GLN
2	F	75	THR
2	F	78	LYS
2	F	80	LYS
2	F	82	GLN
2	F	88	TYR
2	F	89	VAL
2	F	90	GLU
2	F	98	GLU
2	F	100	ASN
2	F	104	MET
2	F	107	GLU
2	F	108	ILE
2	F	109	ARG
2	F	112	LEU
2	F	114	THR
2	F	120	THR
2	F	132	GLU
2	F	134	SER
2	F	135	ASN
2	F	146	MET
2	F	147	VAL
1	G	7	SER
1	G	8	ASP

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Mol	Chain	Res	Type
1	G	12	PHE
1	G	15	VAL
1	G	17	LYS
1	G	21	ASN
1	G	22	ASN
1	G	24	LEU
1	G	26	GLN
1	G	33	LYS
1	G	37	VAL
1	G	41	LYS
1	G	42	HIS
1	G	52	GLU
1	G	53	LYS
1	G	61	LEU
1	G	62	GLN
1	G	66	LYS
1	G	71	SER
1	G	73	ASP
1	G	77	LYS
1	G	78	MET
1	G	79	ASN
1	G	82	LYS
1	G	84	SER
1	G	86	VAL
1	G	89	MET
1	G	92	LEU
1	G	93	THR
1	G	95	LEU
1	G	99	SER
1	G	106	GLU
1	G	107	ARG
1	G	112	LEU
1	G	113	ILE
1	G	117	SER
1	G	120	PHE
1	G	121	CYS
1	G	127	TYR
1	G	134	SER
1	G	144	LYS
1	G	145	LYS
1	G	146	ARG
1	G	148	GLU

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Mol	Chain	Res	Type
1	G	162	ARG
1	G	163	SER
1	G	178	GLU
1	G	183	LYS
1	G	194	LEU
1	G	199	SER
1	G	200	SER
1	G	201	HIS
1	G	211	GLN
1	G	216	SER
1	G	222	LYS
1	G	226	GLN
1	G	228	ASN
1	G	230	ILE
1	G	234	PHE
1	G	238	LYS
1	G	239	THR
1	G	247	ARG
1	G	250	LYS
1	G	254	ILE
1	G	258	VAL
1	G	259	THR
1	G	262	ILE
1	G	263	VAL
1	G	266	ASN
1	G	269	THR
1	G	271	LEU
1	G	272	LEU
1	G	274	LYS
1	G	282	LYS
1	G	286	THR
1	G	298	SER
1	G	299	GLU
1	G	302	ARG
1	G	312	ASN
1	G	313	TYR
1	G	314	THR
1	G	316	LEU
1	G	317	SER
1	G	320	HIS
1	G	329	ASP
1	G	331	MET

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Mol	Chain	Res	Type
1	G	335	THR
1	G	336	LEU
1	G	342	MET
1	G	346	GLU
1	G	347	GLU
1	G	351	SER
1	G	352	ILE
1	G	357	SER
1	G	358	SER
1	G	360	LEU
1	G	362	LEU
1	G	366	VAL
1	G	368	LYS
1	G	369	LYS
1	G	370	GLU
1	G	371	ARG
1	G	372	ASN
1	G	378	MET
1	G	382	THR
1	G	391	MET
1	G	395	VAL
1	G	399	THR
1	G	401	SER
1	G	402	ILE
1	G	406	ARG
1	G	407	ILE
1	G	408	LYS
1	G	411	ARG
1	G	412	ASP
1	G	415	GLN
1	G	416	LYS
1	G	419	THR
1	G	420	LYS
1	G	427	ILE
1	G	428	GLU
1	G	432	LYS
1	G	437	ARG
1	G	443	LEU
1	G	444	THR
1	G	445	ARG
1	G	447	ASN
1	G	448	LYS

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Mol	Chain	Res	Type
1	G	451	ASP
1	G	459	SER
1	G	461	LEU
1	G	465	ASP
1	G	471	ILE
1	G	473	GLU
1	G	474	ILE
1	G	482	ILE
1	G	485	THR
1	G	488	LYS
1	G	489	LEU
1	G	492	LEU
1	G	494	ASN
1	G	496	THR
1	G	497	MET
1	G	502	GLN
1	G	503	GLU
1	G	504	GLU
1	G	506	GLN
1	G	513	ASN
1	G	521	LEU
1	G	522	GLN
1	G	530	ARG
1	G	543	GLU
1	G	544	GLU
1	G	545	CYS
1	G	547	PHE
1	G	549	LYS
1	G	553	THR
1	G	560	ILE
1	G	561	GLN
1	G	563	GLN
1	G	565	ASN
1	G	568	LYS
1	G	573	LYS
1	G	574	GLN
1	G	575	LEU
1	G	576	LYS
1	G	577	ASP
1	G	578	LYS
1	G	579	THR
1	G	583	ILE

