



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Aug 17, 2017 – 04:34 PM EDT

PDB ID : 2YMN  
EMDB ID: : EMD-2209  
Title : Organization of the Influenza Virus Replication Machinery  
Authors : Moeller, A.; Kirchdoerfer, R.N.; Potter, C.S.; Carragher, B.; Wilson, I.A.  
Deposited on : unknown  
Resolution : 20.00 Å(reported)  
Based on PDB ID : 2IQH

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report  
for a publicly released PDB/EMDB entry.

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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20029824

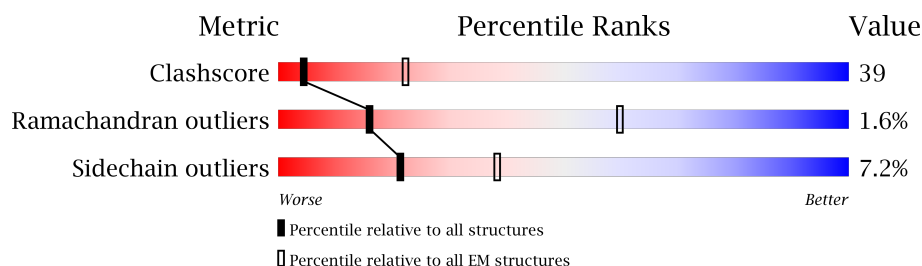
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 20.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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

Mol	Chain	Length	Quality of chain
1	A	498	41% 35% 5% 20%
1	B	498	45% 32% . 20%
1	C	498	35% 43% 5% 18%
1	D	498	38% 37% 5% 20%
1	E	498	39% 36% 5% 20%
1	F	498	40% 35% 5% 20%

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 18994 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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.

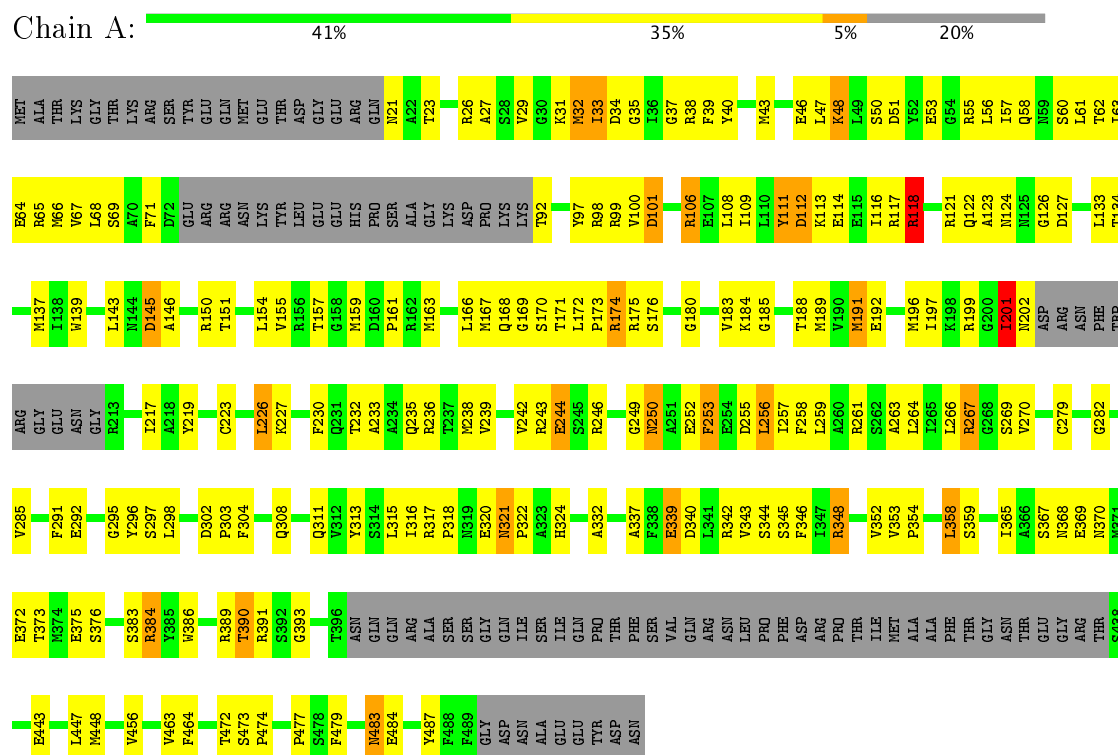
- Molecule 1 is a protein called NUCLEOPROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	399	Total	C	N	O	S	0	0
			3151	1954	586	586	25		
1	B	399	Total	C	N	O	S	0	0
			3151	1954	586	586	25		
1	C	409	Total	C	N	O	S	0	0
			3239	2007	605	602	25		
1	D	399	Total	C	N	O	S	0	0
			3151	1954	586	586	25		
1	E	399	Total	C	N	O	S	0	0
			3151	1954	586	586	25		
1	F	399	Total	C	N	O	S	0	0
			3151	1954	586	586	25		

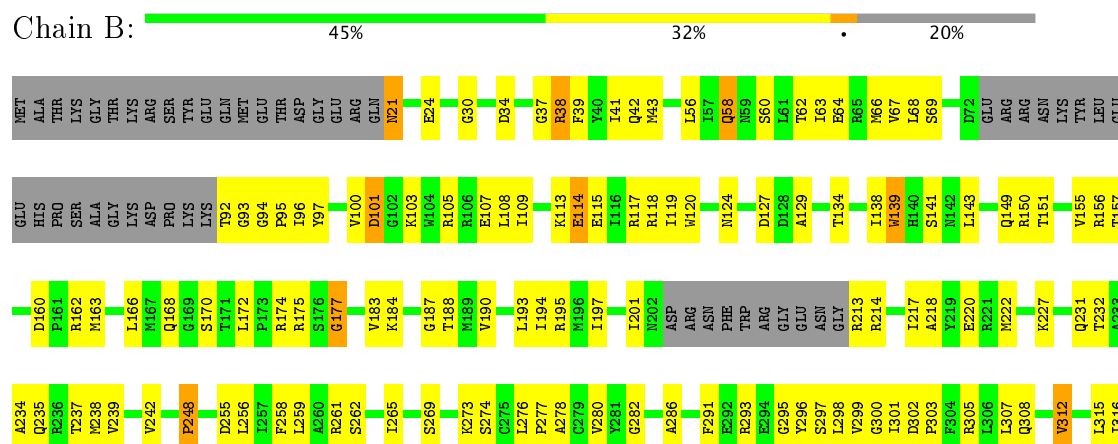
### 3 Residue-property plots

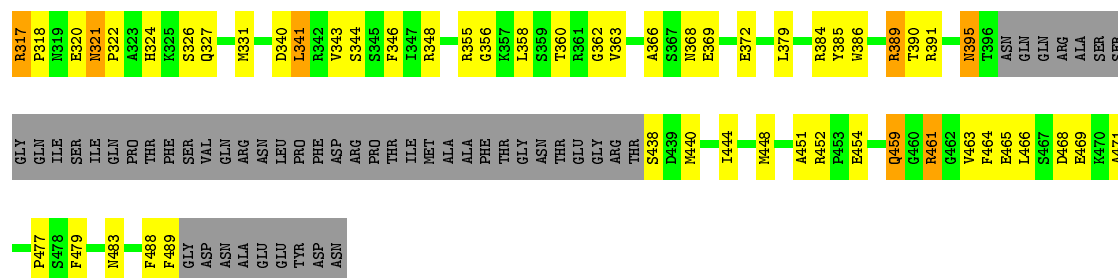
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

#### • Molecule 1: NUCLEOPROTEIN

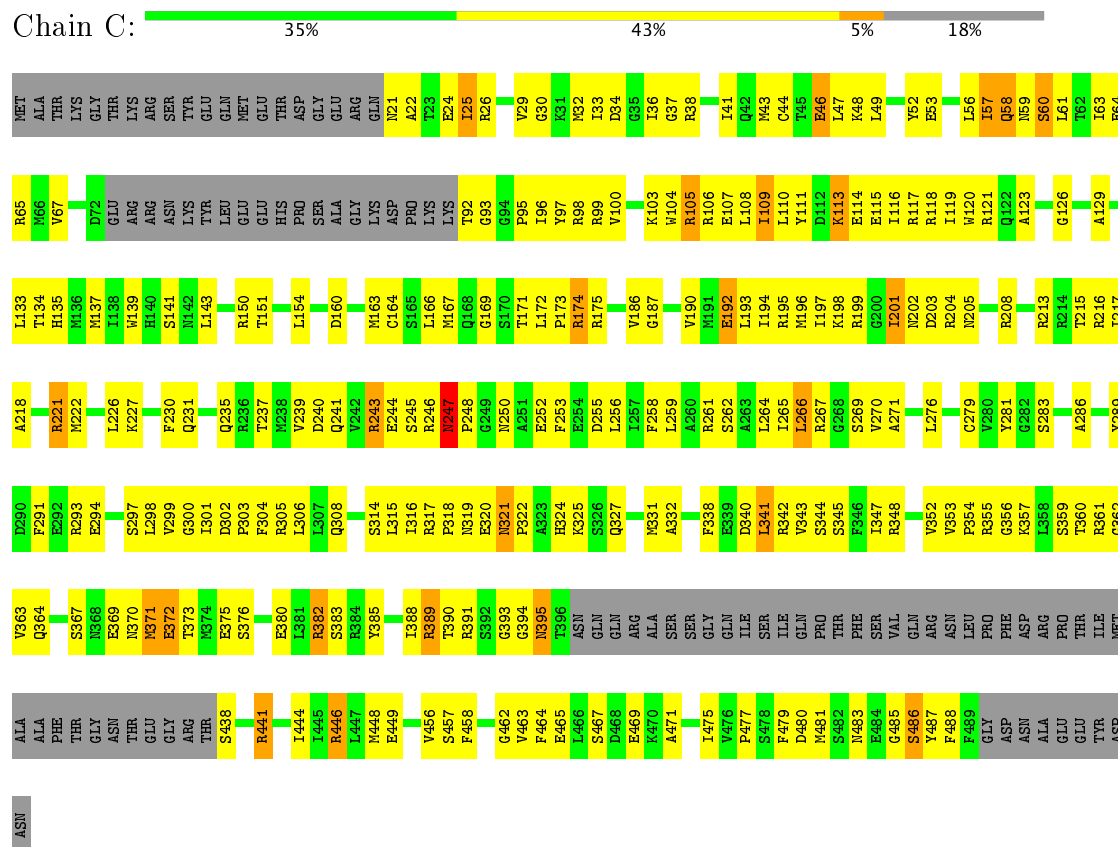


#### • Molecule 1: NUCLEOPROTEIN

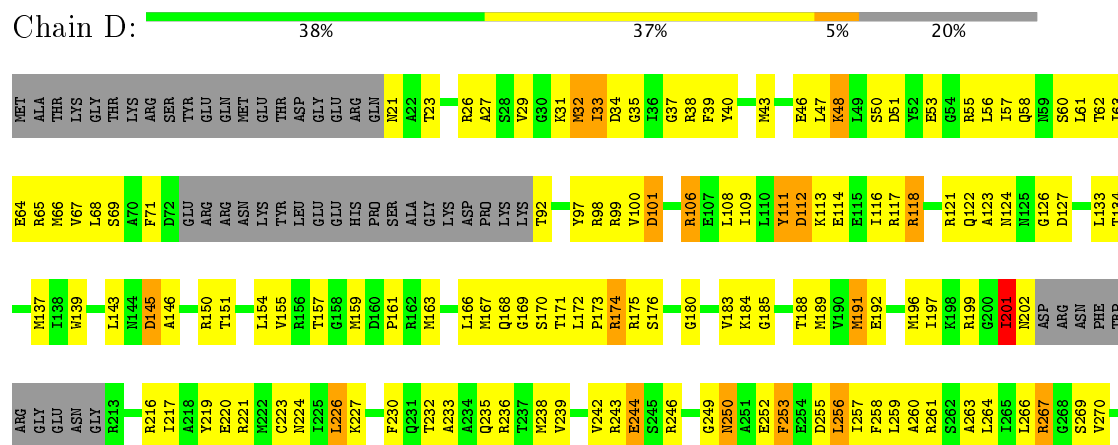


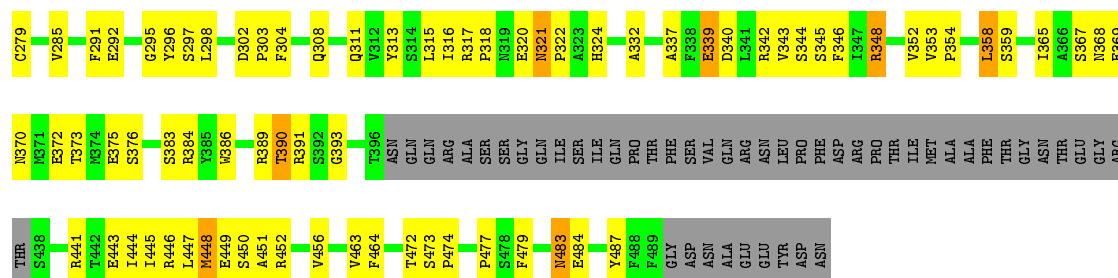


## • Molecule 1: NUCLEOPROTEIN

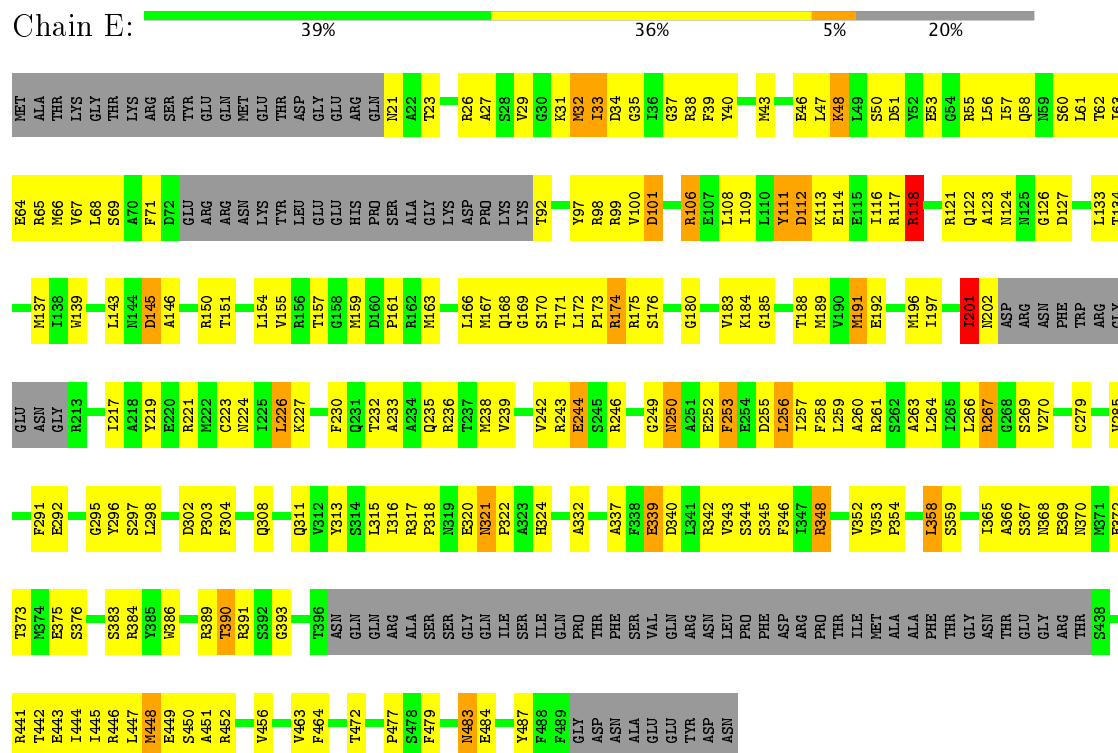


## • Molecule 1: NUCLEOPROTEIN

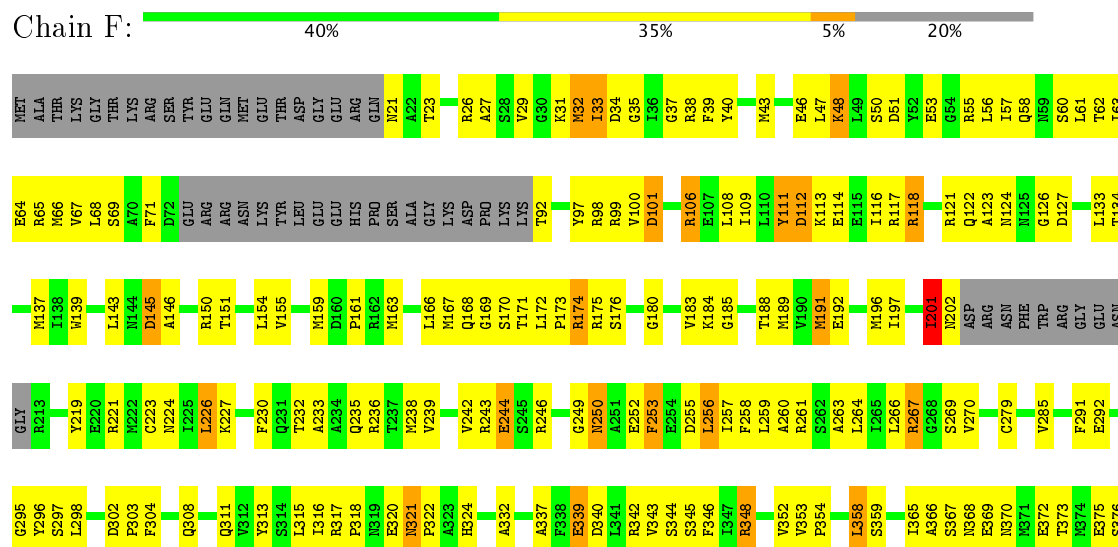


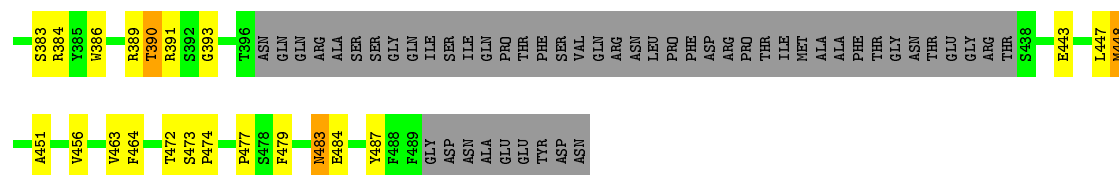


## • Molecule 1: NUCLEOPROTEIN



## • Molecule 1: NUCLEOPROTEIN





## 4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=Not provided°, rise=Not provided Å, axial sym=Not provided	Depositor
Number of segments used	31573	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	WHOLEIMAGE	Depositor
Microscope	FEI TECNAI 20	Depositor
Voltage (kV)	120	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	15	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	50000	Depositor
Image detector	GENERIC CCD	Depositor



