



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Aug 24, 2017 – 12:41 PM EDT

PDB ID : 5A7X
EMDB ID: : EMD-3086
Title : negative stain EM of BG505 SOSIP.664 in complex with sCD4, 17b, and 8ANC195
Authors : Scharf, L.; Wang, H.; Gao, H.; Chen, S.; McDowall, A.; Bjorkman, P.
Deposited on : unknown
Resolution : 17.00 Å(reported)

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

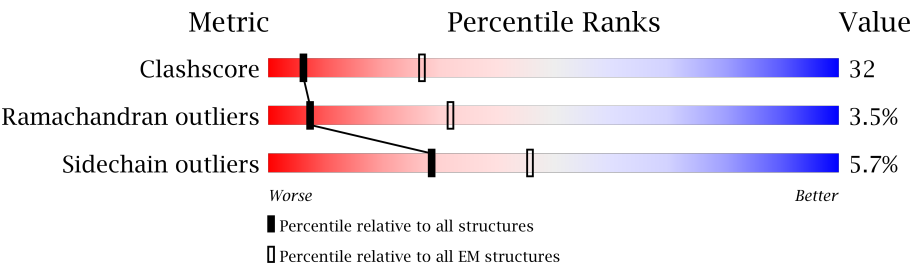
MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 17.00 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 ≥ 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	313	<div><div>41%</div><div>52%</div><div>• •</div></div>
1	E	313	<div><div>40%</div><div>53%</div><div>• •</div></div>
1	I	313	<div><div>41%</div><div>52%</div><div>• •</div></div>
2	B	181	<div><div>34%</div><div>55%</div><div>9% •</div></div>
2	F	181	<div><div>35%</div><div>53%</div><div>10% •</div></div>
2	J	181	<div><div>35%</div><div>54%</div><div>10% •</div></div>
3	C	214	<div><div>34%</div><div>57%</div><div>8% •</div></div>
3	G	214	<div><div>34%</div><div>58%</div><div>7% •</div></div>
3	K	214	<div><div>34%</div><div>57%</div><div>8% •</div></div>

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Mol	Chain	Length	Quality of chain
4	D	229	
4	H	229	
4	L	229	
5	M	215	
5	O	215	
5	Q	215	
6	N	244	
6	P	244	
6	R	244	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	NAG	A	588	X	-	-	-
7	NAG	A	741	X	-	-	-
7	NAG	E	588	X	-	-	-
7	NAG	E	741	X	-	-	-
7	NAG	I	588	X	-	-	-
7	NAG	I	741	X	-	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 31872 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 HIV-1 YU2 GP120.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	306	Total	C	N	O	S	0	0
			2385	1494	417	454	20		
1	E	306	Total	C	N	O	S	0	0
			2385	1494	417	454	20		
1	I	306	Total	C	N	O	S	0	0
			2385	1494	417	454	20		

- Molecule 2 is a protein called T-CELL SURFACE GLYCOPROTEIN CD4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	181	Total	C	N	O	S	0	0
			1412	885	247	276	4		
2	F	181	Total	C	N	O	S	0	0
			1412	885	247	276	4		
2	J	181	Total	C	N	O	S	0	0
			1412	885	247	276	4		

- Molecule 3 is a protein called FAB OF BROADLY NEUTRALIZING ANTIBODY 17B.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	214	Total	C	N	O	S	0	0
			1647	1028	282	332	5		
3	G	214	Total	C	N	O	S	0	0
			1647	1028	282	332	5		
3	K	214	Total	C	N	O	S	0	0
			1647	1028	282	332	5		

- Molecule 4 is a protein called FAB OF BROADLY NEUTRALIZING ANTIBODY 17B.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	229	Total	C	N	O	S	0	0
			1722	1086	289	342	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	229	Total	C	N	O	S	0	0
			1722	1086	289	342	5		
4	L	229	Total	C	N	O	S	0	0
			1722	1086	289	342	5		

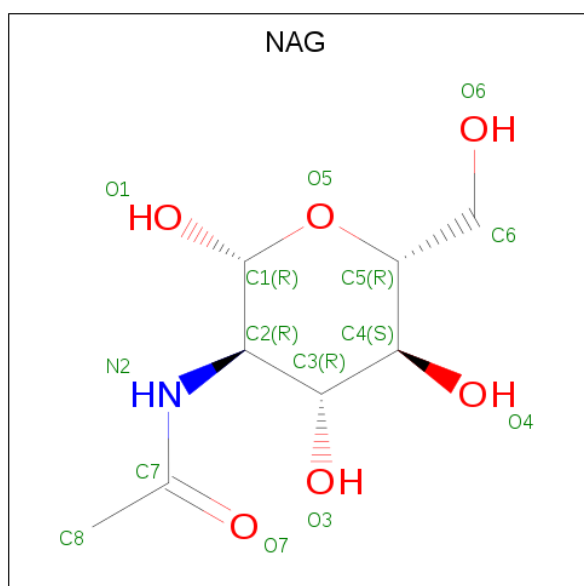
- Molecule 5 is a protein called FAB OF BROADLY NEUTRALIZING ANTIBODY 8ANC195.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	214	Total	C	N	O	S	0	0
			1605	1002	273	325	5		
5	O	214	Total	C	N	O	S	0	0
			1605	1002	273	325	5		
5	Q	214	Total	C	N	O	S	0	0
			1605	1002	273	325	5		

- Molecule 6 is a protein called FAB OF BROADLY NEUTRALIZING ANTIBODY 8ANC195.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	224	Total	C	N	O	S	0	0
			1643	1046	273	319	5		
6	P	224	Total	C	N	O	S	0	0
			1643	1046	273	319	5		
6	R	224	Total	C	N	O	S	0	0
			1643	1046	273	319	5		

- Molecule 7 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	N	O	0
			196	112	14	70	
7	A	1	Total	C	N	O	0
			196	112	14	70	
7	A	1	Total	C	N	O	0
			196	112	14	70	
7	A	1	Total	C	N	O	0
			196	112	14	70	
7	A	1	Total	C	N	O	0
			196	112	14	70	
7	A	1	Total	C	N	O	0
			196	112	14	70	
7	A	1	Total	C	N	O	0
			196	112	14	70	
7	A	1	Total	C	N	O	0
			196	112	14	70	
7	A	1	Total	C	N	O	0
			196	112	14	70	
7	A	1	Total	C	N	O	0
			196	112	14	70	
7	A	1	Total	C	N	O	0
			196	112	14	70	
7	E	1	Total	C	N	O	0
			196	112	14	70	
7	E	1	Total	C	N	O	0
			196	112	14	70	
7	E	1	Total	C	N	O	0
			196	112	14	70	
7	E	1	Total	C	N	O	0
			196	112	14	70	
7	E	1	Total	C	N	O	0
			196	112	14	70	
7	E	1	Total	C	N	O	0
			196	112	14	70	
7	E	1	Total	C	N	O	0
			196	112	14	70	

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Mol	Chain	Residues	Atoms				AltConf
7	E	1	Total	C	N	O	0
			196	112	14	70	
7	E	1	Total	C	N	O	0
			196	112	14	70	
7	E	1	Total	C	N	O	0
			196	112	14	70	
7	E	1	Total	C	N	O	0
			196	112	14	70	
7	E	1	Total	C	N	O	0
			196	112	14	70	
7	E	1	Total	C	N	O	0
			196	112	14	70	
7	I	1	Total	C	N	O	0
			196	112	14	70	
7	I	1	Total	C	N	O	0
			196	112	14	70	
7	I	1	Total	C	N	O	0
			196	112	14	70	
7	I	1	Total	C	N	O	0
			196	112	14	70	
7	I	1	Total	C	N	O	0
			196	112	14	70	
7	I	1	Total	C	N	O	0
			196	112	14	70	
7	I	1	Total	C	N	O	0
			196	112	14	70	
7	I	1	Total	C	N	O	0
			196	112	14	70	
7	I	1	Total	C	N	O	0
			196	112	14	70	
7	I	1	Total	C	N	O	0
			196	112	14	70	
7	I	1	Total	C	N	O	0
			196	112	14	70	
7	N	1	Total	C	N	O	0
			14	8	1	5	

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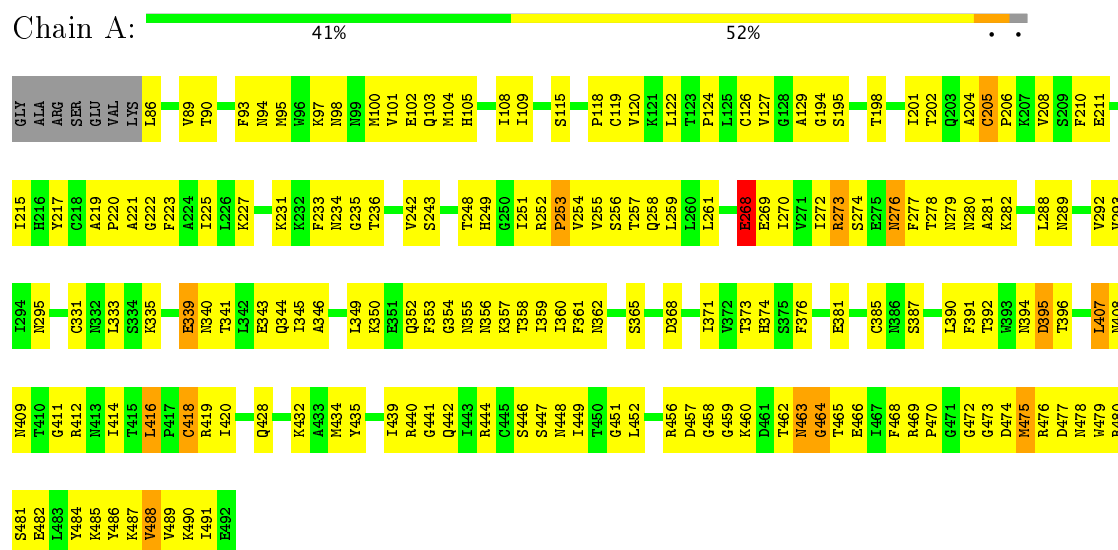
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Mol	Chain	Residues	Atoms				AltConf
7	P	1	Total	C	N	O	0
			14	8	1	5	
7	R	1	Total	C	N	O	0
			14	8	1	5	

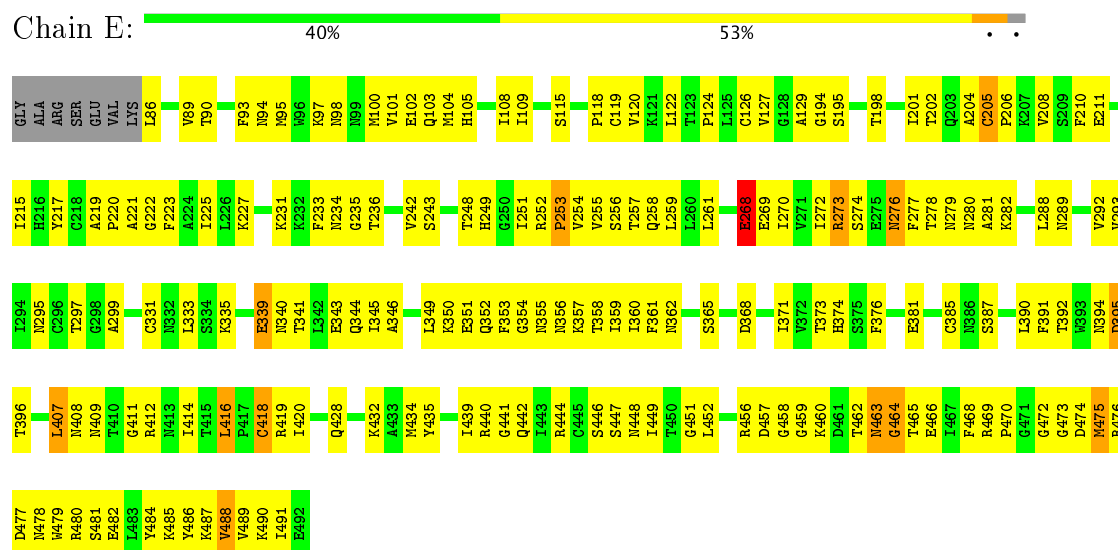
3 Residue-property plots

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: HIV-1 YU2 GP120

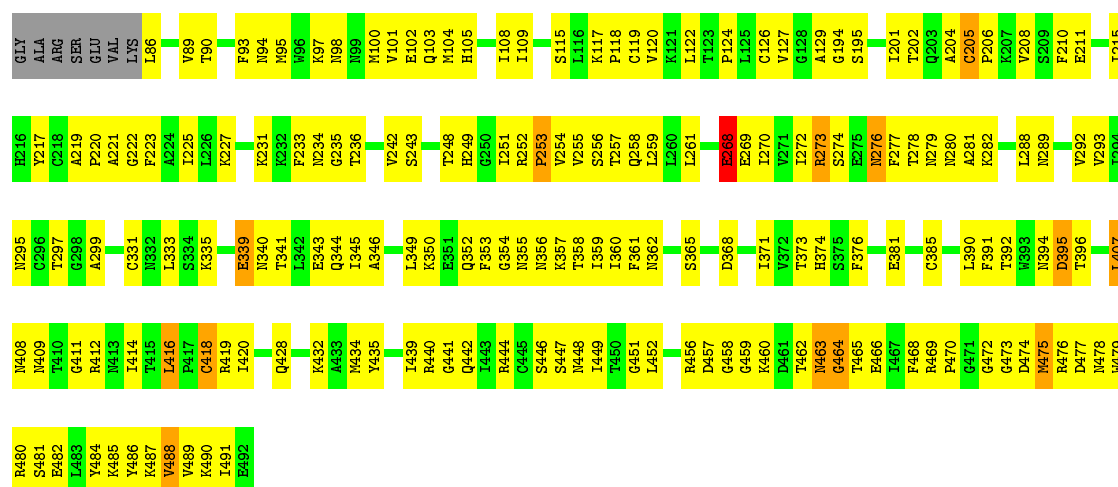


• Molecule 1: HIV-1 YU2 GP120



• Molecule 1: HIV-1 YU2 GP120





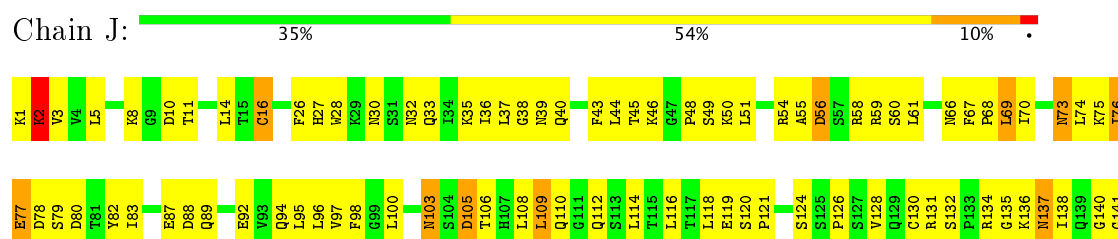
• Molecule 2: T-CELL SURFACE GLYCOPROTEIN CD4

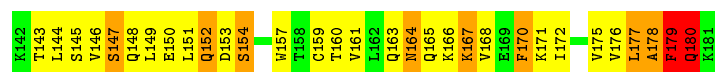


• Molecule 2: T-CELL SURFACE GLYCOPROTEIN CD4



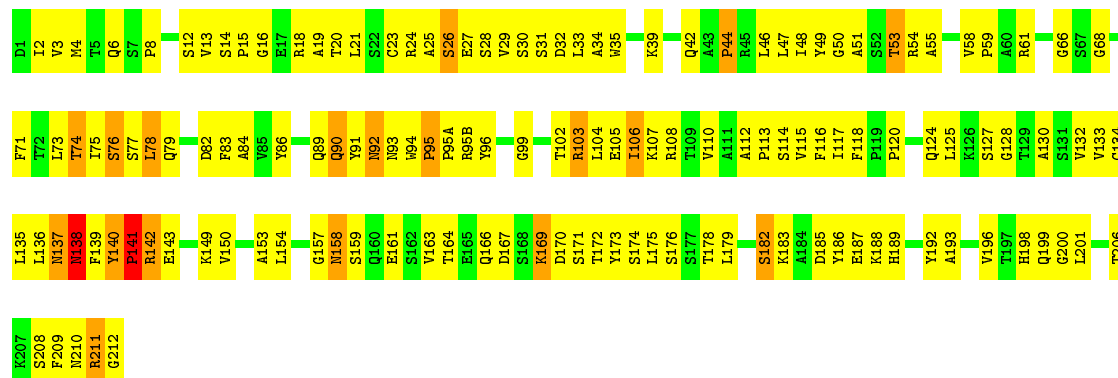
• Molecule 2: T-CELL SURFACE GLYCOPROTEIN CD4





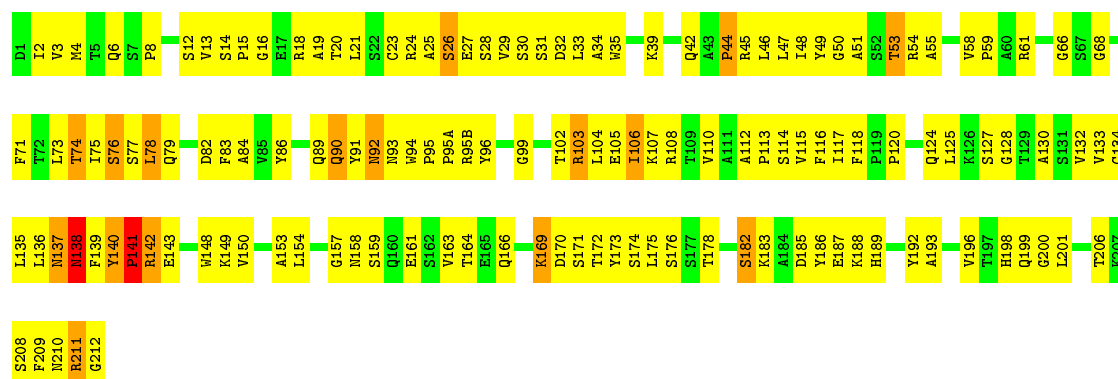
• Molecule 3: FAB OF BROADLY NEUTRALIZING ANTIBODY 17B

Chain C: 34% 57% 8%



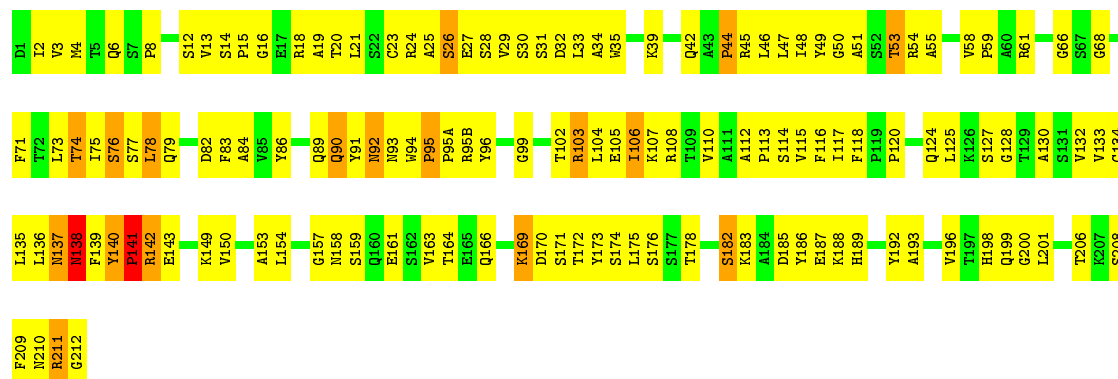
• Molecule 3: FAB OF BROADLY NEUTRALIZING ANTIBODY 17B

Chain G: 34% 58% 7%

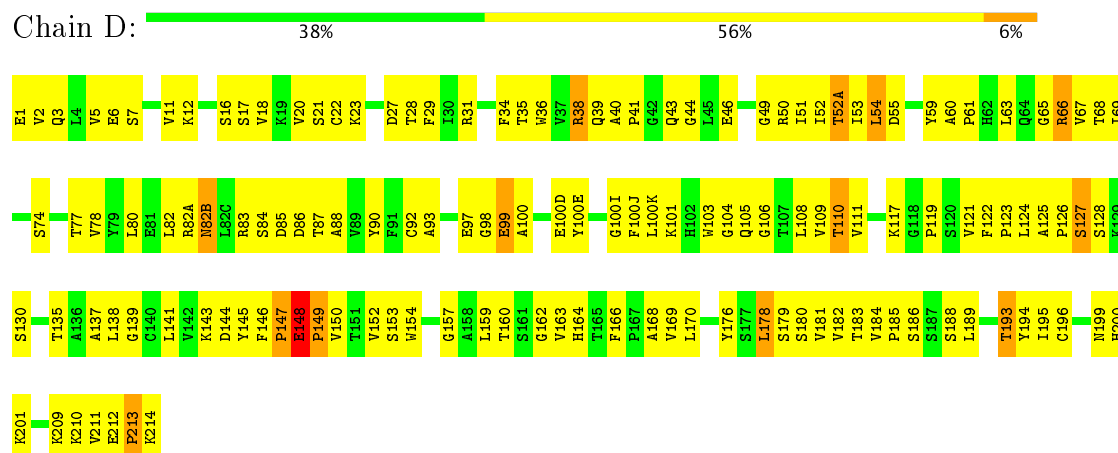


• Molecule 3: FAB OF BROADLY NEUTRALIZING ANTIBODY 17B

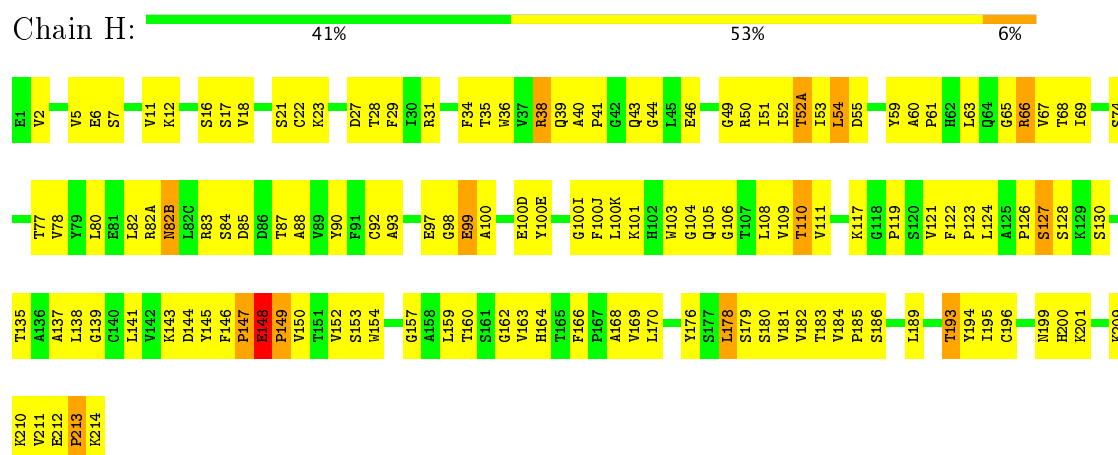
Chain K: 34% 57% 8%



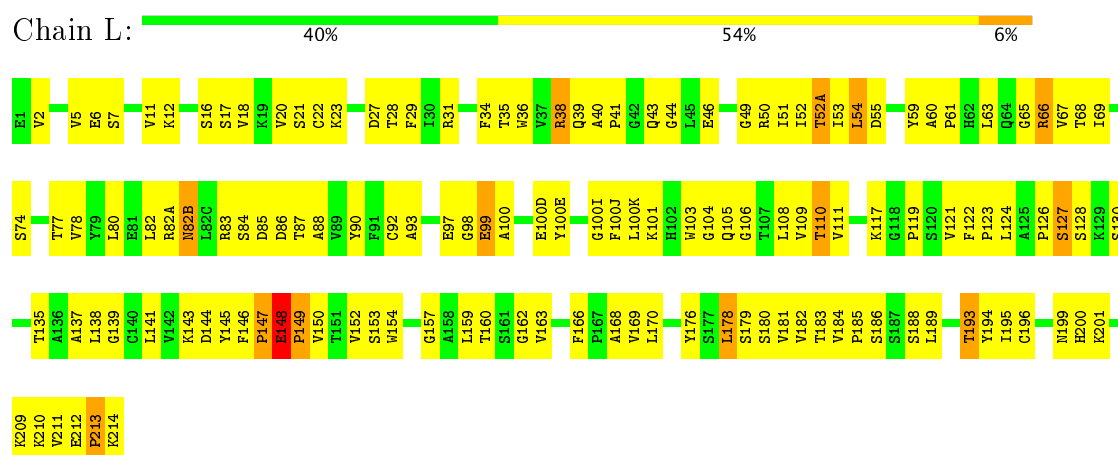
• Molecule 4: FAB OF BROADLY NEUTRALIZING ANTIBODY 17B



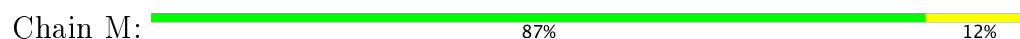
• Molecule 4: FAB OF BROADLY NEUTRALIZING ANTIBODY 17B



• Molecule 4: FAB OF BROADLY NEUTRALIZING ANTIBODY 17B

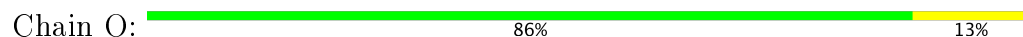


• Molecule 5: FAB OF BROADLY NEUTRALIZING ANTIBODY 8ANC195

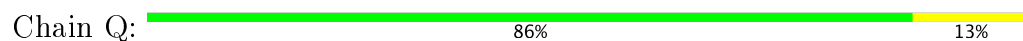




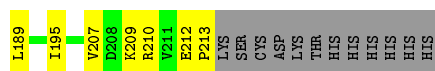
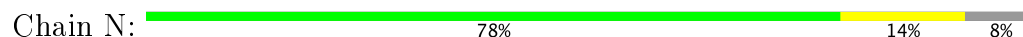
- Molecule 5: FAB OF BROADLY NEUTRALIZING ANTIBODY 8ANC195



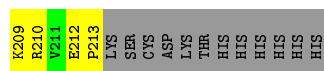
- Molecule 5: FAB OF BROADLY NEUTRALIZING ANTIBODY 8ANC195