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Mol	Chain	Res	Type
1	G	586	TYR
1	G	591	THR
1	G	595	SER
1	G	599	THR
1	G	603	ASP
1	G	607	ASP
1	G	610	THR
1	G	611	SER
1	G	613	LEU
1	G	615	GLN
1	G	616	SER
1	G	617	SER
1	G	619	LYS
1	G	621	VAL
1	G	623	ASP
1	G	624	LEU
1	G	626	LYS
1	G	630	ARG
1	G	657	ARG
1	G	661	GLN
1	G	662	LEU
1	G	664	LYS
1	G	665	GLU
1	G	668	THR
1	G	673	THR
1	G	678	ASN
1	G	683	ARG
1	G	685	ILE
1	G	686	ILE
1	G	690	GLU
1	G	701	VAL
1	G	702	LEU
1	G	704	GLN
1	G	718	ARG
1	G	721	PHE
1	G	724	ARG
1	G	728	GLN
1	G	729	GLU
1	G	731	ARG
1	G	733	ARG
1	G	735	GLU
1	G	740	ASN

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Mol	Chain	Res	Type
1	G	744	LYS
1	G	751	GLN
1	G	753	CYS
1	G	755	LEU
1	G	762	LEU
1	G	768	ARG
1	G	771	GLN
1	G	773	LYS
1	G	777	ARG
1	G	778	THR
1	G	781	LEU
1	G	784	LEU
1	G	789	ASP
1	G	790	LEU
1	G	791	LYS
1	G	793	THR
1	G	794	ASP
1	G	795	VAL
1	G	797	ILE
1	G	800	GLN
1	G	804	ARG
1	G	809	ARG
1	G	812	PHE
1	G	814	LYS
1	G	815	ARG
1	G	818	GLN
1	G	819	LEU
2	H	10	GLU
2	H	20	ARG
2	H	21	THR
2	H	23	ASP
2	H	25	LYS
2	H	26	ILE
2	H	28	TYR
2	H	40	GLN
2	H	43	THR
2	H	49	LYS
2	H	50	VAL
2	H	51	LEU
2	H	53	ASN
2	H	57	ASP
2	H	60	ASN

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Mol	Chain	Res	Type
2	H	67	GLU
2	H	68	GLN
2	H	73	MET
2	H	74	GLN
2	H	75	THR
2	H	78	LYS
2	H	80	LYS
2	H	82	GLN
2	H	86	GLU
2	H	88	TYR
2	H	89	VAL
2	H	90	GLU
2	H	93	ARG
2	H	98	GLU
2	H	100	ASN
2	H	104	MET
2	H	107	GLU
2	H	108	ILE
2	H	109	ARG
2	H	112	LEU
2	H	114	THR
2	H	120	THR
2	H	132	GLU
2	H	134	SER
2	H	135	ASN
2	H	146	MET
2	H	147	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (128) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	96	ASN
1	A	102	HIS
1	A	166	GLN
1	A	223	GLN
1	A	226	GLN
1	A	244	ASN
1	A	266	ASN
1	A	288	HIS
1	A	311	ASN
1	A	312	ASN

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Mol	Chain	Res	Type
1	A	326	GLN
1	A	361	GLN
1	A	375	GLN
1	A	422	GLN
1	A	447	ASN
1	A	494	ASN
1	A	495	HIS
1	A	533	ASN
1	A	601	ASN
1	A	661	GLN
1	A	678	ASN
1	A	728	GLN
1	A	771	GLN
1	A	783	HIS
2	B	7	GLN
2	B	44	ASN
2	B	60	ASN
1	C	26	GLN
1	C	79	ASN
1	C	96	ASN
1	C	102	HIS
1	C	103	ASN
1	C	166	GLN
1	C	223	GLN
1	C	226	GLN
1	C	244	ASN
1	C	266	ASN
1	C	288	HIS
1	C	311	ASN
1	C	312	ASN
1	C	326	GLN
1	C	361	GLN
1	C	375	GLN
1	C	422	GLN
1	C	447	ASN
1	C	494	ASN
1	C	495	HIS
1	C	533	ASN
1	C	565	ASN
1	C	601	ASN
1	C	615	GLN
1	C	661	GLN