## 5 Model quality

### 5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
1	A	0.92	1/3200 (0.0%)	0.92	8/4299 (0.2%)
1	B	0.97	3/3200 (0.1%)	0.92	3/4299 (0.1%)
1	C	0.84	4/3292 (0.1%)	0.88	4/4424 (0.1%)
1	D	0.92	1/3200 (0.0%)	0.92	6/4299 (0.1%)
1	E	0.92	1/3200 (0.0%)	0.92	7/4299 (0.2%)
1	F	0.92	1/3200 (0.0%)	0.92	6/4299 (0.1%)
All	All	0.92	11/19292 (0.1%)	0.91	34/25919 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	1
1	E	0	1
1	F	0	1
All	All	0	4

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	201	ILE	C-N	-13.48	1.03	1.34
1	C	202	ASN	C-N	-7.92	1.15	1.34
1	C	201	ILE	C-N	-7.91	1.15	1.34
1	B	312	VAL	CB-CG2	-5.83	1.40	1.52
1	C	247	ASN	CB-CG	5.77	1.64	1.51
1	A	201	ILE	C-N	-5.26	1.22	1.34
1	E	201	ILE	C-N	-5.26	1.22	1.34
1	B	312	VAL	CB-CG1	-5.25	1.41	1.52
1	C	192	GLU	CG-CD	5.25	1.59	1.51
1	D	201	ILE	C-N	-5.24	1.22	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	201	ILE	C-N	-5.22	1.22	1.34

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	201	ILE	O-C-N	-6.22	112.74	122.70
1	E	201	ILE	O-C-N	-6.22	112.75	122.70
1	A	201	ILE	O-C-N	-6.20	112.78	122.70
1	F	201	ILE	O-C-N	-6.19	112.79	122.70
1	C	201	ILE	O-C-N	-6.14	112.88	122.70
1	C	221	ARG	NE-CZ-NH1	-6.11	117.25	120.30
1	B	38	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	C	341	LEU	CB-CG-CD1	-5.84	101.06	111.00
1	F	358	LEU	CB-CG-CD2	-5.73	101.26	111.00
1	A	358	LEU	CB-CG-CD2	-5.71	101.30	111.00
1	E	358	LEU	CB-CG-CD2	-5.70	101.32	111.00
1	D	358	LEU	CB-CG-CD2	-5.69	101.32	111.00
1	D	66	MET	CG-SD-CE	5.52	109.03	100.20
1	E	66	MET	CG-SD-CE	5.51	109.02	100.20
1	F	66	MET	CG-SD-CE	5.50	109.00	100.20
1	A	66	MET	CG-SD-CE	5.50	108.99	100.20
1	E	256	LEU	CA-CB-CG	5.40	127.72	115.30
1	F	256	LEU	CA-CB-CG	5.40	127.72	115.30
1	A	256	LEU	CA-CB-CG	5.40	127.71	115.30
1	D	256	LEU	CA-CB-CG	5.37	127.65	115.30
1	C	201	ILE	CA-C-N	5.34	128.94	117.20
1	D	145	ASP	CB-CG-OD1	5.33	123.10	118.30
1	A	145	ASP	CB-CG-OD1	5.32	123.09	118.30
1	E	226	LEU	CA-CB-CG	5.31	127.52	115.30
1	B	299	VAL	CG1-CB-CG2	-5.31	102.41	110.90
1	B	38	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	F	226	LEU	CA-CB-CG	5.31	127.50	115.30
1	F	145	ASP	CB-CG-OD1	5.29	123.06	118.30
1	D	226	LEU	CA-CB-CG	5.29	127.47	115.30
1	A	226	LEU	CA-CB-CG	5.29	127.47	115.30
1	E	145	ASP	CB-CG-OD1	5.26	123.03	118.30
1	A	118	ARG	NE-CZ-NH1	-5.08	117.76	120.30
1	E	118	ARG	NE-CZ-NH1	-5.06	117.77	120.30
1	A	384	ARG	NE-CZ-NH2	-5.01	117.80	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	201	ILE	Mainchain
1	D	201	ILE	Mainchain
1	E	201	ILE	Mainchain
1	F	201	ILE	Mainchain

## 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	3151	0	3148	210	0
1	B	3151	0	3145	192	0
1	C	3239	0	3220	257	0
1	D	3151	0	3146	340	0
1	E	3151	0	3141	398	0
1	F	3151	0	3145	297	0
All	All	18994	0	18945	1463	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 39.

All (1463) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:447:LEU:HD21	1:F:367:SER:CB	1.13	1.61
1:D:446:ARG:H	1:E:368:ASN:CB	1.01	1.60
1:D:447:LEU:HD21	1:E:367:SER:CB	1.14	1.59
1:D:447:LEU:CD2	1:E:367:SER:HB2	1.27	1.59
1:E:446:ARG:H	1:F:368:ASN:CB	1.04	1.58
1:E:447:LEU:CD2	1:F:367:SER:HB2	1.27	1.58
1:D:446:ARG:NH2	1:E:365:ILE:CG2	1.69	1.54
1:B:213:ARG:NH1	1:D:243:ARG:CD	1.69	1.49
1:E:447:LEU:HG	1:F:367:SER:C	1.29	1.49
1:D:447:LEU:HG	1:E:367:SER:C	1.28	1.44
1:E:446:ARG:N	1:F:368:ASN:CB	1.80	1.42
1:D:446:ARG:N	1:E:368:ASN:HB3	1.32	1.42
1:E:446:ARG:N	1:F:368:ASN:HB3	1.31	1.39
1:B:213:ARG:NH1	1:D:243:ARG:HD3	1.06	1.37