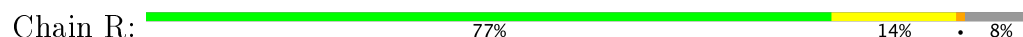
- Molecule 6: FAB OF BROADLY NEUTRALIZING ANTIBODY 8ANC195



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- Molecule 6: FAB OF BROADLY NEUTRALIZING ANTIBODY 8ANC195



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	7174	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	INDIVIDUAL PARTICLES	Depositor
Microscope	FEI TECNAI 12	Depositor
Voltage (kV)	120	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	42000	Depositor
Image detector	GATAN ULTRASCAN 1000 (2k x 2k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.46	0/2432	0.66	0/3296
1	E	0.46	0/2432	0.66	0/3296
1	I	0.46	0/2432	0.66	0/3296
2	B	0.41	0/1432	0.72	2/1930 (0.1%)
2	F	0.41	0/1432	0.72	2/1930 (0.1%)
2	J	0.41	0/1432	0.72	2/1930 (0.1%)
3	C	0.43	0/1684	0.86	3/2288 (0.1%)
3	G	0.43	0/1684	0.86	3/2288 (0.1%)
3	K	0.43	0/1684	0.87	3/2288 (0.1%)
4	D	0.42	0/1762	0.64	0/2399
4	H	0.42	0/1762	0.64	0/2399
4	L	0.42	0/1762	0.64	0/2399
5	M	0.51	0/1640	0.60	0/2232
5	O	0.51	0/1640	0.60	0/2232
5	Q	0.51	0/1640	0.60	0/2232
6	N	0.54	1/1687 (0.1%)	0.60	1/2310 (0.0%)
6	P	0.54	1/1687 (0.1%)	0.61	1/2310 (0.0%)
6	R	0.54	1/1687 (0.1%)	0.60	1/2310 (0.0%)
All	All	0.46	3/31911 (0.0%)	0.68	18/43365 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	P	213	PRO	N-CD	5.15	1.55	1.47
6	N	213	PRO	N-CD	5.15	1.55	1.47
6	R	213	PRO	N-CD	5.07	1.54	1.47

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	140	TYR	C-N-CD	-21.39	73.54	120.60
3	K	140	TYR	C-N-CD	-21.37	73.58	120.60
3	G	140	TYR	C-N-CD	-21.37	73.59	120.60
3	K	140	TYR	C-N-CA	13.74	179.70	122.00
3	G	140	TYR	C-N-CA	13.72	179.63	122.00
3	C	140	TYR	C-N-CA	13.72	179.62	122.00
2	F	179	PHE	N-CA-C	-9.53	85.27	111.00
2	J	179	PHE	N-CA-C	-9.52	85.30	111.00
2	B	179	PHE	N-CA-C	-9.52	85.31	111.00
2	B	180	GLN	N-CA-C	8.14	132.99	111.00
2	F	180	GLN	N-CA-C	8.12	132.93	111.00
2	J	180	GLN	N-CA-C	8.12	132.92	111.00
6	P	212	GLU	C-N-CD	5.54	140.02	128.40
6	R	212	GLU	C-N-CD	5.51	139.98	128.40
6	N	212	GLU	C-N-CD	5.50	139.94	128.40
3	C	141	PRO	N-CA-C	-5.45	97.93	112.10
3	K	141	PRO	N-CA-C	-5.44	97.96	112.10
3	G	141	PRO	N-CA-C	-5.44	97.96	112.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2385	0	2327	209	0
1	E	2385	0	2327	210	0
1	I	2385	0	2327	207	0
2	B	1412	0	1444	149	0
2	F	1412	0	1444	147	0
2	J	1412	0	1444	144	0
3	C	1647	0	1593	172	0
3	G	1647	0	1593	172	0
3	K	1647	0	1593	170	0
4	D	1722	0	1691	152	0
4	H	1722	0	1691	149	0
4	L	1722	0	1691	148	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	M	1605	0	1521	12	0
5	O	1605	0	1521	14	0
5	Q	1605	0	1521	14	0
6	N	1643	0	1586	21	0
6	P	1643	0	1586	19	0
6	R	1643	0	1586	21	0
7	A	196	0	182	20	0
7	E	196	0	182	19	0
7	I	196	0	182	20	0
7	N	14	0	13	0	0
7	P	14	0	13	0	0
7	R	14	0	13	0	0
All	All	31872	0	31071	2030	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 32.