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Mol	Chain	Res	Type
1	C	678	ASN
1	C	728	GLN
1	C	751	GLN
1	C	771	GLN
1	C	783	HIS
1	C	802	GLN
2	D	7	GLN
2	D	44	ASN
2	D	60	ASN
2	D	135	ASN
1	E	26	GLN
1	E	79	ASN
1	E	96	ASN
1	E	102	HIS
1	E	103	ASN
1	E	166	GLN
1	E	223	GLN
1	E	226	GLN
1	E	266	ASN
1	E	311	ASN
1	E	312	ASN
1	E	326	GLN
1	E	361	GLN
1	E	375	GLN
1	E	422	GLN
1	E	447	ASN
1	E	494	ASN
1	E	495	HIS
1	E	533	ASN
1	E	601	ASN
1	E	614	ASN
1	E	661	GLN
1	E	678	ASN
1	E	680	ASN
1	E	699	HIS
1	E	728	GLN
1	E	751	GLN
1	E	771	GLN
1	E	783	HIS
1	E	802	GLN
2	F	7	GLN
2	F	44	ASN

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Mol	Chain	Res	Type
2	F	53	ASN
2	F	60	ASN
2	F	135	ASN
1	G	26	GLN
1	G	79	ASN
1	G	96	ASN
1	G	166	GLN
1	G	223	GLN
1	G	244	ASN
1	G	266	ASN
1	G	288	HIS
1	G	311	ASN
1	G	312	ASN
1	G	361	GLN
1	G	422	GLN
1	G	447	ASN
1	G	494	ASN
1	G	495	HIS
1	G	533	ASN
1	G	565	ASN
1	G	601	ASN
1	G	661	GLN
1	G	678	ASN
1	G	728	GLN
1	G	751	GLN
1	G	771	GLN
1	G	783	HIS
1	G	802	GLN
1	G	816	GLN
2	H	7	GLN
2	H	44	ASN
2	H	60	ASN
2	H	135	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	$\# Z  > 2$
4	ALF	C	999	1,3,5,6	0,4,4	0.00	-	-		
5	ADP	G	998	3,4	24,29,29	0.79	0	29,45,45	1.25	3 (10%)
4	ALF	A	999	1,3,5,6	0,4,4	0.00	-	-		
5	ADP	A	998	3,4	24,29,29	0.80	0	29,45,45	1.25	3 (10%)
4	ALF	G	999	1,3,5,6	0,4,4	0.00	-	-		
5	ADP	C	998	3,4	24,29,29	0.79	0	29,45,45	1.26	3 (10%)
4	ALF	E	999	1,3,5,6	0,4,4	0.00	-	-		
5	ADP	E	998	3,4	24,29,29	0.78	0	29,45,45	1.25	3 (10%)

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
5	ADP	G	998	3,4	-	5/12/32/32	0/3/3/3
5	ADP	A	998	3,4	-	5/12/32/32	0/3/3/3
5	ADP	C	998	3,4	-	5/12/32/32	0/3/3/3
5	ADP	E	998	3,4	-	5/12/32/32	0/3/3/3

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	998	ADP	C5-C6-N6	2.86	124.70	120.35
5	G	998	ADP	C5-C6-N6	2.84	124.67	120.35
5	E	998	ADP	C5-C6-N6	2.83	124.65	120.35
5	A	998	ADP	C5-C6-N6	2.81	124.63	120.35
5	E	998	ADP	O3'-C3'-C2'	2.48	119.84	111.82
5	A	998	ADP	O3'-C3'-C2'	2.46	119.79	111.82
5	G	998	ADP	O3'-C3'-C2'	2.46	119.79	111.82
5	C	998	ADP	O3'-C3'-C2'	2.46	119.77	111.82
5	C	998	ADP	O2B-PB-O3A	2.27	112.24	104.64
5	A	998	ADP	O2B-PB-O3A	2.26	112.20	104.64
5	E	998	ADP	O2B-PB-O3A	2.25	112.18	104.64
5	G	998	ADP	O2B-PB-O3A	2.25	112.18	104.64

There are no chirality outliers.