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:446:ARG:NH2	1:E:365:ILE:HG22	1.26	1.37
1:D:446:ARG:N	1:E:368:ASN:CB	1.78	1.37
1:D:447:LEU:CG	1:E:367:SER:O	1.75	1.34
1:E:447:LEU:CG	1:F:367:SER:O	1.74	1.33
1:E:447:LEU:CG	1:F:367:SER:C	1.95	1.33
1:E:442:THR:O	1:F:368:ASN:CB	1.66	1.33
1:D:447:LEU:CG	1:E:367:SER:C	1.96	1.31
1:B:213:ARG:NH2	1:D:220:GLU:HG2	1.45	1.31
1:D:447:LEU:CA	1:E:367:SER:O	1.79	1.30
1:E:447:LEU:CA	1:F:367:SER:O	1.81	1.27
1:D:446:ARG:NH2	1:E:365:ILE:CB	1.69	1.27
1:E:447:LEU:CD2	1:F:367:SER:O	1.83	1.25
1:B:213:ARG:NE	1:D:220:GLU:CD	1.89	1.25
1:E:447:LEU:HD21	1:F:367:SER:CA	1.66	1.25
1:D:446:ARG:NE	1:E:365:ILE:HG22	1.48	1.24
1:D:447:LEU:CD2	1:E:367:SER:CB	1.96	1.23
1:E:447:LEU:CD2	1:F:367:SER:CB	1.96	1.22
1:C:208:ARG:NE	1:D:199:ARG:HH21	1.34	1.22
1:D:447:LEU:CD2	1:E:367:SER:O	1.87	1.22
1:D:447:LEU:HD21	1:E:367:SER:CA	1.69	1.22
1:B:213:ARG:NH1	1:D:243:ARG:CG	2.01	1.21
1:D:446:ARG:CZ	1:E:365:ILE:HG22	1.30	1.21
1:E:447:LEU:CD2	1:F:367:SER:CA	2.19	1.21
1:D:446:ARG:N	1:E:368:ASN:CA	1.92	1.19
1:D:446:ARG:CZ	1:E:365:ILE:CG2	1.95	1.19
1:E:447:LEU:HD23	1:F:367:SER:O	1.39	1.18
1:D:447:LEU:CD2	1:E:367:SER:CA	2.21	1.17
1:E:447:LEU:HD11	1:F:367:SER:OG	1.48	1.14
1:D:447:LEU:HD11	1:E:367:SER:OG	1.47	1.12
1:D:452:ARG:NH2	1:E:372:GLU:HB2	1.64	1.12
1:E:447:LEU:CD2	1:F:367:SER:C	2.15	1.11
1:B:213:ARG:CD	1:D:220:GLU:OE2	1.96	1.11
1:E:452:ARG:NH2	1:F:372:GLU:HB2	1.65	1.11
1:D:446:ARG:NH2	1:E:365:ILE:HB	1.54	1.10
1:D:447:LEU:HD23	1:E:367:SER:O	1.44	1.09
1:D:446:ARG:HB3	1:E:368:ASN:N	1.67	1.06
1:D:447:LEU:CG	1:E:367:SER:HB2	1.85	1.06
1:E:442:THR:O	1:F:368:ASN:HB2	1.39	1.06
1:E:447:LEU:CB	1:F:367:SER:O	2.05	1.04
1:E:446:ARG:HB3	1:F:368:ASN:HB2	1.35	1.03
1:E:446:ARG:HB2	1:F:369:GLU:HG3	1.39	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:ILE:HG21	1:D:217:ILE:HG12	1.38	1.03
1:D:447:LEU:CB	1:E:367:SER:O	2.05	1.03
1:D:447:LEU:HA	1:E:367:SER:O	1.52	1.03
1:E:447:LEU:CG	1:F:367:SER:HB2	1.89	1.03
1:E:446:ARG:N	1:F:368:ASN:CA	1.96	1.02
1:E:446:ARG:CB	1:F:368:ASN:HB2	1.89	1.02
1:D:446:ARG:HB3	1:E:368:ASN:HB2	1.38	1.02
1:D:447:LEU:CD2	1:E:367:SER:C	2.19	1.01
1:E:447:LEU:HA	1:F:367:SER:O	1.52	1.01
1:B:213:ARG:NE	1:D:220:GLU:OE2	1.94	1.01
1:F:483:ASN:H	1:F:483:ASN:HD22	1.09	1.01
1:D:446:ARG:HB2	1:E:369:GLU:HG3	1.39	1.00
1:D:446:ARG:CB	1:E:368:ASN:HB2	1.91	0.99
1:A:483:ASN:HD22	1:A:483:ASN:H	1.09	0.98
1:E:447:LEU:HG	1:F:368:ASN:N	1.78	0.98
1:E:483:ASN:H	1:E:483:ASN:HD22	1.09	0.98
1:B:213:ARG:CZ	1:D:220:GLU:CG	2.41	0.97
1:D:483:ASN:H	1:D:483:ASN:HD22	1.09	0.97
1:E:111:TYR:HB3	1:E:116:ILE:HD11	1.46	0.96
1:D:446:ARG:CB	1:E:368:ASN:CB	2.42	0.96
1:D:447:LEU:HG	1:E:368:ASN:N	1.81	0.96
1:B:213:ARG:NH2	1:D:220:GLU:CG	2.29	0.96
1:F:189:MET:HE1	1:F:192:GLU:OE1	1.66	0.96
1:D:447:LEU:CG	1:E:367:SER:CB	2.41	0.95
1:D:111:TYR:HB3	1:D:116:ILE:HD11	1.47	0.95
1:E:446:ARG:HB3	1:F:368:ASN:CB	1.80	0.95
1:A:111:TYR:HB3	1:A:116:ILE:HD11	1.47	0.95
1:D:226:LEU:HD13	1:D:230:PHE:HE1	1.31	0.95
1:F:111:TYR:HB3	1:F:116:ILE:HD11	1.46	0.94
1:B:213:ARG:HE	1:D:220:GLU:CD	1.65	0.94
1:E:446:ARG:CB	1:F:368:ASN:CB	2.41	0.94
1:B:100:VAL:CG2	1:B:105:ARG:HD3	1.98	0.94
1:D:452:ARG:HH22	1:E:372:GLU:CB	1.81	0.94
1:C:208:ARG:NE	1:D:199:ARG:NH2	2.15	0.94
1:F:58:GLN:HG3	1:F:315:LEU:HG	1.50	0.93
1:D:58:GLN:HG3	1:D:315:LEU:HG	1.50	0.93
1:C:465:GLU:HG3	1:C:467:SER:H	1.32	0.93
1:E:226:LEU:HD13	1:E:230:PHE:HE1	1.31	0.93
1:E:452:ARG:HH22	1:F:372:GLU:CB	1.82	0.93
1:A:226:LEU:HD13	1:A:230:PHE:HE1	1.31	0.92
1:A:58:GLN:HG3	1:A:315:LEU:HG	1.50	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:447:LEU:CG	1:F:367:SER:CB	2.44	0.92
1:E:446:ARG:HB3	1:F:368:ASN:N	1.70	0.91
1:C:353:VAL:HG22	1:C:354:PRO:HD2	1.52	0.91
1:D:452:ARG:NH2	1:E:372:GLU:CB	2.34	0.91
1:A:189:MET:HE1	1:A:192:GLU:OE1	1.71	0.91
1:C:341:LEU:HB2	1:C:486:SER:HA	1.53	0.91
1:E:58:GLN:HG3	1:E:315:LEU:HG	1.50	0.90
1:D:189:MET:HE1	1:D:192:GLU:OE1	1.71	0.90
1:E:452:ARG:NH2	1:F:372:GLU:CB	2.33	0.90
1:E:446:ARG:CB	1:F:369:GLU:HG3	2.02	0.90
1:F:226:LEU:HD13	1:F:230:PHE:HE1	1.31	0.89
1:E:446:ARG:HB2	1:F:369:GLU:CG	2.03	0.89
1:D:447:LEU:N	1:E:367:SER:O	2.05	0.89
1:E:452:ARG:HH21	1:F:372:GLU:HB2	1.37	0.89
1:D:446:ARG:HB2	1:E:369:GLU:CG	2.03	0.88
1:E:442:THR:O	1:F:368:ASN:HB3	1.74	0.88
1:B:213:ARG:CG	1:D:220:GLU:OE2	2.22	0.87
1:D:446:ARG:CB	1:E:369:GLU:HG3	2.03	0.87
1:B:21:ASN:CB	1:B:24:GLU:HG3	2.04	0.87
1:E:189:MET:HE1	1:E:192:GLU:OE1	1.73	0.87
1:D:447:LEU:HD11	1:E:367:SER:CB	2.05	0.86
1:F:250:ASN:HA	1:F:253:PHE:HB3	1.58	0.86
1:A:250:ASN:HA	1:A:253:PHE:HB3	1.58	0.86
1:B:213:ARG:CZ	1:D:220:GLU:HG2	2.02	0.85
1:B:213:ARG:HH21	1:D:220:GLU:HG2	1.38	0.85
1:E:447:LEU:N	1:F:367:SER:O	2.09	0.85
1:D:446:ARG:HE	1:E:365:ILE:HG22	1.40	0.85
1:C:276:LEU:HB2	1:C:281:TYR:HE1	1.41	0.85
1:B:217:ILE:CG2	1:D:217:ILE:HG12	2.07	0.85
1:E:449:GLU:C	1:F:370:ASN:HB3	1.94	0.84
1:D:452:ARG:HH21	1:E:372:GLU:HB2	1.38	0.84
1:E:308:GLN:HE22	1:E:383:SER:H	1.24	0.84
1:E:446:ARG:CG	1:F:369:GLU:HG3	2.06	0.84
1:B:360:THR:HG22	1:B:362:GLY:H	1.43	0.84
1:E:250:ASN:HA	1:E:253:PHE:HB3	1.58	0.84
1:F:308:GLN:HE22	1:F:383:SER:H	1.24	0.84
1:D:250:ASN:HA	1:D:253:PHE:HB3	1.58	0.84
1:A:308:GLN:HE22	1:A:383:SER:H	1.24	0.83
1:E:447:LEU:HD11	1:F:367:SER:CB	2.07	0.83
1:B:42:GLN:HG2	1:B:119:ILE:HD11	1.59	0.83
1:B:96:ILE:HG13	1:B:109:ILE:HD12	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:446:ARG:CG	1:E:369:GLU:HG3	2.09	0.82
1:B:217:ILE:HB	1:D:217:ILE:HD11	1.60	0.82
1:D:446:ARG:NE	1:E:365:ILE:CG2	2.24	0.82
1:D:308:GLN:HE22	1:D:383:SER:H	1.24	0.82
1:E:443:GLU:OE2	1:F:366:ALA:HB1	1.79	0.82
1:C:106:ARG:HH12	1:C:367:SER:HA	1.45	0.81
1:C:231:GLN:NE2	1:C:269:SER:HB2	1.96	0.80
1:D:114:GLU:HB3	1:D:117:ARG:HH21	1.46	0.80
1:D:447:LEU:CD1	1:E:367:SER:HB2	2.10	0.80
1:D:121:ARG:HG2	1:D:121:ARG:HH11	1.47	0.80
1:D:443:GLU:OE2	1:E:366:ALA:HB1	1.82	0.80
1:E:114:GLU:HB3	1:E:117:ARG:HH21	1.46	0.80
1:F:114:GLU:HB3	1:F:117:ARG:HH21	1.46	0.80
1:A:114:GLU:HB3	1:A:117:ARG:HH21	1.46	0.80
1:A:114:GLU:HA	1:A:117:ARG:HE	1.47	0.80
1:D:114:GLU:HA	1:D:117:ARG:HE	1.47	0.80
1:D:71:PHE:HE1	1:D:117:ARG:HA	1.48	0.79
1:A:121:ARG:HG2	1:A:121:ARG:HH11	1.47	0.79
1:B:213:ARG:NH1	1:D:243:ARG:HG2	1.96	0.79
1:B:231:GLN:NE2	1:B:269:SER:HB3	1.97	0.79
1:F:227:LYS:HE3	1:F:236:ARG:HB3	1.64	0.79
1:F:114:GLU:HA	1:F:117:ARG:HE	1.47	0.79
1:A:324:HIS:HD2	1:A:359:SER:H	1.30	0.79
1:E:121:ARG:HG2	1:E:121:ARG:HH11	1.47	0.79
1:A:227:LYS:HE3	1:A:236:ARG:HB3	1.65	0.79
1:B:324:HIS:CD2	1:B:358:LEU:HD12	2.17	0.79
1:E:71:PHE:HE1	1:E:117:ARG:HA	1.48	0.79
1:E:443:GLU:HA	1:F:366:ALA:HB1	1.65	0.79
1:D:443:GLU:HA	1:E:366:ALA:HB1	1.64	0.78
1:B:265:ILE:HD11	1:B:448:MET:HG2	1.63	0.78
1:D:447:LEU:CD1	1:E:367:SER:CB	2.60	0.78
1:B:213:ARG:HG2	1:D:220:GLU:OE2	1.83	0.78
1:F:121:ARG:HH11	1:F:121:ARG:HG2	1.47	0.78
1:D:446:ARG:HB3	1:E:368:ASN:CB	1.83	0.78
1:B:217:ILE:HG13	1:B:218:ALA:H	1.49	0.78
1:C:33:ILE:HD12	1:C:281:TYR:HE2	1.49	0.78
1:F:71:PHE:HE1	1:F:117:ARG:HA	1.48	0.78
1:A:114:GLU:CB	1:A:117:ARG:HH21	1.97	0.78
1:E:446:ARG:CB	1:F:368:ASN:N	2.42	0.78
1:D:163:MET:HE3	1:D:261:ARG:HG2	1.66	0.77
1:E:114:GLU:HA	1:E:117:ARG:HE	1.47	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:317:ARG:HD3	1:E:369:GLU:OE1	1.84	0.77
1:F:324:HIS:HD2	1:F:359:SER:H	1.30	0.77
1:A:317:ARG:HD3	1:A:369:GLU:OE1	1.84	0.77
1:A:71:PHE:HE1	1:A:117:ARG:HA	1.48	0.77
1:E:447:LEU:CD1	1:F:367:SER:HB2	2.13	0.77
1:E:340:ASP:O	1:E:343:VAL:HG12	1.85	0.77
1:E:483:ASN:HD22	1:E:483:ASN:N	1.82	0.77
1:F:114:GLU:CB	1:F:117:ARG:HH21	1.97	0.77
1:B:213:ARG:CZ	1:D:220:GLU:CD	2.52	0.77
1:E:447:LEU:CD1	1:F:367:SER:CB	2.62	0.77
1:D:114:GLU:CB	1:D:117:ARG:HH21	1.97	0.77
1:D:317:ARG:HD3	1:D:369:GLU:OE1	1.83	0.77
1:D:390:THR:HG22	1:D:391:ARG:H	1.49	0.77
1:F:340:ASP:O	1:F:343:VAL:HG12	1.85	0.77
1:D:324:HIS:HD2	1:D:359:SER:H	1.30	0.77
1:F:111:TYR:HB3	1:F:116:ILE:CD1	2.15	0.77
1:B:317:ARG:HG2	1:B:320:GLU:OE2	1.85	0.77
1:E:227:LYS:HE3	1:E:236:ARG:HB3	1.65	0.77
1:F:317:ARG:HD3	1:F:369:GLU:OE1	1.84	0.77
1:E:114:GLU:CB	1:E:117:ARG:HH21	1.97	0.77
1:E:390:THR:HG22	1:E:391:ARG:H	1.50	0.77
1:D:227:LYS:HE3	1:D:236:ARG:HB3	1.65	0.76
1:F:483:ASN:HD22	1:F:483:ASN:N	1.82	0.76
1:A:111:TYR:HB3	1:A:116:ILE:CD1	2.15	0.76
1:C:327:GLN:O	1:C:331:MET:HG3	1.84	0.76
1:C:154:LEU:HD21	1:C:167:MET:CE	2.15	0.76
1:E:111:TYR:HB3	1:E:116:ILE:CD1	2.15	0.76
1:F:390:THR:HG22	1:F:391:ARG:H	1.50	0.76
1:D:340:ASP:O	1:D:343:VAL:HG12	1.85	0.76
1:D:483:ASN:HD22	1:D:483:ASN:N	1.82	0.76
1:D:111:TYR:HB3	1:D:116:ILE:CD1	2.15	0.76
1:A:340:ASP:O	1:A:343:VAL:HG12	1.85	0.76
1:B:213:ARG:HD3	1:D:220:GLU:OE2	1.84	0.76
1:E:324:HIS:HD2	1:E:359:SER:H	1.30	0.75
1:D:449:GLU:C	1:E:370:ASN:HB3	1.94	0.75
1:C:276:LEU:HB2	1:C:281:TYR:CE1	2.20	0.75
1:E:447:LEU:HD21	1:F:367:SER:HB3	1.60	0.75
1:A:390:THR:HG22	1:A:391:ARG:H	1.50	0.75
1:E:447:LEU:CD1	1:F:367:SER:OG	2.33	0.75
1:B:21:ASN:HB3	1:B:24:GLU:HG3	1.67	0.75
1:F:242:VAL:HG11	1:F:256:LEU:HD21	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:447:LEU:HD21	1:E:367:SER:HB3	1.58	0.75
1:D:449:GLU:OE2	1:E:370:ASN:ND2	2.17	0.75
1:D:242:VAL:HG11	1:D:256:LEU:HD21	1.68	0.74
1:A:163:MET:HE3	1:A:261:ARG:HG2	1.68	0.74
1:D:232:THR:OG1	1:D:235:GLN:HG3	1.87	0.74
1:A:242:VAL:HG11	1:A:256:LEU:HD21	1.68	0.74
1:E:450:SER:OG	1:F:370:ASN:HA	1.87	0.74
1:C:353:VAL:CG2	1:C:354:PRO:HD2	2.17	0.74
1:F:232:THR:OG1	1:F:235:GLN:HG3	1.87	0.74
1:A:483:ASN:HD22	1:A:483:ASN:N	1.82	0.74
1:B:217:ILE:HG13	1:B:218:ALA:N	2.02	0.74
1:D:174:ARG:N	1:D:174:ARG:HD3	2.03	0.74
1:F:163:MET:HE3	1:F:261:ARG:HG2	1.68	0.74
1:A:174:ARG:N	1:A:174:ARG:HD3	2.03	0.74
1:E:342:ARG:HB3	1:E:479:PHE:CE2	2.23	0.74
1:A:232:THR:OG1	1:A:235:GLN:HG3	1.87	0.73
1:E:174:ARG:HD3	1:E:174:ARG:N	2.03	0.73
1:D:446:ARG:CB	1:E:368:ASN:N	2.39	0.73
1:B:160:ASP:HB3	1:B:163:MET:HG3	1.69	0.73
1:B:324:HIS:HD2	1:B:358:LEU:HD12	1.53	0.73
1:D:446:ARG:H	1:E:368:ASN:HB3	0.57	0.73
1:E:242:VAL:HG11	1:E:256:LEU:HD21	1.68	0.73
1:D:447:LEU:CD1	1:E:367:SER:OG	2.32	0.73
1:C:267:ARG:O	1:C:395:ASN:ND2	2.21	0.73
1:E:232:THR:OG1	1:E:235:GLN:HG3	1.87	0.73
1:A:71:PHE:CE1	1:A:117:ARG:HA	2.24	0.73
1:E:446:ARG:HB3	1:F:368:ASN:H	1.51	0.73
1:C:243:ARG:HG2	1:C:243:ARG:HH11	1.53	0.73
1:F:483:ASN:H	1:F:483:ASN:ND2	1.86	0.73
1:E:163:MET:HE3	1:E:261:ARG:HG2	1.69	0.72
1:F:342:ARG:HB3	1:F:479:PHE:CE2	2.23	0.72
1:A:342:ARG:HB3	1:A:479:PHE:CE2	2.23	0.72
1:D:71:PHE:CE1	1:D:117:ARG:HA	2.24	0.72
1:E:226:LEU:HD13	1:E:230:PHE:CE1	2.22	0.72
1:D:342:ARG:HB3	1:D:479:PHE:CE2	2.23	0.72
1:F:174:ARG:HD3	1:F:174:ARG:N	2.03	0.72
1:D:226:LEU:HD13	1:D:230:PHE:CE1	2.22	0.72
1:C:208:ARG:CZ	1:D:199:ARG:NH2	2.52	0.72
1:C:104:TRP:CZ2	1:C:376:SER:HB3	2.25	0.72
1:C:33:ILE:HG23	1:C:281:TYR:CD2	2.25	0.72
1:E:71:PHE:CE1	1:E:117:ARG:HA	2.24	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:71:PHE:CE1	1:F:117:ARG:HA	2.24	0.72
1:F:226:LEU:HD13	1:F:230:PHE:CE1	2.22	0.72
1:C:221:ARG:HG2	1:C:221:ARG:HH11	1.55	0.71
1:E:446:ARG:H	1:F:368:ASN:HB3	0.55	0.71
1:B:321:ASN:HD22	1:B:322:PRO:CD	2.03	0.71
1:C:270:VAL:HG12	1:C:271:ALA:N	2.05	0.71
1:B:100:VAL:HG21	1:B:105:ARG:HD3	1.70	0.71
1:E:483:ASN:ND2	1:E:483:ASN:H	1.86	0.71
1:D:450:SER:OG	1:E:370:ASN:HA	1.91	0.71
1:F:324:HIS:CD2	1:F:359:SER:H	2.09	0.71
1:A:296:TYR:CD1	1:A:302:ASP:HB3	2.26	0.71
1:E:296:TYR:CD1	1:E:302:ASP:HB3	2.26	0.71
1:A:235:GLN:O	1:A:239:VAL:HG23	1.91	0.71
1:D:235:GLN:O	1:D:239:VAL:HG23	1.91	0.71
1:C:198:LYS:HD3	1:C:201:ILE:HD12	1.70	0.71
1:C:299:VAL:O	1:C:388:ILE:HG23	1.89	0.71
1:D:447:LEU:HG	1:E:367:SER:O	1.59	0.71
1:D:445:ILE:C	1:E:368:ASN:HB3	2.10	0.71
1:C:199:ARG:HG2	1:C:199:ARG:HH11	1.56	0.70
1:E:445:ILE:N	1:F:368:ASN:HB3	2.06	0.70
1:B:155:VAL:HG23	1:B:156:ARG:N	2.06	0.70
1:E:267:ARG:HG3	1:E:393:GLY:O	1.92	0.70
1:E:324:HIS:CD2	1:E:359:SER:H	2.09	0.70
1:D:445:ILE:N	1:E:368:ASN:HB3	2.05	0.70
1:F:267:ARG:HG3	1:F:393:GLY:O	1.91	0.70
1:E:235:GLN:O	1:E:239:VAL:HG23	1.91	0.70
1:A:324:HIS:CD2	1:A:359:SER:H	2.09	0.70
1:B:227:LYS:HB2	1:B:239:VAL:HG11	1.74	0.70
1:D:296:TYR:CD1	1:D:302:ASP:HB3	2.26	0.70
1:E:446:ARG:CB	1:F:369:GLU:CG	2.62	0.70
1:C:63:ILE:O	1:C:67:VAL:HG23	1.92	0.69
1:C:246:ARG:HG2	1:C:246:ARG:HH11	1.56	0.69
1:D:446:ARG:H	1:E:368:ASN:HB2	1.44	0.69
1:E:443:GLU:OE1	1:F:367:SER:OG	2.11	0.69
1:B:92:THR:HG22	1:B:93:GLY:N	2.06	0.69
1:C:198:LYS:HA	1:C:201:ILE:HD12	1.74	0.69
1:A:267:ARG:HG3	1:A:393:GLY:O	1.92	0.69
1:D:267:ARG:HG3	1:D:393:GLY:O	1.92	0.69
1:F:296:TYR:CD1	1:F:302:ASP:HB3	2.26	0.69
1:D:37:GLY:HA3	1:D:285:VAL:HG21	1.75	0.69
1:E:37:GLY:HA3	1:E:285:VAL:HG21	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:ASN:HB2	1:B:24:GLU:HG3	1.73	0.69
1:B:213:ARG:HH21	1:D:216:ARG:CZ	2.06	0.69
1:B:213:ARG:CZ	1:D:220:GLU:CB	2.69	0.69
1:E:447:LEU:HD23	1:F:367:SER:C	1.97	0.69
1:F:235:GLN:O	1:F:239:VAL:HG23	1.91	0.69
1:B:321:ASN:HD22	1:B:322:PRO:HD2	1.58	0.69
1:C:93:GLY:HA3	1:C:110:LEU:HD23	1.75	0.69
1:C:192:GLU:O	1:C:195:ARG:HG2	1.92	0.68
1:D:443:GLU:OE1	1:E:367:SER:OG	2.12	0.68
1:D:324:HIS:CD2	1:D:359:SER:H	2.09	0.68
1:B:138:ILE:HD12	1:B:183:VAL:HG21	1.76	0.68
1:C:44:CYS:HA	1:C:49:LEU:HD12	1.75	0.68
1:E:445:ILE:C	1:F:368:ASN:HB3	2.11	0.68
1:A:226:LEU:HD13	1:A:230:PHE:CE1	2.22	0.68
1:C:289:TYR:CE1	1:C:294:GLU:HG2	2.27	0.68
1:E:449:GLU:OE2	1:F:370:ASN:ND2	2.19	0.68
1:A:37:GLY:HA3	1:A:285:VAL:HG21	1.75	0.68
1:E:446:ARG:CG	1:F:369:GLU:CG	2.56	0.68
1:A:483:ASN:H	1:A:483:ASN:ND2	1.86	0.68
1:F:92:THR:N	1:F:113:LYS:HG2	2.09	0.68
1:F:37:GLY:HA3	1:F:285:VAL:HG21	1.75	0.68
1:E:452:ARG:HH22	1:F:372:GLU:HB3	1.59	0.67
1:A:92:THR:N	1:A:113:LYS:HG2	2.09	0.67
1:B:213:ARG:CZ	1:D:220:GLU:HB3	2.24	0.67
1:C:193:LEU:O	1:C:197:ILE:HG12	1.94	0.67
1:C:340:ASP:HB3	1:C:343:VAL:HG22	1.75	0.67
1:D:444:ILE:O	1:E:368:ASN:HA	1.94	0.67
1:C:29:VAL:O	1:C:33:ILE:HG12	1.93	0.67
1:D:483:ASN:H	1:D:483:ASN:ND2	1.86	0.67
1:B:156:ARG:HH12	1:B:195:ARG:NH1	1.92	0.67
1:C:113:LYS:HD2	1:C:113:LYS:H	1.59	0.67
1:E:92:THR:N	1:E:113:LYS:HG2	2.09	0.67
1:C:172:LEU:HD12	1:C:173:PRO:HD2	1.76	0.67
1:A:217:ILE:CD1	1:E:217:ILE:CG2	2.43	0.67
1:A:244:GLU:OE1	1:A:244:GLU:HA	1.95	0.67
1:B:217:ILE:CG2	1:D:217:ILE:CG1	2.73	0.67
1:F:151:THR:HG23	1:F:161:PRO:HB3	1.77	0.67
1:B:274:SER:OG	1:B:389:ARG:HD3	1.95	0.67
1:C:33:ILE:HG21	1:C:291:PHE:CD2	2.30	0.67
1:E:151:THR:HG23	1:E:161:PRO:HB3	1.77	0.67
1:C:316:ILE:HD11	1:C:320:GLU:HB2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:244:GLU:OE1	1:F:244:GLU:HA	1.95	0.66
1:C:25:ILE:HG13	1:C:26:ARG:H	1.60	0.66
1:D:92:THR:N	1:D:113:LYS:HG2	2.09	0.66
1:C:96:ILE:HG12	1:C:109:ILE:CG2	2.25	0.66
1:D:452:ARG:HH22	1:E:372:GLU:HB3	1.60	0.66
1:D:244:GLU:HA	1:D:244:GLU:OE1	1.95	0.66
1:E:242:VAL:HG13	1:E:252:GLU:HG3	1.78	0.66
1:A:315:LEU:HD12	1:A:365:ILE:HD13	1.78	0.66
1:A:151:THR:HG23	1:A:161:PRO:HB3	1.77	0.66
1:B:262:SER:HA	1:B:448:MET:CE	2.25	0.66
1:C:154:LEU:HD21	1:C:167:MET:HE3	1.77	0.66
1:C:171:THR:O	1:C:171:THR:HG22	1.96	0.66
1:D:242:VAL:HG13	1:D:252:GLU:HG3	1.78	0.66
1:C:96:ILE:HG12	1:C:109:ILE:HG21	1.77	0.66
1:E:244:GLU:OE1	1:E:244:GLU:HA	1.95	0.66
1:E:444:ILE:O	1:F:368:ASN:HA	1.96	0.65
1:D:447:LEU:HD21	1:E:367:SER:HB2	0.77	0.65
1:D:447:LEU:HD23	1:E:367:SER:CA	2.24	0.65
1:C:360:THR:HG22	1:C:362:GLY:H	1.60	0.65
1:C:46:GLU:HA	1:C:46:GLU:OE1	1.96	0.65
1:D:445:ILE:O	1:E:368:ASN:O	2.13	0.65
1:F:242:VAL:HG13	1:F:252:GLU:HG3	1.78	0.65
1:C:345:SER:HA	1:C:352:VAL:HG23	1.77	0.65
1:C:114:GLU:HG3	1:C:117:ARG:HH21	1.62	0.65
1:D:58:GLN:HG3	1:D:315:LEU:CG	2.26	0.65
1:E:26:ARG:HH11	1:E:295:GLY:HA3	1.62	0.65
1:F:58:GLN:HG3	1:F:315:LEU:CG	2.26	0.65
1:D:375:GLU:OE1	1:D:375:GLU:N	2.30	0.65
1:E:227:LYS:HB2	1:E:239:VAL:HG11	1.79	0.65
1:A:58:GLN:HG3	1:A:315:LEU:CG	2.26	0.64
1:B:69:SER:OG	1:B:92:THR:HG21	1.97	0.64
1:D:227:LYS:HB2	1:D:239:VAL:HG11	1.79	0.64
1:B:113:LYS:O	1:B:117:ARG:HB2	1.97	0.64