All (2030) 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:B:176:VAL:C	2:B:177:LEU:HD12	1.62	1.20
2:J:176:VAL:C	2:J:177:LEU:HD12	1.62	1.19
2:F:176:VAL:C	2:F:177:LEU:HD12	1.62	1.17
2:J:108:LEU:HD21	2:J:112:GLN:HB3	1.28	1.15
2:B:108:LEU:HD21	2:B:112:GLN:HB3	1.28	1.13
6:P:93:THR:HG21	6:P:100(L):PHE:HB3	1.32	1.09
4:L:148:GLU:HG3	4:L:149:PRO:HA	1.34	1.08
4:D:148:GLU:HG3	4:D:149:PRO:HA	1.34	1.07
6:N:93:THR:HG21	6:N:100(L):PHE:HB3	1.32	1.06
2:F:108:LEU:HD21	2:F:112:GLN:HB3	1.28	1.06
6:R:93:THR:HG21	6:R:100(L):PHE:HB3	1.32	1.06
2:B:178:ALA:O	2:B:179:PHE:HD1	1.38	1.06
2:J:178:ALA:O	2:J:179:PHE:HD1	1.38	1.05
2:F:178:ALA:O	2:F:179:PHE:HD1	1.38	1.04
4:H:148:GLU:HG3	4:H:149:PRO:HA	1.34	1.04
6:P:93:THR:CG2	6:P:100(L):PHE:HB3	1.89	1.03
6:R:93:THR:CG2	6:R:100(L):PHE:HB3	1.89	1.02
6:N:93:THR:CG2	6:N:100(L):PHE:HB3	1.89	1.01
2:J:179:PHE:O	2:J:180:GLN:HB2	1.62	0.99
2:B:179:PHE:O	2:B:180:GLN:HB2	1.62	0.98
3:G:94:TRP:CZ3	3:G:95(A):PRO:HG3	1.99	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:94:TRP:CZ3	3:K:95(A):PRO:HG3	1.99	0.98
3:C:94:TRP:CZ3	3:C:95(A):PRO:HG3	1.99	0.97
4:L:127:SER:HB3	4:L:130:SER:HB2	1.48	0.95
2:F:179:PHE:O	2:F:180:GLN:HB2	1.62	0.95
2:F:150:GLU:HB3	2:F:152:GLN:HE22	1.33	0.94
2:J:130:CYS:HA	2:J:159:CYS:HA	1.50	0.94
4:H:127:SER:HB3	4:H:130:SER:HB2	1.49	0.93
4:D:127:SER:HB3	4:D:130:SER:HB2	1.49	0.93
3:K:46:LEU:HD12	4:L:101:LYS:HA	1.50	0.93
2:J:150:GLU:HB3	2:J:152:GLN:HE22	1.33	0.93
2:F:140:GLY:HA3	2:F:144:LEU:HG	1.51	0.93
2:B:150:GLU:HB3	2:B:152:GLN:HE22	1.33	0.92
2:J:140:GLY:HA3	2:J:144:LEU:HG	1.51	0.92
2:F:130:CYS:HA	2:F:159:CYS:HA	1.50	0.92
2:B:130:CYS:HA	2:B:159:CYS:HA	1.50	0.92
2:B:140:GLY:HA3	2:B:144:LEU:HG	1.51	0.91
3:G:46:LEU:HD12	4:H:101:LYS:HA	1.50	0.91
3:C:46:LEU:HD12	4:D:101:LYS:HA	1.50	0.91
2:F:108:LEU:O	2:F:177:LEU:HD13	1.76	0.85
2:J:108:LEU:O	2:J:177:LEU:HD13	1.76	0.85
2:B:128:VAL:HB	2:B:144:LEU:HD11	1.59	0.85
2:J:128:VAL:HB	2:J:144:LEU:HD11	1.59	0.85
4:L:148:GLU:HG3	4:L:149:PRO:CA	2.07	0.85
4:H:148:GLU:HG3	4:H:149:PRO:CA	2.07	0.84
3:K:193:ALA:HA	3:K:208:SER:HB3	1.58	0.84
2:B:150:GLU:HB3	2:B:152:GLN:NE2	1.92	0.84
3:G:193:ALA:HA	3:G:208:SER:HB3	1.58	0.84
2:F:150:GLU:HB3	2:F:152:GLN:NE2	1.92	0.84
2:B:108:LEU:O	2:B:177:LEU:HD13	1.76	0.84
4:D:148:GLU:HG3	4:D:149:PRO:CA	2.07	0.84
2:J:150:GLU:HB3	2:J:152:GLN:NE2	1.92	0.84
3:K:46:LEU:HD22	3:K:55:ALA:HB2	1.60	0.83
4:D:195:ILE:HG12	4:D:210:LYS:HA	1.60	0.83
3:C:193:ALA:HA	3:C:208:SER:HB3	1.58	0.83
4:L:147:PRO:O	4:L:148:GLU:HB2	1.79	0.83
3:C:46:LEU:HD22	3:C:55:ALA:HB2	1.60	0.83
3:K:78:LEU:HD11	3:K:104:LEU:HD21	1.61	0.82
4:H:147:PRO:O	4:H:148:GLU:HB2	1.79	0.82
2:B:178:ALA:O	2:B:179:PHE:CD1	2.30	0.82
4:L:195:ILE:HG12	4:L:210:LYS:HA	1.60	0.82
3:C:29:VAL:HG13	3:C:92:ASN:HB3	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:29:VAL:HG13	3:G:92:ASN:HB3	1.62	0.82
4:H:195:ILE:HG12	4:H:210:LYS:HA	1.60	0.81
3:C:78:LEU:HD11	3:C:104:LEU:HD21	1.62	0.81
7:E:963:NAG:H3	7:E:963:NAG:H82	1.62	0.81
2:F:128:VAL:HB	2:F:144:LEU:HD11	1.59	0.81
3:G:46:LEU:HD22	3:G:55:ALA:HB2	1.60	0.81
7:I:963:NAG:H3	7:I:963:NAG:H82	1.62	0.81
3:C:140:TYR:CG	3:C:141:PRO:HD3	2.16	0.81
3:G:78:LEU:HD11	3:G:104:LEU:HD21	1.61	0.81
2:F:131:ARG:CZ	2:F:137:ASN:HB3	2.12	0.80
2:B:131:ARG:CZ	2:B:137:ASN:HB3	2.12	0.80
3:C:49:TYR:O	3:C:53:THR:HG23	1.82	0.80
2:J:131:ARG:CZ	2:J:137:ASN:HB3	2.12	0.80
3:G:140:TYR:CG	3:G:141:PRO:HD3	2.16	0.80
2:J:178:ALA:O	2:J:179:PHE:CD1	2.30	0.80
3:K:29:VAL:HG13	3:K:92:ASN:HB3	1.62	0.80
7:A:963:NAG:H3	7:A:963:NAG:H82	1.62	0.80
2:F:178:ALA:O	2:F:179:PHE:CD1	2.30	0.80
3:G:49:TYR:O	3:G:53:THR:HG23	1.82	0.79
3:K:140:TYR:CG	3:K:141:PRO:HD3	2.16	0.79
4:H:39:GLN:HE21	4:H:44:GLY:HA2	1.47	0.79
1:A:280:ASN:O	2:B:35:LYS:HD2	1.82	0.79
1:E:280:ASN:O	2:F:35:LYS:HD2	1.82	0.79
3:K:49:TYR:O	3:K:53:THR:HG23	1.82	0.79
4:D:147:PRO:O	4:D:148:GLU:HB2	1.79	0.79
4:D:39:GLN:HE21	4:D:44:GLY:HA2	1.48	0.79
1:I:412:ARG:HA	7:I:908:NAG:O6	1.83	0.78
1:A:412:ARG:HA	7:A:908:NAG:O6	1.83	0.78
1:E:412:ARG:HA	7:E:908:NAG:O6	1.83	0.78
6:P:52:TRP:HE1	6:P:97:THR:HG21	1.49	0.78
4:D:163:VAL:HG12	4:D:182:VAL:HB	1.66	0.78
1:E:273:ARG:HH11	1:E:273:ARG:HG2	1.49	0.78
1:I:280:ASN:O	2:J:35:LYS:HD2	1.82	0.78
6:N:126:PRO:HG3	6:N:138:LEU:HB3	1.66	0.78
4:L:163:VAL:HG12	4:L:182:VAL:HB	1.66	0.78
6:P:126:PRO:HG3	6:P:138:LEU:HB3	1.66	0.78
4:H:163:VAL:HG12	4:H:182:VAL:HB	1.66	0.77
6:N:52:TRP:HE1	6:N:97:THR:HG21	1.49	0.77
4:L:39:GLN:HE21	4:L:44:GLY:HA2	1.47	0.77
1:E:95:MET:HE1	1:E:273:ARG:HH11	1.50	0.77
1:A:273:ARG:HG2	1:A:273:ARG:HH11	1.49	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:141:PRO:HB3	3:C:143:GLU:OE2	1.85	0.76
6:R:126:PRO:HG3	6:R:138:LEU:HB3	1.66	0.76
1:A:392:THR:HG22	7:A:894:NAG:HN2	1.50	0.76
1:E:269:GLU:HA	1:E:289:ASN:ND2	2.01	0.76
6:R:52:TRP:HE1	6:R:97:THR:HG21	1.49	0.76
3:G:141:PRO:HB3	3:G:143:GLU:OE2	1.85	0.76
1:A:269:GLU:HA	1:A:289:ASN:ND2	2.01	0.76
3:K:198:HIS:CD2	3:K:199:GLN:H	2.05	0.75
1:I:95:MET:HE1	1:I:273:ARG:HH11	1.51	0.75
1:I:269:GLU:HA	1:I:289:ASN:ND2	2.01	0.75
1:E:392:THR:HG22	7:E:894:NAG:HN2	1.50	0.75
3:C:198:HIS:CD2	3:C:199:GLN:H	2.04	0.75
3:K:141:PRO:HB3	3:K:143:GLU:OE2	1.85	0.75
6:N:93:THR:HG21	6:N:100(L):PHE:CB	2.14	0.75
6:P:93:THR:HG21	6:P:100(L):PHE:CB	2.14	0.75
1:I:463:ASN:O	1:I:465:THR:HG22	1.87	0.75
1:A:95:MET:HE1	1:A:273:ARG:HH11	1.51	0.74
1:A:460:LYS:HB2	2:B:32:ASN:O	1.87	0.74
1:E:95:MET:CE	1:E:484:TYR:HB2	2.18	0.74
1:I:460:LYS:HB2	2:J:32:ASN:O	1.87	0.74
2:F:61:LEU:HB3	2:F:66:ASN:HB3	1.69	0.74
3:K:113:PRO:HD3	3:K:198:HIS:ND1	2.02	0.74
1:I:273:ARG:HG2	1:I:273:ARG:HH11	1.49	0.74
1:I:95:MET:CE	1:I:484:TYR:HB2	2.18	0.74
1:A:95:MET:CE	1:A:484:TYR:HB2	2.18	0.74
3:G:198:HIS:CD2	3:G:199:GLN:H	2.04	0.73
3:G:113:PRO:HD3	3:G:198:HIS:ND1	2.02	0.73
1:A:463:ASN:O	1:A:465:THR:HG22	1.87	0.73
2:B:178:ALA:HB1	2:B:180:GLN:H	1.53	0.73
2:J:76:ILE:H	2:J:76:ILE:HD12	1.54	0.73
1:E:463:ASN:O	1:E:465:THR:HG22	1.87	0.73
1:I:392:THR:HG22	7:I:894:NAG:HN2	1.50	0.73
1:E:460:LYS:HB2	2:F:32:ASN:O	1.87	0.73
3:K:198:HIS:H	3:K:201:LEU:HD12	1.54	0.73
2:B:76:ILE:HD12	2:B:76:ILE:H	1.54	0.73
3:C:113:PRO:HD3	3:C:198:HIS:ND1	2.02	0.73
4:H:135:THR:HA	4:H:185:PRO:HA	1.71	0.73
6:R:93:THR:HG21	6:R:100(L):PHE:CB	2.14	0.73
2:B:77:GLU:CD	2:B:77:GLU:H	1.91	0.73
3:C:198:HIS:H	3:C:201:LEU:HD12	1.54	0.72
2:J:178:ALA:HB1	2:J:180:GLN:H	1.53	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:76:ILE:H	2:F:76:ILE:HD12	1.54	0.72
2:J:61:LEU:HB3	2:J:66:ASN:HB3	1.69	0.72
3:G:198:HIS:H	3:G:201:LEU:HD12	1.54	0.72
2:B:154:SER:HB2	2:B:176:VAL:H	1.55	0.72
3:K:175:LEU:HD12	3:K:176:SER:H	1.54	0.72
3:C:175:LEU:HD12	3:C:176:SER:H	1.54	0.72
3:G:175:LEU:HD12	3:G:176:SER:H	1.54	0.72
3:G:32:ASP:HB2	3:G:92:ASN:HB2	1.72	0.72
2:J:77:GLU:CD	2:J:77:GLU:H	1.91	0.72
2:F:176:VAL:C	2:F:177:LEU:CD1	2.53	0.72
2:F:77:GLU:H	2:F:77:GLU:CD	1.91	0.72
2:B:61:LEU:HB3	2:B:66:ASN:HB3	1.69	0.71
4:D:135:THR:HA	4:D:185:PRO:HA	1.71	0.71
2:J:154:SER:HB2	2:J:176:VAL:H	1.55	0.71
2:F:178:ALA:HB1	2:F:180:GLN:H	1.53	0.71
4:L:135:THR:HA	4:L:185:PRO:HA	1.71	0.71
2:F:161:VAL:O	2:F:167:LYS:HA	1.90	0.71
3:G:93:ASN:ND2	3:G:95(B):ARG:HB2	2.05	0.71
3:G:94:TRP:HA	3:G:95:PRO:C	2.11	0.71
4:L:182:VAL:HG22	4:L:184:VAL:HG13	1.72	0.71
4:H:182:VAL:HG22	4:H:184:VAL:HG13	1.72	0.71
2:F:154:SER:HB2	2:F:176:VAL:H	1.55	0.71
3:G:154:LEU:O	3:G:154:LEU:HD13	1.91	0.71
3:K:154:LEU:O	3:K:154:LEU:HD13	1.91	0.71
2:B:36:ILE:HG22	2:B:37:LEU:HD22	1.72	0.71
3:G:46:LEU:HD12	4:H:101:LYS:CA	2.21	0.71
4:H:146:PHE:CD1	4:H:147:PRO:HA	2.26	0.71
2:J:36:ILE:HG22	2:J:37:LEU:HD22	1.72	0.71
3:C:93:ASN:ND2	3:C:95(B):ARG:HB2	2.05	0.71
3:C:94:TRP:HA	3:C:95:PRO:C	2.11	0.71
4:H:126:PRO:HG3	4:H:138:LEU:HD13	1.73	0.71
2:B:177:LEU:N	2:B:177:LEU:HD12	2.06	0.70
4:D:146:PHE:CD1	4:D:147:PRO:HA	2.26	0.70
4:L:126:PRO:HG3	4:L:138:LEU:HD13	1.73	0.70
3:K:93:ASN:ND2	3:K:95(B):ARG:HB2	2.05	0.70
4:L:99:GLU:N	4:L:100(D):GLU:OE1	2.25	0.70
2:F:177:LEU:N	2:F:177:LEU:HD12	2.06	0.70
4:L:146:PHE:CD1	4:L:147:PRO:HA	2.26	0.70
3:C:20:THR:HG23	3:C:74:THR:HG23	1.74	0.70
4:D:126:PRO:HG3	4:D:138:LEU:HD13	1.73	0.70
3:K:94:TRP:HA	3:K:95:PRO:C	2.11	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:11:VAL:HG21	4:H:147:PRO:HG3	1.74	0.70
2:J:161:VAL:O	2:J:167:LYS:HA	1.90	0.70
3:C:154:LEU:O	3:C:154:LEU:HD13	1.91	0.70
2:F:36:ILE:HG22	2:F:37:LEU:HD22	1.72	0.70
4:H:82(B):ASN:N	4:H:82(B):ASN:HD22	1.90	0.70
4:D:82(B):ASN:HD22	4:D:82(B):ASN:N	1.90	0.70
1:E:440:ARG:HD2	1:E:442:GLN:O	1.92	0.70
2:J:176:VAL:C	2:J:177:LEU:CD1	2.53	0.70
1:I:440:ARG:HD2	1:I:442:GLN:O	1.92	0.70
2:J:3:VAL:HG22	2:J:94:GLN:HB3	1.74	0.70
2:B:161:VAL:O	2:B:167:LYS:HA	1.90	0.70
4:D:11:VAL:HG21	4:D:147:PRO:HG3	1.74	0.70
1:E:95:MET:HE2	1:E:484:TYR:HB2	1.73	0.70
3:K:32:ASP:HB2	3:K:92:ASN:HB2	1.72	0.70
4:D:99:GLU:N	4:D:100(D):GLU:OE1	2.24	0.69
2:J:177:LEU:HD12	2:J:177:LEU:N	2.06	0.69
4:D:182:VAL:HG22	4:D:184:VAL:HG13	1.72	0.69
3:C:182:SER:OG	3:C:185:ASP:HB3	1.93	0.69
3:C:32:ASP:HB2	3:C:92:ASN:HB2	1.72	0.69
3:C:46:LEU:HD12	4:D:101:LYS:CA	2.21	0.69
4:H:99:GLU:N	4:H:100(D):GLU:OE1	2.25	0.69
3:K:20:THR:HG23	3:K:74:THR:HG23	1.74	0.69
3:C:149:LYS:HE2	3:C:154:LEU:HD23	1.74	0.69
2:F:3:VAL:HG22	2:F:94:GLN:HB3	1.74	0.69
2:B:3:VAL:HG22	2:B:94:GLN:HB3	1.74	0.69
3:G:182:SER:OG	3:G:185:ASP:HB3	1.93	0.69
2:J:128:VAL:HA	2:J:160:THR:O	1.93	0.69
4:L:11:VAL:HG21	4:L:147:PRO:HG3	1.74	0.69
3:K:46:LEU:HD12	4:L:101:LYS:CA	2.21	0.69
6:P:68:LEU:HD12	6:P:81:GLU:OE1	1.93	0.69
6:R:68:LEU:HD12	6:R:81:GLU:OE1	1.93	0.69
6:R:81:GLU:OE2	6:R:82(A):LYS:HE2	1.93	0.69
2:B:134:ARG:HE	2:B:152:GLN:HB2	1.58	0.69
2:F:134:ARG:HE	2:F:152:GLN:HB2	1.58	0.69
3:G:149:LYS:HE2	3:G:154:LEU:HD23	1.74	0.69
1:A:440:ARG:HD2	1:A:442:GLN:O	1.92	0.69
5:M:10:THR:HG22	5:M:103:LYS:HB3	1.75	0.69
4:H:124:LEU:HD11	4:H:141:LEU:HB2	1.75	0.68
5:Q:155:GLN:HE21	5:Q:158:ASN:HD21	1.40	0.68
5:M:155:GLN:HE21	5:M:158:ASN:HD21	1.40	0.68
4:L:82(B):ASN:HD22	4:L:82(B):ASN:N	1.90	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:P:81:GLU:OE2	6:P:82(A):LYS:HE2	1.93	0.68
2:B:128:VAL:HA	2:B:160:THR:O	1.93	0.68
2:F:154:SER:HB2	2:F:176:VAL:HG23	1.75	0.68
1:I:288:LEU:HD12	1:I:449:ILE:O	1.93	0.68
1:A:288:LEU:HD12	1:A:449:ILE:O	1.93	0.68
2:J:140:GLY:CA	2:J:144:LEU:HG	2.24	0.68
5:O:10:THR:HG22	5:O:103:LYS:HB3	1.75	0.68
3:K:149:LYS:HE2	3:K:154:LEU:HD23	1.74	0.68
6:N:68:LEU:HD12	6:N:81:GLU:OE1	1.93	0.68
1:E:439:ILE:HD12	1:E:440:ARG:N	2.09	0.68
3:G:20:THR:HG23	3:G:74:THR:HG23	1.74	0.68
6:N:81:GLU:OE2	6:N:82(A):LYS:HE2	1.93	0.68
5:O:155:GLN:HE21	5:O:158:ASN:HD21	1.40	0.68
2:B:154:SER:HB2	2:B:176:VAL:HG23	1.75	0.68
3:K:133:VAL:HG21	4:L:141:LEU:HD13	1.76	0.68
5:Q:10:THR:HG22	5:Q:103:LYS:HB3	1.75	0.68
3:C:133:VAL:HG21	4:D:141:LEU:HD13	1.76	0.67
2:J:103:ASN:N	2:J:103:ASN:HD22	1.90	0.67
2:J:134:ARG:HE	2:J:152:GLN:HB2	1.58	0.67
2:F:128:VAL:HA	2:F:160:THR:O	1.93	0.67
1:A:202:THR:HG22	3:C:95:PRO:HG3	1.76	0.67
4:D:119:PRO:HB3	4:D:145:TYR:HB3	1.77	0.67
1:E:288:LEU:HD12	1:E:449:ILE:O	1.93	0.67
3:K:182:SER:OG	3:K:185:ASP:HB3	1.93	0.67
2:B:103:ASN:N	2:B:103:ASN:HD22	1.90	0.67
3:C:12:SER:HB2	3:C:107:LYS:HB2	1.77	0.67
1:I:202:THR:HG22	3:K:95:PRO:HG3	1.76	0.67
4:D:159:LEU:HD21	4:D:184:VAL:HG11	1.77	0.67
4:D:7:SER:HB3	4:D:21:SER:OG	1.95	0.67
4:H:159:LEU:HD21	4:H:184:VAL:HG11	1.77	0.67
4:H:7:SER:HB3	4:H:21:SER:OG	1.95	0.67
1:I:95:MET:HE2	1:I:235:GLY:HA3	1.76	0.67
1:A:439:ILE:HD12	1:A:440:ARG:N	2.09	0.67
2:F:176:VAL:O	2:F:177:LEU:HD12	1.95	0.67
2:B:140:GLY:CA	2:B:144:LEU:HG	2.24	0.67
3:K:140:TYR:CD2	3:K:141:PRO:HD3	2.29	0.67
4:L:7:SER:HB3	4:L:21:SER:OG	1.95	0.67
1:A:127:VAL:HG23	1:A:129:ALA:H	1.60	0.67
4:L:159:LEU:HD21	4:L:184:VAL:HG11	1.77	0.67
1:I:439:ILE:HD12	1:I:440:ARG:N	2.09	0.67
3:K:39:LYS:HB2	3:K:42:GLN:OE1	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:124:LEU:HD11	4:L:141:LEU:HB2	1.75	0.67
3:C:140:TYR:CD2	3:C:141:PRO:HD3	2.29	0.66
3:C:39:LYS:HB2	3:C:42:GLN:OE1	1.95	0.66
1:E:202:THR:HG22	3:G:95:PRO:HG3	1.76	0.66
2:F:140:GLY:CA	2:F:144:LEU:HG	2.24	0.66
3:G:133:VAL:HG21	4:H:141:LEU:HD13	1.76	0.66
4:H:119:PRO:HB3	4:H:145:TYR:HB3	1.77	0.66
3:G:39:LYS:HB2	3:G:42:GLN:OE1	1.95	0.66
4:L:119:PRO:HB3	4:L:145:TYR:HB3	1.77	0.66
2:B:98:PHE:HB3	2:B:118:LEU:HD11	1.77	0.66
4:D:124:LEU:HD11	4:D:141:LEU:HB2	1.75	0.66
2:F:103:ASN:N	2:F:103:ASN:HD22	1.91	0.66
2:J:154:SER:HB2	2:J:176:VAL:HG23	1.75	0.66
2:J:50:LYS:HG2	2:J:50:LYS:O	1.95	0.66
4:D:100:ALA:HA	4:D:100(D):GLU:O	1.96	0.66
3:G:12:SER:HB2	3:G:107:LYS:HB2	1.77	0.66
3:G:140:TYR:CD2	3:G:141:PRO:HD3	2.29	0.66
3:K:12:SER:HB2	3:K:107:LYS:HB2	1.77	0.66
1:A:475:MET:O	1:A:478:ASN:HB2	1.95	0.66
3:C:159:SER:HA	3:C:178:THR:O	1.96	0.66
2:F:50:LYS:O	2:F:50:LYS:HG2	1.95	0.66
1:I:475:MET:O	1:I:478:ASN:HB2	1.95	0.66
4:L:36:TRP:CE2	4:L:80:LEU:HB2	2.31	0.66
2:B:50:LYS:HG2	2:B:50:LYS:O	1.95	0.66
3:C:91:TYR:HA	3:C:96:TYR:CD1	2.31	0.66
1:E:475:MET:O	1:E:478:ASN:HB2	1.95	0.66
4:H:100:ALA:HA	4:H:100(D):GLU:O	1.96	0.66
1:I:127:VAL:HG23	1:I:129:ALA:H	1.60	0.66
2:J:154:SER:CB	2:J:176:VAL:H	2.09	0.66
1:I:419:ARG:NH2	4:L:99:GLU:OE1	2.29	0.66
2:B:154:SER:CB	2:B:176:VAL:H	2.09	0.66
5:Q:151:ASP:OD2	5:Q:189:HIS:ND1	2.26	0.66
2:F:75:LYS:HB3	2:F:77:GLU:OE2	1.96	0.65
3:K:159:SER:HA	3:K:178:THR:O	1.96	0.65
5:O:151:ASP:OD2	5:O:189:HIS:ND1	2.26	0.65
1:A:95:MET:HE2	1:A:235:GLY:HA3	1.77	0.65
2:B:176:VAL:C	2:B:177:LEU:CD1	2.53	0.65
4:D:12:LYS:O	4:D:111:VAL:HA	1.96	0.65
1:A:419:ARG:NH2	4:D:99:GLU:OE1	2.29	0.65
1:A:459:GLY:O	1:A:462:THR:HG23	1.96	0.65
1:A:487:LYS:HG3	1:A:487:LYS:O	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:98:PHE:HB3	2:F:118:LEU:HD11	1.77	0.65
3:K:91:TYR:HA	3:K:96:TYR:CD1	2.31	0.65
1:A:95:MET:HE2	1:A:484:TYR:HB2	1.79	0.65
4:L:100:ALA:HA	4:L:100(D):GLU:O	1.96	0.65
2:B:176:VAL:O	2:B:177:LEU:HD12	1.95	0.65
1:E:419:ARG:NH2	4:H:99:GLU:OE1	2.29	0.65
2:J:75:LYS:HB3	2:J:77:GLU:OE2	1.96	0.65
1:E:127:VAL:HG23	1:E:129:ALA:H	1.60	0.65
3:G:91:TYR:HA	3:G:96:TYR:CD1	2.31	0.65
1:A:339:GLU:O	1:A:343:GLU:HG3	1.97	0.65
2:B:75:LYS:HB3	2:B:77:GLU:OE2	1.96	0.65
4:D:36:TRP:CE2	4:D:80:LEU:HB2	2.31	0.65
2:F:154:SER:CB	2:F:176:VAL:H	2.09	0.65
4:H:12:LYS:O	4:H:111:VAL:HA	1.96	0.65
1:I:339:GLU:O	1:I:343:GLU:HG3	1.97	0.65
1:I:487:LYS:HG3	1:I:487:LYS:O	1.97	0.65
2:J:98:PHE:HB3	2:J:118:LEU:HD11	1.77	0.65
3:G:159:SER:HA	3:G:178:THR:O	1.96	0.65
4:H:36:TRP:CE2	4:H:80:LEU:HB2	2.31	0.65
1:I:459:GLY:O	1:I:462:THR:HG23	1.97	0.65
1:A:205:CYS:N	1:A:206:PRO:HD3	2.12	0.64
4:H:150:VAL:HG23	4:H:199:ASN:O	1.97	0.64
4:L:12:LYS:O	4:L:111:VAL:HA	1.96	0.64
1:E:487:LYS:HG3	1:E:487:LYS:O	1.97	0.64
3:G:18:ARG:HA	3:G:76:SER:O	1.97	0.64
1:I:205:CYS:N	1:I:206:PRO:HD3	2.12	0.64
3:K:18:ARG:HA	3:K:76:SER:O	1.97	0.64
1:E:339:GLU:O	1:E:343:GLU:HG3	1.97	0.64
3:G:193:ALA:CA	3:G:208:SER:HB3	2.27	0.64
2:J:176:VAL:O	2:J:177:LEU:HD12	1.94	0.64
1:A:119:CYS:HB2	1:A:434:MET:HE2	1.80	0.64
1:E:205:CYS:N	1:E:206:PRO:HD3	2.13	0.64
1:E:459:GLY:O	1:E:462:THR:HG23	1.96	0.64
4:H:138:LEU:HD12	4:H:211:VAL:CG1	2.28	0.64
4:L:138:LEU:HD12	4:L:211:VAL:HG11	1.80	0.64
4:L:138:LEU:HD12	4:L:211:VAL:CG1	2.28	0.64
1:I:119:CYS:HB2	1:I:434:MET:HE2	1.80	0.64
4:L:154:TRP:HB2	4:L:159:LEU:O	1.98	0.64
1:A:280:ASN:HD22	1:A:458:GLY:N	1.95	0.64
4:H:138:LEU:HD12	4:H:211:VAL:HG11	1.80	0.64
1:A:279:ASN:HD22	1:A:282:LYS:HG2	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:138:LEU:HD12	4:D:211:VAL:CG1	2.28	0.64
4:H:154:TRP:HB2	4:H:159:LEU:O	1.98	0.64
1:I:456:ARG:HB3	1:I:468:PHE:CE2	2.33	0.64
3:C:86:TYR:HE2	3:C:104:LEU:HD22	1.63	0.64
6:P:100:LYS:HB2	6:P:100(A):TRP:CE3	2.33	0.63
1:E:280:ASN:HD22	1:E:458:GLY:N	1.95	0.63
4:L:40:ALA:HB3	4:L:43:GLN:HG3	1.81	0.63
1:A:335:LYS:HD3	1:A:407:LEU:O	1.98	0.63
1:A:456:ARG:HB3	1:A:468:PHE:CE2	2.33	0.63
1:E:456:ARG:HB3	1:E:468:PHE:CE2	2.33	0.63
1:I:280:ASN:HD22	1:I:458:GLY:N	1.95	0.63
6:R:100:LYS:HB2	6:R:100(A):TRP:CE3	2.33	0.63
4:D:150:VAL:HG23	4:D:199:ASN:O	1.97	0.63
4:D:138:LEU:HD12	4:D:211:VAL:HG11	1.80	0.63
1:E:391:PHE:CD2	1:E:470:PRO:HG3	2.34	0.63
2:F:163:GLN:HG3	2:F:164:ASN:OD1	1.99	0.63
3:G:185:ASP:OD1	3:G:185:ASP:O	2.16	0.63
1:I:272:ILE:O	1:I:272:ILE:HG13	1.99	0.63
1:I:95:MET:HE2	1:I:484:TYR:HB2	1.80	0.63
3:K:86:TYR:HE2	3:K:104:LEU:HD22	1.63	0.63
1:E:335:LYS:HD3	1:E:407:LEU:O	1.98	0.63
1:E:353:PHE:CE1	1:E:456:ARG:HD3	2.34	0.63
1:A:272:ILE:O	1:A:272:ILE:HG13	1.99	0.62
2:B:114:LEU:O	2:B:145:SER:HA	1.99	0.62
2:F:114:LEU:O	2:F:145:SER:HA	1.99	0.62
2:B:163:GLN:HG3	2:B:164:ASN:OD1	1.99	0.62
1:E:279:ASN:HD22	1:E:282:LYS:HG2	1.63	0.62
2:F:131:ARG:NH1	2:F:137:ASN:HB3	2.14	0.62
1:I:391:PHE:CD2	1:I:470:PRO:HG3	2.34	0.62
1:A:215:ILE:HG12	1:A:251:ILE:O	1.99	0.62
3:G:46:LEU:CD1	4:H:101:LYS:HA	2.27	0.62
3:K:185:ASP:O	3:K:185:ASP:OD1	2.17	0.62
3:K:46:LEU:CD1	4:L:101:LYS:HA	2.28	0.62
2:B:131:ARG:NH1	2:B:137:ASN:HB3	2.14	0.62
3:C:18:ARG:HA	3:C:76:SER:O	1.98	0.62
1:E:215:ILE:HG12	1:E:251:ILE:O	1.99	0.62
1:I:335:LYS:HD3	1:I:407:LEU:O	1.98	0.62
3:K:187:GLU:HA	3:K:211:ARG:NH1	2.15	0.62
4:L:150:VAL:HG23	4:L:199:ASN:O	1.97	0.62
6:N:100:LYS:HB2	6:N:100(A):TRP:CE3	2.33	0.62
1:E:119:CYS:HB2	1:E:434:MET:HE2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:95:MET:HE2	1:E:235:GLY:HA3	1.82	0.62
1:I:215:ILE:HG12	1:I:251:ILE:O	1.99	0.62
1:I:353:PHE:CE1	1:I:456:ARG:HD3	2.34	0.62
2:J:163:GLN:HG3	2:J:164:ASN:OD1	1.99	0.62
3:C:185:ASP:O	3:C:185:ASP:OD1	2.16	0.62
3:C:93:ASN:HD21	3:C:95(B):ARG:HB2	1.65	0.62
4:D:98:GLY:O	4:D:100:ALA:N	2.32	0.62
1:A:391:PHE:CD2	1:A:470:PRO:HG3	2.34	0.62
4:D:154:TRP:HB2	4:D:159:LEU:O	1.98	0.62
1:A:353:PHE:CE1	1:A:456:ARG:HD3	2.34	0.62
1:I:279:ASN:HD22	1:I:282:LYS:HG2	1.63	0.62
5:M:151:ASP:OD2	5:M:189:HIS:ND1	2.26	0.62
3:G:86:TYR:HE2	3:G:104:LEU:HD22	1.63	0.62
4:H:108:LEU:HD12	4:H:109:VAL:H	1.65	0.62