All (20) torsion outliers are listed below:

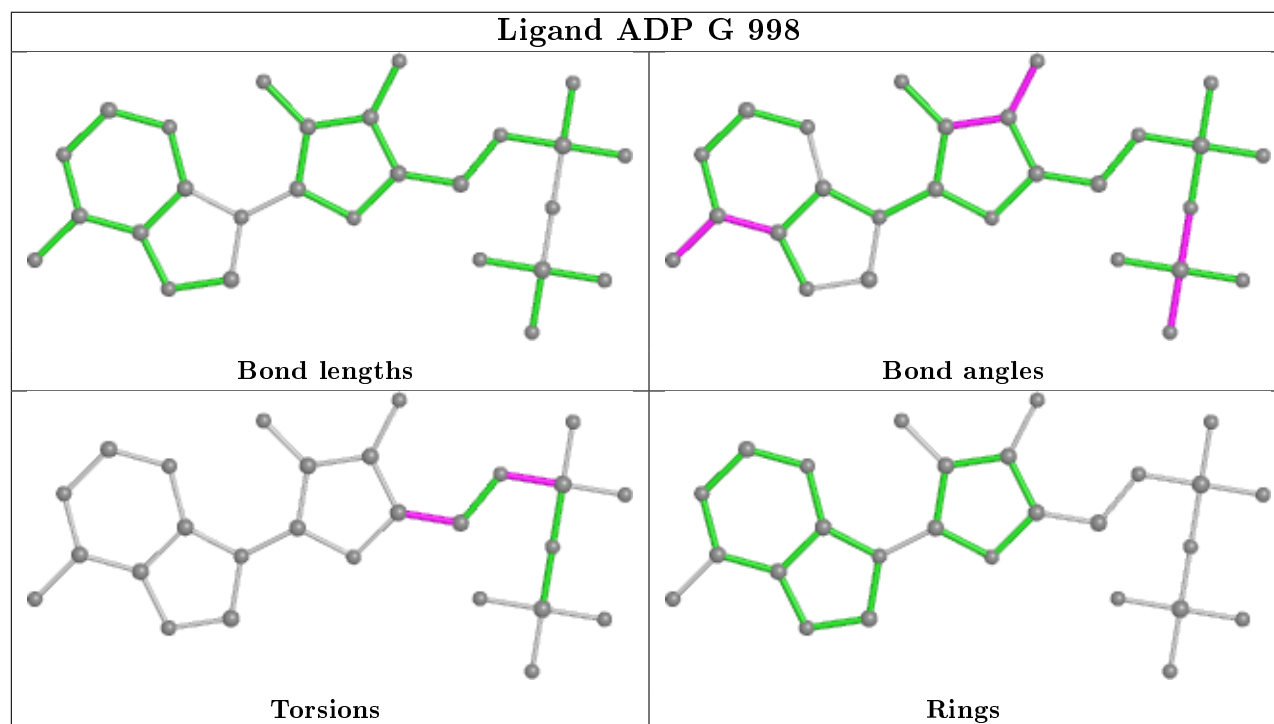
Mol	Chain	Res	Type	Atoms
5	G	998	ADP	C5'-O5'-PA-O1A
5	G	998	ADP	C5'-O5'-PA-O2A
5	A	998	ADP	C5'-O5'-PA-O1A
5	A	998	ADP	C5'-O5'-PA-O2A
5	C	998	ADP	C5'-O5'-PA-O1A
5	C	998	ADP	C5'-O5'-PA-O2A
5	E	998	ADP	C5'-O5'-PA-O1A
5	E	998	ADP	C5'-O5'-PA-O2A
5	G	998	ADP	O4'-C4'-C5'-O5'
5	G	998	ADP	C3'-C4'-C5'-O5'
5	A	998	ADP	O4'-C4'-C5'-O5'
5	A	998	ADP	C3'-C4'-C5'-O5'
5	C	998	ADP	O4'-C4'-C5'-O5'
5	C	998	ADP	C3'-C4'-C5'-O5'
5	E	998	ADP	O4'-C4'-C5'-O5'
5	E	998	ADP	C3'-C4'-C5'-O5'
5	G	998	ADP	C5'-O5'-PA-O3A
5	A	998	ADP	C5'-O5'-PA-O3A
5	C	998	ADP	C5'-O5'-PA-O3A
5	E	998	ADP	C5'-O5'-PA-O3A

There are no ring outliers.