1:F:315:LEU:HD12	1:F:365:ILE:HD13	1.78	0.64
1:F:375:GLU:OE1	1:F:375:GLU:N	2.30	0.64
1:A:375:GLU:N	1:A:375:GLU:OE1	2.30	0.64
1:D:315:LEU:HD12	1:D:365:ILE:HD13	1.78	0.64
1:E:375:GLU:OE1	1:E:375:GLU:N	2.30	0.64
1:D:447:LEU:CG	1:E:367:SER:CA	2.67	0.64
1:A:227:LYS:HB2	1:A:239:VAL:HG11	1.79	0.64
1:D:151:THR:HG23	1:D:161:PRO:HB3	1.77	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:ILE:CD1	1:C:111:TYR:HB2	2.27	0.64
1:D:26:ARG:HH11	1:D:295:GLY:HA3	1.62	0.64
1:E:315:LEU:HD12	1:E:365:ILE:HD13	1.78	0.64
1:E:62:THR:O	1:E:65:ARG:HG2	1.98	0.64
1:E:443:GLU:OE2	1:F:366:ALA:CB	2.45	0.64
1:A:242:VAL:HG13	1:A:252:GLU:HG3	1.78	0.64
1:F:62:THR:O	1:F:65:ARG:HG2	1.98	0.64
1:D:447:LEU:HD23	1:E:367:SER:C	2.01	0.64
1:F:197:ILE:HG23	1:F:201:ILE:HG13	1.80	0.64
1:F:26:ARG:HH11	1:F:295:GLY:HA3	1.62	0.64
1:B:95:PRO:HA	1:B:108:LEU:HD23	1.80	0.63
1:D:62:THR:O	1:D:65:ARG:HG2	1.98	0.63
1:F:342:ARG:HB3	1:F:479:PHE:CD2	2.34	0.63
1:A:197:ILE:HG23	1:A:201:ILE:HG13	1.80	0.63
1:E:111:TYR:CB	1:E:116:ILE:HD11	2.26	0.63
1:C:194:ILE:HD12	1:C:253:PHE:HD1	1.63	0.63
1:C:221:ARG:NH1	1:C:221:ARG:HG2	2.14	0.63
1:E:58:GLN:HG3	1:E:315:LEU:CG	2.26	0.63
1:A:26:ARG:HH11	1:A:295:GLY:HA3	1.62	0.63
1:F:227:LYS:HB2	1:F:239:VAL:HG11	1.79	0.63
1:C:325:LYS:HG2	1:C:360:THR:HG21	1.79	0.63
1:C:340:ASP:OD1	1:C:486:SER:HB3	1.99	0.63
1:E:344:SER:O	1:E:348:ARG:HB2	1.99	0.63
1:E:342:ARG:HB3	1:E:479:PHE:CD2	2.34	0.63
1:E:447:LEU:HD23	1:F:367:SER:CA	2.23	0.63
1:A:154:LEU:HD21	1:A:167:MET:HG2	1.81	0.63
1:A:62:THR:O	1:A:65:ARG:HG2	1.98	0.63
1:C:151:THR:HA	1:C:154:LEU:HD12	1.81	0.63
1:C:243:ARG:HG2	1:C:243:ARG:NH1	2.10	0.63
1:C:246:ARG:NH1	1:C:246:ARG:HG2	2.12	0.63
1:D:344:SER:O	1:D:348:ARG:HB2	1.99	0.63
1:A:344:SER:O	1:A:348:ARG:HB2	1.99	0.62
1:C:240:ASP:HA	1:C:243:ARG:NH1	2.14	0.62
1:F:97:TYR:CE2	1:F:106:ARG:HG3	2.34	0.62
1:A:342:ARG:HB3	1:A:479:PHE:CD2	2.34	0.62
1:C:208:ARG:CD	1:D:199:ARG:HH21	2.08	0.62
1:C:208:ARG:HE	1:D:199:ARG:HH21	1.38	0.62
1:E:197:ILE:HG23	1:E:201:ILE:HG13	1.80	0.62
1:E:450:SER:N	1:F:370:ASN:HB3	2.13	0.62
1:B:297:SER:O	1:B:303:PRO:HD3	1.99	0.62
1:B:237:THR:HB	1:B:440:MET:SD	2.39	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:445:ILE:O	1:F:368:ASN:O	2.17	0.62
1:A:111:TYR:CB	1:A:116:ILE:HD11	2.26	0.62
1:A:176:SER:OG	1:A:180:GLY:HA3	1.99	0.62
1:D:197:ILE:HG23	1:D:201:ILE:HG13	1.80	0.62
1:E:180:GLY:O	1:E:183:VAL:HG12	2.00	0.62
1:D:97:TYR:CE2	1:D:106:ARG:HG3	2.34	0.62
1:D:342:ARG:HB3	1:D:479:PHE:CD2	2.34	0.62
1:F:344:SER:O	1:F:348:ARG:HB2	1.99	0.62
1:B:120:TRP:CZ2	1:B:129:ALA:HB3	2.34	0.62
1:B:459:GLN:H	1:B:459:GLN:HE21	1.48	0.62
1:D:180:GLY:O	1:D:183:VAL:HG12	2.00	0.62
1:F:176:SER:OG	1:F:180:GLY:HA3	1.99	0.62
1:A:121:ARG:HB3	1:A:126:GLY:HA2	1.82	0.61
1:A:180:GLY:O	1:A:183:VAL:HG12	2.00	0.61
1:B:238:MET:O	1:B:242:VAL:HG23	2.00	0.61
1:E:154:LEU:HD21	1:E:167:MET:HG2	1.81	0.61
1:D:111:TYR:CB	1:D:116:ILE:HD11	2.26	0.61
1:A:97:TYR:CE2	1:A:106:ARG:HG3	2.34	0.61
1:E:176:SER:OG	1:E:180:GLY:HA3	1.99	0.61
1:D:176:SER:OG	1:D:180:GLY:HA3	1.99	0.61
1:F:111:TYR:CB	1:F:116:ILE:HD11	2.26	0.61
1:C:154:LEU:HD21	1:C:167:MET:HE1	1.80	0.61
1:E:92:THR:N	1:E:113:LYS:HZ3	1.99	0.61
1:F:121:ARG:NH1	1:F:121:ARG:HG2	2.15	0.61
1:B:151:THR:O	1:B:155:VAL:HG13	2.00	0.61
1:B:348:ARG:HH11	1:B:348:ARG:HG2	1.66	0.61
1:E:97:TYR:CE2	1:E:106:ARG:HG3	2.35	0.61
1:E:242:VAL:HG11	1:E:256:LEU:CD2	2.31	0.61
1:C:265:ILE:HG13	1:C:266:LEU:H	1.66	0.60
1:A:321:ASN:HB3	1:A:324:HIS:HB2	1.83	0.60
1:E:121:ARG:NH1	1:E:121:ARG:HG2	2.15	0.60
1:E:121:ARG:HB3	1:E:126:GLY:HA2	1.82	0.60
1:F:154:LEU:HD21	1:F:167:MET:HG2	1.81	0.60
1:D:121:ARG:HB3	1:D:126:GLY:HA2	1.82	0.60
1:D:154:LEU:HD21	1:D:167:MET:HG2	1.81	0.60
1:E:321:ASN:HB3	1:E:324:HIS:HB2	1.83	0.60
1:E:43:MET:O	1:E:47:LEU:HD23	2.02	0.60
1:F:121:ARG:HB3	1:F:126:GLY:HA2	1.82	0.60
1:E:446:ARG:CA	1:F:368:ASN:CB	2.50	0.60
1:D:450:SER:N	1:E:370:ASN:HB3	2.16	0.60
1:C:231:GLN:HG3	1:C:395:ASN:OD1	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:ASP:O	1:A:258:PHE:HB3	2.02	0.60
1:C:380:GLU:OE2	1:C:382:ARG:HD3	2.02	0.60
1:C:98:ARG:O	1:C:105:ARG:N	2.28	0.60
1:D:238:MET:HE1	1:D:259:LEU:HD13	1.83	0.60
1:F:180:GLY:O	1:F:183:VAL:HG12	2.00	0.60
1:F:43:MET:O	1:F:47:LEU:HD23	2.02	0.60
1:A:121:ARG:NH1	1:A:121:ARG:HG2	2.15	0.60
1:F:242:VAL:HG11	1:F:256:LEU:CD2	2.31	0.60
1:B:213:ARG:NH1	1:D:220:GLU:HB3	2.15	0.60
1:D:255:ASP:O	1:D:258:PHE:HB3	2.02	0.60
1:A:92:THR:N	1:A:113:LYS:HZ3	1.99	0.60
1:B:341:LEU:HD11	1:B:488:PHE:HA	1.84	0.60
1:E:447:LEU:CG	1:F:367:SER:CA	2.68	0.60
1:F:238:MET:HE1	1:F:259:LEU:HD13	1.84	0.60
1:C:438:SER:HB3	1:C:441:ARG:HG3	1.84	0.59
1:D:242:VAL:HG11	1:D:256:LEU:CD2	2.31	0.59
1:D:444:ILE:C	1:E:368:ASN:HA	2.22	0.59
1:F:255:ASP:O	1:F:258:PHE:HB3	2.02	0.59
1:C:270:VAL:O	1:C:391:ARG:HA	2.03	0.59
1:D:321:ASN:HB3	1:D:324:HIS:HB2	1.83	0.59
1:D:443:GLU:OE2	1:E:366:ALA:CB	2.48	0.59
1:D:92:THR:N	1:D:113:LYS:HZ3	1.99	0.59
1:E:255:ASP:O	1:E:258:PHE:HB3	2.02	0.59
1:C:199:ARG:HG2	1:C:199:ARG:NH1	2.18	0.59
1:D:43:MET:O	1:D:47:LEU:HD23	2.02	0.59
1:D:443:GLU:CD	1:E:367:SER:HG	2.06	0.59
1:F:92:THR:N	1:F:113:LYS:HZ3	2.01	0.59
1:A:43:MET:O	1:A:47:LEU:HD23	2.02	0.59
1:B:100:VAL:HG22	1:B:105:ARG:HD3	1.84	0.59
1:F:339:GLU:OE1	1:F:340:ASP:N	2.35	0.59
1:B:464:PHE:CZ	1:B:471:ALA:HB1	2.37	0.58
1:C:33:ILE:HG21	1:C:291:PHE:CE2	2.38	0.58
1:F:298:LEU:HD12	1:F:298:LEU:N	2.19	0.58
1:A:242:VAL:HG11	1:A:256:LEU:CD2	2.31	0.58
1:B:346:PHE:CZ	1:B:477:PRO:HB3	2.37	0.58
1:D:339:GLU:OE1	1:D:340:ASP:N	2.35	0.58
1:E:298:LEU:HD12	1:E:298:LEU:N	2.19	0.58
1:F:321:ASN:HB3	1:F:324:HIS:HB2	1.83	0.58
1:A:238:MET:HE1	1:A:259:LEU:HD13	1.85	0.58
1:B:265:ILE:HD11	1:B:448:MET:CG	2.31	0.58
1:B:355:ARG:HG2	1:B:489:PHE:HE2	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:324:HIS:CD2	1:C:359:SER:H	2.22	0.58
1:D:121:ARG:HG2	1:D:121:ARG:NH1	2.15	0.58
1:D:150:ARG:O	1:D:154:LEU:HG	2.04	0.58
1:C:208:ARG:CZ	1:D:199:ARG:HH21	2.02	0.58
1:C:283:SER:O	1:C:286:ALA:HB3	2.04	0.58
1:C:61:LEU:HA	1:C:64:GLU:OE1	2.03	0.58
1:E:150:ARG:O	1:E:154:LEU:HG	2.04	0.58
1:C:21:ASN:OD1	1:C:22:ALA:N	2.33	0.58
1:A:339:GLU:OE1	1:A:340:ASP:N	2.35	0.58
1:B:317:ARG:O	1:B:320:GLU:HB2	2.04	0.58
1:B:321:ASN:HB3	1:B:324:HIS:HB2	1.85	0.58
1:B:321:ASN:OD1	1:B:324:HIS:ND1	2.37	0.58
1:C:240:ASP:O	1:C:244:GLU:HG2	2.03	0.58
1:E:447:LEU:HD21	1:F:367:SER:HB2	0.76	0.58
1:A:61:LEU:HA	1:A:64:GLU:OE1	2.04	0.58
1:C:382:ARG:HH11	1:C:382:ARG:HG2	1.68	0.57
1:D:346:PHE:CE2	1:D:477:PRO:HB3	2.39	0.57
1:E:267:ARG:HB2	1:E:393:GLY:HA3	1.86	0.57
1:E:61:LEU:HA	1:E:64:GLU:OE1	2.04	0.57
1:A:150:ARG:O	1:A:154:LEU:HG	2.04	0.57
1:A:267:ARG:HB2	1:A:393:GLY:HA3	1.86	0.57
1:F:150:ARG:O	1:F:154:LEU:HG	2.04	0.57
1:F:346:PHE:CE2	1:F:477:PRO:HB3	2.39	0.57
1:A:346:PHE:CE2	1:A:477:PRO:HB3	2.39	0.57
1:B:155:VAL:HG23	1:B:156:ARG:H	1.68	0.57
1:D:447:LEU:CD2	1:E:367:SER:HA	2.28	0.57
1:D:61:LEU:HA	1:D:64:GLU:OE1	2.04	0.57
1:E:346:PHE:CE2	1:E:477:PRO:HB3	2.39	0.57
1:B:115:GLU:HA	1:B:115:GLU:OE1	2.04	0.57
1:D:298:LEU:N	1:D:298:LEU:HD12	2.19	0.57
1:D:267:ARG:HB2	1:D:393:GLY:HA3	1.86	0.57
1:F:61:LEU:HA	1:F:64:GLU:OE1	2.04	0.57
1:B:372:GLU:HA	1:B:372:GLU:OE1	2.04	0.57
1:D:370:ASN:HD22	1:D:372:GLU:HB3	1.70	0.57
1:A:217:ILE:HD11	1:E:217:ILE:CA	1.96	0.57
1:C:25:ILE:HG13	1:C:26:ARG:N	2.20	0.57
1:D:71:PHE:CE1	1:D:117:ARG:HG2	2.40	0.57
1:F:370:ASN:HD22	1:F:372:GLU:HB3	1.70	0.57
1:F:71:PHE:CE1	1:F:117:ARG:HG2	2.40	0.57
1:E:196:MET:CE	1:E:219:TYR:HB2	2.35	0.57
1:F:267:ARG:HB2	1:F:393:GLY:HA3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:46:GLU:O	1:F:48:LYS:HG2	2.05	0.57
1:C:475:ILE:O	1:C:477:PRO:HD3	2.05	0.57
1:C:371:MET:HG2	1:C:371:MET:O	2.05	0.56
1:D:196:MET:CE	1:D:219:TYR:HB2	2.35	0.56
1:B:213:ARG:CZ	1:D:243:ARG:HG2	2.34	0.56
1:D:31:LYS:HD3	1:D:292:GLU:OE2	2.05	0.56
1:D:321:ASN:HD22	1:D:322:PRO:HD2	1.70	0.56
1:D:445:ILE:CA	1:E:368:ASN:HB3	2.35	0.56
1:E:31:LYS:HD3	1:E:292:GLU:OE2	2.05	0.56
1:E:321:ASN:HD22	1:E:322:PRO:HD2	1.70	0.56
1:E:446:ARG:CD	1:F:369:GLU:HG3	2.35	0.56
1:F:321:ASN:HD22	1:F:322:PRO:HD2	1.70	0.56
1:A:298:LEU:HD12	1:A:298:LEU:N	2.19	0.56
1:E:230:PHE:HB3	1:E:235:GLN:HB3	1.88	0.56
1:A:238:MET:O	1:A:242:VAL:HG23	2.05	0.56
1:B:139:TRP:CZ2	1:B:277:PRO:HG3	2.40	0.56
1:C:216:ARG:NH2	1:C:243:ARG:O	2.37	0.56
1:C:246:ARG:C	1:C:248:PRO:HD3	2.26	0.56
1:D:46:GLU:O	1:D:48:LYS:HG2	2.05	0.56
1:F:230:PHE:HB3	1:F:235:GLN:HB3	1.88	0.56
1:F:196:MET:CE	1:F:219:TYR:HB2	2.35	0.56
1:C:353:VAL:HG22	1:C:354:PRO:CD	2.32	0.56
1:D:443:GLU:CD	1:E:367:SER:H	2.09	0.56
1:A:196:MET:CE	1:A:219:TYR:HB2	2.35	0.56
1:A:31:LYS:HD3	1:A:292:GLU:OE2	2.05	0.56
1:C:197:ILE:HD12	1:C:248:PRO:HB3	1.86	0.56
1:E:444:ILE:C	1:F:368:ASN:HA	2.26	0.56
1:D:449:GLU:C	1:E:370:ASN:CB	2.71	0.56
1:A:46:GLU:O	1:A:48:LYS:HG2	2.05	0.56
1:B:231:GLN:HE22	1:B:269:SER:HB3	1.70	0.56
1:C:464:PHE:N	1:C:464:PHE:CD2	2.73	0.56
1:E:71:PHE:CE1	1:E:117:ARG:HG2	2.40	0.56
1:E:446:ARG:HD2	1:F:369:GLU:HG3	1.87	0.56
1:B:214:ARG:HG2	1:B:214:ARG:HH11	1.71	0.56
1:B:366:ALA:HB3	1:B:369:GLU:HG3	1.87	0.56
1:B:346:PHE:CE2	1:B:477:PRO:HB3	2.41	0.56
1:C:109:ILE:HD11	1:C:111:TYR:HB2	1.88	0.56
1:C:270:VAL:CG1	1:C:271:ALA:N	2.69	0.56
1:D:230:PHE:HB3	1:D:235:GLN:HB3	1.88	0.56
1:D:353:VAL:HG13	1:D:354:PRO:HD2	1.88	0.56
1:D:447:LEU:HG	1:E:367:SER:CA	2.25	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:97:TYR:N	1:D:97:TYR:CD1	2.74	0.56
1:E:450:SER:N	1:F:370:ASN:CB	2.69	0.56
1:A:71:PHE:CE1	1:A:117:ARG:HG2	2.40	0.56
1:E:238:MET:O	1:E:242:VAL:HG23	2.06	0.56
1:E:339:GLU:OE1	1:E:340:ASP:N	2.35	0.56
1:E:46:GLU:O	1:E:48:LYS:HG2	2.05	0.56
1:B:21:ASN:HB3	1:B:24:GLU:CG	2.36	0.55
1:C:198:LYS:HD3	1:C:201:ILE:CD1	2.37	0.55
1:E:447:LEU:CD2	1:F:367:SER:HA	2.28	0.55
1:A:263:ALA:HA	1:A:266:LEU:O	2.06	0.55
1:A:370:ASN:HD22	1:A:372:GLU:HB3	1.70	0.55
1:D:243:ARG:HG2	1:D:243:ARG:O	2.06	0.55
1:E:370:ASN:HD22	1:E:372:GLU:HB3	1.70	0.55
1:F:238:MET:O	1:F:242:VAL:HG23	2.06	0.55
1:F:243:ARG:HG2	1:F:243:ARG:O	2.06	0.55
1:F:321:ASN:HD22	1:F:322:PRO:CD	2.20	0.55
1:A:39:PHE:CZ	1:A:67:VAL:HG21	2.42	0.55
1:D:321:ASN:HD22	1:D:322:PRO:CD	2.20	0.55
1:F:31:LYS:HD3	1:F:292:GLU:OE2	2.05	0.55
1:D:39:PHE:CZ	1:D:67:VAL:HG21	2.42	0.55
1:E:449:GLU:C	1:F:370:ASN:CB	2.71	0.55
1:A:353:VAL:HG13	1:A:354:PRO:HD2	1.88	0.55
1:B:56:LEU:HD11	1:B:315:LEU:HG	1.89	0.55
1:B:39:PHE:CE2	1:B:67:VAL:HG21	2.42	0.55
1:D:263:ALA:HA	1:D:266:LEU:O	2.06	0.55
1:E:447:LEU:HD21	1:F:367:SER:HA	1.80	0.55
1:D:238:MET:O	1:D:242:VAL:HG23	2.05	0.55
1:E:443:GLU:CD	1:F:367:SER:H	2.10	0.55
1:A:230:PHE:HB3	1:A:235:GLN:HB3	1.88	0.55
1:E:243:ARG:HG2	1:E:243:ARG:O	2.06	0.55
1:E:263:ALA:HA	1:E:266:LEU:O	2.06	0.55
1:E:321:ASN:HD22	1:E:322:PRO:CD	2.20	0.55
1:F:263:ALA:HA	1:F:266:LEU:O	2.06	0.55
1:F:311:GLN:HG3	1:F:313:TYR:CZ	2.42	0.55
1:A:252:GLU:O	1:A:255:ASP:N	2.40	0.55
1:C:190:VAL:HG13	1:C:256:LEU:HB3	1.88	0.55
1:E:39:PHE:CZ	1:E:67:VAL:HG21	2.42	0.55
1:A:311:GLN:HG3	1:A:313:TYR:CZ	2.42	0.55
1:A:321:ASN:HD22	1:A:322:PRO:HD2	1.70	0.55
1:A:97:TYR:N	1:A:97:TYR:CD1	2.74	0.55
1:A:308:GLN:HE22	1:A:383:SER:N	2.01	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:253:PHE:CD2	1:D:253:PHE:C	2.81	0.55
1:F:252:GLU:O	1:F:255:ASP:N	2.40	0.55
1:F:39:PHE:CZ	1:F:67:VAL:HG21	2.42	0.55
1:F:97:TYR:N	1:F:97:TYR:CD1	2.74	0.55
1:B:465:GLU:HB2	1:B:468:ASP:HB2	1.88	0.54
1:C:369:GLU:HG3	1:C:370:ASN:H	1.72	0.54
1:C:348:ARG:NH2	1:C:380:GLU:O	2.40	0.54
1:C:46:GLU:C	1:C:48:LYS:H	2.11	0.54
1:B:134:THR:CG2	1:B:177:GLY:H	2.19	0.54
1:C:348:ARG:HA	1:C:383:SER:OG	2.07	0.54
1:D:252:GLU:O	1:D:255:ASP:N	2.40	0.54
1:E:252:GLU:O	1:E:255:ASP:N	2.40	0.54
1:C:341:LEU:CB	1:C:486:SER:HA	2.32	0.54
1:E:311:GLN:HG3	1:E:313:TYR:CZ	2.42	0.54
1:A:189:MET:CE	1:A:192:GLU:OE1	2.52	0.54
1:A:321:ASN:HD22	1:A:322:PRO:CD	2.20	0.54
1:B:190:VAL:O	1:B:194:ILE:HD13	2.08	0.54
1:D:311:GLN:HG3	1:D:313:TYR:CZ	2.42	0.54
1:A:243:ARG:O	1:A:243:ARG:HG2	2.06	0.54
1:A:253:PHE:CD2	1:A:253:PHE:C	2.81	0.54
1:C:321:ASN:HB3	1:C:324:HIS:CG	2.43	0.54
1:D:100:VAL:HG12	1:D:101:ASP:N	2.22	0.54
1:E:238:MET:HE1	1:E:259:LEU:HD13	1.90	0.54
1:E:53:GLU:OE2	1:E:99:ARG:N	2.41	0.54
1:C:33:ILE:HG23	1:C:281:TYR:CE2	2.43	0.54
1:E:189:MET:CE	1:E:192:GLU:OE1	2.52	0.54
1:E:445:ILE:CA	1:F:368:ASN:HB3	2.37	0.54
1:B:303:PRO:HG2	1:B:389:ARG:HH12	1.72	0.54
1:C:143:LEU:HA	1:C:332:ALA:CB	2.38	0.54
1:D:53:GLU:OE2	1:D:99:ARG:N	2.41	0.54
1:E:100:VAL:HG12	1:E:101:ASP:N	2.22	0.54
1:A:100:VAL:HG12	1:A:101:ASP:N	2.22	0.54
1:B:155:VAL:CG2	1:B:156:ARG:N	2.71	0.54
1:B:34:ASP:OD1	1:B:38:ARG:NH2	2.41	0.54
1:F:353:VAL:HG13	1:F:354:PRO:HD2	1.88	0.53
1:C:107:GLU:O	1:C:109:ILE:N	2.41	0.53
1:C:38:ARG:HD2	1:C:123:ALA:O	2.08	0.53
1:E:253:PHE:CD2	1:E:253:PHE:C	2.81	0.53
1:E:97:TYR:N	1:E:97:TYR:CD1	2.74	0.53
1:F:100:VAL:HG12	1:F:101:ASP:N	2.22	0.53
1:B:276:LEU:HD13	1:B:280:VAL:HG11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:303:PRO:HG2	1:C:389:ARG:HH12	1.72	0.53
1:D:450:SER:N	1:E:370:ASN:CB	2.71	0.53
1:E:353:VAL:HG13	1:E:354:PRO:HD2	1.89	0.53
1:C:194:ILE:HD11	1:C:256:LEU:HB2	1.89	0.53
1:C:58:GLN:HG3	1:C:315:LEU:HG	1.90	0.53
1:D:71:PHE:CD1	1:D:117:ARG:HG2	2.44	0.53
1:F:53:GLU:OE2	1:F:99:ARG:N	2.41	0.53
1:B:213:ARG:NH1	1:D:243:ARG:HG3	2.15	0.53
1:C:321:ASN:HB3	1:C:324:HIS:CD2	2.42	0.53
1:D:167:MET:HG3	1:D:170:SER:HB3	1.91	0.53
1:F:253:PHE:C	1:F:253:PHE:CD2	2.81	0.53
1:F:270:VAL:N	1:F:391:ARG:O	2.42	0.53
1:B:355:ARG:HG2	1:B:489:PHE:CE2	2.43	0.53
1:B:291:PHE:O	1:B:295:GLY:N	2.40	0.53
1:C:344:SER:O	1:C:347:ILE:HG22	2.08	0.53
1:E:444:ILE:C	1:F:368:ASN:CB	2.77	0.53
1:C:121:ARG:HB3	1:C:126:GLY:HA2	1.91	0.53
1:D:189:MET:CE	1:D:192:GLU:OE1	2.52	0.53
1:A:217:ILE:HD12	1:E:217:ILE:CG2	2.36	0.53
1:A:100:VAL:O	1:A:101:ASP:C	2.48	0.53
1:F:317:ARG:HB2	1:F:320:GLU:HG3	1.91	0.53
1:A:71:PHE:CD1	1:A:117:ARG:HG2	2.44	0.53
1:A:167:MET:HG3	1:A:170:SER:HB3	1.91	0.53
1:A:317:ARG:HB2	1:A:320:GLU:HG3	1.91	0.53
1:B:327:GLN:O	1:B:331:MET:HG3	2.09	0.53
1:C:227:LYS:HB2	1:C:239:VAL:HG11	1.89	0.53
1:C:302:ASP:O	1:C:306:LEU:HD13	2.09	0.53
1:D:232:THR:HG1	1:D:235:GLN:HG3	1.72	0.53
1:D:308:GLN:HE22	1:D:383:SER:N	2.01	0.53
1:D:343:VAL:HG13	1:D:344:SER:N	2.24	0.53
1:D:446:ARG:CD	1:E:369:GLU:HG3	2.39	0.53
1:A:232:THR:O	1:A:236:ARG:HG3	2.09	0.52
1:D:444:ILE:C	1:E:368:ASN:CB	2.77	0.52
1:F:343:VAL:HG13	1:F:344:SER:N	2.24	0.52
1:B:265:ILE:HD11	1:B:448:MET:CB	2.39	0.52
1:C:355:ARG:HB2	1:C:488:PHE:CE2	2.44	0.52
1:D:270:VAL:N	1:D:391:ARG:O	2.42	0.52
1:E:343:VAL:HG13	1:E:344:SER:N	2.24	0.52
1:F:71:PHE:CD1	1:F:117:ARG:HG2	2.44	0.52
1:C:106:ARG:NH1	1:C:367:SER:HA	2.21	0.52
1:D:232:THR:O	1:D:236:ARG:HG3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:ARG:CZ	1:D:243:ARG:CG	2.85	0.52
1:F:370:ASN:ND2	1:F:372:GLU:HB3	2.25	0.52
1:B:69:SER:OG	1:B:92:THR:CG2	2.58	0.52
1:C:61:LEU:HD23	1:C:64:GLU:OE1	2.09	0.52
1:E:146:ALA:HB2	1:E:337:ALA:HB2	1.92	0.52
1:E:71:PHE:CD1	1:E:117:ARG:HG2	2.44	0.52
1:F:232:THR:O	1:F:236:ARG:HG3	2.09	0.52
1:F:342:ARG:HB3	1:F:479:PHE:HE2	1.73	0.52
1:A:270:VAL:N	1:A:391:ARG:O	2.42	0.52
1:C:270:VAL:HG12	1:C:271:ALA:H	1.74	0.52
1:C:342:ARG:HB3	1:C:479:PHE:CD2	2.45	0.52
1:D:134:THR:O	1:D:137:MET:HB3	2.10	0.52
1:E:100:VAL:O	1:E:101:ASP:C	2.48	0.52
1:F:39:PHE:CE2	1:F:67:VAL:HG21	2.45	0.52
1:C:267:ARG:HG3	1:C:393:GLY:O	2.09	0.52
1:E:317:ARG:HB2	1:E:320:GLU:HG3	1.92	0.52
1:E:232:THR:O	1:E:236:ARG:HG3	2.09	0.52
1:D:443:GLU:HG3	1:E:367:SER:OG	2.10	0.52
1:A:134:THR:O	1:A:137:MET:HB3	2.10	0.52
1:A:343:VAL:HG13	1:A:344:SER:N	2.24	0.52
1:A:39:PHE:CE2	1:A:67:VAL:HG21	2.45	0.52
1:C:192:GLU:HB3	1:C:222:MET:HE1	1.91	0.52
1:D:449:GLU:HB3	1:E:370:ASN:N	2.25	0.52
1:F:146:ALA:HB2	1:F:337:ALA:HB2	1.92	0.52
1:A:111:TYR:CD2	1:A:116:ILE:HD11	2.45	0.52
1:B:197:ILE:HG23	1:B:248:PRO:HB2	1.91	0.52
1:B:324:HIS:HD2	1:B:358:LEU:HA	1.75	0.52
1:B:386:TRP:NE1	1:B:464:PHE:HB2	2.25	0.52
1:D:39:PHE:CE2	1:D:67:VAL:HG21	2.45	0.52