1:I:100:MET:HE1	1:I:487:LYS:N	2.15	0.62
2:J:170:PHE:O	2:J:172:ILE:HG12	2.00	0.62
2:B:170:PHE:O	2:B:172:ILE:HG12	2.00	0.61
4:H:98:GLY:O	4:H:100:ALA:N	2.32	0.61
3:G:187:GLU:HA	3:G:211:ARG:NH1	2.15	0.61
4:H:40:ALA:HB3	4:H:43:GLN:HG3	1.80	0.61
2:J:114:LEU:O	2:J:145:SER:HA	1.99	0.61
2:J:177:LEU:CD1	2:J:177:LEU:N	2.64	0.61
1:E:272:ILE:O	1:E:272:ILE:HG13	1.99	0.61
1:A:365:SER:HB2	2:B:46:LYS:O	2.00	0.61
2:B:58:ARG:HG2	2:B:61:LEU:HG	1.82	0.61
4:D:40:ALA:HB3	4:D:43:GLN:HG3	1.81	0.61
4:D:50:ARG:NH2	4:D:97:GLU:OE2	2.33	0.61
1:E:279:ASN:HB3	1:E:282:LYS:HG2	1.82	0.61
1:E:280:ASN:HD22	1:E:458:GLY:CA	2.14	0.61
4:L:50:ARG:NH2	4:L:97:GLU:OE2	2.33	0.61
4:D:126:PRO:HG3	4:D:138:LEU:CD1	2.30	0.61
1:I:115:SER:O	1:I:208:VAL:HG11	2.00	0.61
4:L:126:PRO:HG3	4:L:138:LEU:CD1	2.31	0.61
3:C:193:ALA:CA	3:C:208:SER:HB3	2.27	0.61
2:F:177:LEU:N	2:F:177:LEU:CD1	2.64	0.61
3:K:2:ILE:HG12	3:K:27:GLU:OE1	2.01	0.61
2:B:26:PHE:CE1	2:B:39:ASN:HB3	2.36	0.61
3:C:187:GLU:HA	3:C:211:ARG:NH1	2.15	0.61
4:D:108:LEU:HD12	4:D:109:VAL:H	1.65	0.61
1:E:115:SER:O	1:E:208:VAL:HG11	2.00	0.61
3:G:93:ASN:HD21	3:G:95(B):ARG:HB2	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:131:ARG:NH1	2:J:137:ASN:HB3	2.14	0.61
3:K:193:ALA:CA	3:K:208:SER:HB3	2.27	0.61
1:A:280:ASN:HD22	1:A:458:GLY:CA	2.14	0.61
1:A:456:ARG:HB3	1:A:468:PHE:CD2	2.36	0.61
3:C:135:LEU:HD23	3:C:136:LEU:N	2.16	0.61
1:E:456:ARG:HB3	1:E:468:PHE:CD2	2.36	0.61
1:E:100:MET:HE1	1:E:487:LYS:N	2.16	0.61
2:F:58:ARG:HG2	2:F:61:LEU:HG	1.82	0.61
3:K:189:HIS:O	3:K:211:ARG:NE	2.34	0.61
1:A:373:THR:HB	1:A:385:CYS:O	2.01	0.60
3:G:78:LEU:HD11	3:G:104:LEU:CD2	2.31	0.60
1:A:115:SER:O	1:A:208:VAL:HG11	2.00	0.60
1:E:255:VAL:HG13	1:E:475:MET:SD	2.41	0.60
3:K:48:ILE:HD13	3:K:54:ARG:HA	1.84	0.60
1:A:100:MET:HE1	1:A:487:LYS:N	2.15	0.60
3:C:136:LEU:HD22	3:C:175:LEU:HD23	1.82	0.60
4:D:212:GLU:C	4:D:214:LYS:H	2.05	0.60
4:L:108:LEU:HD12	4:L:109:VAL:H	1.65	0.60
4:L:212:GLU:C	4:L:214:LYS:H	2.05	0.60
1:A:255:VAL:HG13	1:A:475:MET:SD	2.41	0.60
1:A:279:ASN:HB3	1:A:282:LYS:HG2	1.82	0.60
2:B:177:LEU:N	2:B:177:LEU:CD1	2.64	0.60
3:C:48:ILE:HD13	3:C:54:ARG:HA	1.84	0.60
2:F:170:PHE:O	2:F:172:ILE:HG12	2.00	0.60
3:G:2:ILE:HG12	3:G:27:GLU:OE1	2.01	0.60
1:I:279:ASN:HB3	1:I:282:LYS:HG2	1.82	0.60
2:J:120:SER:OG	2:J:121:PRO:HD2	2.01	0.60
2:F:26:PHE:CE1	2:F:39:ASN:HB3	2.36	0.60
4:H:126:PRO:HG3	4:H:138:LEU:CD1	2.30	0.60
4:H:38:ARG:HD2	4:H:46:GLU:OE1	2.01	0.60
1:I:255:VAL:HG13	1:I:475:MET:SD	2.41	0.60
2:J:58:ARG:HG2	2:J:61:LEU:HG	1.82	0.60
1:A:280:ASN:HD22	1:A:458:GLY:H	1.49	0.60
4:D:38:ARG:HD2	4:D:46:GLU:OE1	2.01	0.60
4:H:212:GLU:C	4:H:214:LYS:H	2.05	0.60
4:H:50:ARG:NH2	4:H:97:GLU:OE2	2.33	0.60
4:L:108:LEU:HD12	4:L:109:VAL:N	2.17	0.60
4:L:38:ARG:HD2	4:L:46:GLU:OE1	2.01	0.60
1:E:365:SER:HB2	2:F:46:LYS:O	2.00	0.60
1:I:280:ASN:HD22	1:I:458:GLY:CA	2.14	0.60
2:J:26:PHE:CE1	2:J:39:ASN:HB3	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:135:LEU:HD23	3:K:136:LEU:N	2.16	0.60
3:K:136:LEU:HD22	3:K:175:LEU:HD23	1.82	0.60
3:G:135:LEU:HD23	3:G:136:LEU:N	2.16	0.60
3:G:136:LEU:HD22	3:G:175:LEU:HD23	1.82	0.60
1:I:365:SER:HB2	2:J:46:LYS:O	2.00	0.60
1:I:391:PHE:CG	1:I:470:PRO:HG3	2.37	0.60
3:K:78:LEU:HD11	3:K:104:LEU:CD2	2.31	0.60
3:C:78:LEU:HD11	3:C:104:LEU:CD2	2.31	0.60
1:E:391:PHE:CG	1:E:470:PRO:HG3	2.37	0.60
1:E:280:ASN:HD22	1:E:458:GLY:H	1.49	0.60
3:G:48:ILE:HD13	3:G:54:ARG:HA	1.84	0.60
1:I:451:GLY:C	1:I:452:LEU:HD12	2.23	0.60
3:C:2:ILE:HG12	3:C:27:GLU:OE1	2.01	0.60
1:E:373:THR:HB	1:E:385:CYS:O	2.01	0.60
3:G:189:HIS:O	3:G:211:ARG:NE	2.34	0.60
3:K:139:PHE:HE1	3:K:175:LEU:H	1.50	0.60
1:A:86:LEU:HA	1:A:243:SER:CB	2.32	0.59
3:C:189:HIS:O	3:C:211:ARG:NE	2.34	0.59
4:H:108:LEU:HD12	4:H:109:VAL:N	2.17	0.59
1:A:451:GLY:C	1:A:452:LEU:HD12	2.23	0.59
3:C:78:LEU:CD1	3:C:104:LEU:HD21	2.33	0.59
1:I:456:ARG:HB3	1:I:468:PHE:CD2	2.36	0.59
1:I:280:ASN:HD22	1:I:458:GLY:H	1.49	0.59
6:N:100:LYS:HB2	6:N:100(A):TRP:CZ3	2.37	0.59
2:B:120:SER:OG	2:B:121:PRO:HD2	2.01	0.59
2:B:55:ALA:O	2:B:56:ASP:HB2	2.02	0.59
2:F:55:ALA:O	2:F:56:ASP:HB2	2.02	0.59
4:H:141:LEU:HD12	4:H:179:SER:OG	2.03	0.59
1:I:86:LEU:HA	1:I:243:SER:CB	2.32	0.59
3:K:93:ASN:HD21	3:K:95(B):ARG:HB2	1.65	0.59
4:L:141:LEU:HD12	4:L:179:SER:OG	2.03	0.59
1:A:391:PHE:CG	1:A:470:PRO:HG3	2.37	0.59
1:E:451:GLY:C	1:E:452:LEU:HD12	2.23	0.59
2:B:8:LYS:HD2	2:B:76:ILE:HG13	1.85	0.59
1:E:86:LEU:HA	1:E:243:SER:CB	2.32	0.59
2:J:2:LYS:HD3	2:J:3:VAL:H	1.67	0.59
1:A:448:ASN:ND2	7:A:948:NAG:H82	2.18	0.59
4:D:108:LEU:HD12	4:D:109:VAL:N	2.17	0.59
2:J:55:ALA:O	2:J:56:ASP:HB2	2.02	0.59
6:R:100:LYS:HB2	6:R:100(A):TRP:CZ3	2.37	0.59
2:F:120:SER:OG	2:F:121:PRO:HD2	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:139:PHE:HE1	3:G:175:LEU:H	1.50	0.59
1:I:94:ASN:ND2	1:I:97:LYS:HB3	2.18	0.59
3:K:44:PRO:HD2	4:L:103:TRP:CE3	2.38	0.59
2:B:2:LYS:HD3	2:B:3:VAL:H	1.67	0.59
2:F:2:LYS:HD3	2:F:3:VAL:H	1.67	0.59
3:G:116:PHE:CD2	4:H:137:ALA:HB3	2.38	0.59
1:A:242:VAL:HG22	1:A:243:SER:N	2.18	0.58
1:I:124:PRO:CG	2:J:60:SER:HA	2.33	0.58
6:P:100:LYS:HB2	6:P:100(A):TRP:CZ3	2.38	0.58
1:A:278:THR:HG22	7:A:776:NAG:O6	2.03	0.58
3:C:46:LEU:CD1	4:D:101:LYS:HA	2.28	0.58
2:F:164:ASN:O	2:F:166:LYS:N	2.36	0.58
1:E:368:ASP:CG	2:F:59:ARG:HH22	2.07	0.58
1:I:242:VAL:HG22	1:I:243:SER:N	2.18	0.58
3:K:116:PHE:CD2	4:L:137:ALA:HB3	2.38	0.58
1:A:371:ILE:HD12	1:A:472:GLY:O	2.04	0.58
1:E:371:ILE:HD12	1:E:472:GLY:O	2.04	0.58
1:E:94:ASN:ND2	1:E:97:LYS:HB3	2.18	0.58
1:I:276:ASN:OD1	1:I:278:THR:HB	2.03	0.58
1:I:373:THR:HB	1:I:385:CYS:O	2.01	0.58
4:L:60:ALA:HB3	4:L:63:LEU:HD12	1.85	0.58
1:A:124:PRO:CG	2:B:60:SER:HA	2.33	0.58
3:C:139:PHE:HE1	3:C:175:LEU:H	1.50	0.58
3:G:78:LEU:CD1	3:G:104:LEU:HD21	2.33	0.58
3:G:29:VAL:HG11	3:G:90:GLN:HG2	1.85	0.58
1:I:448:ASN:ND2	7:I:948:NAG:H82	2.18	0.58
3:K:193:ALA:HA	3:K:208:SER:CB	2.32	0.58
1:E:448:ASN:ND2	7:E:948:NAG:H82	2.18	0.58
1:A:94:ASN:ND2	1:A:97:LYS:HB3	2.18	0.58
2:B:164:ASN:O	2:B:166:LYS:N	2.37	0.58
3:C:198:HIS:HB3	3:C:201:LEU:HG	1.86	0.58
1:E:124:PRO:CG	2:F:60:SER:HA	2.33	0.58
3:G:193:ALA:HA	3:G:208:SER:CB	2.32	0.58
3:C:29:VAL:HG11	3:C:90:GLN:HG2	1.85	0.58
1:E:104:MET:O	1:E:108:ILE:HG12	2.04	0.58
1:E:242:VAL:HG22	1:E:243:SER:N	2.18	0.58
2:F:8:LYS:HD2	2:F:76:ILE:HG13	1.85	0.58
3:G:44:PRO:HD2	4:H:103:TRP:CE3	2.38	0.58
1:I:278:THR:HG22	7:I:776:NAG:O6	2.03	0.58
1:I:368:ASP:CG	2:J:59:ARG:HH22	2.06	0.58
3:K:29:VAL:HG12	3:K:29:VAL:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:141:LEU:HD12	4:D:179:SER:OG	2.03	0.58
3:G:59:PRO:HB3	3:G:61:ARG:NH1	2.19	0.58
1:I:279:ASN:HD22	1:I:282:LYS:CG	2.17	0.58
3:K:59:PRO:HB3	3:K:61:ARG:NH1	2.19	0.58
3:K:78:LEU:CD1	3:K:104:LEU:HD21	2.32	0.58
4:D:214:LYS:O	4:D:214:LYS:HD3	2.04	0.58
1:E:279:ASN:HD22	1:E:282:LYS:HD3	1.68	0.58
1:A:104:MET:O	1:A:108:ILE:HG12	2.04	0.57
3:G:29:VAL:O	3:G:29:VAL:HG12	2.04	0.57
2:J:8:LYS:HD2	2:J:76:ILE:HG13	1.85	0.57
3:K:29:VAL:HG11	3:K:90:GLN:HG2	1.85	0.57
1:A:279:ASN:HD22	1:A:282:LYS:HD3	1.68	0.57
4:D:51:ILE:O	4:D:51:ILE:HG23	2.04	0.57
1:E:276:ASN:OD1	1:E:278:THR:HB	2.03	0.57
3:G:94:TRP:HA	3:G:95:PRO:O	2.05	0.57
1:I:104:MET:HA	1:I:217:TYR:OH	2.04	0.57
1:I:100:MET:HE1	1:I:486:TYR:C	2.25	0.57
4:L:6:GLU:OE2	4:L:106:GLY:N	2.36	0.57
1:A:233:PHE:CE2	1:A:235:GLY:HA2	2.39	0.57
1:A:276:ASN:OD1	1:A:278:THR:HB	2.03	0.57
3:C:18:ARG:HG3	3:C:75:ILE:O	2.04	0.57
1:I:273:ARG:HG2	1:I:273:ARG:NH1	2.20	0.57
5:Q:22:SER:CB	5:Q:72:THR:HG22	2.34	0.57
1:A:104:MET:HA	1:A:217:TYR:OH	2.04	0.57
3:C:116:PHE:CD2	4:D:137:ALA:HB3	2.38	0.57
1:E:278:THR:HG22	7:E:776:NAG:O6	2.03	0.57
1:E:279:ASN:HD22	1:E:282:LYS:CG	2.17	0.57
2:F:76:ILE:N	2:F:76:ILE:HD12	2.19	0.57
1:I:104:MET:O	1:I:108:ILE:HG12	2.04	0.57
1:I:371:ILE:HD12	1:I:472:GLY:O	2.04	0.57
2:J:76:ILE:H	2:J:76:ILE:CD1	2.13	0.57
3:K:18:ARG:HG3	3:K:75:ILE:O	2.04	0.57
3:K:94:TRP:HA	3:K:95:PRO:O	2.05	0.57
3:C:59:PRO:HB3	3:C:61:ARG:NH1	2.19	0.57
3:C:44:PRO:HD2	4:D:103:TRP:CE3	2.38	0.57
2:F:178:ALA:CB	2:F:180:GLN:H	2.18	0.57
2:F:83:ILE:HG23	2:F:92:GLU:HG3	1.87	0.57
4:L:193:THR:HB	4:L:210:LYS:HE2	1.86	0.57
2:B:83:ILE:HG23	2:B:92:GLU:HG3	1.87	0.57
3:C:143:GLU:OE1	3:C:143:GLU:N	2.37	0.57
4:D:60:ALA:HB3	4:D:63:LEU:HD12	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:100:MET:HE1	1:E:486:TYR:C	2.25	0.57
3:G:18:ARG:HG3	3:G:75:ILE:O	2.04	0.57
4:H:60:ALA:HB3	4:H:63:LEU:HD12	1.85	0.57
4:L:214:LYS:O	4:L:214:LYS:HD3	2.04	0.57
4:L:98:GLY:O	4:L:100:ALA:N	2.32	0.57
1:A:466:GLU:HB3	1:A:468:PHE:CE1	2.40	0.57
1:E:233:PHE:CE2	1:E:235:GLY:HA2	2.39	0.57
1:E:466:GLU:HB3	1:E:468:PHE:CE1	2.39	0.57
3:G:198:HIS:CD2	3:G:199:GLN:N	2.72	0.57
3:K:189:HIS:HB2	3:K:192:TYR:OH	2.05	0.57
5:O:22:SER:CB	5:O:72:THR:HG22	2.35	0.57
2:B:178:ALA:CB	2:B:180:GLN:H	2.18	0.57
3:C:29:VAL:HG12	3:C:29:VAL:O	2.04	0.57
4:H:51:ILE:HG23	4:H:51:ILE:O	2.04	0.57
2:J:178:ALA:CB	2:J:180:GLN:H	2.18	0.57
4:D:126:PRO:HG3	4:D:138:LEU:CB	2.35	0.57
4:D:193:THR:HB	4:D:210:LYS:HE2	1.86	0.57
3:K:8:PRO:O	3:K:102:THR:HG23	2.05	0.57
4:L:126:PRO:HG3	4:L:138:LEU:CB	2.35	0.57
3:C:189:HIS:HB2	3:C:192:TYR:OH	2.05	0.57
1:E:108:ILE:HD12	1:E:253:PRO:CB	2.35	0.57
4:H:214:LYS:O	4:H:214:LYS:HD3	2.04	0.57
5:M:22:SER:CB	5:M:72:THR:HG22	2.34	0.57
3:G:189:HIS:HB2	3:G:192:TYR:OH	2.05	0.56
2:J:164:ASN:O	2:J:166:LYS:N	2.37	0.56
2:J:83:ILE:HG23	2:J:92:GLU:HG3	1.87	0.56
3:K:198:HIS:HB3	3:K:201:LEU:HG	1.86	0.56
3:C:193:ALA:HA	3:C:208:SER:CB	2.32	0.56
3:G:198:HIS:HB3	3:G:201:LEU:HG	1.86	0.56
1:I:233:PHE:CE2	1:I:235:GLY:HA2	2.39	0.56
1:I:466:GLU:HB3	1:I:468:PHE:CE1	2.40	0.56
1:A:279:ASN:HD22	1:A:282:LYS:CG	2.17	0.56
1:A:368:ASP:CG	2:B:59:ARG:HH22	2.07	0.56
1:A:100:MET:HE1	1:A:486:TYR:C	2.25	0.56
3:C:8:PRO:O	3:C:102:THR:HG23	2.05	0.56
3:C:135:LEU:HD12	4:D:181:VAL:HG11	1.86	0.56
3:C:136:LEU:HD22	3:C:175:LEU:HB3	1.87	0.56
2:F:16:CYS:HB2	2:F:28:TRP:CZ2	2.41	0.56
3:K:135:LEU:HD12	4:L:181:VAL:HG11	1.86	0.56
5:Q:22:SER:HB2	5:Q:72:THR:HG22	1.87	0.56
1:A:122:LEU:HD11	4:D:54:LEU:HG	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ILE:HD12	1:A:253:PRO:CB	2.35	0.56
2:B:16:CYS:HB2	2:B:28:TRP:CZ2	2.41	0.56
3:C:141:PRO:C	3:C:143:GLU:H	2.08	0.56
4:D:12:LYS:HE2	4:D:17:SER:O	2.05	0.56
4:D:6:GLU:OE2	4:D:106:GLY:N	2.36	0.56
2:F:44:LEU:HD12	2:F:45:THR:N	2.21	0.56
1:I:122:LEU:HD11	4:L:54:LEU:HG	1.86	0.56
1:I:204:ALA:C	1:I:206:PRO:HD3	2.26	0.56
3:K:136:LEU:HD22	3:K:175:LEU:HB3	1.87	0.56
1:A:204:ALA:C	1:A:206:PRO:HD3	2.26	0.56
1:E:104:MET:HA	1:E:217:TYR:OH	2.04	0.56
3:G:141:PRO:C	3:G:143:GLU:H	2.08	0.56
3:G:136:LEU:HD22	3:G:175:LEU:HB3	1.87	0.56
4:H:12:LYS:HE2	4:H:17:SER:O	2.05	0.56
1:I:279:ASN:HD22	1:I:282:LYS:HD3	1.69	0.56
4:L:51:ILE:HG23	4:L:51:ILE:O	2.04	0.56
4:H:92:CYS:O	4:H:104:GLY:N	2.38	0.56
3:C:94:TRP:HA	3:C:95:PRO:O	2.05	0.56
3:G:135:LEU:HD12	4:H:181:VAL:HG11	1.86	0.56
2:J:26:PHE:CE2	2:J:67:PHE:HB3	2.41	0.56
2:J:76:ILE:N	2:J:76:ILE:HD12	2.19	0.56
2:B:76:ILE:N	2:B:76:ILE:HD12	2.19	0.56
4:H:193:THR:HB	4:H:210:LYS:HE2	1.86	0.56
1:I:279:ASN:HD22	1:I:282:LYS:CD	2.19	0.56
2:J:70:ILE:N	2:J:70:ILE:HD12	2.21	0.56
1:A:273:ARG:NH1	1:A:273:ARG:HG2	2.20	0.56
1:A:394:ASN:C	1:A:396:THR:H	2.09	0.56
2:B:44:LEU:HD12	2:B:45:THR:N	2.21	0.56
2:B:70:ILE:N	2:B:70:ILE:HD12	2.21	0.56
1:E:279:ASN:HD22	1:E:282:LYS:CD	2.19	0.56
2:F:26:PHE:CE2	2:F:67:PHE:HB3	2.41	0.56
1:I:108:ILE:HD12	1:I:253:PRO:CB	2.35	0.56
4:L:52:ILE:HG23	4:L:100(E):TYR:CZ	2.41	0.56
1:A:394:ASN:O	1:A:396:THR:N	2.37	0.56
3:C:15:PRO:HD3	3:C:106:ILE:HG22	1.88	0.56
4:H:126:PRO:HG3	4:H:138:LEU:CB	2.35	0.56
4:H:52:ILE:HG23	4:H:100(E):TYR:CZ	2.41	0.56
4:L:168:ALA:HA	4:L:178:LEU:HB3	1.88	0.56
2:B:26:PHE:CE2	2:B:67:PHE:HB3	2.41	0.56
1:E:122:LEU:HD11	4:H:54:LEU:HG	1.86	0.56
3:K:198:HIS:CD2	3:K:199:GLN:N	2.72	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:52:ILE:HG23	4:D:100(E):TYR:CZ	2.41	0.55
2:J:16:CYS:HB2	2:J:28:TRP:CZ2	2.41	0.55
3:K:141:PRO:C	3:K:143:GLU:H	2.08	0.55
1:E:204:ALA:C	1:E:206:PRO:HD3	2.26	0.55
3:G:8:PRO:O	3:G:102:THR:HG23	2.05	0.55
2:J:44:LEU:HD12	2:J:45:THR:N	2.21	0.55
3:C:135:LEU:HD11	4:D:181:VAL:HG21	1.88	0.55
3:C:198:HIS:CD2	3:C:199:GLN:N	2.72	0.55
1:E:254:VAL:HG11	1:E:261:LEU:HB2	1.89	0.55
1:I:371:ILE:HD11	1:I:473:GLY:HA3	1.89	0.55
3:K:135:LEU:HD11	4:L:181:VAL:HG21	1.89	0.55
4:L:12:LYS:HE2	4:L:17:SER:O	2.05	0.55
2:B:76:ILE:CD1	2:B:76:ILE:H	2.14	0.55
4:D:168:ALA:HA	4:D:178:LEU:HB3	1.88	0.55
2:F:76:ILE:HA	2:F:97:VAL:HB	1.89	0.55
2:B:103:ASN:N	2:B:103:ASN:ND2	2.55	0.55
2:J:76:ILE:HA	2:J:97:VAL:HB	1.89	0.55
3:K:176:SER:HB2	4:L:166:PHE:CE2	2.42	0.55
2:F:70:ILE:N	2:F:70:ILE:HD12	2.21	0.55
4:H:146:PHE:CG	4:H:147:PRO:HA	2.42	0.55
1:I:254:VAL:HG11	1:I:261:LEU:HB2	1.89	0.55
2:J:138:ILE:HD13	2:J:146:VAL:HG22	1.88	0.55
4:L:146:PHE:CG	4:L:147:PRO:HA	2.42	0.55
1:A:254:VAL:HG11	1:A:261:LEU:HB2	1.89	0.55
1:A:279:ASN:HD22	1:A:282:LYS:CD	2.19	0.55
2:B:138:ILE:HD13	2:B:146:VAL:HG22	1.88	0.55
4:H:97:GLU:HA	4:H:97:GLU:OE1	2.07	0.55
5:O:22:SER:HB2	5:O:72:THR:HG22	1.88	0.55
1:A:371:ILE:HD11	1:A:473:GLY:HA3	1.88	0.55
4:D:5:VAL:O	4:D:22:CYS:HA	2.07	0.55
4:D:67:VAL:HG22	4:D:68:THR:N	2.22	0.55
1:E:394:ASN:C	1:E:396:THR:H	2.09	0.55
3:G:135:LEU:HD11	4:H:181:VAL:HG21	1.89	0.55
3:G:176:SER:HB2	4:H:166:PHE:CE2	2.42	0.55
1:I:394:ASN:O	1:I:396:THR:N	2.37	0.55
2:F:36:ILE:HD13	2:F:49:SER:CB	2.37	0.55
4:H:82(B):ASN:N	4:H:82(B):ASN:ND2	2.55	0.55
2:J:108:LEU:HD23	2:J:109:LEU:N	2.22	0.55
3:C:135:LEU:HD23	3:C:135:LEU:C	2.28	0.55
1:I:129:ALA:O	1:I:195:SER:N	2.40	0.55
3:K:192:TYR:HB2	3:K:209:PHE:CE1	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:22:SER:HB2	5:M:72:THR:HG22	1.88	0.55
1:E:129:ALA:O	1:E:195:SER:N	2.40	0.54
4:H:154:TRP:CZ2	4:H:196:CYS:HB3	2.42	0.54
2:J:132:SER:HB3	2:J:136:LYS:HB2	1.89	0.54
4:H:5:VAL:O	4:H:22:CYS:HA	2.07	0.54
4:D:146:PHE:CG	4:D:147:PRO:HA	2.42	0.54
3:G:141:PRO:C	3:G:143:GLU:N	2.61	0.54
3:K:141:PRO:C	3:K:143:GLU:N	2.61	0.54
1:A:129:ALA:O	1:A:195:SER:N	2.40	0.54
2:B:76:ILE:HA	2:B:97:VAL:HB	1.89	0.54
3:C:116:PHE:CE2	4:D:137:ALA:HB3	2.43	0.54
2:F:138:ILE:HD13	2:F:146:VAL:HG22	1.88	0.54
3:G:192:TYR:HB2	3:G:209:PHE:CE1	2.42	0.54
1:A:105:HIS:O	1:A:109:ILE:HG13	2.08	0.54
2:B:108:LEU:HD23	2:B:109:LEU:N	2.22	0.54
2:B:36:ILE:HD13	2:B:49:SER:CB	2.37	0.54
3:C:176:SER:HB2	4:D:166:PHE:CE2	2.42	0.54
3:C:192:TYR:HB2	3:C:209:PHE:CE1	2.42	0.54
4:D:82(B):ASN:ND2	4:D:82(B):ASN:N	2.55	0.54
2:F:132:SER:HB3	2:F:136:LYS:HB2	1.89	0.54
3:K:15:PRO:HD3	3:K:106:ILE:HG22	1.88	0.54
3:K:163:VAL:HG12	3:K:164:THR:N	2.23	0.54
4:L:93:ALA:HB3	4:L:100(K):LEU:HD13	1.90	0.54
4:L:16:SER:OG	4:L:17:SER:N	2.40	0.54
4:L:5:VAL:O	4:L:22:CYS:HA	2.07	0.54
4:L:82(B):ASN:N	4:L:82(B):ASN:ND2	2.55	0.54
1:A:118:PRO:HG3	1:A:435:TYR:CZ	2.42	0.54
3:C:135:LEU:CD1	4:D:181:VAL:HG21	2.37	0.54
2:F:103:ASN:N	2:F:103:ASN:ND2	2.55	0.54
3:G:21:LEU:N	3:G:21:LEU:HD12	2.23	0.54
4:L:154:TRP:CZ2	4:L:196:CYS:HB3	2.42	0.54
1:E:105:HIS:O	1:E:109:ILE:HG13	2.08	0.54
1:E:273:ARG:NH1	1:E:273:ARG:HG2	2.20	0.54
3:G:135:LEU:HD23	3:G:135:LEU:C	2.28	0.54
3:G:163:VAL:HG12	3:G:164:THR:N	2.23	0.54
1:I:118:PRO:HG3	1:I:435:TYR:CZ	2.42	0.54
2:B:178:ALA:CB	2:B:180:GLN:HA	2.38	0.54
1:E:371:ILE:HD11	1:E:473:GLY:HA3	1.88	0.54
3:G:135:LEU:CD1	4:H:181:VAL:HG21	2.37	0.54
3:G:116:PHE:CE2	4:H:137:ALA:HB3	2.43	0.54
4:H:212:GLU:O	4:H:214:LYS:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:116:PHE:CE2	4:L:137:ALA:HB3	2.43	0.54
3:K:135:LEU:CD1	4:L:181:VAL:HG21	2.37	0.54
4:D:154:TRP:CZ2	4:D:196:CYS:HB3	2.42	0.54
3:G:149:LYS:HA	3:G:153:ALA:O	2.08	0.54
2:J:178:ALA:CB	2:J:180:GLN:HA	2.38	0.54
3:K:135:LEU:C	3:K:135:LEU:HD23	2.28	0.54
3:K:3:VAL:N	3:K:26:SER:OG	2.35	0.54
4:L:67:VAL:HG22	4:L:68:THR:N	2.22	0.54
1:A:452:LEU:N	1:A:452:LEU:HD12	2.23	0.54
2:F:108:LEU:HD23	2:F:109:LEU:N	2.22	0.54
2:F:176:VAL:CA	2:F:177:LEU:HD12	2.36	0.54
4:H:67:VAL:HG22	4:H:68:THR:N	2.22	0.54
1:I:104:MET:HE2	1:I:215:ILE:HD11	1.90	0.54
2:J:103:ASN:N	2:J:103:ASN:ND2	2.55	0.54
2:J:36:ILE:HD13	2:J:49:SER:CB	2.37	0.54
3:K:29:VAL:CG1	3:K:90:GLN:HG2	2.38	0.54
1:A:101:VAL:HG13	1:A:479:TRP:HB2	1.90	0.53
1:E:118:PRO:HG3	1:E:435:TYR:CZ	2.42	0.53
7:E:894:NAG:O3	7:E:894:NAG:H83	2.08	0.53
3:G:15:PRO:HD3	3:G:106:ILE:HG22	1.88	0.53
1:I:349:LEU:HD22	1:I:468:PHE:CE2	2.44	0.53
3:K:106:ILE:HG13	3:K:166:GLN:HE21	1.73	0.53
1:A:349:LEU:HD22	1:A:468:PHE:CE2	2.44	0.53
7:A:894:NAG:H83	7:A:894:NAG:O3	2.08	0.53
3:C:21:LEU:HD12	3:C:21:LEU:N	2.22	0.53
4:D:16:SER:OG	4:D:17:SER:N	2.39	0.53
3:G:106:ILE:HG13	3:G:166:GLN:HE21	1.73	0.53
1:I:105:HIS:O	1:I:109:ILE:HG13	2.08	0.53
1:I:452:LEU:N	1:I:452:LEU:HD12	2.23	0.53
3:C:163:VAL:HG12	3:C:164:THR:N	2.23	0.53
1:E:101:VAL:HG13	1:E:479:TRP:HB2	1.90	0.53
4:H:168:ALA:HA	4:H:178:LEU:HB3	1.89	0.53
1:I:394:ASN:C	1:I:396:THR:H	2.09	0.53
3:K:149:LYS:HA	3:K:153:ALA:O	2.08	0.53
1:A:86:LEU:HA	1:A:243:SER:HB2	1.91	0.53
4:D:66:ARG:O	4:D:82:LEU:HD23	2.09	0.53
1:E:349:LEU:HD22	1:E:468:PHE:CE2	2.44	0.53
3:K:21:LEU:HD12	3:K:21:LEU:N	2.22	0.53
1:A:219:ALA:HB2	1:A:225:ILE:HG13	1.91	0.53
3:C:113:PRO:HD2	3:C:201:LEU:HG	1.91	0.53
4:D:93:ALA:HB3	4:D:100(K):LEU:HD13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:178:ALA:CB	2:F:180:GLN:HA	2.38	0.53
3:G:29:VAL:CG1	3:G:90:GLN:HG2	2.39	0.53
3:K:113:PRO:HD2	3:K:201:LEU:HG	1.91	0.53
4:L:97:GLU:OE1	4:L:97:GLU:HA	2.07	0.53
1:A:280:ASN:ND2	1:A:458:GLY:HA3	2.24	0.53
2:B:132:SER:HB3	2:B:136:LYS:HB2	1.89	0.53
1:E:371:ILE:CD1	1:E:473:GLY:HA3	2.39	0.53
1:E:452:LEU:N	1:E:452:LEU:HD12	2.23	0.53
1:E:474:ASP:O	1:E:476:ARG:N	2.42	0.53
3:G:150:VAL:HG13	3:G:192:TYR:CE1	2.44	0.53
3:G:150:VAL:O	3:G:153:ALA:HB3	2.09	0.53
1:A:242:VAL:CG2	1:A:243:SER:N	2.72	0.53
3:C:117:ILE:HD11	3:C:132:VAL:CG1	2.39	0.53
3:C:150:VAL:HG13	3:C:192:TYR:CE1	2.44	0.53
2:F:98:PHE:CD2	2:F:161:VAL:HG11	2.44	0.53