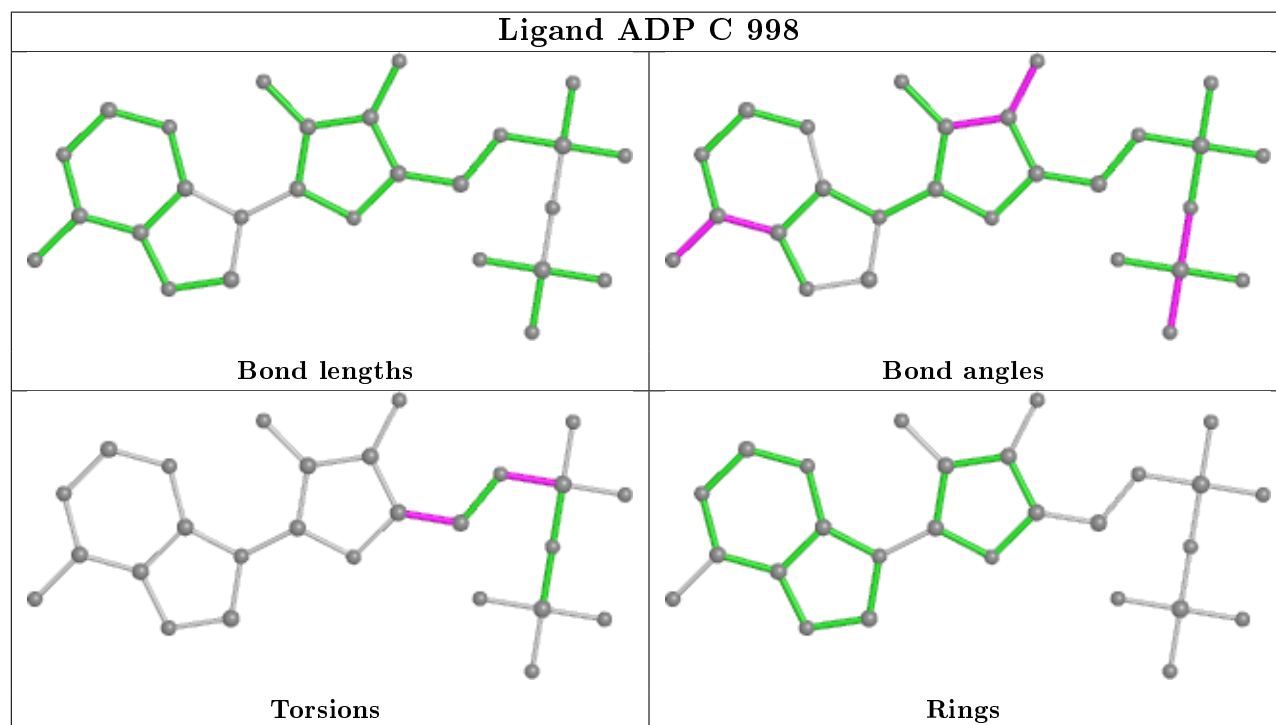
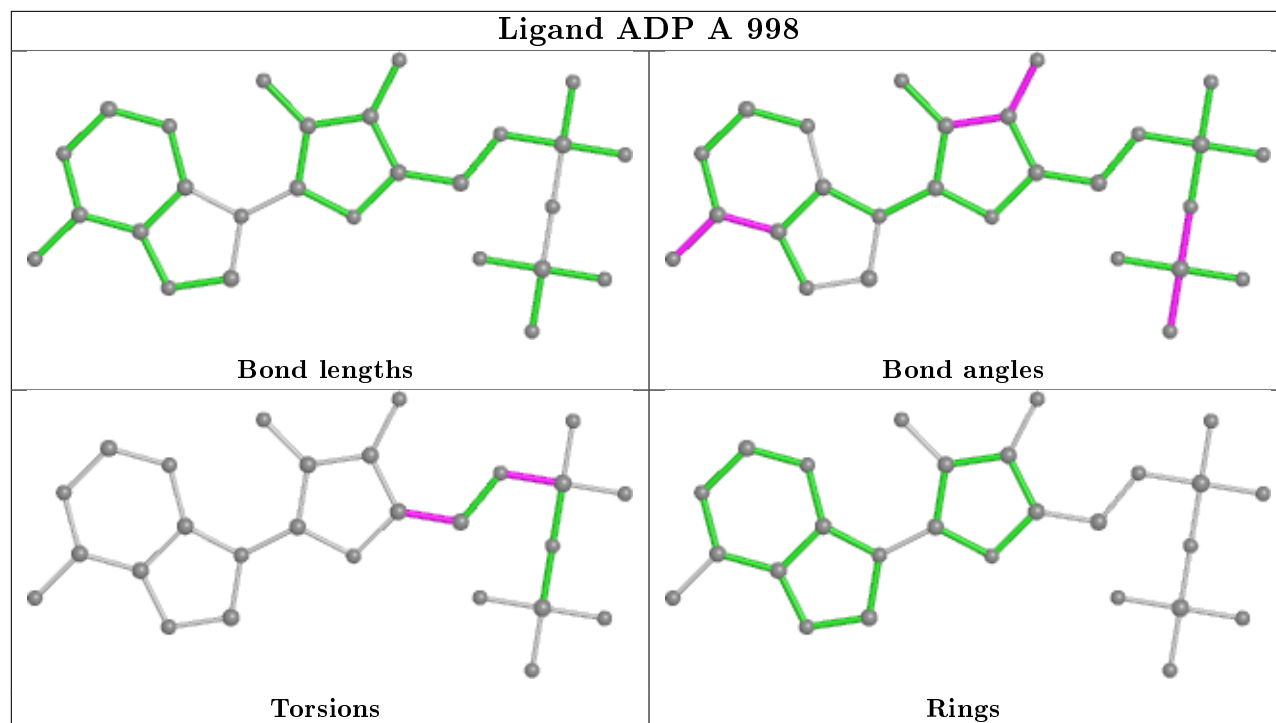
8 monomers are involved in 12 short contacts:

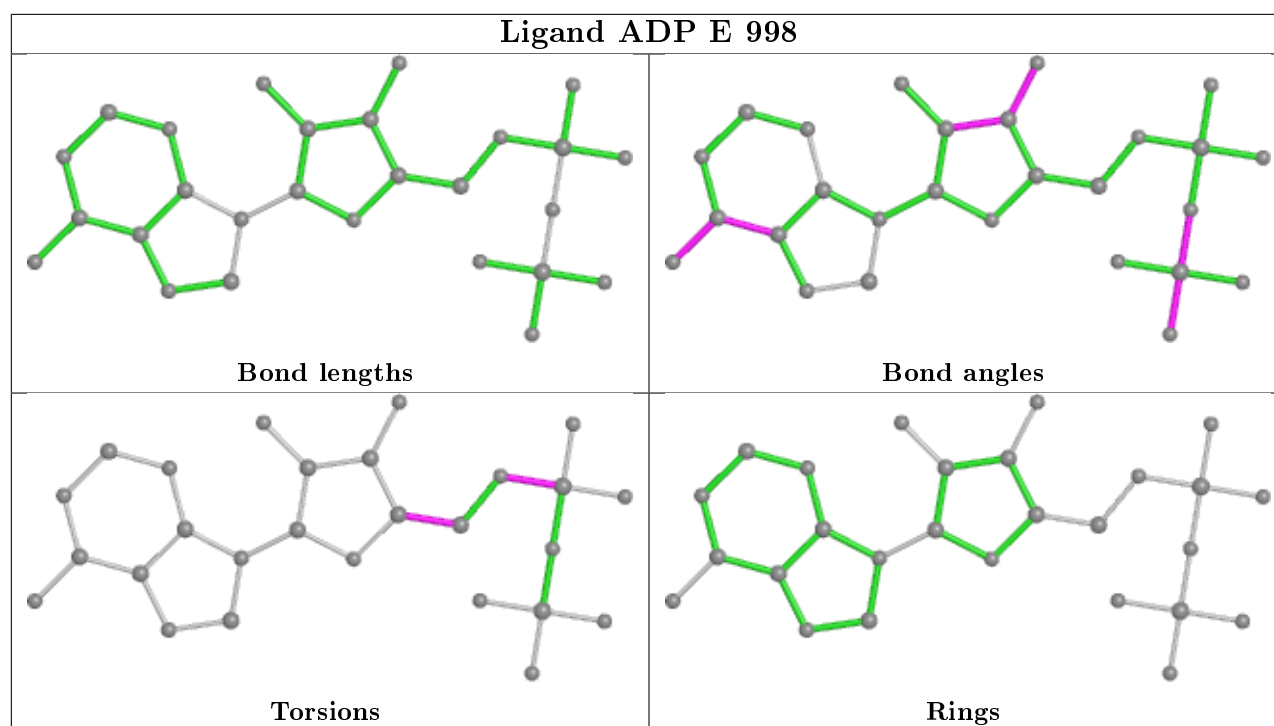
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	999	ALF	1	0
5	G	998	ADP	3	0
4	A	999	ALF	1	0
5	A	998	ADP	1	0
4	G	999	ALF	1	0
5	C	998	ADP	4	0
4	E	999	ALF	1	0
5	E	998	ADP	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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.