1:D:446:ARG:HD2	1:E:369:GLU:HG3	1.91	0.52
1:E:370:ASN:ND2	1:E:372:GLU:HB3	2.25	0.52
1:F:111:TYR:CD2	1:F:116:ILE:HD11	2.45	0.52
1:F:168:GLN:O	1:F:184:LYS:HA	2.10	0.52
1:F:308:GLN:HE22	1:F:383:SER:N	2.01	0.52
1:D:168:GLN:O	1:D:184:LYS:HA	2.11	0.52
1:D:445:ILE:N	1:E:368:ASN:CB	2.72	0.52
1:E:134:THR:O	1:E:137:MET:HB3	2.10	0.52
1:E:168:GLN:O	1:E:184:LYS:HA	2.10	0.52
1:E:270:VAL:N	1:E:391:ARG:O	2.42	0.52
1:E:308:GLN:HE22	1:E:383:SER:N	2.01	0.52
1:E:29:VAL:O	1:E:32:MET:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:100:VAL:O	1:F:101:ASP:C	2.48	0.52
1:F:69:SER:OG	1:F:92:THR:HG21	2.10	0.52
1:D:111:TYR:CD2	1:D:116:ILE:HD11	2.45	0.51
1:D:315:LEU:HB2	1:D:365:ILE:HD11	1.92	0.51
1:D:146:ALA:HB2	1:D:337:ALA:HB2	1.92	0.51
1:A:168:GLN:O	1:A:184:LYS:HA	2.11	0.51
1:C:174:ARG:HD3	1:C:175:ARG:H	1.75	0.51
1:D:69:SER:OG	1:D:92:THR:HG21	2.10	0.51
1:E:167:MET:HG3	1:E:170:SER:HB3	1.91	0.51
1:E:296:TYR:CE1	1:E:302:ASP:HB3	2.45	0.51
1:A:370:ASN:ND2	1:A:372:GLU:HB3	2.25	0.51
1:C:261:ARG:O	1:C:264:LEU:HB2	2.10	0.51
1:D:100:VAL:O	1:D:101:ASP:C	2.48	0.51
1:E:111:TYR:CD2	1:E:116:ILE:HD11	2.45	0.51
1:A:38:ARG:NH1	1:A:123:ALA:O	2.44	0.51
1:B:60:SER:OG	1:B:278:ALA:HB3	2.11	0.51
1:D:370:ASN:ND2	1:D:372:GLU:HB3	2.24	0.51
1:F:35:GLY:HA3	1:F:124:ASN:OD1	2.11	0.51
1:F:296:TYR:CE1	1:F:302:ASP:HB3	2.46	0.51
1:F:29:VAL:O	1:F:32:MET:HG3	2.10	0.51
1:A:223:CYS:O	1:A:226:LEU:HB3	2.11	0.51
1:A:315:LEU:HB2	1:A:365:ILE:HD11	1.92	0.51
1:A:69:SER:OG	1:A:92:THR:HG21	2.10	0.51
1:B:134:THR:HG23	1:B:177:GLY:H	1.76	0.51
1:B:385:TYR:HB3	1:B:463:VAL:CG1	2.40	0.51
1:D:223:CYS:O	1:D:226:LEU:HB3	2.11	0.51
1:D:29:VAL:O	1:D:32:MET:HG3	2.10	0.51
1:D:35:GLY:HA3	1:D:124:ASN:OD1	2.11	0.51
1:E:315:LEU:HB2	1:E:365:ILE:HD11	1.92	0.51
1:E:445:ILE:N	1:F:368:ASN:CB	2.74	0.51
1:E:302:ASP:HB2	1:E:303:PRO:HD3	1.93	0.51
1:E:450:SER:HA	1:F:370:ASN:HB2	1.93	0.51
1:F:38:ARG:NH1	1:F:123:ALA:O	2.44	0.51
1:F:134:THR:O	1:F:137:MET:HB3	2.10	0.51
1:F:223:CYS:O	1:F:226:LEU:HB3	2.11	0.51
1:A:146:ALA:HB2	1:A:337:ALA:HB2	1.92	0.51
1:B:303:PRO:CG	1:B:389:ARG:HH12	2.24	0.51
1:C:265:ILE:HD11	1:C:448:MET:CE	2.40	0.51
1:A:171:THR:O	1:A:173:PRO:HD3	2.11	0.51
1:C:291:PHE:HE2	1:C:306:LEU:HD21	1.74	0.51
1:D:317:ARG:HB2	1:D:320:GLU:HG3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:447:LEU:HD21	1:E:367:SER:HA	1.80	0.51
1:E:253:PHE:O	1:E:257:ILE:HG13	2.11	0.51
1:E:321:ASN:HD22	1:E:322:PRO:N	2.09	0.51
1:F:171:THR:O	1:F:173:PRO:HD3	2.11	0.51
1:F:302:ASP:HB2	1:F:303:PRO:HD3	1.93	0.51
1:A:29:VAL:O	1:A:32:MET:HG3	2.10	0.51
1:D:171:THR:O	1:D:173:PRO:HD3	2.11	0.51
1:D:441:ARG:O	1:E:368:ASN:OD1	2.29	0.51
1:E:223:CYS:O	1:E:226:LEU:HB3	2.11	0.51
1:E:69:SER:OG	1:E:92:THR:HG21	2.10	0.51
1:A:35:GLY:HA3	1:A:124:ASN:OD1	2.11	0.51
1:B:343:VAL:HG23	1:B:344:SER:N	2.26	0.51
1:C:57:ILE:HG22	1:C:58:GLN:N	2.26	0.51
1:D:291:PHE:O	1:D:295:GLY:N	2.42	0.51
1:D:296:TYR:CE1	1:D:302:ASP:HB3	2.45	0.51
1:E:171:THR:O	1:E:173:PRO:HD3	2.11	0.51
1:A:296:TYR:CE1	1:A:302:ASP:HB3	2.46	0.50
1:A:311:GLN:HG3	1:A:313:TYR:OH	2.12	0.50
1:C:100:VAL:O	1:C:100:VAL:HG23	2.11	0.50
1:D:38:ARG:NH1	1:D:123:ALA:O	2.44	0.50
1:E:39:PHE:CE2	1:E:67:VAL:HG21	2.45	0.50
1:F:106:ARG:NH1	1:F:367:SER:HA	2.26	0.50
1:D:253:PHE:O	1:D:257:ILE:HG13	2.11	0.50
1:E:106:ARG:NH1	1:E:367:SER:HA	2.26	0.50
1:F:167:MET:HG3	1:F:170:SER:HB3	1.91	0.50
1:F:311:GLN:HG3	1:F:313:TYR:OH	2.12	0.50
1:F:321:ASN:HD22	1:F:322:PRO:N	2.09	0.50
1:A:137:MET:CE	1:A:175:ARG:HE	2.25	0.50
1:C:243:ARG:O	1:C:243:ARG:HG3	2.11	0.50
1:E:311:GLN:HG3	1:E:313:TYR:OH	2.12	0.50
1:E:443:GLU:CD	1:F:367:SER:HG	2.11	0.50
1:C:52:TYR:HE2	1:C:104:TRP:HH2	1.59	0.50
1:C:231:GLN:HG3	1:C:395:ASN:CG	2.31	0.50
1:D:118:ARG:HH21	1:D:122:GLN:HG3	1.77	0.50
1:D:302:ASP:HB2	1:D:303:PRO:HD3	1.93	0.50
1:F:315:LEU:HB2	1:F:365:ILE:HD11	1.92	0.50
1:A:196:MET:HE3	1:A:219:TYR:HB2	1.93	0.50
1:A:291:PHE:O	1:A:295:GLY:N	2.42	0.50
1:B:385:TYR:HB3	1:B:463:VAL:HG12	1.93	0.50
1:C:319:ASN:HD22	1:C:319:ASN:N	2.08	0.50
1:E:38:ARG:NH1	1:E:123:ALA:O	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:ASP:HB2	1:A:303:PRO:HD3	1.93	0.50
1:B:321:ASN:HD22	1:B:322:PRO:N	2.09	0.50
1:B:461:ARG:HD2	1:B:461:ARG:N	2.26	0.50
1:D:446:ARG:CZ	1:E:365:ILE:HG23	2.25	0.50
1:E:35:GLY:HA3	1:E:124:ASN:OD1	2.11	0.50
1:E:137:MET:CE	1:E:175:ARG:HE	2.25	0.50
1:F:253:PHE:O	1:F:257:ILE:HG13	2.11	0.50
1:A:217:ILE:HD11	1:E:217:ILE:HA	1.89	0.50
1:B:234:ALA:HB1	1:B:444:ILE:CG1	2.41	0.50
1:D:63:ILE:O	1:D:67:VAL:HG23	2.12	0.50
1:F:118:ARG:HH21	1:F:122:GLN:HG3	1.77	0.50
1:A:106:ARG:NH1	1:A:367:SER:HA	2.26	0.50
1:B:454:GLU:CD	1:B:454:GLU:H	2.15	0.50
1:C:37:GLY:O	1:C:41:ILE:HG13	2.12	0.50
1:C:98:ARG:NE	1:C:107:GLU:OE2	2.44	0.50
1:D:106:ARG:NH1	1:D:367:SER:HA	2.26	0.50
1:D:321:ASN:HD22	1:D:322:PRO:N	2.09	0.50
1:E:196:MET:HE3	1:E:219:TYR:HB2	1.94	0.50
1:F:137:MET:CE	1:F:175:ARG:HE	2.25	0.50
1:A:58:GLN:HE21	1:A:58:GLN:HA	1.77	0.50
1:B:214:ARG:NH1	1:B:214:ARG:HG2	2.27	0.50
1:D:137:MET:CE	1:D:175:ARG:HE	2.25	0.50
1:C:321:ASN:HD22	1:C:322:PRO:HD2	1.76	0.49
1:E:63:ILE:O	1:E:67:VAL:HG23	2.12	0.49
1:A:232:THR:HG1	1:A:235:GLN:HG3	1.77	0.49
1:E:232:THR:HG1	1:E:235:GLN:HG3	1.77	0.49
1:A:253:PHE:O	1:A:257:ILE:HG13	2.11	0.49
1:B:262:SER:HA	1:B:448:MET:HE3	1.93	0.49
1:C:345:SER:CB	1:C:352:VAL:H	2.24	0.49
1:C:394:GLY:O	1:C:395:ASN:O	2.30	0.49
1:A:53:GLU:OE2	1:A:99:ARG:N	2.41	0.49
1:B:316:ILE:CG1	1:B:320:GLU:HB3	2.42	0.49
1:F:58:GLN:HA	1:F:58:GLN:HE21	1.77	0.49
1:A:63:ILE:O	1:A:67:VAL:HG23	2.12	0.49
1:B:96:ILE:HG13	1:B:109:ILE:CD1	2.40	0.49
1:D:311:GLN:HG3	1:D:313:TYR:OH	2.12	0.49
1:E:238:MET:HE3	1:E:255:ASP:OD1	2.13	0.49
1:E:449:GLU:HB3	1:F:370:ASN:N	2.26	0.49
1:B:30:GLY:O	1:B:34:ASP:HB2	2.12	0.49
1:C:250:ASN:HA	1:C:253:PHE:HB3	1.93	0.49
1:C:265:ILE:HG13	1:C:266:LEU:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:342:ARG:HB3	1:D:479:PHE:HE2	1.73	0.49
1:E:58:GLN:HE21	1:E:58:GLN:HA	1.77	0.49
1:A:321:ASN:HD22	1:A:322:PRO:N	2.09	0.49
1:D:166:LEU:HD21	1:D:264:LEU:HD23	1.95	0.49
1:C:100:VAL:O	1:C:103:LYS:O	2.30	0.49
1:C:113:LYS:CD	1:C:113:LYS:H	2.22	0.49
1:C:300:GLY:O	1:C:303:PRO:HD2	2.12	0.49
1:C:143:LEU:HA	1:C:332:ALA:HB1	1.95	0.49
1:F:56:LEU:HG	1:F:58:GLN:HG2	1.95	0.49
1:C:121:ARG:O	1:C:126:GLY:N	2.37	0.49
1:C:291:PHE:CE2	1:C:306:LEU:HD21	2.48	0.49
1:E:298:LEU:CD1	1:E:298:LEU:N	2.76	0.49
1:E:56:LEU:HG	1:E:58:GLN:HG2	1.95	0.49
1:B:190:VAL:HG13	1:B:256:LEU:HB3	1.94	0.48
1:C:22:ALA:O	1:C:25:ILE:HG12	2.13	0.48
1:C:38:ARG:CD	1:C:123:ALA:O	2.61	0.48
1:C:262:SER:HA	1:C:448:MET:HE3	1.94	0.48
1:D:56:LEU:HG	1:D:58:GLN:HG2	1.95	0.48
1:F:63:ILE:O	1:F:67:VAL:HG23	2.12	0.48
1:A:298:LEU:CD1	1:A:298:LEU:N	2.76	0.48
1:B:97:TYR:CD1	1:B:97:TYR:N	2.81	0.48
1:C:289:TYR:CZ	1:C:294:GLU:HG2	2.48	0.48
1:E:291:PHE:O	1:E:295:GLY:N	2.42	0.48
1:E:447:LEU:HG	1:F:367:SER:CA	2.28	0.48
1:C:174:ARG:HD3	1:C:175:ARG:N	2.28	0.48
1:C:265:ILE:HD11	1:C:448:MET:HE3	1.94	0.48
1:D:58:GLN:HA	1:D:58:GLN:HE21	1.77	0.48
1:F:298:LEU:N	1:F:298:LEU:CD1	2.76	0.48
1:A:118:ARG:HH21	1:A:122:GLN:HG3	1.77	0.48
1:A:345:SER:HA	1:A:352:VAL:HG23	1.96	0.48
1:C:321:ASN:HD22	1:C:322:PRO:CD	2.26	0.48
1:C:370:ASN:OD1	1:C:373:THR:HG23	2.12	0.48
1:D:298:LEU:N	1:D:298:LEU:CD1	2.76	0.48
1:E:118:ARG:HH21	1:E:122:GLN:HG3	1.77	0.48
1:B:155:VAL:CG2	1:B:156:ARG:H	2.26	0.48
1:B:157:THR:HG22	1:B:194:ILE:HG21	1.96	0.48
1:C:171:THR:CG2	1:C:171:THR:O	2.60	0.48
1:E:189:MET:HB2	1:E:226:LEU:HD23	1.96	0.48
1:E:316:ILE:HG22	1:E:376:SER:HA	1.95	0.48
1:E:163:MET:CE	1:E:261:ARG:HG2	2.43	0.48
1:F:196:MET:HE1	1:F:219:TYR:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:LEU:O	1:C:143:LEU:HD12	2.13	0.48
1:C:195:ARG:CG	1:C:196:MET:N	2.76	0.48
1:C:43:MET:CE	1:C:119:ILE:HG21	2.44	0.48
1:D:196:MET:HE1	1:D:219:TYR:HB2	1.95	0.48
1:E:267:ARG:H	1:E:267:ARG:HG2	1.42	0.48
1:D:446:ARG:CG	1:E:369:GLU:CG	2.59	0.48
1:E:443:GLU:HG3	1:F:367:SER:OG	2.13	0.48
1:F:143:LEU:HA	1:F:332:ALA:HB2	1.96	0.48
1:A:189:MET:HB2	1:A:226:LEU:HD23	1.95	0.48
1:A:166:LEU:HD21	1:A:264:LEU:HD23	1.95	0.48
1:B:37:GLY:HA2	1:B:282:GLY:N	2.29	0.48
1:B:37:GLY:O	1:B:41:ILE:HG13	2.13	0.48
1:B:386:TRP:HB3	1:B:466:LEU:CD2	2.44	0.48
1:C:196:MET:O	1:C:197:ILE:C	2.50	0.48
1:D:226:LEU:HD12	1:D:239:VAL:HG13	1.96	0.48
1:E:345:SER:HA	1:E:352:VAL:HG23	1.96	0.48
1:B:168:GLN:O	1:B:184:LYS:HA	2.13	0.48
1:D:345:SER:HA	1:D:352:VAL:HG23	1.96	0.48
1:F:345:SER:HA	1:F:352:VAL:HG23	1.96	0.48
1:F:318:PRO:HD3	1:F:373:THR:O	2.14	0.48
1:A:163:MET:CE	1:A:261:ARG:HG2	2.43	0.48
1:A:316:ILE:HG22	1:A:376:SER:HA	1.95	0.48
1:B:258:PHE:O	1:B:261:ARG:HB3	2.14	0.48
1:B:348:ARG:HG2	1:B:348:ARG:NH1	2.29	0.48
1:F:189:MET:CE	1:F:192:GLU:OE1	2.52	0.48
1:F:189:MET:HB2	1:F:226:LEU:HD23	1.96	0.48
1:B:43:MET:HA	1:B:43:MET:CE	2.44	0.47
1:C:141:SER:OG	1:C:169:GLY:HA2	2.14	0.47
1:D:318:PRO:HD3	1:D:373:THR:O	2.14	0.47
1:E:166:LEU:HD21	1:E:264:LEU:HD23	1.95	0.47
1:F:163:MET:CE	1:F:261:ARG:HG2	2.43	0.47
1:C:135:HIS:HE1	1:C:298:LEU:CD2	2.27	0.47
1:D:450:SER:HA	1:E:370:ASN:HB2	1.96	0.47
1:B:124:ASN:O	1:B:127:ASP:OD2	2.32	0.47
1:B:143:LEU:HD11	1:B:363:VAL:HG21	1.96	0.47
1:B:293:ARG:HG3	1:B:293:ARG:HH11	1.80	0.47
1:C:22:ALA:O	1:C:25:ILE:CG1	2.62	0.47
1:A:56:LEU:HG	1:A:58:GLN:HG2	1.95	0.47
1:C:230:PHE:CD1	1:C:235:GLN:HB3	2.49	0.47
1:C:49:LEU:HD22	1:C:53:GLU:HB3	1.97	0.47
1:F:174:ARG:HD3	1:F:175:ARG:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:ARG:HH12	1:A:367:SER:HA	1.79	0.47
1:B:166:LEU:HB3	1:B:187:GLY:H	1.78	0.47
1:B:190:VAL:HG12	1:B:194:ILE:HD13	1.97	0.47
1:B:92:THR:OG1	1:B:113:LYS:HG2	2.15	0.47
1:D:316:ILE:HG22	1:D:376:SER:HA	1.95	0.47
1:E:197:ILE:HG23	1:E:201:ILE:CG1	2.45	0.47
1:E:318:PRO:HD3	1:E:373:THR:O	2.14	0.47
1:F:106:ARG:HH12	1:F:367:SER:HA	1.79	0.47
1:A:226:LEU:HD12	1:A:239:VAL:HG13	1.95	0.47
1:A:297:SER:C	1:A:298:LEU:HD12	2.35	0.47
1:B:62:THR:HG23	1:B:94:GLY:HA3	1.97	0.47
1:D:170:SER:HA	1:D:188:THR:HG23	1.97	0.47
1:D:446:ARG:NH1	1:E:366:ALA:CA	1.96	0.47
1:F:197:ILE:HG23	1:F:201:ILE:CG1	2.45	0.47
1:F:226:LEU:HD12	1:F:239:VAL:HG13	1.95	0.47
1:A:318:PRO:HD3	1:A:373:THR:O	2.14	0.47
1:B:326:SER:HA	1:B:379:LEU:HD22	1.96	0.47
1:C:340:ASP:HA	1:C:486:SER:HB2	1.95	0.47
1:C:345:SER:HB3	1:C:352:VAL:H	1.79	0.47
1:D:40:TYR:CE2	1:D:279:CYS:HA	2.50	0.47
1:F:166:LEU:HD21	1:F:264:LEU:HD23	1.95	0.47
1:A:217:ILE:HD13	1:E:217:ILE:HG21	1.96	0.47
1:A:443:GLU:O	1:A:447:LEU:HG	2.15	0.47
1:C:385:TYR:HB3	1:C:463:VAL:CG1	2.45	0.47
1:F:443:GLU:O	1:F:447:LEU:HG	2.15	0.47
1:A:40:TYR:CE2	1:A:279:CYS:HA	2.50	0.47
1:C:252:GLU:H	1:C:252:GLU:CD	2.17	0.47
1:C:341:LEU:HD12	1:C:485:GLY:O	2.14	0.47
1:D:106:ARG:HH12	1:D:367:SER:HA	1.79	0.47
1:E:143:LEU:HA	1:E:332:ALA:HB2	1.96	0.47
1:A:304:PHE:CE2	1:A:386:TRP:HA	2.50	0.47
1:B:234:ALA:HB1	1:B:444:ILE:HG12	1.97	0.47
1:C:204:ARG:O	1:C:205:ASN:HB2	2.15	0.47
1:C:247:ASN:O	1:C:248:PRO:C	2.53	0.47
1:C:258:PHE:HE2	1:C:444:ILE:HD12	1.80	0.47
1:D:189:MET:HB2	1:D:226:LEU:HD23	1.95	0.47
1:D:386:TRP:NE1	1:D:464:PHE:HB2	2.30	0.47
1:E:174:ARG:HD3	1:E:175:ARG:H	1.80	0.47
1:E:106:ARG:HH12	1:E:367:SER:HA	1.79	0.47
1:A:143:LEU:HA	1:A:332:ALA:HB2	1.96	0.47
1:A:174:ARG:HD3	1:A:175:ARG:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:297:SER:O	1:C:303:PRO:HG3	2.14	0.47
1:C:477:PRO:HB2	1:C:479:PHE:CE1	2.49	0.47
1:C:92:THR:HG21	1:C:116:ILE:HD12	1.95	0.47
1:E:441:ARG:O	1:F:368:ASN:OD1	2.33	0.47
1:F:316:ILE:HG22	1:F:376:SER:HA	1.95	0.47
1:D:443:GLU:CD	1:E:367:SER:OG	2.52	0.46
1:E:114:GLU:HA	1:E:117:ARG:NE	2.24	0.46
1:E:170:SER:HA	1:E:188:THR:HG23	1.97	0.46
1:E:40:TYR:CE2	1:E:279:CYS:HA	2.50	0.46
1:B:262:SER:HA	1:B:448:MET:HE1	1.94	0.46
1:C:104:TRP:CZ2	1:C:376:SER:CB	2.96	0.46
1:D:297:SER:C	1:D:298:LEU:HD12	2.35	0.46
1:E:304:PHE:CE2	1:E:386:TRP:HA	2.50	0.46
1:A:386:TRP:NE1	1:A:464:PHE:HB2	2.30	0.46
1:B:296:TYR:CE1	1:B:302:ASP:HB3	2.51	0.46
1:D:114:GLU:HA	1:D:117:ARG:NE	2.24	0.46
1:E:226:LEU:HD12	1:E:239:VAL:HG13	1.96	0.46
1:F:297:SER:C	1:F:298:LEU:HD12	2.35	0.46
1:C:193:LEU:HD21	1:C:222:MET:HB2	1.98	0.46
1:C:438:SER:HB3	1:C:441:ARG:CG	2.44	0.46
1:D:446:ARG:CA	1:E:368:ASN:CB	2.51	0.46
1:B:141:SER:HB2	1:B:172:LEU:HD12	1.98	0.46
1:B:193:LEU:O	1:B:197:ILE:HG12	2.16	0.46
1:B:217:ILE:HG22	1:D:217:ILE:CG1	2.44	0.46
1:B:232:THR:OG1	1:B:235:GLN:HG3	2.16	0.46
1:C:208:ARG:HH11	1:C:208:ARG:HG2	1.80	0.46
1:C:33:ILE:HD12	1:C:281:TYR:CE2	2.40	0.46
1:D:39:PHE:CE1	1:D:43:MET:HE2	2.51	0.46
1:D:53:GLU:OE2	1:D:98:ARG:HA	2.15	0.46
1:E:297:SER:C	1:E:298:LEU:HD12	2.35	0.46
1:E:443:GLU:CD	1:F:367:SER:OG	2.53	0.46
1:F:53:GLU:OE2	1:F:98:ARG:HA	2.15	0.46
1:C:116:ILE:O	1:C:119:ILE:HG22	2.16	0.46
1:C:457:SER:O	1:C:458:PHE:HB2	2.16	0.46
1:D:143:LEU:HA	1:D:332:ALA:HB2	1.96	0.46
1:E:487:TYR:CD2	1:E:487:TYR:N	2.84	0.46
1:E:53:GLU:OE2	1:E:98:ARG:HA	2.15	0.46
1:F:487:TYR:N	1:F:487:TYR:CD2	2.84	0.46
1:B:301:ILE:O	1:B:302:ASP:C	2.54	0.46
1:E:324:HIS:HD2	1:E:358:LEU:HA	1.81	0.46
1:E:386:TRP:NE1	1:E:464:PHE:HB2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:40:TYR:CE2	1:F:279:CYS:HA	2.50	0.46
1:F:291:PHE:O	1:F:295:GLY:N	2.42	0.46
1:F:304:PHE:CE2	1:F:386:TRP:HA	2.50	0.46
1:A:39:PHE:CZ	1:A:67:VAL:CG2	2.99	0.46
1:C:58:GLN:HE22	1:C:363:VAL:HG13	1.81	0.46
1:D:174:ARG:HD3	1:D:175:ARG:H	1.80	0.46
1:D:196:MET:HE3	1:D:219:TYR:HB2	1.97	0.46
1:F:232:THR:OG1	1:F:235:GLN:CG	2.61	0.46
1:F:56:LEU:O	1:F:58:GLN:N	2.49	0.46
1:A:114:GLU:HA	1:A:117:ARG:NE	2.24	0.46
1:A:170:SER:HA	1:A:188:THR:HG23	1.97	0.46
1:A:197:ILE:HG23	1:A:201:ILE:CG1	2.45	0.46
1:B:300:GLY:O	1:B:303:PRO:HD2	2.16	0.46
1:B:93:GLY:HA2	1:B:109:ILE:O	2.15	0.46
1:C:56:LEU:HD22	1:C:104:TRP:CZ3	2.50	0.46
1:D:368:ASN:HD22	1:D:368:ASN:N	2.13	0.46
1:D:443:GLU:O	1:D:447:LEU:HG	2.15	0.46
1:D:39:PHE:CZ	1:D:67:VAL:CG2	2.99	0.46
1:E:443:GLU:O	1:E:447:LEU:HG	2.15	0.46
1:A:39:PHE:CE1	1:A:43:MET:HE2	2.51	0.46
1:A:56:LEU:O	1:A:58:GLN:N	2.49	0.46
1:C:115:GLU:OE2	1:C:118:ARG:NH2	2.48	0.46
1:E:196:MET:HE1	1:E:219:TYR:HB2	1.98	0.46
1:E:39:PHE:CE1	1:E:43:MET:HE2	2.51	0.46
1:F:170:SER:HA	1:F:188:THR:HG23	1.97	0.46
1:F:386:TRP:NE1	1:F:464:PHE:HB2	2.30	0.46
1:F:39:PHE:CZ	1:F:67:VAL:CG2	2.99	0.46
1:A:324:HIS:HD2	1:A:358:LEU:HA	1.81	0.45
1:A:269:SER:HA	1:A:391:ARG:O	2.17	0.45
1:C:129:ALA:O	1:C:133:LEU:HG	2.16	0.45
1:C:301:ILE:HG12	1:C:305:ARG:HG3	1.99	0.45
1:D:304:PHE:CE2	1:D:386:TRP:HA	2.50	0.45
1:E:269:SER:HA	1:E:391:ARG:O	2.17	0.45
1:E:342:ARG:HB3	1:E:479:PHE:HE2	1.73	0.45
1:A:342:ARG:HB3	1:A:479:PHE:HE2	1.73	0.45
1:A:368:ASN:N	1:A:368:ASN:HD22	2.13	0.45
1:C:30:GLY:HA2	1:C:291:PHE:HB3	1.98	0.45
1:C:58:GLN:CA	1:C:58:GLN:HE21	2.29	0.45
1:E:39:PHE:CZ	1:E:67:VAL:CG2	2.99	0.45
1:A:53:GLU:OE2	1:A:98:ARG:HA	2.15	0.45
1:B:156:ARG:NH1	1:B:195:ARG:NH1	2.61	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:TYR:HB3	1:C:116:ILE:HD11	1.97	0.45
1:B:276:LEU:HD22	1:B:307:LEU:HD21	1.99	0.45
1:C:164:CYS:C	1:C:166:LEU:N	2.68	0.45
1:C:230:PHE:CE1	1:C:259:LEU:HD12	2.52	0.45
1:C:240:ASP:HA	1:C:243:ARG:HH12	1.80	0.45
1:F:39:PHE:CE1	1:F:43:MET:HE2	2.51	0.45
1:B:232:THR:CG2	1:B:235:GLN:HE21	2.30	0.45
1:B:302:ASP:N	1:B:303:PRO:HD2	2.31	0.45
1:B:58:GLN:HG3	1:B:315:LEU:HD12	1.98	0.45
1:B:92:THR:CG2	1:B:93:GLY:N	2.74	0.45
1:C:215:THR:O	1:C:218:ALA:N	2.50	0.45
1:C:438:SER:HB3	1:C:441:ARG:CD	2.47	0.45
1:D:297:SER:O	1:D:303:PRO:HG3	2.16	0.45
1:D:143:LEU:HA	1:D:332:ALA:CB	2.47	0.45
1:E:223:CYS:O	1:E:227:LYS:N	2.45	0.45
1:E:56:LEU:O	1:E:58:GLN:N	2.49	0.45
1:C:247:ASN:N	1:C:248:PRO:HD3	2.31	0.45
1:D:324:HIS:HD2	1:D:358:LEU:HA	1.81	0.45
1:D:56:LEU:O	1:D:57:ILE:C	2.54	0.45
1:D:56:LEU:O	1:D:58:GLN:N	2.49	0.45
1:E:297:SER:O	1:E:303:PRO:HG3	2.16	0.45
1:A:174:ARG:CD	1:A:175:ARG:H	2.30	0.45
1:A:232:THR:OG1	1:A:235:GLN:CG	2.61	0.45
1:B:451:ALA:O	1:B:452:ARG:HD3	2.17	0.45
1:C:164:CYS:O	1:C:166:LEU:N	2.50	0.45
1:C:24:GLU:O	1:C:25:ILE:C	2.54	0.45
1:C:265:ILE:CG1	1:C:266:LEU:H	2.29	0.45