1:I:407:LEU:HB3	7:I:894:NAG:H81	1.91	0.53
7:I:894:NAG:H83	7:I:894:NAG:O3	2.08	0.53
3:K:150:VAL:HG13	3:K:192:TYR:CE1	2.44	0.53
1:A:395:ASP:O	1:A:395:ASP:OD1	2.27	0.53
3:C:124:GLN:HG3	4:D:122:PHE:CD2	2.44	0.53
3:C:149:LYS:HA	3:C:153:ALA:O	2.08	0.53
3:G:113:PRO:HD2	3:G:201:LEU:HG	1.91	0.53
4:H:66:ARG:O	4:H:82:LEU:HD23	2.09	0.53
1:I:474:ASP:O	1:I:476:ARG:N	2.42	0.53
2:J:98:PHE:CD2	2:J:161:VAL:HG11	2.44	0.53
3:K:117:ILE:HD11	3:K:132:VAL:CG1	2.39	0.53
1:A:474:ASP:O	1:A:476:ARG:N	2.42	0.53
3:C:141:PRO:C	3:C:143:GLU:N	2.61	0.53
1:E:120:VAL:HA	1:E:201:ILE:O	2.09	0.53
1:E:395:ASP:O	1:E:395:ASP:OD1	2.27	0.53
1:E:124:PRO:CB	2:F:60:SER:HA	2.39	0.53
1:I:219:ALA:HB2	1:I:225:ILE:HG13	1.91	0.53
1:I:395:ASP:O	1:I:395:ASP:OD1	2.27	0.53
4:L:66:ARG:O	4:L:82:LEU:HD23	2.09	0.53
6:R:6:GLN:HB3	6:R:107:THR:HG22	1.91	0.53
3:C:150:VAL:O	3:C:153:ALA:HB3	2.09	0.52
3:C:106:ILE:HG13	3:C:166:GLN:HE21	1.73	0.52
4:D:97:GLU:HA	4:D:97:GLU:OE1	2.07	0.52
3:G:135:LEU:C	3:G:136:LEU:HD12	2.29	0.52
2:J:10:ASP:O	2:J:74:LEU:HB2	2.09	0.52
4:L:29:PHE:CE2	4:L:52(A):THR:HG21	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:VAL:HA	1:A:201:ILE:O	2.09	0.52
2:B:176:VAL:CA	2:B:177:LEU:HD12	2.36	0.52
3:G:117:ILE:HD11	3:G:132:VAL:CG1	2.39	0.52
1:I:242:VAL:CG2	1:I:243:SER:N	2.72	0.52
4:L:35:THR:HG23	4:L:49:GLY:O	2.09	0.52
1:A:124:PRO:CB	2:B:60:SER:HA	2.39	0.52
4:D:85:ASP:N	4:D:85:ASP:OD1	2.41	0.52
3:G:115:VAL:HG22	3:G:196:VAL:HG21	1.90	0.52
4:H:139:GLY:HA2	4:H:154:TRP:CH2	2.44	0.52
1:I:120:VAL:HA	1:I:201:ILE:O	2.09	0.52
1:I:101:VAL:HG13	1:I:479:TRP:HB2	1.90	0.52
3:K:124:GLN:HG3	4:L:122:PHE:CD2	2.44	0.52
3:K:143:GLU:OE1	3:K:143:GLU:N	2.38	0.52
4:L:212:GLU:O	4:L:214:LYS:N	2.41	0.52
1:A:457:ASP:OD2	1:A:469:ARG:NE	2.39	0.52
2:B:98:PHE:CD2	2:B:161:VAL:HG11	2.44	0.52
4:D:139:GLY:HA2	4:D:154:TRP:CH2	2.45	0.52
1:E:269:GLU:HA	7:E:789:NAG:C1	2.40	0.52
4:H:93:ALA:HB3	4:H:100(K):LEU:HD13	1.90	0.52
4:D:35:THR:HG23	4:D:49:GLY:O	2.09	0.52
1:E:120:VAL:CG1	1:E:434:MET:HB3	2.40	0.52
1:E:407:LEU:HB3	7:E:894:NAG:H81	1.91	0.52
2:F:154:SER:HB2	2:F:176:VAL:CG2	2.39	0.52
4:H:2:VAL:HG13	4:H:27:ASP:HB3	1.91	0.52
1:I:280:ASN:ND2	1:I:458:GLY:HA3	2.24	0.52
1:I:269:GLU:HA	7:I:789:NAG:C1	2.39	0.52
2:J:176:VAL:CA	2:J:177:LEU:HD12	2.36	0.52
3:K:150:VAL:O	3:K:153:ALA:HB3	2.09	0.52
1:A:280:ASN:ND2	1:A:458:GLY:CA	2.73	0.52
2:B:10:ASP:O	2:B:74:LEU:HB2	2.09	0.52
3:C:29:VAL:CG1	3:C:90:GLN:HG2	2.38	0.52
4:D:29:PHE:CE2	4:D:52(A):THR:HG21	2.44	0.52
1:E:394:ASN:O	1:E:396:THR:N	2.37	0.52
2:F:10:ASP:O	2:F:74:LEU:HB2	2.09	0.52
3:G:124:GLN:HG3	4:H:122:PHE:CD2	2.44	0.52
4:H:16:SER:OG	4:H:17:SER:N	2.40	0.52
1:I:120:VAL:CG1	1:I:434:MET:HB3	2.40	0.52
1:I:86:LEU:HA	1:I:243:SER:HB2	1.91	0.52
3:K:136:LEU:HB2	3:K:175:LEU:HB3	1.92	0.52
1:A:269:GLU:HA	7:A:789:NAG:C1	2.40	0.52
1:A:407:LEU:HB3	7:A:894:NAG:H81	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:33:LEU:HD22	3:C:89:GLN:O	2.10	0.52
1:E:242:VAL:CG2	1:E:243:SER:N	2.72	0.52
3:G:3:VAL:N	3:G:26:SER:OG	2.35	0.52
3:G:48:ILE:CD1	3:G:54:ARG:HG2	2.40	0.52
1:I:124:PRO:CB	2:J:60:SER:HA	2.39	0.52
4:D:189:LEU:HD23	4:D:194:TYR:HE2	1.75	0.52
1:E:219:ALA:HB2	1:E:225:ILE:HG13	1.91	0.52
1:E:353:PHE:CZ	1:E:456:ARG:HD3	2.45	0.52
1:I:353:PHE:CZ	1:I:456:ARG:HD3	2.45	0.52
1:I:371:ILE:CD1	1:I:473:GLY:HA3	2.39	0.52
4:D:92:CYS:O	4:D:104:GLY:N	2.38	0.52
3:G:142:ARG:CG	3:G:163:VAL:HG11	2.40	0.52
3:G:118:PHE:CD2	4:H:124:LEU:HD23	2.45	0.52
4:H:35:THR:HG23	4:H:49:GLY:O	2.10	0.52
3:C:115:VAL:HG22	3:C:196:VAL:HG21	1.90	0.52
3:C:142:ARG:CG	3:C:163:VAL:HG11	2.40	0.52
1:E:280:ASN:ND2	1:E:458:GLY:HA3	2.24	0.52
1:I:385:CYS:HA	1:I:418:CYS:HA	1.92	0.52
3:K:135:LEU:C	3:K:136:LEU:HD12	2.29	0.52
3:K:115:VAL:HG22	3:K:196:VAL:HG21	1.90	0.52
3:K:48:ILE:CD1	3:K:54:ARG:HG2	2.40	0.52
3:K:118:PHE:CD2	4:L:124:LEU:HD23	2.45	0.52
3:C:48:ILE:CD1	3:C:54:ARG:HG2	2.40	0.51
3:C:118:PHE:CD2	4:D:124:LEU:HD23	2.45	0.51
2:J:154:SER:HB2	2:J:176:VAL:CG2	2.39	0.51
1:A:353:PHE:CZ	1:A:456:ARG:HD3	2.45	0.51
1:A:371:ILE:CD1	1:A:473:GLY:HA3	2.39	0.51
2:B:108:LEU:HD23	2:B:108:LEU:C	2.31	0.51
4:D:2:VAL:HG13	4:D:27:ASP:HB3	1.91	0.51
3:G:33:LEU:HD22	3:G:89:GLN:O	2.10	0.51
1:I:280:ASN:ND2	1:I:458:GLY:CA	2.73	0.51
2:J:108:LEU:C	2:J:108:LEU:HD23	2.31	0.51
1:A:86:LEU:HA	1:A:243:SER:HB3	1.92	0.51
3:C:135:LEU:C	3:C:136:LEU:HD12	2.29	0.51
1:E:346:ALA:O	1:E:350:LYS:HG2	2.10	0.51
3:G:143:GLU:OE1	3:G:143:GLU:N	2.38	0.51
4:H:29:PHE:CE2	4:H:52(A):THR:HG21	2.44	0.51
3:K:33:LEU:HD22	3:K:89:GLN:O	2.10	0.51
6:R:35:VAL:HB	6:R:51:ILE:HG22	1.93	0.51
1:A:346:ALA:O	1:A:350:LYS:HG2	2.10	0.51
1:E:295:ASN:O	1:E:331:CYS:HA	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:186:TYR:O	3:G:192:TYR:OH	2.29	0.51
4:H:135:THR:HG22	4:H:185:PRO:CA	2.41	0.51
1:I:295:ASN:O	1:I:331:CYS:HA	2.10	0.51
3:K:175:LEU:CD1	3:K:176:SER:H	2.23	0.51
4:L:41:PRO:C	4:L:43:GLN:H	2.14	0.51
2:F:108:LEU:HD23	2:F:108:LEU:C	2.31	0.51
2:F:100:LEU:HD12	2:F:170:PHE:CB	2.41	0.51
3:G:136:LEU:HB2	3:G:175:LEU:HB3	1.92	0.51
3:G:78:LEU:HD23	3:G:79:GLN:N	2.26	0.51
2:J:76:ILE:HG12	2:J:119:GLU:OE2	2.11	0.51
2:J:26:PHE:CZ	2:J:67:PHE:HB3	2.46	0.51
4:L:139:GLY:HA2	4:L:154:TRP:CH2	2.44	0.51
4:L:189:LEU:HD23	4:L:194:TYR:HE2	1.75	0.51
4:L:5:VAL:O	4:L:23:LYS:N	2.43	0.51
1:A:120:VAL:CG1	1:A:434:MET:HB3	2.40	0.51
1:A:95:MET:HA	1:A:98:ASN:HB2	1.93	0.51
3:C:175:LEU:CD1	3:C:176:SER:H	2.23	0.51
1:E:104:MET:HE2	1:E:215:ILE:HD11	1.91	0.51
4:H:41:PRO:C	4:H:43:GLN:H	2.14	0.51
1:I:457:ASP:HB3	2:J:48:PRO:HG2	1.93	0.51
3:K:142:ARG:CG	3:K:163:VAL:HG11	2.40	0.51
4:L:141:LEU:HD12	4:L:179:SER:HG	1.74	0.51
2:B:69:LEU:C	2:B:69:LEU:HD22	2.31	0.51
4:D:66:ARG:HB2	4:D:66:ARG:HH11	1.76	0.51
1:E:86:LEU:HA	1:E:243:SER:HB3	1.92	0.51
2:F:69:LEU:C	2:F:69:LEU:HD22	2.31	0.51
4:H:12:LYS:HG3	4:H:18:VAL:HB	1.93	0.51
4:L:12:LYS:HG3	4:L:18:VAL:HB	1.93	0.51
2:B:76:ILE:HG12	2:B:119:GLU:OE2	2.11	0.51
4:D:135:THR:HG22	4:D:185:PRO:CA	2.41	0.51
1:E:457:ASP:HB3	2:F:48:PRO:HG2	1.93	0.51
1:E:86:LEU:HA	1:E:243:SER:HB2	1.91	0.51
4:H:77:THR:HG22	4:H:78:VAL:N	2.26	0.51
2:J:79:SER:O	2:J:80:ASP:HB2	2.10	0.51
4:L:2:VAL:HG13	4:L:27:ASP:HB3	1.91	0.51
4:L:40:ALA:O	4:L:43:GLN:HB2	2.11	0.51
4:L:92:CYS:O	4:L:104:GLY:N	2.38	0.51
2:B:154:SER:HB2	2:B:176:VAL:N	2.25	0.51
2:B:79:SER:O	2:B:80:ASP:HB2	2.10	0.51
3:C:136:LEU:HB2	3:C:175:LEU:HB3	1.92	0.51
4:H:40:ALA:O	4:H:43:GLN:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:346:ALA:O	1:I:350:LYS:HG2	2.10	0.51
1:I:95:MET:HA	1:I:98:ASN:HB2	1.93	0.51
1:A:252:ARG:O	1:A:254:VAL:N	2.44	0.51
1:A:357:LYS:HG3	1:A:464:GLY:CA	2.41	0.51
4:D:212:GLU:O	4:D:214:LYS:N	2.41	0.51
4:H:189:LEU:HD23	4:H:194:TYR:HE2	1.75	0.51
4:L:77:THR:HG22	4:L:78:VAL:N	2.26	0.51
2:B:100:LEU:HD12	2:B:170:PHE:CB	2.41	0.50
3:C:3:VAL:N	3:C:26:SER:OG	2.34	0.50
4:D:36:TRP:CD2	4:D:80:LEU:HB2	2.46	0.50
4:H:66:ARG:HB2	4:H:66:ARG:HH11	1.76	0.50
1:I:357:LYS:HG3	1:I:464:GLY:CA	2.41	0.50
4:L:27:ASP:CG	4:L:28:THR:H	2.14	0.50
4:D:27:ASP:CG	4:D:28:THR:H	2.15	0.50
1:I:222:GLY:HA2	1:I:491:ILE:CG2	2.42	0.50
2:J:69:LEU:C	2:J:69:LEU:HD22	2.31	0.50
6:N:195:ILE:HG12	6:N:210:ARG:CA	2.41	0.50
6:N:35:VAL:HB	6:N:51:ILE:HG22	1.92	0.50
6:P:6:GLN:HB3	6:P:107:THR:HG22	1.91	0.50
1:A:95:MET:HE3	1:A:234:ASN:O	2.12	0.50
1:A:295:ASN:O	1:A:331:CYS:HA	2.10	0.50
1:E:249:HIS:O	1:E:251:ILE:HG13	2.12	0.50
1:E:280:ASN:ND2	1:E:458:GLY:CA	2.73	0.50
3:G:175:LEU:CD1	3:G:176:SER:H	2.23	0.50
1:I:86:LEU:HA	1:I:243:SER:HB3	1.92	0.50
6:N:6:GLN:HB3	6:N:107:THR:HG22	1.91	0.50
6:P:195:ILE:HG12	6:P:210:ARG:CA	2.41	0.50
6:P:35:VAL:HB	6:P:51:ILE:HG22	1.92	0.50
5:Q:22:SER:HA	5:Q:72:THR:HG22	1.94	0.50
6:R:195:ILE:HG12	6:R:210:ARG:CA	2.41	0.50
3:C:115:VAL:CG2	3:C:196:VAL:HG21	2.42	0.50
4:D:41:PRO:C	4:D:43:GLN:H	2.14	0.50
3:K:138:ASN:N	3:K:138:ASN:OD1	2.44	0.50
5:M:22:SER:HA	5:M:72:THR:HG22	1.94	0.50
3:K:169:LYS:HE3	3:K:169:LYS:HA	1.94	0.50
3:K:186:TYR:O	3:K:192:TYR:OH	2.29	0.50
4:L:135:THR:HG22	4:L:185:PRO:CA	2.41	0.50
1:A:86:LEU:HD11	7:A:741:NAG:O7	2.12	0.50
2:B:161:VAL:HB	2:B:168:VAL:HG22	1.94	0.50
2:B:154:SER:HB2	2:B:176:VAL:CG2	2.39	0.50
4:D:40:ALA:O	4:D:43:GLN:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:95:MET:HE3	1:E:234:ASN:O	2.10	0.50
1:E:95:MET:HE1	1:E:273:ARG:HG2	1.93	0.50
1:E:385:CYS:HA	1:E:418:CYS:HA	1.92	0.50
1:E:357:LYS:HG3	1:E:464:GLY:CA	2.41	0.50
1:I:360:ILE:HG22	1:I:361:PHE:N	2.27	0.50
1:E:457:ASP:OD2	1:E:469:ARG:NE	2.39	0.50
3:G:115:VAL:CG2	3:G:196:VAL:HG21	2.42	0.50
4:H:6:GLU:OE2	4:H:106:GLY:N	2.36	0.50
1:I:249:HIS:O	1:I:251:ILE:HG13	2.12	0.50
1:I:252:ARG:O	1:I:254:VAL:N	2.44	0.50
1:I:100:MET:CG	1:I:488:VAL:HG12	2.42	0.50
1:I:95:MET:HE3	1:I:234:ASN:O	2.12	0.50
3:K:115:VAL:CG2	3:K:196:VAL:HG21	2.42	0.50
3:C:169:LYS:HA	3:C:169:LYS:HE3	1.94	0.50
3:C:78:LEU:HD23	3:C:79:GLN:N	2.26	0.50
4:D:39:GLN:NE2	4:D:44:GLY:HA2	2.23	0.50
2:F:26:PHE:CZ	2:F:67:PHE:HB3	2.46	0.50
2:F:5:LEU:HD22	2:F:96:LEU:HB2	1.94	0.50
3:G:46:LEU:HD13	4:H:101:LYS:HD2	1.94	0.50
4:H:52:ILE:HG23	4:H:100(E):TYR:OH	2.12	0.50
4:H:36:TRP:CD2	4:H:80:LEU:HB2	2.47	0.50
4:H:85:ASP:OD1	4:H:85:ASP:N	2.41	0.50
4:L:36:TRP:CD2	4:L:80:LEU:HB2	2.46	0.50
6:R:40:ALA:O	6:R:43:GLN:HB2	2.12	0.50
2:B:26:PHE:CZ	2:B:67:PHE:HB3	2.46	0.50
4:D:147:PRO:HG2	4:D:148:GLU:H	1.77	0.50
4:D:52:ILE:HG23	4:D:100(E):TYR:OH	2.12	0.50
1:E:222:GLY:HA2	1:E:491:ILE:CG2	2.42	0.50
1:E:252:ARG:O	1:E:254:VAL:N	2.44	0.50
1:E:95:MET:HA	1:E:98:ASN:HB2	1.93	0.50
2:J:161:VAL:HB	2:J:168:VAL:HG22	1.94	0.50
4:L:66:ARG:HH11	4:L:66:ARG:HB2	1.76	0.50
5:O:22:SER:HA	5:O:72:THR:HG22	1.94	0.50
1:A:385:CYS:HA	1:A:418:CYS:HA	1.92	0.49
1:A:222:GLY:HA2	1:A:491:ILE:CG2	2.42	0.49
4:D:12:LYS:HG3	4:D:18:VAL:HB	1.93	0.49
2:F:79:SER:O	2:F:80:ASP:HB2	2.11	0.49
1:I:360:ILE:CG2	1:I:361:PHE:N	2.75	0.49
1:I:86:LEU:HD11	7:I:741:NAG:O7	2.12	0.49
1:I:411:GLY:O	7:I:908:NAG:O6	2.30	0.49
3:K:78:LEU:HD23	3:K:79:GLN:N	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:147:PRO:HG2	4:L:148:GLU:H	1.77	0.49
1:A:95:MET:HE1	1:A:273:ARG:NH1	2.24	0.49
2:B:164:ASN:C	2:B:166:LYS:H	2.15	0.49
4:D:77:THR:HG22	4:D:78:VAL:N	2.26	0.49
4:H:27:ASP:CG	4:H:28:THR:H	2.14	0.49
6:P:40:ALA:O	6:P:43:GLN:HB2	2.12	0.49
5:Q:54:LEU:HD21	5:Q:60:SER:HA	1.94	0.49
2:B:5:LEU:HD22	2:B:96:LEU:HB2	1.94	0.49
3:C:19:ALA:HB1	3:C:104:LEU:HD11	1.95	0.49
1:E:360:ILE:CG2	1:E:361:PHE:N	2.75	0.49
2:F:76:ILE:HG12	2:F:119:GLU:OE2	2.11	0.49
2:J:100:LEU:HD12	2:J:170:PHE:CB	2.41	0.49
2:J:5:LEU:HD22	2:J:96:LEU:HB2	1.94	0.49
3:C:105:GLU:HG2	3:C:106:ILE:N	2.27	0.49
1:E:360:ILE:HG22	1:E:361:PHE:N	2.27	0.49
4:H:182:VAL:O	4:H:182:VAL:HG13	2.12	0.49
4:L:52:ILE:HG23	4:L:100(E):TYR:OH	2.12	0.49
1:A:457:ASP:HB3	2:B:48:PRO:HG2	1.93	0.49
3:G:47:LEU:HD11	3:G:86:TYR:CE1	2.48	0.49
2:J:154:SER:HB2	2:J:176:VAL:N	2.25	0.49
3:K:47:LEU:HD11	3:K:86:TYR:CE1	2.48	0.49
1:A:344:GLN:HG2	7:A:789:NAG:C8	2.43	0.49
1:A:100:MET:CG	1:A:488:VAL:HG12	2.42	0.49
4:H:141:LEU:HD12	4:H:179:SER:HG	1.77	0.49
4:H:147:PRO:HG2	4:H:148:GLU:H	1.78	0.49
1:I:344:GLN:HG2	7:I:789:NAG:C8	2.43	0.49
1:I:95:MET:HE1	1:I:273:ARG:NH1	2.24	0.49
3:K:193:ALA:HB1	3:K:206:THR:HG23	1.94	0.49
3:C:186:TYR:O	3:C:192:TYR:OH	2.29	0.49
1:E:361:PHE:C	1:E:362:ASN:HD22	2.16	0.49
2:F:161:VAL:HB	2:F:168:VAL:HG22	1.93	0.49
3:G:19:ALA:HB1	3:G:104:LEU:HD11	1.95	0.49
1:I:292:VAL:HG12	1:I:333:LEU:HD11	1.95	0.49
1:I:457:ASP:OD2	1:I:469:ARG:NE	2.38	0.49
2:J:2:LYS:CD	2:J:3:VAL:H	2.26	0.49
1:A:360:ILE:CG2	1:A:361:PHE:N	2.75	0.49
1:A:360:ILE:HG22	1:A:361:PHE:N	2.27	0.49
2:B:2:LYS:CD	2:B:3:VAL:H	2.26	0.49
3:C:138:ASN:N	3:C:138:ASN:OD1	2.45	0.49
3:C:46:LEU:HD13	4:D:101:LYS:HD2	1.94	0.49
1:E:292:VAL:HG12	1:E:333:LEU:HD11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:77:GLU:OE1	2:F:77:GLU:N	2.45	0.49
3:G:66:GLY:HA3	3:G:71:PHE:HA	1.95	0.49
1:I:361:PHE:C	1:I:362:ASN:HD22	2.16	0.49
2:J:164:ASN:C	2:J:166:LYS:H	2.15	0.49
4:L:182:VAL:HG13	4:L:182:VAL:O	2.12	0.49
1:A:344:GLN:HG2	7:A:789:NAG:H83	1.95	0.49
2:B:178:ALA:HB3	2:B:180:GLN:HA	1.95	0.49
3:C:47:LEU:HD11	3:C:86:TYR:CE1	2.48	0.49
4:D:5:VAL:O	4:D:23:LYS:N	2.43	0.49
1:E:109:ILE:HG23	1:E:428:GLN:HG2	1.95	0.49
1:E:344:GLN:HG2	7:E:789:NAG:H83	1.95	0.49
1:E:95:MET:CE	1:E:235:GLY:HA3	2.43	0.49
4:H:66:ARG:HH11	4:H:66:ARG:CB	2.26	0.49
3:K:117:ILE:HD11	3:K:132:VAL:HG12	1.95	0.49
6:N:40:ALA:O	6:N:43:GLN:HB2	2.12	0.49
1:A:249:HIS:O	1:A:251:ILE:HG13	2.12	0.49
1:E:414:ILE:HG22	1:E:416:LEU:HD13	1.95	0.49
1:E:86:LEU:HD11	7:E:741:NAG:O7	2.12	0.49
3:G:169:LYS:HE3	3:G:169:LYS:HA	1.94	0.49
1:I:414:ILE:HG22	1:I:416:LEU:HD13	1.95	0.49
2:J:77:GLU:OE1	2:J:77:GLU:N	2.45	0.49
5:M:54:LEU:HD21	5:M:60:SER:HA	1.94	0.49
2:B:77:GLU:N	2:B:77:GLU:OE1	2.45	0.48
3:C:174:SER:O	4:D:166:PHE:HE2	1.96	0.48
4:D:182:VAL:O	4:D:182:VAL:HG13	2.12	0.48
4:D:66:ARG:HH11	4:D:66:ARG:CB	2.26	0.48
3:G:174:SER:O	4:H:166:PHE:HE2	1.96	0.48
1:A:292:VAL:HG12	1:A:333:LEU:HD11	1.95	0.48
1:A:361:PHE:C	1:A:362:ASN:HD22	2.16	0.48
1:E:100:MET:CG	1:E:488:VAL:HG12	2.42	0.48
2:F:178:ALA:HB3	2:F:180:GLN:HA	1.95	0.48
3:G:47:LEU:HD11	3:G:86:TYR:HE1	1.78	0.48
3:K:186:TYR:CE1	3:K:192:TYR:CE2	3.01	0.48
5:O:54:LEU:HD21	5:O:60:SER:HA	1.94	0.48
1:A:456:ARG:HD2	1:A:468:PHE:CZ	2.48	0.48
3:G:138:ASN:OD1	3:G:138:ASN:N	2.44	0.48
4:H:214:LYS:C	4:H:214:LYS:HD3	2.34	0.48
3:K:19:ALA:HB1	3:K:104:LEU:HD11	1.95	0.48
4:L:162:GLY:O	4:L:182:VAL:HG23	2.13	0.48
4:D:126:PRO:CG	4:D:138:LEU:HD13	2.43	0.48
4:D:162:GLY:O	4:D:182:VAL:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:344:GLN:HG2	7:E:789:NAG:C8	2.43	0.48
2:F:164:ASN:C	2:F:166:LYS:H	2.15	0.48
4:H:84:SER:HA	4:H:111:VAL:O	2.13	0.48
3:K:105:GLU:HG2	3:K:106:ILE:N	2.27	0.48
3:K:66:GLY:HA3	3:K:71:PHE:HA	1.95	0.48
4:L:84:SER:HA	4:L:111:VAL:O	2.14	0.48
3:C:193:ALA:HB1	3:C:206:THR:HG23	1.94	0.48
3:G:193:ALA:HB1	3:G:206:THR:HG23	1.94	0.48
4:H:5:VAL:O	4:H:23:LYS:N	2.43	0.48
3:K:142:ARG:N	3:K:143:GLU:OE1	2.47	0.48
1:A:124:PRO:HB3	2:B:60:SER:HA	1.96	0.48
2:F:154:SER:HB2	2:F:176:VAL:N	2.25	0.48
3:G:142:ARG:N	3:G:143:GLU:OE1	2.47	0.48
4:H:162:GLY:O	4:H:182:VAL:HG23	2.13	0.48
1:I:344:GLN:HG2	7:I:789:NAG:H83	1.95	0.48
3:K:47:LEU:HD11	3:K:86:TYR:HE1	1.78	0.48
4:L:121:VAL:HG11	4:L:196:CYS:SG	2.54	0.48
3:C:142:ARG:N	3:C:143:GLU:OE1	2.47	0.48
3:C:186:TYR:CE1	3:C:192:TYR:CE2	3.01	0.48
3:C:66:GLY:HA3	3:C:71:PHE:HA	1.95	0.48
1:E:269:GLU:HG2	7:E:789:NAG:HN2	1.79	0.48
1:E:272:ILE:O	1:E:272:ILE:CG1	2.62	0.48
3:G:186:TYR:CE1	3:G:192:TYR:CE2	3.01	0.48
4:L:126:PRO:CG	4:L:138:LEU:HD13	2.43	0.48
4:L:214:LYS:C	4:L:214:LYS:HD3	2.34	0.48
1:A:414:ILE:HG22	1:A:416:LEU:HD13	1.95	0.48
2:B:10:ASP:OD1	2:B:11:THR:N	2.41	0.48
4:D:214:LYS:C	4:D:214:LYS:HD3	2.34	0.48
3:G:120:PRO:HD3	3:G:132:VAL:HG22	1.96	0.48
3:G:187:GLU:O	3:G:211:ARG:NH1	2.47	0.48
3:G:33:LEU:HG	3:G:71:PHE:CG	2.49	0.48
4:H:117:LYS:O	4:H:117:LYS:HG3	2.14	0.48
1:I:119:CYS:N	1:I:205:CYS:SG	2.87	0.48
4:L:65:GLY:O	4:L:82(A):ARG:NH1	2.47	0.48
1:A:104:MET:HE2	1:A:215:ILE:HD11	1.95	0.48
3:C:24:ARG:HG3	3:C:24:ARG:HH11	1.78	0.48
3:C:33:LEU:HG	3:C:71:PHE:CG	2.49	0.48
4:D:121:VAL:HG11	4:D:196:CYS:SG	2.54	0.48
4:D:66:ARG:HA	4:D:82(A):ARG:HH11	1.79	0.48
2:F:151:LEU:HA	2:F:176:VAL:HG11	1.96	0.48
2:J:160:THR:HG23	2:J:167:LYS:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:178:ALA:HB3	2:J:180:GLN:HA	1.95	0.48
2:J:83:ILE:HG23	2:J:92:GLU:CG	2.44	0.48
3:K:187:GLU:O	3:K:211:ARG:NH1	2.47	0.48
3:K:24:ARG:HG3	3:K:24:ARG:HH11	1.78	0.48
3:K:33:LEU:HG	3:K:71:PHE:CG	2.49	0.48
3:K:174:SER:O	4:L:166:PHE:HE2	1.96	0.48
6:N:35(A):ASN:O	6:N:93:THR:HB	2.13	0.48
1:A:411:GLY:O	7:A:908:NAG:O6	2.30	0.48
1:E:411:GLY:O	7:E:908:NAG:O6	2.30	0.48
1:E:456:ARG:HD2	1:E:468:PHE:CZ	2.48	0.48
4:H:121:VAL:HG11	4:H:196:CYS:SG	2.54	0.48
6:N:13:LYS:O	6:N:16:SER:OG	2.27	0.48
6:P:35(A):ASN:O	6:P:93:THR:HB	2.13	0.48
6:R:35(A):ASN:O	6:R:93:THR:HB	2.13	0.48
2:B:98:PHE:HE1	2:B:120:SER:HG	1.61	0.47
3:C:117:ILE:HD11	3:C:132:VAL:HG12	1.95	0.47
3:C:47:LEU:HD11	3:C:86:TYR:HE1	1.78	0.47
1:I:456:ARG:HD2	1:I:468:PHE:CZ	2.48	0.47
3:K:105:GLU:HG3	3:K:166:GLN:NE2	2.29	0.47
4:L:66:ARG:HA	4:L:82(A):ARG:HH11	1.79	0.47
1:A:102:GLU:OE1	1:A:476:ARG:NE	2.43	0.47
3:C:120:PRO:HD3	3:C:132:VAL:HG22	1.96	0.47
3:C:105:GLU:HG3	3:C:166:GLN:NE2	2.29	0.47
1:E:119:CYS:N	1:E:205:CYS:SG	2.87	0.47
1:E:335:LYS:HD3	1:E:408:ASN:HA	1.96	0.47
3:G:137:ASN:ND2	3:G:138:ASN:OD1	2.48	0.47
3:G:91:TYR:O	3:G:91:TYR:CD1	2.67	0.47
3:K:46:LEU:HD13	4:L:101:LYS:HD2	1.94	0.47
1:A:119:CYS:N	1:A:205:CYS:SG	2.87	0.47
2:B:83:ILE:HA	2:B:92:GLU:HA	1.97	0.47
4:D:65:GLY:O	4:D:82(A):ARG:NH1	2.47	0.47
2:F:2:LYS:CD	2:F:3:VAL:H	2.26	0.47
2:F:83:ILE:HA	2:F:92:GLU:HA	1.97	0.47
4:H:65:GLY:O	4:H:82(A):ARG:NH1	2.47	0.47
4:H:66:ARG:NH1	4:H:66:ARG:HB2	2.29	0.47
4:L:117:LYS:HG3	4:L:117:LYS:O	2.14	0.47
4:L:38:ARG:HB3	4:L:90:TYR:CD2	2.49	0.47
4:L:66:ARG:NH1	4:L:66:ARG:HB2	2.29	0.47
3:C:137:ASN:ND2	3:C:138:ASN:OD1	2.47	0.47
3:C:187:GLU:O	3:C:211:ARG:NH1	2.47	0.47
1:E:105:HIS:HB2	1:E:479:TRP:CD1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:117:ILE:HD11	3:G:132:VAL:HG12	1.95	0.47
1:I:269:GLU:HG2	7:I:789:NAG:HN2	1.79	0.47
2:J:151:LEU:HA	2:J:176:VAL:HG11	1.96	0.47
3:K:48:ILE:HG22	3:K:49:TYR:N	2.29	0.47
4:L:66:ARG:CB	4:L:66:ARG:HH11	2.26	0.47
1:A:124:PRO:HG2	2:B:60:SER:HA	1.96	0.47
2:B:178:ALA:HB1	2:B:180:GLN:N	2.26	0.47
2:B:3:VAL:HG22	2:B:94:GLN:CB	2.44	0.47
3:C:83:PHE:O	3:C:84:ALA:HB2	2.15	0.47
1:E:100:MET:HG3	1:E:488:VAL:HG12	1.97	0.47
2:F:130:CYS:CA	2:F:159:CYS:HA	2.34	0.47
2:F:98:PHE:HE1	2:F:120:SER:HG	1.61	0.47
4:H:38:ARG:HB3	4:H:90:TYR:CD2	2.49	0.47
1:A:109:ILE:HG23	1:A:428:GLN:HG2	1.95	0.47
1:A:215:ILE:HG13	1:A:215:ILE:O	2.15	0.47
1:A:371:ILE:HD11	2:B:43:PHE:CD2	2.50	0.47
3:C:91:TYR:O	3:C:91:TYR:CD1	2.67	0.47
4:D:66:ARG:NH1	4:D:66:ARG:HB2	2.29	0.47