1:D:232:THR:OG1	1:D:235:GLN:CG	2.61	0.45
1:F:174:ARG:CD	1:F:175:ARG:H	2.30	0.45
1:F:232:THR:HG1	1:F:235:GLN:HG3	1.82	0.45
1:F:324:HIS:HD2	1:F:358:LEU:HA	1.81	0.45
1:D:92:THR:CA	1:D:113:LYS:HZ3	2.30	0.45
1:F:297:SER:O	1:F:303:PRO:HG3	2.16	0.45
1:F:269:SER:HA	1:F:391:ARG:O	2.16	0.45
1:A:111:TYR:HD2	1:A:116:ILE:HD11	1.81	0.45
1:E:92:THR:CA	1:E:113:LYS:HZ3	2.30	0.45
1:A:297:SER:O	1:A:303:PRO:HG3	2.16	0.45
1:A:68:LEU:HD21	1:A:133:LEU:O	2.17	0.45
1:C:95:PRO:HB2	1:C:97:TYR:HE2	1.81	0.45
1:D:487:TYR:CD2	1:D:487:TYR:N	2.84	0.45
1:E:143:LEU:HA	1:E:332:ALA:CB	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:223:CYS:O	1:F:227:LYS:N	2.45	0.45
1:F:143:LEU:HA	1:F:332:ALA:CB	2.47	0.45
1:B:170:SER:HA	1:B:188:THR:HG23	1.99	0.44
1:C:34:ASP:OD2	1:C:291:PHE:HB2	2.16	0.44
1:C:356:GLY:O	1:C:357:LYS:HG3	2.17	0.44
1:D:269:SER:HA	1:D:391:ARG:O	2.16	0.44
1:E:145:ASP:OD2	1:E:169:GLY:N	2.48	0.44
1:E:34:ASP:OD2	1:E:291:PHE:HB2	2.18	0.44
1:B:321:ASN:ND2	1:B:322:PRO:HD2	2.27	0.44
1:D:34:ASP:OD2	1:D:291:PHE:HB2	2.18	0.44
1:F:68:LEU:HD21	1:F:133:LEU:O	2.17	0.44
1:A:386:TRP:CE2	1:A:464:PHE:HB2	2.53	0.44
1:B:37:GLY:CA	1:B:282:GLY:HA2	2.47	0.44
1:B:269:SER:HB2	1:B:391:ARG:O	2.17	0.44
1:C:247:ASN:HD22	1:C:247:ASN:C	2.20	0.44
1:C:44:CYS:SG	1:C:49:LEU:HD12	2.58	0.44
1:E:68:LEU:HD21	1:E:133:LEU:O	2.17	0.44
1:A:143:LEU:HA	1:A:332:ALA:CB	2.47	0.44
1:B:100:VAL:O	1:B:101:ASP:C	2.56	0.44
1:B:193:LEU:HA	1:B:222:MET:HE3	2.00	0.44
1:B:312:VAL:O	1:B:379:LEU:HB2	2.18	0.44
1:C:456:VAL:HG13	1:C:456:VAL:O	2.17	0.44
1:D:68:LEU:HD21	1:D:133:LEU:O	2.17	0.44
1:E:232:THR:OG1	1:E:235:GLN:CG	2.61	0.44
1:F:196:MET:HE3	1:F:219:TYR:HB2	1.98	0.44
1:A:235:GLN:HE21	1:A:266:LEU:HB2	1.83	0.44
1:B:193:LEU:HD23	1:B:222:MET:HE2	1.98	0.44
1:C:160:ASP:O	1:C:163:MET:HG3	2.18	0.44
1:C:216:ARG:NH1	1:C:245:SER:O	2.49	0.44
1:E:174:ARG:CD	1:E:175:ARG:H	2.30	0.44
1:F:386:TRP:CE2	1:F:464:PHE:HB2	2.53	0.44
1:F:50:SER:OG	1:F:53:GLU:HG3	2.18	0.44
1:F:92:THR:CA	1:F:113:LYS:HZ3	2.31	0.44
1:C:52:TYR:HE2	1:C:104:TRP:CH2	2.36	0.44
1:C:205:ASN:N	1:C:205:ASN:ND2	2.64	0.44
1:C:485:GLY:O	1:C:487:TYR:N	2.51	0.44
1:D:386:TRP:CE2	1:D:464:PHE:HB2	2.53	0.44
1:F:47:LEU:HD11	1:F:109:ILE:CD1	2.48	0.44
1:A:267:ARG:HG2	1:A:267:ARG:H	1.42	0.44
1:A:487:TYR:CD2	1:A:487:TYR:N	2.84	0.44
1:C:204:ARG:O	1:C:205:ASN:CB	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:LEU:HD12	1:C:364:GLN:HG2	2.00	0.44
1:E:26:ARG:NH1	1:E:295:GLY:C	2.71	0.44
1:F:235:GLN:HE21	1:F:266:LEU:HB2	1.83	0.44
1:F:34:ASP:OD2	1:F:291:PHE:HB2	2.18	0.44
1:A:172:LEU:HD12	1:A:173:PRO:HD2	2.00	0.44
1:D:111:TYR:HD2	1:D:116:ILE:HD11	1.81	0.44
1:F:172:LEU:HD12	1:F:173:PRO:HD2	2.00	0.44
1:F:253:PHE:C	1:F:253:PHE:HD2	2.22	0.44
1:F:185:GLY:HA2	1:F:270:VAL:HG21	2.00	0.44
1:E:446:ARG:HB2	1:F:368:ASN:HB2	1.89	0.44
1:B:317:ARG:HG2	1:B:317:ARG:H	1.62	0.44
1:C:98:ARG:HB2	1:C:105:ARG:HB2	1.99	0.44
1:D:174:ARG:CD	1:D:175:ARG:H	2.30	0.44
1:A:145:ASP:OD2	1:A:169:GLY:N	2.48	0.43
1:A:56:LEU:O	1:A:57:ILE:C	2.54	0.43
1:B:103:LYS:HD3	1:B:372:GLU:OE1	2.18	0.43
1:C:135:HIS:CE1	1:C:298:LEU:HD21	2.53	0.43
1:C:25:ILE:O	1:C:29:VAL:HG23	2.17	0.43
1:C:320:GLU:OE1	1:C:325:LYS:NZ	2.51	0.43
1:C:462:GLY:O	1:C:464:PHE:CE2	2.71	0.43
1:C:58:GLN:CA	1:C:58:GLN:NE2	2.81	0.43
1:E:386:TRP:CE2	1:E:464:PHE:HB2	2.53	0.43
1:E:50:SER:OG	1:E:53:GLU:HG3	2.18	0.43
1:F:26:ARG:NH1	1:F:295:GLY:C	2.71	0.43
1:F:56:LEU:O	1:F:57:ILE:C	2.54	0.43
1:A:253:PHE:HD2	1:A:253:PHE:C	2.22	0.43
1:A:50:SER:OG	1:A:53:GLU:HG3	2.18	0.43
1:B:459:GLN:H	1:B:459:GLN:NE2	2.15	0.43
1:C:270:VAL:CG1	1:C:271:ALA:H	2.29	0.43
1:C:338:PHE:CD1	1:C:338:PHE:N	2.87	0.43
1:C:58:GLN:HE21	1:C:58:GLN:HA	1.82	0.43
1:E:342:ARG:CB	1:E:479:PHE:CE2	3.00	0.43
1:A:112:ASP:O	1:A:113:LYS:C	2.56	0.43
1:B:384:ARG:HH11	1:B:384:ARG:HG2	1.84	0.43
1:B:41:ILE:HD11	1:B:286:ALA:N	2.32	0.43
1:C:164:CYS:C	1:C:166:LEU:H	2.21	0.43
1:C:195:ARG:HG2	1:C:196:MET:N	2.33	0.43
1:C:262:SER:HA	1:C:448:MET:CE	2.47	0.43
1:C:293:ARG:HG2	1:C:293:ARG:HH11	1.83	0.43
1:C:46:GLU:O	1:C:48:LYS:N	2.51	0.43
1:D:47:LEU:HD11	1:D:109:ILE:CD1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:197:ILE:HG23	1:D:201:ILE:CG1	2.45	0.43
1:A:47:LEU:HD11	1:A:109:ILE:CD1	2.48	0.43
1:A:34:ASP:OD2	1:A:291:PHE:HB2	2.18	0.43
1:B:255:ASP:O	1:B:258:PHE:HB3	2.17	0.43
1:B:39:PHE:CZ	1:B:67:VAL:CG2	3.01	0.43
1:B:63:ILE:O	1:B:67:VAL:HG23	2.18	0.43
1:C:61:LEU:O	1:C:65:ARG:HG3	2.18	0.43
1:D:50:SER:OG	1:D:53:GLU:HG3	2.18	0.43
1:E:47:LEU:HD11	1:E:109:ILE:CD1	2.48	0.43
1:E:235:GLN:HE21	1:E:266:LEU:HB2	1.83	0.43
1:E:447:LEU:N	1:F:367:SER:C	2.56	0.43
1:A:92:THR:CA	1:A:113:LYS:HZ3	2.30	0.43
1:B:68:LEU:C	1:B:175:ARG:HH22	2.22	0.43
1:D:174:ARG:HD3	1:D:174:ARG:H	1.82	0.43
1:E:172:LEU:HD12	1:E:173:PRO:HD2	2.00	0.43
1:E:317:ARG:HB3	1:E:318:PRO:HD2	2.01	0.43
1:F:317:ARG:HB3	1:F:318:PRO:HD2	2.01	0.43
1:A:33:ILE:HG22	1:A:34:ASP:N	2.34	0.43
1:B:115:GLU:CA	1:B:115:GLU:OE1	2.66	0.43
1:B:37:GLY:HA2	1:B:282:GLY:CA	2.49	0.43
1:C:213:ARG:O	1:C:217:ILE:HG13	2.19	0.43
1:D:112:ASP:O	1:D:113:LYS:C	2.56	0.43
1:D:253:PHE:C	1:D:253:PHE:HD2	2.22	0.43
1:E:390:THR:HG22	1:E:391:ARG:N	2.28	0.43
1:F:111:TYR:HD2	1:F:116:ILE:HD11	1.81	0.43
1:F:33:ILE:HG22	1:F:34:ASP:N	2.34	0.43
1:A:26:ARG:NH1	1:A:295:GLY:C	2.71	0.43
1:A:324:HIS:HD2	1:A:359:SER:N	2.08	0.43
1:C:446:ARG:O	1:C:449:GLU:HB3	2.19	0.43
1:E:37:GLY:HA3	1:E:285:VAL:CG2	2.46	0.43
1:E:56:LEU:O	1:E:57:ILE:C	2.54	0.43
1:A:51:ASP:O	1:A:55:ARG:HG3	2.19	0.43
1:B:118:ARG:HD2	1:B:119:ILE:N	2.33	0.43
1:C:97:TYR:HA	1:C:105:ARG:O	2.19	0.43
1:A:196:MET:HE1	1:A:219:TYR:HB2	1.99	0.43
1:A:317:ARG:HB2	1:A:320:GLU:CG	2.49	0.43
1:B:92:THR:HG22	1:B:93:GLY:H	1.80	0.43
1:C:32:MET:O	1:C:36:ILE:HG13	2.19	0.43
1:D:145:ASP:OD2	1:D:169:GLY:N	2.48	0.43
1:D:37:GLY:HA3	1:D:285:VAL:CG2	2.46	0.43
1:D:303:PRO:HD2	1:D:389:ARG:HH22	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:112:ASP:O	1:E:113:LYS:C	2.56	0.43
1:E:33:ILE:HG21	1:E:291:PHE:CG	2.54	0.43
1:A:238:MET:HE3	1:A:255:ASP:OD1	2.18	0.43
1:A:33:ILE:HG21	1:A:291:PHE:CG	2.54	0.43
1:A:58:GLN:NE2	1:A:58:GLN:HA	2.34	0.43
1:B:68:LEU:HB3	1:B:175:ARG:NH2	2.34	0.43
1:D:33:ILE:HG21	1:D:291:PHE:CG	2.54	0.43
1:D:58:GLN:HA	1:D:58:GLN:NE2	2.34	0.43
1:F:264:LEU:HA	1:F:264:LEU:HD23	1.73	0.43
1:D:26:ARG:NH1	1:D:295:GLY:C	2.71	0.42
1:D:33:ILE:HG22	1:D:34:ASP:N	2.34	0.42
1:E:58:GLN:NE2	1:E:58:GLN:HA	2.34	0.42
1:F:473:SER:HA	1:F:474:PRO:HD3	1.63	0.42
1:F:51:ASP:O	1:F:55:ARG:HG3	2.19	0.42
1:F:40:TYR:CE1	1:F:63:ILE:HD12	2.54	0.42
1:A:199:ARG:HD3	1:A:199:ARG:HA	1.95	0.42
1:B:395:ASN:HD22	1:B:395:ASN:C	2.22	0.42
1:C:205:ASN:N	1:C:205:ASN:HD22	2.17	0.42
1:D:185:GLY:HA2	1:D:270:VAL:HG21	2.00	0.42
1:D:317:ARG:HB3	1:D:318:PRO:HD2	2.01	0.42
1:D:342:ARG:CB	1:D:479:PHE:CE2	3.00	0.42
1:E:111:TYR:HD2	1:E:116:ILE:HD11	1.81	0.42
1:F:33:ILE:HG21	1:F:291:PHE:CG	2.54	0.42
1:A:114:GLU:HB3	1:A:117:ARG:NH2	2.26	0.42
1:A:185:GLY:HA2	1:A:270:VAL:HG21	2.00	0.42
1:A:303:PRO:HD2	1:A:389:ARG:HH22	1.84	0.42
1:C:316:ILE:HG13	1:C:320:GLU:OE1	2.19	0.42
1:D:235:GLN:HE21	1:D:266:LEU:HB2	1.83	0.42
1:E:185:GLY:HA2	1:E:270:VAL:HG21	2.00	0.42
1:E:33:ILE:HG22	1:E:34:ASP:N	2.34	0.42
1:E:447:LEU:HG	1:F:368:ASN:CA	2.46	0.42
1:B:114:GLU:HA	1:B:117:ARG:NE	2.34	0.42
1:B:234:ALA:CB	1:B:444:ILE:HG12	2.50	0.42
1:C:33:ILE:HG23	1:C:281:TYR:HD2	1.78	0.42
1:D:163:MET:CE	1:D:261:ARG:HG2	2.42	0.42
1:D:444:ILE:C	1:E:368:ASN:CA	2.87	0.42
1:E:303:PRO:HD2	1:E:389:ARG:HH22	1.84	0.42
1:E:51:ASP:O	1:E:55:ARG:HG3	2.19	0.42
1:F:124:ASN:O	1:F:127:ASP:HB2	2.20	0.42
1:A:60:SER:O	1:A:64:GLU:HG3	2.20	0.42
1:C:139:TRP:CZ2	1:C:143:LEU:HD22	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:317:ARG:HB2	1:C:318:PRO:HD2	2.01	0.42
1:C:382:ARG:NH1	1:C:382:ARG:HG2	2.33	0.42
1:A:40:TYR:CE1	1:A:63:ILE:HD12	2.54	0.42
1:C:192:GLU:HA	1:C:195:ARG:HD3	2.00	0.42
1:C:237:THR:O	1:C:241:GLN:HG3	2.19	0.42
1:C:265:ILE:HD11	1:C:448:MET:CG	2.50	0.42
1:C:438:SER:HB3	1:C:441:ARG:HD2	2.01	0.42
1:D:172:LEU:HD12	1:D:173:PRO:HD2	2.00	0.42
1:E:40:TYR:CE1	1:E:63:ILE:HD12	2.54	0.42
1:F:221:ARG:O	1:F:224:ASN:N	2.53	0.42
1:F:303:PRO:HD2	1:F:389:ARG:HH22	1.84	0.42
1:A:124:ASN:O	1:A:127:ASP:HB2	2.20	0.42
1:B:238:MET:SD	1:B:259:LEU:CD1	3.08	0.42
1:B:320:GLU:OE1	1:B:360:THR:HG23	2.19	0.42
1:B:64:GLU:O	1:B:68:LEU:HG	2.19	0.42
1:C:120:TRP:CZ2	1:C:129:ALA:HB3	2.55	0.42
1:C:265:ILE:CG1	1:C:266:LEU:N	2.83	0.42
1:C:60:SER:HB3	1:C:279:CYS:HB3	2.02	0.42
1:C:46:GLU:C	1:C:48:LYS:N	2.73	0.42
1:D:159:MET:SD	1:D:191:MET:HG3	2.60	0.42
1:D:230:PHE:CE2	1:D:259:LEU:HG	2.55	0.42
1:D:60:SER:O	1:D:64:GLU:HG3	2.20	0.42
1:E:122:GLN:OE1	1:E:122:GLN:HA	2.20	0.42
1:E:230:PHE:CE2	1:E:259:LEU:HG	2.55	0.42
1:F:112:ASP:O	1:F:113:LYS:C	2.56	0.42
1:A:174:ARG:HD3	1:A:174:ARG:H	1.83	0.42
1:C:150:ARG:HD3	1:C:150:ARG:HA	1.81	0.42
1:C:464:PHE:CE1	1:C:471:ALA:HB1	2.55	0.42
1:D:317:ARG:HB2	1:D:320:GLU:CG	2.49	0.42
1:D:51:ASP:O	1:D:55:ARG:HG3	2.19	0.42
1:D:446:ARG:HB2	1:E:368:ASN:HB2	1.89	0.42
1:F:122:GLN:HA	1:F:122:GLN:OE1	2.20	0.42
1:F:267:ARG:H	1:F:267:ARG:HG2	1.42	0.42
1:B:273:LYS:HB3	1:B:298:LEU:HD23	2.01	0.42
1:C:134:THR:HA	1:C:137:MET:HE3	2.02	0.42
1:C:235:GLN:O	1:C:239:VAL:HG23	2.20	0.42
1:D:151:THR:O	1:D:155:VAL:HG22	2.20	0.42
1:E:151:THR:O	1:E:155:VAL:HG22	2.20	0.42
1:E:159:MET:SD	1:E:191:MET:HG3	2.60	0.42
1:E:317:ARG:HB2	1:E:320:GLU:CG	2.49	0.42
1:E:324:HIS:CD2	1:E:358:LEU:HA	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:PRO:HG2	1:B:389:ARG:NH1	2.34	0.42
1:D:473:SER:HA	1:D:474:PRO:HD3	1.63	0.42
1:E:253:PHE:HD2	1:E:253:PHE:C	2.21	0.42
1:F:346:PHE:HE2	1:F:463:VAL:HG21	1.85	0.42
1:A:122:GLN:OE1	1:A:122:GLN:HA	2.20	0.41
1:B:321:ASN:HA	1:B:322:PRO:HD3	1.97	0.41
1:C:342:ARG:C	1:C:344:SER:H	2.23	0.41
1:C:463:VAL:HG12	1:C:464:PHE:N	2.35	0.41
1:D:122:GLN:OE1	1:D:122:GLN:HA	2.20	0.41
1:F:151:THR:O	1:F:155:VAL:HG22	2.20	0.41
1:F:230:PHE:CE2	1:F:259:LEU:HG	2.55	0.41
1:F:60:SER:O	1:F:64:GLU:HG3	2.20	0.41
1:B:242:VAL:HG12	1:B:242:VAL:O	2.20	0.41
1:B:58:GLN:HG2	1:B:58:GLN:H	1.63	0.41
1:D:264:LEU:HA	1:D:264:LEU:HD23	1.74	0.41
1:D:40:TYR:CE1	1:D:63:ILE:HD12	2.54	0.41
1:E:124:ASN:O	1:E:127:ASP:HB2	2.20	0.41
1:D:449:GLU:HB3	1:E:369:GLU:C	2.41	0.41
1:E:346:PHE:HE2	1:E:463:VAL:HG21	1.85	0.41
1:F:324:HIS:CD2	1:F:358:LEU:HA	2.55	0.41
1:A:346:PHE:HE2	1:A:463:VAL:HG21	1.85	0.41
1:B:160:ASP:C	1:B:162:ARG:H	2.24	0.41
1:B:66:MET:HA	1:B:92:THR:HG21	2.02	0.41
1:C:195:ARG:NH2	1:C:222:MET:HE1	2.35	0.41
1:C:370:ASN:ND2	1:C:372:GLU:H	2.18	0.41
1:B:217:ILE:CB	1:D:217:ILE:HD11	2.42	0.41
1:D:230:PHE:CZ	1:D:259:LEU:HG	2.55	0.41
1:D:201:ILE:HG21	1:D:249:GLY:HA2	2.02	0.41
1:D:324:HIS:CD2	1:D:358:LEU:HA	2.55	0.41
1:F:317:ARG:HB2	1:F:320:GLU:CG	2.49	0.41
1:A:159:MET:SD	1:A:191:MET:HG3	2.60	0.41
1:A:230:PHE:CE2	1:A:259:LEU:HG	2.55	0.41
1:B:235:GLN:O	1:B:239:VAL:HG23	2.18	0.41
1:B:386:TRP:HB3	1:B:466:LEU:HD21	2.02	0.41
1:F:168:GLN:HE21	1:F:183:VAL:HG22	1.85	0.41
1:A:168:GLN:HE21	1:A:183:VAL:HG22	1.86	0.41
1:C:385:TYR:HB3	1:C:463:VAL:HG12	2.02	0.41
1:C:56:LEU:HG	1:C:58:GLN:HG2	2.02	0.41
1:D:264:LEU:O	1:D:267:ARG:NH1	2.54	0.41
1:E:221:ARG:O	1:E:224:ASN:N	2.53	0.41
1:F:230:PHE:CZ	1:F:259:LEU:HG	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:ILE:HG21	1:E:217:ILE:HD13	1.22	0.41
1:A:264:LEU:O	1:A:267:ARG:NH1	2.54	0.41
1:A:317:ARG:HB3	1:A:318:PRO:HD2	2.01	0.41
1:B:149:GLN:HG2	1:B:151:THR:HG23	2.02	0.41
1:C:174:ARG:HD3	1:C:174:ARG:N	2.36	0.41
1:E:264:LEU:O	1:E:267:ARG:NH1	2.54	0.41
1:A:37:GLY:HA3	1:A:285:VAL:CG2	2.46	0.41
1:C:121:ARG:HH11	1:C:121:ARG:HG3	1.86	0.41
1:C:166:LEU:HB3	1:C:187:GLY:H	1.86	0.41
1:D:58:GLN:HE21	1:D:58:GLN:CA	2.31	0.41
1:E:174:ARG:HD3	1:E:174:ARG:H	1.82	0.41
1:F:145:ASP:OD2	1:F:169:GLY:N	2.48	0.41
1:F:238:MET:HE3	1:F:255:ASP:OD1	2.20	0.41
1:A:201:ILE:HG21	1:A:249:GLY:HA2	2.02	0.41
1:A:230:PHE:CZ	1:A:259:LEU:HG	2.55	0.41
1:D:116:ILE:N	1:D:116:ILE:HD12	2.36	0.41
1:D:221:ARG:O	1:D:224:ASN:N	2.53	0.41
1:E:168:GLN:HE21	1:E:183:VAL:HG22	1.85	0.41
1:E:26:ARG:HH11	1:E:295:GLY:CA	2.32	0.41
1:E:302:ASP:N	1:E:303:PRO:CD	2.84	0.41
1:E:321:ASN:C	1:E:321:ASN:HD22	2.24	0.41
1:B:41:ILE:CD1	1:B:286:ALA:HB2	2.51	0.41
1:C:134:THR:HA	1:C:137:MET:CE	2.50	0.41
1:C:97:TYR:CD2	1:C:97:TYR:N	2.88	0.41
1:D:168:GLN:HE21	1:D:183:VAL:HG22	1.85	0.41
1:D:223:CYS:O	1:D:227:LYS:N	2.45	0.41
1:E:168:GLN:NE2	1:E:183:VAL:HG22	2.36	0.41
1:E:23:THR:O	1:E:27:ALA:HB3	2.21	0.41
1:E:444:ILE:C	1:F:368:ASN:CA	2.89	0.41
1:F:159:MET:SD	1:F:191:MET:HG3	2.60	0.41
1:F:23:THR:O	1:F:27:ALA:HB3	2.21	0.41
1:A:151:THR:O	1:A:155:VAL:HG22	2.20	0.41
1:C:342:ARG:C	1:C:344:SER:N	2.73	0.41
1:C:43:MET:HE1	1:C:119:ILE:HG21	2.03	0.41
1:D:124:ASN:O	1:D:127:ASP:HB2	2.20	0.41
1:D:267:ARG:HG2	1:D:267:ARG:H	1.42	0.41
1:D:390:THR:HG22	1:D:391:ARG:N	2.27	0.41
1:E:116:ILE:HD12	1:E:116:ILE:N	2.36	0.41
1:F:168:GLN:NE2	1:F:183:VAL:HG22	2.36	0.41
1:F:58:GLN:NE2	1:F:58:GLN:HA	2.34	0.41
1:A:116:ILE:N	1:A:116:ILE:HD12	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:VAL:HG12	1:A:161:PRO:HD3	2.03	0.41
1:A:168:GLN:NE2	1:A:183:VAL:HG22	2.36	0.41
1:A:23:THR:O	1:A:27:ALA:HB3	2.21	0.41
1:A:37:GLY:HA2	1:A:282:GLY:HA2	2.03	0.41
1:A:473:SER:HA	1:A:474:PRO:HD3	1.63	0.41
1:C:121:ARG:HG3	1:C:121:ARG:NH1	2.36	0.41
1:C:246:ARG:CG	1:C:246:ARG:HH11	2.31	0.41
1:C:304:PHE:O	1:C:308:GLN:HB2	2.21	0.41
1:D:23:THR:O	1:D:27:ALA:HB3	2.21	0.41
1:D:58:GLN:CA	1:D:58:GLN:NE2	2.84	0.41
1:E:201:ILE:HG21	1:E:249:GLY:HA2	2.02	0.41
1:F:448:MET:O	1:F:451:ALA:HB3	2.21	0.41
1:A:321:ASN:C	1:A:321:ASN:HD22	2.24	0.40
1:D:257:ILE:O	1:D:260:ALA:HB3	2.21	0.40
1:D:448:MET:O	1:D:451:ALA:HB3	2.21	0.40
1:D:446:ARG:HD2	1:E:366:ALA:HB3	1.86	0.40
1:F:116:ILE:N	1:F:116:ILE:HD12	2.36	0.40
1:F:121:ARG:NH1	1:F:121:ARG:CG	2.83	0.40
1:F:155:VAL:HG12	1:F:161:PRO:HD3	2.03	0.40
1:F:201:ILE:HG21	1:F:249:GLY:HA2	2.02	0.40
1:F:302:ASP:N	1:F:303:PRO:CD	2.84	0.40
1:A:121:ARG:O	1:A:122:GLN:C	2.60	0.40
1:A:324:HIS:CD2	1:A:358:LEU:HA	2.55	0.40
1:B:358:LEU:HD12	1:B:358:LEU:HA	1.97	0.40
1:B:62:THR:O	1:B:66:MET:HG3	2.21	0.40
1:D:238:MET:HE3	1:D:255:ASP:OD1	2.21	0.40
1:E:60:SER:O	1:E:64:GLU:HG3	2.20	0.40
1:F:238:MET:CE	1:F:255:ASP:OD1	2.69	0.40
1:F:37:GLY:HA3	1:F:285:VAL:CG2	2.46	0.40
1:A:157:THR:HB	1:A:159:MET:HG3	2.04	0.40
1:C:186:VAL:O	1:C:190:VAL:HG23	2.22	0.40
1:C:361:ARG:HA	1:C:361:ARG:HD3	1.80	0.40
1:D:315:LEU:HD12	1:D:365:ILE:CD1	2.50	0.40
1:D:346:PHE:HE2	1:D:463:VAL:HG21	1.85	0.40
1:E:155:VAL:HG12	1:E:161:PRO:HD3	2.03	0.40
1:E:446:ARG:HG3	1:F:369:GLU:HB2	1.01	0.40
1:F:257:ILE:O	1:F:260:ALA:HB3	2.21	0.40
1:F:264:LEU:O	1:F:267:ARG:NH1	2.54	0.40
1:F:342:ARG:CB	1:F:479:PHE:CE2	3.00	0.40
1:B:238:MET:SD	1:B:259:LEU:HD11	2.62	0.40
1:C:104:TRP:HZ2	1:C:376:SER:CB	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:157:THR:HB	1:D:159:MET:HG3	2.04	0.40
1:F:121:ARG:O	1:F:122:GLN:C	2.60	0.40
1:F:242:VAL:HG13	1:F:252:GLU:CG	2.50	0.40
1:F:321:ASN:C	1:F:321:ASN:HD22	2.24	0.40
1:E:446:ARG:HD2	1:F:366:ALA:HB3	1.85	0.40
1:A:223:CYS:O	1:A:227:LYS:N	2.45	0.40
1:C:172:LEU:HD12	1:C:172:LEU:HA	1.88	0.40
1:C:195:ARG:HG2	1:C:196:MET:H	1.87	0.40
1:D:238:MET:CE	1:D:255:ASP:OD1	2.70	0.40
1:E:157:THR:HB	1:E:159:MET:HG3	2.04	0.40
1:E:257:ILE:O	1:E:260:ALA:HB3	2.21	0.40
1:D:443:GLU:OE2	1:E:366:ALA:CA	2.70	0.40
1:E:448:MET:O	1:E:451:ALA:HB3	2.21	0.40
1:F:114:GLU:HB3	1:F:117:ARG:NH2	2.26	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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	391/498 (78%)	339 (87%)	47 (12%)	5 (1%)	14	56
1	B	391/498 (78%)	341 (87%)	41 (10%)	9 (2%)	7	43
1	C	403/498 (81%)	332 (82%)	63 (16%)	8 (2%)	9	46
1	D	391/498 (78%)	339 (87%)	47 (12%)	5 (1%)	14	56
1	E	391/498 (78%)	339 (87%)	47 (12%)	5 (1%)	14	56
1	F	391/498 (78%)	339 (87%)	47 (12%)	5 (1%)	14	56
All	All	2358/2988 (79%)	2029 (86%)	292 (12%)	37 (2%)	16	51

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	203	ASP
1	C	395	ASN
1	C	486	SER
1	A	233	ALA
1	A	472	THR
1	B	150	ARG
1	B	177	GLY
1	C	25	ILE
1	D	233	ALA
1	D	472	THR
1	E	233	ALA
1	E	472	THR
1	F	233	ALA
1	F	472	THR
1	A	101	ASP
1	A	250	ASN
1	B	101	ASP
1	B	341	LEU
1	C	108	LEU
1	C	480	ASP
1	D	101	ASP
1	D	250	ASN
1	E	101	ASP
1	E	250	ASN
1	F	101	ASP
1	F	250	ASN
1	B	340	ASP
1	B	469	GLU
1	A	448	MET
1	B	318	PRO
1	C	47	LEU
1	C	266	LEU
1	D	448	MET
1	E	448	MET
1	F	448	MET
1	B	248	PRO
1	B	356	GLY

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.



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	338/422 (80%)	313 (93%)	25 (7%)	16	48
1	B	338/422 (80%)	318 (94%)	20 (6%)	23	55
1	C	346/422 (82%)	319 (92%)	27 (8%)	15	46
1	D	338/422 (80%)	313 (93%)	25 (7%)	16	48
1	E	338/422 (80%)	313 (93%)	25 (7%)	16	48
1	F	338/422 (80%)	313 (93%)	25 (7%)	16	48
All	All	2036/2532 (80%)	1889 (93%)	147 (7%)	21	49