1:E:371:ILE:HD11	2:F:43:PHE:CD2	2.49	0.47
3:G:105:GLU:HG2	3:G:106:ILE:N	2.27	0.47
3:G:24:ARG:HH11	3:G:24:ARG:HG3	1.78	0.47
1:I:124:PRO:HG2	2:J:60:SER:HA	1.97	0.47
1:I:231:LYS:HB2	1:I:268:GLU:HB2	1.96	0.47
1:I:272:ILE:CG1	1:I:272:ILE:O	2.62	0.47
3:K:120:PRO:HD3	3:K:132:VAL:HG22	1.96	0.47
3:K:198:HIS:HD2	3:K:199:GLN:H	1.59	0.47
1:A:105:HIS:HB2	1:A:479:TRP:CD1	2.49	0.47
1:A:227:LYS:HE3	1:A:485:LYS:HE3	1.96	0.47
3:C:198:HIS:HD2	3:C:199:GLN:H	1.59	0.47
4:D:137:ALA:HA	4:D:183:THR:HA	1.97	0.47
4:D:38:ARG:HB3	4:D:90:TYR:CD2	2.49	0.47
1:E:227:LYS:HE3	1:E:485:LYS:HE3	1.96	0.47
3:G:105:GLU:HG3	3:G:166:GLN:NE2	2.29	0.47
3:G:48:ILE:HG22	3:G:49:TYR:N	2.29	0.47
3:G:133:VAL:CG2	4:H:141:LEU:HD13	2.45	0.47
1:I:119:CYS:HB3	3:K:94:TRP:NE1	2.30	0.47
1:I:256:SER:HB2	1:I:376:PHE:HB3	1.96	0.47
2:B:83:ILE:HG23	2:B:92:GLU:CG	2.44	0.47
4:D:117:LYS:HG3	4:D:117:LYS:O	2.14	0.47
4:D:84:SER:HA	4:D:111:VAL:O	2.13	0.47
1:E:381:GLU:HB3	1:E:420:ILE:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:28:TRP:HB2	2:F:37:LEU:HD23	1.97	0.47
3:G:91:TYR:HB2	4:H:100(I):GLY:HA3	1.97	0.47
1:I:109:ILE:HG23	1:I:428:GLN:HG2	1.95	0.47
2:J:98:PHE:HE1	2:J:120:SER:HG	1.61	0.47
1:A:221:ALA:C	1:A:223:PHE:H	2.17	0.47
1:E:268:GLU:HB3	1:E:269:GLU:H	1.51	0.47
2:F:178:ALA:HB1	2:F:180:GLN:N	2.25	0.47
4:H:66:ARG:HA	4:H:82(A):ARG:HH11	1.79	0.47
1:I:95:MET:CE	1:I:235:GLY:HA3	2.43	0.47
3:K:137:ASN:ND2	3:K:138:ASN:OD1	2.48	0.47
4:L:189:LEU:HB3	4:L:213:PRO:CG	2.45	0.47
6:R:38:ARG:HB3	6:R:48:ILE:HD11	1.97	0.47
1:A:272:ILE:O	1:A:272:ILE:CG1	2.62	0.47
1:A:335:LYS:HD3	1:A:408:ASN:HA	1.96	0.47
3:C:114:SER:O	3:C:116:PHE:CD1	2.68	0.47
4:D:189:LEU:HB3	4:D:213:PRO:CG	2.45	0.47
1:E:119:CYS:HB3	3:G:94:TRP:NE1	2.30	0.47
1:E:221:ALA:C	1:E:223:PHE:H	2.17	0.47
2:F:100:LEU:HB2	2:F:170:PHE:CD1	2.50	0.47
2:F:108:LEU:O	2:F:109:LEU:O	2.33	0.47
3:G:114:SER:O	3:G:116:PHE:CD1	2.68	0.47
1:I:102:GLU:OE1	1:I:476:ARG:NE	2.43	0.47
1:I:279:ASN:ND2	1:I:282:LYS:HG2	2.30	0.47
1:I:259:LEU:HB2	1:I:374:HIS:CE1	2.50	0.47
1:I:105:HIS:HB2	1:I:479:TRP:CD1	2.49	0.47
1:I:227:LYS:HE3	1:I:485:LYS:HE3	1.96	0.47
2:J:114:LEU:HD11	2:J:116:LEU:HD21	1.97	0.47
3:K:28:SER:HA	3:K:68:GLY:O	2.15	0.47
1:A:256:SER:HB2	1:A:376:PHE:HB3	1.96	0.47
1:A:231:LYS:HB2	1:A:268:GLU:HB2	1.96	0.47
3:C:183:LYS:C	3:C:183:LYS:HD3	2.35	0.47
3:G:183:LYS:HD3	3:G:183:LYS:C	2.35	0.47
3:K:91:TYR:O	3:K:91:TYR:CD1	2.67	0.47
3:K:94:TRP:CE3	3:K:95(A):PRO:HG3	2.49	0.47
4:L:7:SER:HB3	4:L:21:SER:H	1.80	0.47
5:M:145:LYS:HB3	5:M:197:THR:OG1	2.15	0.47
1:A:269:GLU:HG2	7:A:789:NAG:HN2	1.79	0.46
2:B:108:LEU:O	2:B:109:LEU:O	2.33	0.46
2:B:151:LEU:HA	2:B:176:VAL:HG11	1.96	0.46
2:F:160:THR:HG23	2:F:167:LYS:HB2	1.96	0.46
1:E:124:PRO:HB3	2:F:60:SER:HA	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:83:ILE:HG23	2:F:92:GLU:CG	2.44	0.46
6:P:38:ARG:HB3	6:P:48:ILE:HD11	1.97	0.46
2:B:154:SER:OG	2:B:175:VAL:HA	2.15	0.46
3:G:193:ALA:CB	3:G:208:SER:HB3	2.45	0.46
3:G:83:PHE:O	3:G:84:ALA:HB2	2.15	0.46
4:H:7:SER:HB3	4:H:21:SER:H	1.80	0.46
2:J:100:LEU:HB2	2:J:170:PHE:CD1	2.50	0.46
2:J:37:LEU:N	2:J:37:LEU:HD23	2.31	0.46
4:L:163:VAL:HG12	4:L:182:VAL:CB	2.42	0.46
1:A:273:ARG:NH1	1:A:484:TYR:CD1	2.84	0.46
1:A:100:MET:HG3	1:A:488:VAL:HG12	1.97	0.46
2:B:120:SER:HG	2:B:121:PRO:HD2	1.81	0.46
3:C:28:SER:HA	3:C:68:GLY:O	2.15	0.46
4:D:126:PRO:O	4:D:128:SER:N	2.48	0.46
3:C:133:VAL:CG2	4:D:141:LEU:HD13	2.44	0.46
4:D:160:THR:O	4:D:163:VAL:HG22	2.15	0.46
4:D:170:LEU:HD13	4:D:176:TYR:CZ	2.50	0.46
1:E:390:LEU:HG	1:E:416:LEU:HD21	1.98	0.46
3:K:114:SER:O	3:K:116:PHE:CD1	2.68	0.46
3:K:193:ALA:CB	3:K:208:SER:HB3	2.45	0.46
3:C:193:ALA:CB	3:C:208:SER:HB3	2.45	0.46
3:C:48:ILE:HG22	3:C:49:TYR:N	2.29	0.46
3:C:91:TYR:HB2	4:D:100(I):GLY:HA3	1.97	0.46
1:E:280:ASN:O	2:F:35:LYS:CD	2.60	0.46
1:E:465:THR:HG23	1:E:465:THR:O	2.16	0.46
2:F:76:ILE:CD1	2:F:76:ILE:H	2.14	0.46
1:I:93:PHE:CE2	1:I:487:LYS:HG2	2.51	0.46
2:J:108:LEU:HD22	2:J:149:LEU:HD23	1.98	0.46
3:K:83:PHE:O	3:K:84:ALA:HB2	2.15	0.46
4:L:126:PRO:HG3	4:L:138:LEU:HB3	1.98	0.46
4:L:170:LEU:HD13	4:L:176:TYR:CZ	2.50	0.46
4:L:137:ALA:HA	4:L:183:THR:HA	1.96	0.46
4:L:39:GLN:NE2	4:L:44:GLY:HA2	2.23	0.46
1:A:119:CYS:HB3	3:C:94:TRP:NE1	2.30	0.46
2:B:100:LEU:HB2	2:B:170:PHE:CD1	2.50	0.46
1:E:124:PRO:HG2	2:F:60:SER:HA	1.96	0.46
3:G:25:ALA:O	3:G:26:SER:O	2.33	0.46
1:I:335:LYS:HD3	1:I:408:ASN:HA	1.96	0.46
1:I:371:ILE:HD11	2:J:43:PHE:CD2	2.50	0.46
1:I:124:PRO:HB3	2:J:60:SER:HA	1.96	0.46
3:K:183:LYS:HD3	3:K:183:LYS:C	2.35	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:LEU:HB2	1:A:374:HIS:CE1	2.50	0.46
2:B:130:CYS:CA	2:B:159:CYS:HA	2.34	0.46
3:C:25:ALA:O	3:C:26:SER:O	2.33	0.46
1:E:93:PHE:CE2	1:E:487:LYS:HG2	2.51	0.46
2:F:110:GLN:HA	2:F:176:VAL:HG13	1.98	0.46
1:I:273:ARG:NH1	1:I:484:TYR:CD1	2.84	0.46
3:K:91:TYR:HB2	4:L:100(I):GLY:HA3	1.97	0.46
1:A:280:ASN:O	2:B:35:LYS:CD	2.60	0.46
1:A:381:GLU:HB3	1:A:420:ILE:HD13	1.96	0.46
2:B:108:LEU:HD22	2:B:149:LEU:HD23	1.97	0.46
2:B:37:LEU:HD23	2:B:37:LEU:N	2.30	0.46
1:E:236:THR:O	1:E:236:THR:HG23	2.16	0.46
1:E:343:GLU:C	1:E:345:ILE:H	2.19	0.46
1:E:354:GLY:O	1:E:357:LYS:HB2	2.16	0.46
1:E:259:LEU:HB2	1:E:374:HIS:CE1	2.50	0.46
3:G:28:SER:HA	3:G:68:GLY:O	2.15	0.46
4:H:126:PRO:CG	4:H:138:LEU:HD13	2.43	0.46
4:H:11:VAL:CG2	4:H:147:PRO:HG3	2.46	0.46
1:I:100:MET:HG3	1:I:488:VAL:HG12	1.96	0.46
3:K:134:CYS:O	3:K:136:LEU:HD12	2.15	0.46
1:A:104:MET:HE2	1:A:217:TYR:HE2	1.81	0.46
1:A:236:THR:HG23	1:A:236:THR:O	2.16	0.46
1:A:412:ARG:HA	7:A:908:NAG:C6	2.46	0.46
1:E:256:SER:HB2	1:E:376:PHE:HB3	1.96	0.46
1:E:231:LYS:HB2	1:E:268:GLU:HB2	1.96	0.46
1:E:100:MET:HE1	1:E:486:TYR:CB	2.46	0.46
1:I:215:ILE:O	1:I:215:ILE:HG13	2.15	0.46
2:J:28:TRP:HB2	2:J:37:LEU:HD23	1.97	0.46
4:L:126:PRO:O	4:L:128:SER:N	2.48	0.46
1:A:95:MET:CE	1:A:235:GLY:HA3	2.43	0.46
2:B:160:THR:HG23	2:B:167:LYS:HB2	1.96	0.46
3:C:134:CYS:O	3:C:136:LEU:HD12	2.15	0.46
4:D:7:SER:HB3	4:D:21:SER:H	1.80	0.46
1:E:215:ILE:O	1:E:215:ILE:HG13	2.15	0.46
1:E:95:MET:CB	1:E:484:TYR:HA	2.46	0.46
4:H:160:THR:O	4:H:163:VAL:HG22	2.15	0.46
1:I:354:GLY:O	1:I:357:LYS:HB2	2.16	0.46
1:I:381:GLU:HB3	1:I:420:ILE:HD13	1.96	0.46
4:L:169:VAL:O	4:L:176:TYR:HA	2.16	0.46
1:A:274:SER:HB3	1:A:277:PHE:CD1	2.51	0.46
1:A:390:LEU:HG	1:A:416:LEU:HD21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:37:LEU:N	2:F:37:LEU:HD23	2.30	0.46
4:H:170:LEU:HD13	4:H:176:TYR:CZ	2.50	0.46
4:H:189:LEU:HB3	4:H:213:PRO:CG	2.45	0.46
1:I:274:SER:HB3	1:I:277:PHE:CD1	2.51	0.46
1:I:343:GLU:C	1:I:345:ILE:H	2.20	0.46
1:I:94:ASN:ND2	1:I:97:LYS:CB	2.79	0.46
2:J:30:ASN:O	2:J:33:GLN:N	2.48	0.46
4:L:160:THR:O	4:L:163:VAL:HG22	2.15	0.46
5:O:145:LYS:HB3	5:O:197:THR:OG1	2.15	0.46
1:A:95:MET:HE1	1:A:273:ARG:HG2	1.99	0.45
2:B:114:LEU:HD11	2:B:116:LEU:HD21	1.97	0.45
2:F:3:VAL:HG22	2:F:94:GLN:CB	2.44	0.45
4:H:126:PRO:O	4:H:128:SER:N	2.48	0.45
1:I:390:LEU:HG	1:I:416:LEU:HD21	1.98	0.45
1:I:95:MET:CB	1:I:484:TYR:HA	2.46	0.45
2:J:108:LEU:O	2:J:109:LEU:O	2.33	0.45
1:A:273:ARG:NH1	1:A:273:ARG:CG	2.78	0.45
1:A:93:PHE:CE2	1:A:487:LYS:HG2	2.51	0.45
1:E:257:THR:O	1:E:258:GLN:HB2	2.16	0.45
2:F:114:LEU:HD11	2:F:116:LEU:HD21	1.97	0.45
2:F:154:SER:OG	2:F:175:VAL:HA	2.15	0.45
3:G:134:CYS:O	3:G:136:LEU:HD12	2.15	0.45
4:H:137:ALA:HA	4:H:183:THR:HA	1.97	0.45
4:H:39:GLN:NE2	4:H:44:GLY:HA2	2.23	0.45
1:I:465:THR:HG23	1:I:465:THR:O	2.16	0.45
2:J:83:ILE:HA	2:J:92:GLU:HA	1.97	0.45
6:N:6:GLN:HB3	6:N:107:THR:CG2	2.47	0.45
6:N:38:ARG:HB3	6:N:48:ILE:HD11	1.97	0.45
1:A:368:ASP:OD2	2:B:59:ARG:NH2	2.43	0.45
2:B:110:GLN:HA	2:B:176:VAL:HG13	1.98	0.45
4:D:100(J):PHE:O	4:D:100(K):LEU:HD23	2.16	0.45
1:E:102:GLU:OE1	1:E:476:ARG:NE	2.43	0.45
1:E:98:ASN:HB3	1:E:101:VAL:HG23	1.99	0.45
6:P:6:GLN:HB3	6:P:107:THR:CG2	2.47	0.45
5:Q:145:LYS:HB3	5:Q:197:THR:OG1	2.15	0.45
1:A:440:ARG:O	1:A:442:GLN:N	2.50	0.45
1:A:465:THR:O	1:A:465:THR:HG23	2.16	0.45
1:A:105:HIS:HB2	1:A:479:TRP:HD1	1.82	0.45
2:B:28:TRP:HB2	2:B:37:LEU:HD23	1.97	0.45
1:E:440:ARG:O	1:E:442:GLN:N	2.50	0.45
1:E:273:ARG:NH1	1:E:484:TYR:CD1	2.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:110:GLN:HA	2:J:176:VAL:HG13	1.98	0.45
1:A:94:ASN:ND2	1:A:97:LYS:CB	2.79	0.45
2:B:30:ASN:O	2:B:33:GLN:N	2.48	0.45
3:C:73:LEU:HD13	3:C:73:LEU:O	2.17	0.45
1:E:412:ARG:HA	7:E:908:NAG:C6	2.46	0.45
1:E:460:LYS:O	1:E:460:LYS:HG3	2.16	0.45
1:I:236:THR:O	1:I:236:THR:HG23	2.16	0.45
1:I:269:GLU:CG	7:I:789:NAG:HN2	2.29	0.45
1:I:460:LYS:O	1:I:460:LYS:HG3	2.16	0.45
2:J:3:VAL:HG22	2:J:94:GLN:CB	2.44	0.45
2:J:54:ARG:NH1	2:J:75:LYS:HG3	2.31	0.45
2:J:94:GLN:HG3	2:J:96:LEU:HD22	1.98	0.45
3:K:112:ALA:HB2	3:K:200:GLY:O	2.17	0.45
3:K:25:ALA:O	3:K:26:SER:O	2.33	0.45
1:A:257:THR:O	1:A:258:GLN:HB2	2.17	0.45
1:A:269:GLU:CG	7:A:789:NAG:HN2	2.29	0.45
1:A:460:LYS:HG3	1:A:460:LYS:O	2.16	0.45
2:B:59:ARG:HG3	2:B:59:ARG:H	1.60	0.45
3:C:33:LEU:C	3:C:33:LEU:HD13	2.37	0.45
1:E:274:SER:HB3	1:E:277:PHE:CD1	2.51	0.45
1:E:98:ASN:ND2	1:E:486:TYR:O	2.50	0.45
1:E:95:MET:HE1	1:E:273:ARG:NH1	2.24	0.45
1:I:448:ASN:OD1	7:I:948:NAG:H2	2.17	0.45
3:K:33:LEU:C	3:K:33:LEU:HD13	2.37	0.45
3:K:3:VAL:HB	3:K:26:SER:OG	2.17	0.45
3:K:133:VAL:CG2	4:L:141:LEU:HD13	2.45	0.45
1:A:95:MET:CB	1:A:484:TYR:HA	2.46	0.45
3:C:48:ILE:CD1	3:C:54:ARG:HA	2.47	0.45
2:F:54:ARG:NH1	2:F:75:LYS:HG3	2.32	0.45
4:H:52(A):THR:O	4:H:55:ASP:N	2.48	0.45
2:J:73:ASN:HA	2:J:73:ASN:HD22	1.65	0.45
4:L:152:VAL:HG11	4:L:180:SER:CB	2.47	0.45
1:A:98:ASN:HB3	1:A:101:VAL:HG23	1.99	0.45
2:B:114:LEU:C	2:B:114:LEU:HD13	2.38	0.45
3:C:103:ARG:HG3	3:C:103:ARG:HH11	1.82	0.45
3:C:112:ALA:HB2	3:C:200:GLY:O	2.17	0.45
3:C:79:GLN:O	3:C:82:ASP:HB2	2.17	0.45
4:D:52(A):THR:O	4:D:55:ASP:N	2.48	0.45
2:F:108:LEU:C	2:F:177:LEU:HD13	2.36	0.45
4:H:119:PRO:HB3	4:H:145:TYR:CB	2.46	0.45
1:I:412:ARG:HA	7:I:908:NAG:C6	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:95:MET:HB3	1:I:484:TYR:HA	1.99	0.45
4:L:59:TYR:CE2	4:L:68:THR:HA	2.52	0.45
1:A:354:GLY:O	1:A:357:LYS:HB2	2.16	0.45
4:D:169:VAL:O	4:D:176:TYR:HA	2.16	0.45
1:E:269:GLU:CG	7:E:789:NAG:HN2	2.29	0.45
1:E:94:ASN:ND2	1:E:97:LYS:CB	2.79	0.45
2:F:108:LEU:HD22	2:F:149:LEU:HD23	1.98	0.45
2:F:30:ASN:O	2:F:33:GLN:N	2.48	0.45
3:G:198:HIS:HD2	3:G:199:GLN:H	1.59	0.45
4:H:59:TYR:CE2	4:H:68:THR:HA	2.52	0.45
1:I:221:ALA:C	1:I:223:PHE:H	2.17	0.45
2:J:146:VAL:O	2:J:147:SER:C	2.56	0.45
2:J:150:GLU:HB2	2:J:153:ASP:OD2	2.17	0.45
1:A:268:GLU:HB3	1:A:269:GLU:H	1.51	0.45
3:C:94:TRP:CE3	3:C:95(A):PRO:HG3	2.49	0.45
4:H:169:VAL:O	4:H:176:TYR:HA	2.16	0.45
1:I:440:ARG:O	1:I:442:GLN:N	2.50	0.45
2:J:154:SER:OG	2:J:175:VAL:HA	2.15	0.45
1:A:279:ASN:ND2	1:A:282:LYS:HG2	2.30	0.44
1:A:343:GLU:C	1:A:345:ILE:H	2.19	0.44
2:B:146:VAL:O	2:B:147:SER:C	2.56	0.44
3:C:3:VAL:HB	3:C:26:SER:OG	2.17	0.44
4:D:11:VAL:CG2	4:D:147:PRO:HG3	2.46	0.44
4:D:34:PHE:CG	4:D:78:VAL:HG21	2.53	0.44
1:E:279:ASN:ND2	1:E:282:LYS:HG2	2.30	0.44
2:F:166:LYS:C	2:F:167:LYS:HD3	2.38	0.44
3:G:86:TYR:CE2	3:G:104:LEU:HD22	2.49	0.44
3:G:163:VAL:HG12	3:G:164:THR:O	2.18	0.44
3:G:3:VAL:HB	3:G:26:SER:OG	2.17	0.44
3:G:50:GLY:O	3:G:51:ALA:HB3	2.17	0.44
4:H:152:VAL:HG11	4:H:180:SER:CB	2.47	0.44
1:I:98:ASN:ND2	1:I:486:TYR:O	2.50	0.44
3:K:120:PRO:HG3	3:K:186:TYR:CZ	2.52	0.44
4:L:28:THR:HB	4:L:31:ARG:HD2	1.99	0.44
2:B:80:ASP:HB3	2:B:82:TYR:CE1	2.52	0.44
4:D:126:PRO:HG3	4:D:138:LEU:HB3	1.98	0.44
2:F:70:ILE:H	2:F:70:ILE:HD12	1.82	0.44
2:F:80:ASP:HB3	2:F:82:TYR:CE1	2.52	0.44
3:G:6:GLN:OE1	3:G:99:GLY:HA3	2.18	0.44
4:H:100(J):PHE:O	4:H:100(K):LEU:HD23	2.16	0.44
1:I:257:THR:O	1:I:258:GLN:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:50:GLY:O	3:K:51:ALA:HB3	2.17	0.44
1:A:221:ALA:C	1:A:223:PHE:N	2.71	0.44
2:B:150:GLU:HB2	2:B:153:ASP:OD2	2.17	0.44
2:B:166:LYS:C	2:B:167:LYS:HD3	2.38	0.44
2:B:54:ARG:NH1	2:B:75:LYS:HG3	2.31	0.44
4:D:199:ASN:HD21	4:D:201:LYS:HG2	1.83	0.44
2:F:28:TRP:CE2	2:F:69:LEU:HB2	2.53	0.44
3:G:16:GLY:HA2	3:G:77:SER:OG	2.18	0.44
3:G:210:ASN:O	3:G:212:GLY:N	2.50	0.44
3:G:73:LEU:HD13	3:G:73:LEU:O	2.17	0.44
4:H:87:THR:HG23	4:H:110:THR:HA	1.99	0.44
4:H:126:PRO:HG3	4:H:138:LEU:HB3	1.98	0.44
4:H:69:ILE:HG12	4:H:80:LEU:HD23	2.00	0.44
1:I:221:ALA:C	1:I:223:PHE:N	2.71	0.44
2:J:108:LEU:C	2:J:177:LEU:HD13	2.36	0.44
3:K:163:VAL:HG12	3:K:164:THR:O	2.18	0.44
3:K:79:GLN:O	3:K:82:ASP:HB2	2.17	0.44
2:B:28:TRP:CE2	2:B:69:LEU:HB2	2.52	0.44
3:C:175:LEU:HD12	3:C:176:SER:N	2.29	0.44
3:C:210:ASN:O	3:C:212:GLY:N	2.51	0.44
4:D:152:VAL:HG11	4:D:180:SER:CB	2.47	0.44
4:D:59:TYR:CE2	4:D:68:THR:HA	2.52	0.44
1:E:448:ASN:OD1	7:E:948:NAG:H2	2.17	0.44
1:E:89:VAL:HG22	1:E:90:THR:N	2.33	0.44
2:F:126:PRO:HB2	2:F:161:VAL:HG13	1.99	0.44
2:F:146:VAL:O	2:F:147:SER:C	2.56	0.44
2:F:94:GLN:HG3	2:F:96:LEU:HD22	1.98	0.44
3:G:175:LEU:HD12	3:G:176:SER:N	2.29	0.44
3:K:124:GLN:O	3:K:127:SER:HB2	2.18	0.44
4:L:100(J):PHE:O	4:L:100(K):LEU:HD23	2.16	0.44
4:L:69:ILE:HG12	4:L:80:LEU:HD23	2.00	0.44
1:A:335:LYS:O	1:A:339:GLU:HB2	2.18	0.44
1:A:100:MET:HE1	1:A:486:TYR:CB	2.47	0.44
2:B:154:SER:HB2	2:B:176:VAL:CB	2.48	0.44
1:E:273:ARG:NH1	1:E:273:ARG:CG	2.78	0.44
1:E:95:MET:HB3	1:E:484:TYR:HA	1.99	0.44
1:I:108:ILE:HD12	1:I:253:PRO:HB2	2.00	0.44
1:I:100:MET:HE1	1:I:486:TYR:CB	2.47	0.44
2:J:80:ASP:HB3	2:J:82:TYR:CE1	2.52	0.44
3:K:16:GLY:HA2	3:K:77:SER:OG	2.18	0.44
3:K:210:ASN:O	3:K:212:GLY:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:CYS:N	1:A:206:PRO:CD	2.81	0.44
3:C:6:GLN:OE1	3:C:99:GLY:HA3	2.18	0.44
1:E:108:ILE:HD12	1:E:253:PRO:HB2	2.00	0.44
3:G:120:PRO:HG3	3:G:186:TYR:CZ	2.52	0.44
4:H:163:VAL:HG12	4:H:182:VAL:CB	2.42	0.44
4:H:199:ASN:HD21	4:H:201:LYS:HG2	1.83	0.44
1:I:98:ASN:HB3	1:I:101:VAL:HG23	1.99	0.44
1:I:335:LYS:O	1:I:339:GLU:HB2	2.18	0.44
2:J:28:TRP:CE2	2:J:69:LEU:HB2	2.52	0.44
1:A:359:ILE:O	1:A:395:ASP:HB2	2.18	0.44
1:A:98:ASN:ND2	1:A:486:TYR:O	2.50	0.44
2:B:78:ASP:O	2:B:95:LEU:HD23	2.18	0.44
3:C:86:TYR:CE2	3:C:104:LEU:HD22	2.49	0.44
4:D:28:THR:HB	4:D:31:ARG:HD2	1.99	0.44
1:E:335:LYS:O	1:E:339:GLU:HB2	2.18	0.44
2:F:114:LEU:HD13	2:F:114:LEU:C	2.38	0.44
2:F:150:GLU:HB2	2:F:153:ASP:OD2	2.17	0.44
3:G:112:ALA:HB2	3:G:200:GLY:O	2.17	0.44
3:G:79:GLN:O	3:G:82:ASP:HB2	2.17	0.44
4:H:34:PHE:CG	4:H:78:VAL:HG21	2.52	0.44
2:J:114:LEU:C	2:J:114:LEU:HD13	2.38	0.44
2:J:130:CYS:CA	2:J:159:CYS:HA	2.34	0.44
2:J:78:ASP:O	2:J:95:LEU:HD23	2.18	0.44
1:A:279:ASN:C	1:A:281:ALA:H	2.22	0.44
1:A:448:ASN:OD1	7:A:948:NAG:H2	2.17	0.44
1:A:95:MET:HB3	1:A:484:TYR:HA	1.99	0.44
4:D:87:THR:HG23	4:D:110:THR:HA	1.99	0.44
4:D:54:LEU:HD12	4:D:54:LEU:HA	1.83	0.44
1:E:108:ILE:HD12	1:E:253:PRO:HB3	1.99	0.44
1:E:105:HIS:HB2	1:E:479:TRP:HD1	1.82	0.44
3:G:103:ARG:HG3	3:G:103:ARG:HH11	1.82	0.44
3:G:33:LEU:C	3:G:33:LEU:HD13	2.37	0.44
1:I:108:ILE:HD12	1:I:253:PRO:HB3	1.99	0.44
1:I:89:VAL:HG22	1:I:90:THR:N	2.33	0.44
3:K:48:ILE:CD1	3:K:54:ARG:HA	2.47	0.44
4:L:199:ASN:HD21	4:L:201:LYS:HG2	1.83	0.44
4:L:7:SER:CB	4:L:21:SER:H	2.31	0.44
1:A:105:HIS:HA	1:A:479:TRP:NE1	2.33	0.44
1:A:221:ALA:O	1:A:223:PHE:HD1	2.01	0.44
1:A:272:ILE:O	1:A:277:PHE:HZ	2.01	0.44
2:B:94:GLN:HG3	2:B:96:LEU:HD22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:120:PRO:HG3	3:C:186:TYR:CZ	2.53	0.44
3:C:163:VAL:HG12	3:C:164:THR:O	2.17	0.44
1:E:359:ILE:O	1:E:395:ASP:HB2	2.18	0.44
2:F:120:SER:HG	2:F:121:PRO:HD2	1.81	0.44
2:F:154:SER:HB2	2:F:176:VAL:CB	2.47	0.44
3:G:48:ILE:CD1	3:G:54:ARG:HA	2.47	0.44
1:I:340:ASN:O	1:I:343:GLU:HB2	2.18	0.44
1:A:95:MET:CE	1:A:273:ARG:HG2	2.48	0.43
1:E:350:LYS:HE2	1:E:359:ILE:HD13	2.00	0.43
2:F:36:ILE:HD13	2:F:49:SER:HB3	2.00	0.43
2:F:5:LEU:HB2	2:F:168:VAL:HG13	2.00	0.43
3:G:124:GLN:O	3:G:127:SER:HB2	2.18	0.43
3:G:4:MET:HE1	3:G:33:LEU:HD23	2.00	0.43
3:G:55:ALA:O	3:G:58:VAL:HG23	2.18	0.43
1:I:359:ILE:O	1:I:395:ASP:HB2	2.18	0.43
1:I:105:HIS:HB2	1:I:479:TRP:HD1	1.82	0.43
2:J:126:PRO:HB2	2:J:161:VAL:HG13	1.99	0.43
2:J:154:SER:HB2	2:J:176:VAL:CB	2.47	0.43
3:K:161:GLU:OE2	3:K:175:LEU:HD21	2.18	0.43
3:K:6:GLN:OE1	3:K:99:GLY:HA3	2.18	0.43
5:O:22:SER:CA	5:O:72:THR:HG22	2.48	0.43
6:R:6:GLN:HB3	6:R:107:THR:CG2	2.47	0.43
1:A:108:ILE:HD12	1:A:253:PRO:HB3	1.99	0.43
1:A:280:ASN:ND2	2:B:35:LYS:HD3	2.33	0.43
4:D:1:GLU:O	4:D:3:GLN:NE2	2.48	0.43
1:I:221:ALA:O	1:I:223:PHE:HD1	2.01	0.43
1:I:350:LYS:HE2	1:I:359:ILE:HD13	2.00	0.43
1:I:95:MET:HE1	1:I:273:ARG:HG2	2.00	0.43
2:J:151:LEU:HD12	2:J:176:VAL:HB	2.00	0.43
2:J:157:TRP:O	2:J:171:LYS:HA	2.18	0.43
2:J:178:ALA:HB1	2:J:180:GLN:N	2.25	0.43
1:I:280:ASN:ND2	2:J:35:LYS:HD3	2.33	0.43
2:J:79:SER:HA	2:J:95:LEU:O	2.18	0.43
3:K:73:LEU:HD13	3:K:73:LEU:O	2.17	0.43
1:A:89:VAL:HG22	1:A:90:THR:N	2.33	0.43
2:B:70:ILE:HD12	2:B:70:ILE:H	1.82	0.43
3:C:143:GLU:CD	3:C:143:GLU:H	2.21	0.43
3:C:167:ASP:OD2	4:D:164:HIS:NE2	2.51	0.43
2:F:14:LEU:HD23	2:F:14:LEU:N	2.33	0.43
2:F:151:LEU:HD12	2:F:176:VAL:HB	2.00	0.43
2:F:36:ILE:HA	2:F:49:SER:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:79:SER:HA	2:F:95:LEU:O	2.18	0.43
1:I:105:HIS:HA	1:I:479:TRP:NE1	2.33	0.43
1:A:108:ILE:HD12	1:A:253:PRO:HB2	2.00	0.43
2:B:151:LEU:HD12	2:B:176:VAL:HB	2.00	0.43
3:G:161:GLU:OE2	3:G:175:LEU:HD21	2.18	0.43
4:H:28:THR:HB	4:H:31:ARG:HD2	1.99	0.43
1:I:446:SER:O	7:I:948:NAG:H62	2.19	0.43
3:K:103:ARG:HG3	3:K:103:ARG:HH11	1.82	0.43
3:K:4:MET:HE1	3:K:33:LEU:HD23	2.00	0.43
4:L:53:ILE:HG23	4:L:54:LEU:N	2.34	0.43
5:O:107:LYS:HG3	5:O:108:ARG:N	2.34	0.43
1:A:476:ARG:HB3	1:A:480:ARG:NH1	2.34	0.43
2:B:176:VAL:HG12	2:B:177:LEU:N	2.34	0.43
4:D:7:SER:CB	4:D:21:SER:H	2.31	0.43
1:E:340:ASN:O	1:E:343:GLU:HB2	2.18	0.43
4:H:145:TYR:CD1	4:H:145:TYR:C	2.92	0.43
2:J:166:LYS:C	2:J:167:LYS:HD3	2.38	0.43
2:J:5:LEU:HB2	2:J:168:VAL:HG13	2.00	0.43
2:F:78:ASP:O	2:F:95:LEU:HD23	2.18	0.43
3:G:135:LEU:O	3:G:136:LEU:HD12	2.19	0.43
1:I:412:ARG:HA	7:I:908:NAG:HO6	1.80	0.43
1:I:95:MET:CE	1:I:273:ARG:HG2	2.49	0.43
2:J:105:ASP:OD1	2:J:106:THR:N	2.52	0.43
3:K:141:PRO:HB3	3:K:143:GLU:CD	2.39	0.43
3:K:142:ARG:HG3	3:K:163:VAL:HG11	2.01	0.43
2:B:126:PRO:HB2	2:B:161:VAL:HG13	1.99	0.43
2:B:157:TRP:O	2:B:171:LYS:HA	2.18	0.43
2:B:79:SER:HA	2:B:95:LEU:O	2.18	0.43
3:C:124:GLN:O	3:C:127:SER:HB2	2.18	0.43
3:C:16:GLY:HA2	3:C:77:SER:OG	2.18	0.43
3:C:50:GLY:O	3:C:51:ALA:HB3	2.17	0.43
4:D:119:PRO:HB3	4:D:145:TYR:CB	2.46	0.43
1:E:446:SER:O	7:E:948:NAG:H62	2.19	0.43
3:G:30:SER:OG	3:G:31:SER:N	2.52	0.43
4:H:7:SER:CB	4:H:21:SER:H	2.31	0.43
4:H:53:ILE:HG23	4:H:54:LEU:N	2.34	0.43
1:I:272:ILE:O	1:I:277:PHE:HZ	2.01	0.43
1:I:279:ASN:C	1:I:281:ALA:H	2.22	0.43
1:I:293:VAL:O	1:I:333:LEU:HD12	2.19	0.43
2:J:79:SER:OG	2:J:96:LEU:HA	2.19	0.43
3:K:143:GLU:CD	3:K:143:GLU:H	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:24:ARG:HH11	3:K:24:ARG:CG	2.32	0.43
4:L:123:PRO:HD3	4:L:209:LYS:HE2	2.01	0.43
4:L:34:PHE:CG	4:L:78:VAL:HG21	2.53	0.43
4:L:87:THR:HG23	4:L:110:THR:HA	2.00	0.43
5:Q:107:LYS:HG3	5:Q:108:ARG:N	2.34	0.43
1:A:252:ARG:O	1:A:254:VAL:HG23	2.19	0.43
2:B:105:ASP:OD1	2:B:106:THR:N	2.52	0.43
3:C:135:LEU:O	3:C:136:LEU:HD12	2.19	0.43
3:C:139:PHE:N	3:C:172:THR:HB	2.34	0.43
3:C:142:ARG:HG3	3:C:163:VAL:HG11	2.00	0.43
3:C:161:GLU:OE2	3:C:175:LEU:HD21	2.18	0.43
3:C:55:ALA:O	3:C:58:VAL:HG23	2.18	0.43
1:E:293:VAL:O	1:E:333:LEU:HD12	2.19	0.43
1:E:280:ASN:ND2	2:F:35:LYS:HD3	2.33	0.43
2:F:27:HIS:CE1	2:F:38:GLY:HA3	2.54	0.43
4:H:146:PHE:H	4:H:200:HIS:HE1	1.67	0.43
3:G:95(B):ARG:HD2	4:H:61:PRO:HG3	2.01	0.43
1:I:252:ARG:O	1:I:254:VAL:HG23	2.18	0.43
3:K:135:LEU:O	3:K:136:LEU:HD12	2.19	0.43
4:L:83:ARG:HB2	4:L:85:ASP:OD1	2.19	0.43
5:M:107:LYS:HG3	5:M:108:ARG:N	2.34	0.43
4:D:53:ILE:HG23	4:D:54:LEU:N	2.34	0.43
4:D:67:VAL:CG2	4:D:68:THR:N	2.82	0.43
1:E:279:ASN:C	1:E:281:ALA:H	2.22	0.43
3:G:143:GLU:H	3:G:143:GLU:CD	2.21	0.43
1:I:205:CYS:N	1:I:206:PRO:CD	2.81	0.43
2:J:36:ILE:HD13	2:J:49:SER:HB3	2.00	0.43
2:J:27:HIS:CE1	2:J:38:GLY:HA3	2.54	0.43
3:K:55:ALA:O	3:K:58:VAL:HG23	2.18	0.43
7:A:762:NAG:O3	7:A:762:NAG:C7	2.67	0.43
3:C:95(B):ARG:HD2	4:D:61:PRO:HG3	2.01	0.43
4:D:83:ARG:HB2	4:D:85:ASP:OD1	2.19	0.43
1:E:252:ARG:O	1:E:254:VAL:HG23	2.18	0.43
1:E:95:MET:CE	1:E:273:ARG:HG2	2.48	0.43
4:L:145:TYR:CD1	4:L:145:TYR:C	2.92	0.43
5:M:22:SER:CA	5:M:72:THR:HG22	2.48	0.43
5:Q:197:THR:HG22	5:Q:204:PRO:HB3	2.00	0.43
6:R:93:THR:HG21	6:R:100(L):PHE:CG	2.54	0.43
2:B:36:ILE:HD13	2:B:49:SER:HB3	2.01	0.42
2:B:5:LEU:HB2	2:B:168:VAL:HG13	2.00	0.42
3:C:188:LYS:HG2	3:C:188:LYS:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:24:ARG:CG	3:C:24:ARG:HH11	2.32	0.42
1:E:356:ASN:HD21	7:E:856:NAG:H4	1.84	0.42
1:E:333:LEU:HD23	1:E:390:LEU:HD21	2.01	0.42
1:E:105:HIS:HA	1:E:479:TRP:NE1	2.33	0.42
3:G:24:ARG:HH11	3:G:24:ARG:CG	2.32	0.42
1:I:356:ASN:HD21	7:I:856:NAG:H4	1.84	0.42
2:J:132:SER:OG	2:J:136:LYS:N	2.45	0.42
2:J:36:ILE:HA	2:J:49:SER:HB3	2.00	0.42
3:K:95(B):ARG:HD2	4:L:61:PRO:HG3	2.01	0.42
4:L:66:ARG:NH2	4:L:86:ASP:OD2	2.42	0.42
5:M:197:THR:HG22	5:M:204:PRO:HB3	2.00	0.42
6:P:93:THR:HG21	6:P:100(L):PHE:CG	2.54	0.42
1:A:340:ASN:O	1:A:343:GLU:HB2	2.18	0.42
2:B:27:HIS:CE1	2:B:38:GLY:HA3	2.54	0.42
2:B:36:ILE:HA	2:B:49:SER:HB3	2.00	0.42
4:D:69:ILE:HG12	4:D:80:LEU:HD23	2.00	0.42
2:F:150:GLU:HB3	2:F:152:GLN:CD	2.38	0.42
2:F:16:CYS:HB2	2:F:28:TRP:HZ2	1.84	0.42
2:F:79:SER:OG	2:F:96:LEU:HA	2.19	0.42
4:L:119:PRO:HB3	4:L:145:TYR:CB	2.46	0.42
1:A:350:LYS:HE2	1:A:359:ILE:HD13	2.00	0.42
1:A:489:VAL:HG22	1:A:490:LYS:N	2.35	0.42
1:A:446:SER:O	7:A:948:NAG:H62	2.19	0.42
4:D:145:TYR:C	4:D:145:TYR:CD1	2.92	0.42
4:D:123:PRO:HD3	4:D:209:LYS:HE2	2.01	0.42
1:E:272:ILE:O	1:E:277:PHE:HZ	2.01	0.42
2:F:157:TRP:O	2:F:171:LYS:HA	2.18	0.42
4:H:178:LEU:C	4:H:178:LEU:HD12	2.40	0.42
1:I:407:LEU:HD23	1:I:407:LEU:N	2.35	0.42
2:J:14:LEU:HD23	2:J:14:LEU:N	2.33	0.42
3:K:188:LYS:HG2	3:K:188:LYS:O	2.19	0.42
1:A:293:VAL:O	1:A:333:LEU:HD12	2.19	0.42
1:A:356:ASN:HD21	7:A:856:NAG:H4	1.84	0.42
3:C:4:MET:HE1	3:C:33:LEU:HD23	2.00	0.42
1:E:119:CYS:HB2	1:E:434:MET:CE	2.48	0.42
1:E:221:ALA:C	1:E:223:PHE:N	2.71	0.42
1:E:222:GLY:HA2	1:E:491:ILE:HG21	2.02	0.42
7:E:762:NAG:C7	7:E:762:NAG:O3	2.67	0.42
1:I:476:ARG:HB3	1:I:480:ARG:NH1	2.34	0.42
4:L:138:LEU:HD12	4:L:211:VAL:HG12	2.01	0.42
4:L:146:PHE:H	4:L:200:HIS:HE1	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:67:VAL:CG2	4:L:68:THR:N	2.82	0.42
5:O:197:THR:HG22	5:O:204:PRO:HB3	2.00	0.42
1:A:222:GLY:HA2	1:A:491:ILE:HG21	2.02	0.42
3:C:141:PRO:HB3	3:C:143:GLU:CD	2.39	0.42
4:D:153:SER:HB3	4:D:157:GLY:HA2	2.01	0.42
1:E:280:ASN:HD22	1:E:458:GLY:HA3	1.82	0.42
3:G:142:ARG:HG3	3:G:163:VAL:HG11	2.01	0.42
4:H:123:PRO:HD3	4:H:209:LYS:HE2	2.01	0.42
4:H:67:VAL:CG2	4:H:68:THR:N	2.82	0.42
4:H:82(A):ARG:O	4:H:82(B):ASN:HB2	2.20	0.42
1:I:95:MET:CE	1:I:273:ARG:HH11	2.28	0.42
1:I:333:LEU:HD23	1:I:390:LEU:HD21	2.01	0.42
1:I:463:ASN:O	1:I:465:THR:N	2.52	0.42
3:K:175:LEU:HD12	3:K:176:SER:N	2.29	0.42
6:N:93:THR:HG21	6:N:100(L):PHE:CG	2.54	0.42
2:B:14:LEU:N	2:B:14:LEU:HD23	2.33	0.42
2:B:108:LEU:C	2:B:177:LEU:HD13	2.36	0.42
3:C:185:ASP:OD1	3:C:189:HIS:CD2	2.73	0.42
4:D:178:LEU:C	4:D:178:LEU:HD12	2.40	0.42
1:E:221:ALA:O	1:E:223:PHE:HD1	2.01	0.42
2:F:176:VAL:HG12	2:F:177:LEU:N	2.34	0.42
3:G:139:PHE:N	3:G:172:THR:HB	2.34	0.42
4:H:153:SER:HB3	4:H:157:GLY:HA2	2.01	0.42
4:H:40:ALA:HB3	4:H:43:GLN:CG	2.49	0.42
7:I:762:NAG:C7	7:I:762:NAG:O3	2.67	0.42
3:K:124:GLN:HE22	3:K:130:ALA:CA	2.32	0.42
3:K:185:ASP:OD1	3:K:189:HIS:CD2	2.73	0.42
3:K:23:CYS:HB2	3:K:35:TRP:CH2	2.55	0.42
6:P:81:GLU:CD	6:P:82(A):LYS:HE2	2.40	0.42
5:Q:22:SER:CA	5:Q:72:THR:HG22	2.48	0.42
6:R:81:GLU:CD	6:R:82(A):LYS:HE2	2.40	0.42
3:C:23:CYS:HB2	3:C:35:TRP:CH2	2.55	0.42
1:E:371:ILE:HD11	1:E:473:GLY:CA	2.49	0.42
3:G:185:ASP:OD1	3:G:189:HIS:CD2	2.73	0.42
3:G:33:LEU:HD13	3:G:34:ALA:N	2.35	0.42
1:I:119:CYS:HB2	1:I:434:MET:CE	2.48	0.42
1:I:480:ARG:O	1:I:482:GLU:N	2.53	0.42
1:I:222:GLY:HA2	1:I:491:ILE:HG21	2.02	0.42
2:J:176:VAL:HG12	2:J:177:LEU:N	2.34	0.42
4:L:153:SER:HB3	4:L:157:GLY:HA2	2.01	0.42
1:A:480:ARG:O	1:A:482:GLU:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:121:PRO:O	2:B:124:SER:HB3	2.20	0.42
3:C:13:VAL:O	3:C:106:ILE:HA	2.20	0.42
4:D:154:TRP:CE2	4:D:196:CYS:HB3	2.55	0.42
1:E:350:LYS:C	1:E:352:GLN:H	2.23	0.42
2:F:105:ASP:OD1	2:F:106:THR:N	2.52	0.42
4:H:83:ARG:HB2	4:H:85:ASP:OD1	2.19	0.42
1:I:371:ILE:HD11	1:I:473:GLY:CA	2.49	0.42
1:A:292:VAL:CG1	1:A:333:LEU:HD11	2.50	0.42
1:A:357:LYS:HG3	1:A:464:GLY:HA3	2.02	0.42
3:C:124:GLN:HE22	3:C:130:ALA:CA	2.32	0.42
4:D:40:ALA:HB3	4:D:43:GLN:CG	2.49	0.42
1:E:205:CYS:N	1:E:206:PRO:CD	2.81	0.42
2:F:10:ASP:OD1	2:F:11:THR:N	2.41	0.42
3:G:124:GLN:HE22	3:G:130:ALA:CA	2.32	0.42
3:G:139:PHE:HE1	3:G:174:SER:HA	1.84	0.42
1:I:268:GLU:HB3	1:I:269:GLU:H	1.51	0.42
3:K:139:PHE:N	3:K:172:THR:HB	2.34	0.42
4:L:7:SER:OG	4:L:20:VAL:HG13	2.20	0.42
4:L:85:ASP:OD1	4:L:85:ASP:N	2.41	0.42
5:M:129:THR:HG22	5:M:130:ALA:N	2.35	0.42
1:A:333:LEU:HD23	1:A:390:LEU:HD21	2.01	0.42
1:A:407:LEU:HD23	1:A:407:LEU:N	2.35	0.42
2:B:79:SER:OG	2:B:96:LEU:HA	2.19	0.42
3:C:82:ASP:O	3:C:104:LEU:HD23	2.20	0.42
4:D:66:ARG:NH2	4:D:86:ASP:OD2	2.42	0.42
1:E:297:THR:C	1:E:299:ALA:H	2.23	0.42
3:G:107:LYS:HG3	3:G:140:TYR:OH	2.20	0.42
4:H:154:TRP:CE2	4:H:196:CYS:HB3	2.55	0.42
1:I:350:LYS:C	1:I:352:GLN:H	2.23	0.42
1:I:357:LYS:HG3	1:I:464:GLY:HA3	2.02	0.42
1:I:489:VAL:HG22	1:I:490:LYS:N	2.35	0.42
2:J:70:ILE:H	2:J:70:ILE:HD12	1.82	0.42
3:K:33:LEU:HD13	3:K:34:ALA:N	2.35	0.42
2:B:179:PHE:O	2:B:180:GLN:CB	2.50	0.41
2:B:36:ILE:HD13	2:B:49:SER:HB2	2.02	0.41
3:C:30:SER:OG	3:C:31:SER:N	2.52	0.41
3:C:33:LEU:HD13	3:C:34:ALA:N	2.35	0.41
4:D:125:ALA:HA	4:D:126:PRO:HD3	1.93	0.41
4:D:143:LYS:HG2	4:D:144:ASP:N	2.35	0.41
1:E:407:LEU:N	1:E:407:LEU:HD23	2.35	0.41
1:E:476:ARG:HB3	1:E:480:ARG:NH1	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:178:ALA:CB	2:F:180:GLN:N	2.81	0.41
3:G:125:LEU:CD1	3:G:130:ALA:HB2	2.50	0.41
3:G:13:VAL:O	3:G:106:ILE:HA	2.19	0.41
3:G:188:LYS:HG2	3:G:188:LYS:O	2.19	0.41
4:H:143:LYS:HG2	4:H:144:ASP:N	2.35	0.41
3:K:82:ASP:O	3:K:104:LEU:HD23	2.20	0.41
4:L:154:TRP:CE2	4:L:196:CYS:HB3	2.55	0.41
6:N:81:GLU:CD	6:N:82(A):LYS:HE2	2.40	0.41
1:A:119:CYS:HB2	1:A:434:MET:CE	2.48	0.41
1:A:350:LYS:C	1:A:352:GLN:H	2.23	0.41
1:A:463:ASN:O	1:A:465:THR:N	2.52	0.41
4:D:82(A):ARG:O	4:D:82(B):ASN:HB2	2.20	0.41
1:E:252:ARG:HA	1:E:253:PRO:HD2	1.91	0.41
1:E:333:LEU:HB3	1:E:414:ILE:HB	2.02	0.41
1:E:477:ASP:O	1:E:480:ARG:HB2	2.20	0.41
2:F:51:LEU:O	2:F:55:ALA:N	2.53	0.41
3:G:23:CYS:HB2	3:G:35:TRP:CH2	2.55	0.41
1:I:477:ASP:O	1:I:480:ARG:HB2	2.20	0.41
2:J:36:ILE:HD13	2:J:49:SER:HB2	2.02	0.41
4:L:88:ALA:O	4:L:108:LEU:HD12	2.21	0.41
6:N:81:GLU:OE2	6:N:82(A):LYS:CE	2.66	0.41
5:Q:121:SER:O	5:Q:125:LEU:HG	2.21	0.41
1:A:274:SER:HB3	1:A:277:PHE:CE1	2.55	0.41
1:A:333:LEU:HB3	1:A:414:ILE:HB	2.02	0.41
7:A:963:NAG:H3	7:A:963:NAG:C8	2.37	0.41
3:C:125:LEU:CD1	3:C:130:ALA:HB2	2.50	0.41
1:E:104:MET:HE2	1:E:217:TYR:HE2	1.85	0.41
1:E:350:LYS:HE2	1:E:357:LYS:O	2.20	0.41
2:F:121:PRO:O	2:F:124:SER:HB3	2.20	0.41
1:I:280:ASN:O	2:J:35:LYS:CD	2.60	0.41
3:K:125:LEU:CD1	3:K:130:ALA:HB2	2.50	0.41
3:K:14:SER:OG	3:K:15:PRO:HD2	2.19	0.41
4:L:178:LEU:HD12	4:L:178:LEU:C	2.40	0.41
4:L:212:GLU:C	4:L:214:LYS:N	2.73	0.41
4:L:52(A):THR:O	4:L:55:ASP:N	2.48	0.41
4:L:5:VAL:HB	4:L:23:LYS:HB3	2.02	0.41
6:P:81:GLU:OE2	6:P:82(A):LYS:CE	2.66	0.41
1:A:350:LYS:HE2	1:A:357:LYS:O	2.20	0.41
1:A:478:ASN:HD22	1:A:478:ASN:N	2.19	0.41
2:B:150:GLU:HB3	2:B:152:GLN:CD	2.38	0.41
2:B:178:ALA:CB	2:B:180:GLN:N	2.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:107:LYS:HG3	3:C:140:TYR:OH	2.20	0.41
3:C:150:VAL:HG11	3:C:189:HIS:CD2	2.56	0.41
4:D:146:PHE:H	4:D:200:HIS:HE1	1.67	0.41
1:E:463:ASN:O	1:E:465:THR:N	2.52	0.41
1:E:480:ARG:O	1:E:482:GLU:N	2.53	0.41
3:K:13:VAL:O	3:K:106:ILE:HA	2.19	0.41
3:K:30:SER:OG	3:K:31:SER:N	2.52	0.41
1:A:248:THR:HG22	1:A:486:TYR:CD2	2.56	0.41
1:A:341:THR:HG22	1:A:345:ILE:HD12	2.03	0.41
2:B:51:LEU:O	2:B:55:ALA:N	2.53	0.41
3:C:105:GLU:OE2	3:C:173:TYR:CE2	2.73	0.41
3:C:105:GLU:OE2	3:C:173:TYR:HE2	2.03	0.41
4:D:138:LEU:H	4:D:138:LEU:HD23	1.85	0.41
4:D:40:ALA:HB1	4:D:41:PRO:HD2	2.02	0.41
1:E:489:VAL:HG22	1:E:490:LYS:N	2.35	0.41
2:F:128:VAL:HG23	2:F:141:GLY:O	2.21	0.41
3:G:105:GLU:OE2	3:G:173:TYR:CE2	2.73	0.41
1:I:333:LEU:HB3	1:I:414:ILE:HB	2.02	0.41
3:K:107:LYS:HG3	3:K:140:TYR:OH	2.20	0.41
3:K:139:PHE:HE1	3:K:174:SER:HA	1.84	0.41
2:B:116:LEU:O	2:B:143:THR:HG23	2.21	0.41
3:C:14:SER:OG	3:C:15:PRO:HD2	2.20	0.41
2:F:116:LEU:O	2:F:143:THR:HG23	2.21	0.41
3:G:141:PRO:HB3	3:G:143:GLU:CD	2.39	0.41
3:G:105:GLU:OE2	3:G:173:TYR:HE2	2.03	0.41
1:I:100:MET:HE1	1:I:486:TYR:HB3	2.03	0.41
2:J:121:PRO:O	2:J:124:SER:HB3	2.20	0.41
4:L:138:LEU:HD23	4:L:138:LEU:H	1.85	0.41
4:L:40:ALA:HB1	4:L:41:PRO:HD2	2.02	0.41
5:O:129:THR:HG22	5:O:130:ALA:N	2.35	0.41
5:Q:124:GLN:HG2	5:Q:129:THR:O	2.21	0.41
1:A:371:ILE:HD11	1:A:473:GLY:CA	2.49	0.41
4:D:88:ALA:O	4:D:108:LEU:HD12	2.21	0.41
1:E:248:THR:HG22	1:E:486:TYR:CD2	2.56	0.41
3:G:82:ASP:O	3:G:104:LEU:HD23	2.20	0.41
3:G:187:GLU:O	3:G:211:ARG:CZ	2.69	0.41
4:H:138:LEU:N	4:H:138:LEU:HD23	2.36	0.41
4:H:138:LEU:H	4:H:138:LEU:HD23	1.85	0.41
4:H:195:ILE:CG1	4:H:210:LYS:HA	2.42	0.41
1:I:270:ILE:HG12	1:I:288:LEU:HA	2.03	0.41
1:I:478:ASN:N	1:I:478:ASN:HD22	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:10:ASP:OD1	2:J:11:THR:N	2.41	0.41
2:J:128:VAL:HG23	2:J:141:GLY:O	2.21	0.41
4:L:54:LEU:HA	4:L:54:LEU:HD12	1.82	0.41
4:L:82(A):ARG:O	4:L:82(B):ASN:HB2	2.20	0.41
6:N:189:LEU:HA	6:N:189:LEU:HD23	1.88	0.41
5:Q:129:THR:HG22	5:Q:130:ALA:N	2.35	0.41
1:A:480:ARG:C	1:A:482:GLU:N	2.74	0.41
1:A:477:ASP:O	1:A:480:ARG:HB2	2.20	0.41
1:A:371:ILE:HG21	2:B:45:THR:HG22	2.03	0.41
4:D:138:LEU:N	4:D:138:LEU:HD23	2.36	0.41
1:E:270:ILE:HG12	1:E:288:LEU:HA	2.03	0.41
2:F:100:LEU:HD12	2:F:170:PHE:CG	2.55	0.41
2:F:2:LYS:HB3	2:F:93:VAL:HG23	2.03	0.41
3:G:45:ARG:NH1	3:G:47:LEU:HD23	2.36	0.41
4:H:54:LEU:HA	4:H:54:LEU:HD12	1.83	0.41
1:I:274:SER:HB3	1:I:277:PHE:CE1	2.55	0.41
1:I:89:VAL:HG22	1:I:90:THR:H	1.86	0.41
2:J:87:GLU:O	2:J:88:ASP:HB2	2.21	0.41
4:L:186:SER:C	4:L:188:SER:H	2.24	0.41
1:A:387:SER:O	1:A:391:PHE:HD1	2.04	0.41
3:C:170:ASP:O	3:C:171:SER:HB2	2.21	0.41
1:E:100:MET:HE1	1:E:486:TYR:HB3	2.02	0.41
3:G:134:CYS:HB2	3:G:148:TRP:CH2	2.56	0.41
4:H:5:VAL:HB	4:H:23:LYS:HB3	2.02	0.41
1:I:297:THR:C	1:I:299:ALA:H	2.24	0.41
1:I:292:VAL:CG1	1:I:333:LEU:HD11	2.50	0.41
1:I:358:THR:O	1:I:359:ILE:HD12	2.21	0.41
2:J:51:LEU:O	2:J:55:ALA:N	2.53	0.41
3:K:105:GLU:OE2	3:K:173:TYR:CE2	2.73	0.41
5:O:121:SER:O	5:O:125:LEU:HG	2.21	0.41
5:O:124:GLN:HG2	5:O:129:THR:O	2.21	0.41
1:A:358:THR:C	1:A:359:ILE:HD12	2.41	0.41
3:C:139:PHE:HE1	3:C:174:SER:HA	1.84	0.41
4:D:212:GLU:C	4:D:214:LYS:N	2.73	0.41
1:E:341:THR:HG22	1:E:345:ILE:HD12	2.03	0.41
2:F:27:HIS:ND1	2:F:38:GLY:HA3	2.36	0.41
3:G:94:TRP:CE3	3:G:95(A):PRO:HG3	2.49	0.41
4:H:143:LYS:HG2	4:H:144:ASP:CG	2.41	0.41
4:H:186:SER:HA	4:H:189:LEU:HG	2.03	0.41
1:I:350:LYS:HE2	1:I:357:LYS:O	2.20	0.41
1:I:358:THR:C	1:I:359:ILE:HD12	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:105:GLU:OE2	3:K:173:TYR:HE2	2.03	0.41
3:K:187:GLU:O	3:K:211:ARG:CZ	2.69	0.41
1:A:270:ILE:HG12	1:A:288:LEU:HA	2.03	0.41
2:B:100:LEU:HD12	2:B:170:PHE:CG	2.56	0.41
3:C:141:PRO:C	3:C:143:GLU:OE1	2.60	0.41
1:A:202:THR:CG2	3:C:95:PRO:HG3	2.48	0.41
4:D:143:LYS:HG2	4:D:144:ASP:CG	2.41	0.41
1:E:274:SER:HB3	1:E:277:PHE:CE1	2.55	0.41
1:E:351:GLU:O	1:E:351:GLU:HG2	2.21	0.41
1:E:358:THR:O	1:E:359:ILE:HD12	2.21	0.41
1:E:371:ILE:HG21	2:F:45:THR:HG22	2.03	0.41
2:F:73:ASN:HA	2:F:73:ASN:HD22	1.65	0.41
3:G:170:ASP:O	3:G:171:SER:HB2	2.21	0.41
4:H:88:ALA:O	4:H:108:LEU:HD12	2.21	0.41
2:J:150:GLU:HB3	2:J:152:GLN:CD	2.38	0.41
2:J:100:LEU:HD12	2:J:170:PHE:CG	2.56	0.41
3:K:141:PRO:O	3:K:143:GLU:N	2.54	0.41
3:K:150:VAL:HG11	3:K:189:HIS:CD2	2.56	0.41
1:I:202:THR:CG2	3:K:95:PRO:HG3	2.48	0.41
2:B:128:VAL:HG23	2:B:141:GLY:O	2.21	0.40
3:C:141:PRO:O	3:C:143:GLU:N	2.54	0.40
4:D:186:SER:HA	4:D:189:LEU:HG	2.03	0.40
4:D:7:SER:OG	4:D:20:VAL:HG13	2.20	0.40
1:E:89:VAL:HG22	1:E:90:THR:H	1.86	0.40
3:G:94:TRP:CA	3:G:95:PRO:O	2.69	0.40
1:I:341:THR:HG22	1:I:345:ILE:CD1	2.51	0.40
2:J:74:LEU:HD12	2:J:74:LEU:HA	1.90	0.40
3:K:170:ASP:O	3:K:171:SER:HB2	2.21	0.40
4:L:138:LEU:HD23	4:L:138:LEU:N	2.36	0.40
6:R:189:LEU:HD23	6:R:189:LEU:HA	1.88	0.40
1:A:394:ASN:C	1:A:396:THR:N	2.74	0.40
1:A:439:ILE:HD12	1:A:439:ILE:C	2.41	0.40
2:B:136:LYS:HB3	2:B:138:ILE:HG23	2.02	0.40
4:D:186:SER:C	4:D:188:SER:H	2.24	0.40
1:E:478:ASN:HD22	1:E:478:ASN:N	2.19	0.40
2:F:10:ASP:CG	2:F:11:THR:H	2.24	0.40
3:G:14:SER:OG	3:G:15:PRO:HD2	2.20	0.40
1:E:202:THR:CG2	3:G:95:PRO:HG3	2.48	0.40
1:I:248:THR:HG22	1:I:486:TYR:CD2	2.56	0.40
3:K:45:ARG:NH1	3:K:47:LEU:HD23	2.36	0.40
6:R:123:PRO:HD3	6:R:209:LYS:HD3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:PHE:HB3	1:A:353:PHE:CZ	2.56	0.40
2:B:16:CYS:HB2	2:B:28:TRP:HZ2	1.84	0.40
2:B:83:ILE:H	2:B:83:ILE:HG13	1.73	0.40
2:B:87:GLU:O	2:B:88:ASP:HB2	2.21	0.40
3:C:158:ASN:O	3:C:179:LEU:HD12	2.22	0.40
4:D:163:VAL:HG12	4:D:182:VAL:CB	2.42	0.40
1:E:358:THR:C	1:E:359:ILE:HD12	2.41	0.40
2:F:36:ILE:HD13	2:F:49:SER:HB2	2.02	0.40
3:G:141:PRO:O	3:G:143:GLU:N	2.54	0.40
4:H:40:ALA:HB1	4:H:41:PRO:HD2	2.02	0.40
1:I:394:ASN:C	1:I:396:THR:N	2.74	0.40
2:J:140:GLY:O	2:J:144:LEU:HD11	2.21	0.40
2:J:54:ARG:HH12	2:J:75:LYS:HG3	1.86	0.40
4:L:143:LYS:HG2	4:L:144:ASP:N	2.35	0.40
4:L:143:LYS:HG2	4:L:144:ASP:CG	2.41	0.40
6:R:146:PHE:HA	6:R:147:PRO:HA	1.88	0.40
1:A:122:LEU:HB3	1:A:198:THR:CG2	2.52	0.40
1:A:335:LYS:CD	1:A:408:ASN:HA	2.52	0.40
2:B:75:LYS:N	2:B:78:ASP:OD2	2.41	0.40
2:B:2:LYS:HB3	2:B:93:VAL:HG23	2.03	0.40
3:C:12:SER:HB3	3:C:105:GLU:OE1	2.22	0.40
1:E:292:VAL:CG1	1:E:333:LEU:HD11	2.50	0.40
1:E:387:SER:O	1:E:391:PHE:HD1	2.04	0.40
2:F:136:LYS:HB3	2:F:138:ILE:HG23	2.02	0.40
3:G:108:ARG:NE	3:G:170:ASP:O	2.54	0.40
3:G:174:SER:HG	4:H:164:HIS:CE1	2.38	0.40
1:I:117:LYS:HA	1:I:118:PRO:HD3	1.85	0.40
2:J:116:LEU:O	2:J:143:THR:HG23	2.21	0.40
3:K:108:ARG:NE	3:K:170:ASP:O	2.54	0.40
3:K:135:LEU:CD2	3:K:137:ASN:N	2.85	0.40
3:C:108:ARG:NE	3:C:170:ASP:O	2.54	0.40
3:C:187:GLU:O	3:C:211:ARG:CZ	2.69	0.40
4:D:139:GLY:HA2	4:D:154:TRP:CZ2	2.57	0.40
1:E:122:LEU:HB3	1:E:198:THR:CG2	2.52	0.40
1:E:439:ILE:HD12	1:E:439:ILE:C	2.41	0.40
2:F:54:ARG:HH12	2:F:75:LYS:HG3	1.86	0.40
3:G:150:VAL:HG11	3:G:189:HIS:CD2	2.56	0.40
4:H:139:GLY:HA2	4:H:154:TRP:CZ2	2.57	0.40
1:I:439:ILE:C	1:I:439:ILE:HD12	2.41	0.40
2:J:27:HIS:ND1	2:J:38:GLY:HA3	2.36	0.40
3:K:150:VAL:O	3:K:153:ALA:CB	2.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	304/313 (97%)	242 (80%)	48 (16%)	14 (5%)	3	28
1	E	304/313 (97%)	242 (80%)	48 (16%)	14 (5%)	3	28
1	I	304/313 (97%)	242 (80%)	48 (16%)	14 (5%)	3	28
2	B	179/181 (99%)	127 (71%)	38 (21%)	14 (8%)	1	18
2	F	179/181 (99%)	127 (71%)	38 (21%)	14 (8%)	1	18
2	J	179/181 (99%)	128 (72%)	37 (21%)	14 (8%)	1	18
3	C	212/214 (99%)	171 (81%)	28 (13%)	13 (6%)	2	22
3	G	212/214 (99%)	171 (81%)	29 (14%)	12 (6%)	2	24
3	K	212/214 (99%)	171 (81%)	28 (13%)	13 (6%)	2	22
4	D	227/229 (99%)	185 (82%)	35 (15%)	7 (3%)	5	37
4	H	227/229 (99%)	185 (82%)	35 (15%)	7 (3%)	5	37
4	L	227/229 (99%)	184 (81%)	36 (16%)	7 (3%)	5	37
5	M	212/215 (99%)	211 (100%)	1 (0%)	0	100	100
5	O	212/215 (99%)	211 (100%)	1 (0%)	0	100	100
5	Q	212/215 (99%)	211 (100%)	1 (0%)	0	100	100
6	N	220/244 (90%)	219 (100%)	1 (0%)	0	100	100
6	P	220/244 (90%)	219 (100%)	1 (0%)	0	100	100
6	R	220/244 (90%)	219 (100%)	1 (0%)	0	100	100
All	All	4062/4188 (97%)	3465 (85%)	454 (11%)	143 (4%)	7	34