All (147) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	32	MET
1	A	33	ILE
1	A	48	LYS
1	A	106	ARG
1	A	108	LEU
1	A	111	TYR
1	A	112	ASP
1	A	118	ARG
1	A	139	TRP
1	A	174	ARG
1	A	191	MET
1	A	202	ASN
1	A	244	GLU
1	A	246	ARG
1	A	253	PHE
1	A	267	ARG
1	A	321	ASN
1	A	339	GLU
1	A	348	ARG
1	A	384	ARG
1	A	390	THR
1	A	456	VAL
1	A	483	ASN
1	A	484	GLU
1	B	21	ASN
1	B	58	GLN

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Mol	Chain	Res	Type
1	B	107	GLU
1	B	114	GLU
1	B	139	TRP
1	B	174	ARG
1	B	220	GLU
1	B	305	ARG
1	B	308	GLN
1	B	317	ARG
1	B	321	ASN
1	B	368	ASN
1	B	389	ARG
1	B	390	THR
1	B	395	ASN
1	B	438	SER
1	B	459	GLN
1	B	461	ARG
1	B	479	PHE
1	B	483	ASN
1	C	46	GLU
1	C	57	ILE
1	C	58	GLN
1	C	59	ASN
1	C	60	SER
1	C	99	ARG
1	C	105	ARG
1	C	109	ILE
1	C	113	LYS
1	C	174	ARG
1	C	226	LEU
1	C	243	ARG
1	C	247	ASN
1	C	255	ASP
1	C	314	SER
1	C	321	ASN
1	C	371	MET
1	C	372	GLU
1	C	375	GLU
1	C	382	ARG
1	C	389	ARG
1	C	390	THR
1	C	441	ARG
1	C	446	ARG

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Mol	Chain	Res	Type
1	C	469	GLU
1	C	481	MET
1	C	483	ASN
1	D	21	ASN
1	D	32	MET
1	D	33	ILE
1	D	48	LYS
1	D	106	ARG
1	D	108	LEU
1	D	111	TYR
1	D	112	ASP
1	D	118	ARG
1	D	139	TRP
1	D	174	ARG
1	D	191	MET
1	D	202	ASN
1	D	244	GLU
1	D	246	ARG
1	D	253	PHE
1	D	267	ARG
1	D	321	ASN
1	D	339	GLU
1	D	348	ARG
1	D	384	ARG
1	D	390	THR
1	D	456	VAL
1	D	483	ASN
1	D	484	GLU
1	E	21	ASN
1	E	32	MET
1	E	33	ILE
1	E	48	LYS
1	E	106	ARG
1	E	108	LEU
1	E	111	TYR
1	E	112	ASP
1	E	118	ARG
1	E	139	TRP
1	E	174	ARG
1	E	191	MET
1	E	202	ASN
1	E	244	GLU

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Mol	Chain	Res	Type
1	E	246	ARG
1	E	253	PHE
1	E	267	ARG
1	E	321	ASN
1	E	339	GLU
1	E	348	ARG
1	E	384	ARG
1	E	390	THR
1	E	456	VAL
1	E	483	ASN
1	E	484	GLU
1	F	21	ASN
1	F	32	MET
1	F	33	ILE
1	F	48	LYS
1	F	106	ARG
1	F	108	LEU
1	F	111	TYR
1	F	112	ASP
1	F	118	ARG
1	F	139	TRP
1	F	174	ARG
1	F	191	MET
1	F	202	ASN
1	F	244	GLU
1	F	246	ARG
1	F	253	PHE
1	F	267	ARG
1	F	321	ASN
1	F	339	GLU
1	F	348	ARG
1	F	384	ARG
1	F	390	THR
1	F	456	VAL
1	F	483	ASN
1	F	484	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	168	GLN

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Mol	Chain	Res	Type
1	A	224	ASN
1	A	272	HIS
1	A	308	GLN
1	A	319	ASN
1	A	321	ASN
1	A	324	HIS
1	A	368	ASN
1	A	370	ASN
1	A	483	ASN
1	B	122	GLN
1	B	142	ASN
1	B	231	GLN
1	B	235	GLN
1	B	241	GLN
1	B	308	GLN
1	B	309	ASN
1	B	311	GLN
1	B	321	ASN
1	B	395	ASN
1	B	459	GLN
1	B	483	ASN
1	C	140	HIS
1	C	142	ASN
1	C	205	ASN
1	C	247	ASN
1	C	308	GLN
1	C	309	ASN
1	C	319	ASN
1	C	321	ASN
1	C	324	HIS
1	C	370	ASN
1	D	21	ASN
1	D	168	GLN
1	D	224	ASN
1	D	272	HIS
1	D	308	GLN
1	D	319	ASN
1	D	321	ASN
1	D	324	HIS
1	D	368	ASN
1	D	370	ASN
1	D	483	ASN

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Mol	Chain	Res	Type
1	E	21	ASN
1	E	168	GLN
1	E	224	ASN
1	E	272	HIS
1	E	308	GLN
1	E	319	ASN
1	E	321	ASN
1	E	324	HIS
1	E	483	ASN
1	F	21	ASN
1	F	168	GLN
1	F	224	ASN
1	F	272	HIS
1	F	308	GLN
1	F	319	ASN
1	F	321	ASN
1	F	324	HIS
1	F	370	ASN
1	F	483	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 ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

### 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	2
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	201:ILE	C	202:ASN	N	1.15
1	C	202:ASN	C	203:ASP	N	1.15
1	B	201:ILE	C	202:ASN	N	1.03