All (143) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	268	GLU

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Mol	Chain	Res	Type
1	A	409	ASN
1	A	475	MET
2	B	109	LEU
2	B	165	GLN
2	B	179	PHE
3	C	26	SER
3	C	76	SER
3	C	138	ASN
4	D	127	SER
1	E	268	GLU
1	E	409	ASN
1	E	475	MET
2	F	109	LEU
2	F	165	GLN
2	F	179	PHE
3	G	26	SER
3	G	76	SER
3	G	138	ASN
4	H	127	SER
1	I	268	GLU
1	I	409	ASN
1	I	475	MET
2	J	109	LEU
2	J	165	GLN
2	J	179	PHE
3	K	26	SER
3	K	76	SER
3	K	138	ASN
4	L	127	SER
1	A	194	GLY
1	A	220	PRO
1	A	253	PRO
1	A	395	ASP
1	A	463	ASN
1	A	464	GLY
2	B	68	PRO
2	B	105	ASP
2	B	178	ALA
2	B	180	GLN
3	C	158	ASN
3	C	211	ARG
4	D	52(A)	THR

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Mol	Chain	Res	Type
4	D	99	GLU
4	D	148	GLU
1	E	194	GLY
1	E	220	PRO
1	E	253	PRO
1	E	395	ASP
1	E	463	ASN
1	E	464	GLY
2	F	68	PRO
2	F	105	ASP
2	F	178	ALA
2	F	180	GLN
3	G	158	ASN
3	G	211	ARG
4	H	52(A)	THR
4	H	99	GLU
4	H	148	GLU
1	I	194	GLY
1	I	220	PRO
1	I	253	PRO
1	I	395	ASP
1	I	463	ASN
1	I	464	GLY
2	J	68	PRO
2	J	105	ASP
2	J	178	ALA
2	J	180	GLN
3	K	158	ASN
3	K	211	ARG
4	L	52(A)	THR
4	L	99	GLU
4	L	148	GLU
1	A	210	PHE
1	A	276	ASN
2	B	154	SER
3	C	78	LEU
1	E	210	PHE
1	E	276	ASN
2	F	154	SER
3	G	78	LEU
1	I	210	PHE
1	I	276	ASN

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Mol	Chain	Res	Type
2	J	154	SER
3	K	78	LEU
4	L	213	PRO
1	A	481	SER
2	B	16	CYS
2	B	164	ASN
3	C	110	VAL
3	C	142	ARG
4	D	193	THR
4	D	213	PRO
1	E	481	SER
2	F	16	CYS
2	F	164	ASN
3	G	110	VAL
3	G	142	ARG
4	H	193	THR
4	H	213	PRO
1	I	481	SER
2	J	16	CYS
2	J	164	ASN
3	K	110	VAL
3	K	142	ARG
4	L	193	THR
1	A	407	LEU
2	B	2	LYS
2	B	56	ASP
2	B	147	SER
3	C	182	SER
1	E	407	LEU
2	F	56	ASP
2	F	147	SER
3	G	182	SER
1	I	407	LEU
2	J	56	ASP
2	J	147	SER
3	K	182	SER
2	B	135	GLY
2	F	2	LYS
2	F	135	GLY
2	J	2	LYS
2	J	135	GLY
1	A	441	GLY

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Mol	Chain	Res	Type
1	E	441	GLY
1	I	441	GLY
3	C	44	PRO
3	G	44	PRO
3	K	44	PRO
3	C	128	GLY
3	G	128	GLY
3	K	128	GLY
3	C	157	GLY
3	G	157	GLY
3	K	157	GLY
4	D	147	PRO
4	H	147	PRO
4	L	147	PRO
3	C	95	PRO
3	K	95	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	271/276 (98%)	257 (95%)	14 (5%)	27	59
1	E	271/276 (98%)	257 (95%)	14 (5%)	27	59
1	I	271/276 (98%)	257 (95%)	14 (5%)	27	59
2	B	164/164 (100%)	149 (91%)	15 (9%)	11	38
2	F	164/164 (100%)	149 (91%)	15 (9%)	11	38
2	J	164/164 (100%)	149 (91%)	15 (9%)	11	38
3	C	184/184 (100%)	174 (95%)	10 (5%)	26	58
3	G	184/184 (100%)	174 (95%)	10 (5%)	26	58
3	K	184/184 (100%)	174 (95%)	10 (5%)	26	58
4	D	193/193 (100%)	183 (95%)	10 (5%)	27	59
4	H	193/193 (100%)	183 (95%)	10 (5%)	27	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	L	193/193 (100%)	183 (95%)	10 (5%)	27	59
5	M	174/182 (96%)	164 (94%)	10 (6%)	24	56
5	O	174/182 (96%)	164 (94%)	10 (6%)	24	56
5	Q	174/182 (96%)	164 (94%)	10 (6%)	24	56
6	N	183/210 (87%)	175 (96%)	8 (4%)	33	63
6	P	183/210 (87%)	175 (96%)	8 (4%)	33	63
6	R	183/210 (87%)	175 (96%)	8 (4%)	33	63
All	All	3507/3627 (97%)	3306 (94%)	201 (6%)	28	56

All (201) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	GLN
1	A	126	CYS
1	A	205	CYS
1	A	211	GLU
1	A	268	GLU
1	A	273	ARG
1	A	339	GLU
1	A	355	ASN
1	A	416	LEU
1	A	418	CYS
1	A	432	LYS
1	A	444	ARG
1	A	447	SER
1	A	488	VAL
2	B	1	LYS
2	B	2	LYS
2	B	40	GLN
2	B	69	LEU
2	B	73	ASN
2	B	76	ILE
2	B	77	GLU
2	B	89	GLN
2	B	103	ASN
2	B	137	ASN
2	B	148	GLN
2	B	152	GLN
2	B	167	LYS
2	B	170	PHE

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Mol	Chain	Res	Type
2	B	177	LEU
3	C	53	THR
3	C	74	THR
3	C	90	GLN
3	C	92	ASN
3	C	103	ARG
3	C	106	ILE
3	C	137	ASN
3	C	138	ASN
3	C	141	PRO
3	C	169	LYS
4	D	38	ARG
4	D	54	LEU
4	D	66	ARG
4	D	74	SER
4	D	82(B)	ASN
4	D	105	GLN
4	D	110	THR
4	D	148	GLU
4	D	149	PRO
4	D	178	LEU
1	E	103	GLN
1	E	126	CYS
1	E	205	CYS
1	E	211	GLU
1	E	268	GLU
1	E	273	ARG
1	E	339	GLU
1	E	355	ASN
1	E	416	LEU
1	E	418	CYS
1	E	432	LYS
1	E	444	ARG
1	E	447	SER
1	E	488	VAL
2	F	1	LYS
2	F	2	LYS
2	F	40	GLN
2	F	69	LEU
2	F	73	ASN
2	F	76	ILE
2	F	77	GLU

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Mol	Chain	Res	Type
2	F	89	GLN
2	F	103	ASN
2	F	137	ASN
2	F	148	GLN
2	F	152	GLN
2	F	167	LYS
2	F	170	PHE
2	F	177	LEU
3	G	53	THR
3	G	74	THR
3	G	90	GLN
3	G	92	ASN
3	G	103	ARG
3	G	106	ILE
3	G	137	ASN
3	G	138	ASN
3	G	141	PRO
3	G	169	LYS
4	H	38	ARG
4	H	54	LEU
4	H	66	ARG
4	H	74	SER
4	H	82(B)	ASN
4	H	105	GLN
4	H	110	THR
4	H	148	GLU
4	H	149	PRO
4	H	178	LEU
1	I	103	GLN
1	I	126	CYS
1	I	205	CYS
1	I	211	GLU
1	I	268	GLU
1	I	273	ARG
1	I	339	GLU
1	I	355	ASN
1	I	416	LEU
1	I	418	CYS
1	I	432	LYS
1	I	444	ARG
1	I	447	SER
1	I	488	VAL

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Mol	Chain	Res	Type
2	J	1	LYS
2	J	2	LYS
2	J	40	GLN
2	J	69	LEU
2	J	73	ASN
2	J	76	ILE
2	J	77	GLU
2	J	89	GLN
2	J	103	ASN
2	J	137	ASN
2	J	148	GLN
2	J	152	GLN
2	J	167	LYS
2	J	170	PHE
2	J	177	LEU
3	K	53	THR
3	K	74	THR
3	K	90	GLN
3	K	92	ASN
3	K	103	ARG
3	K	106	ILE
3	K	137	ASN
3	K	138	ASN
3	K	141	PRO
3	K	169	LYS
4	L	38	ARG
4	L	54	LEU
4	L	66	ARG
4	L	74	SER
4	L	82(B)	ASN
4	L	105	GLN
4	L	110	THR
4	L	148	GLU
4	L	149	PRO
4	L	178	LEU
5	M	7	SER
5	M	19	VAL
5	M	50	ARG
5	M	61	ARG
5	M	78	LEU
5	M	93	THR
5	M	108	ARG

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Mol	Chain	Res	Type
5	M	123	GLU
5	M	146	VAL
5	M	181	LEU
6	N	50	GLN
6	N	66	ARG
6	N	92	CYS
6	N	107	THR
6	N	116	THR
6	N	161	SER
6	N	207	VAL
6	N	209	LYS
5	O	7	SER
5	O	19	VAL
5	O	50	ARG
5	O	61	ARG
5	O	78	LEU
5	O	93	THR
5	O	108	ARG
5	O	123	GLU
5	O	146	VAL
5	O	181	LEU
6	P	50	GLN
6	P	66	ARG
6	P	92	CYS
6	P	107	THR
6	P	116	THR
6	P	161	SER
6	P	207	VAL
6	P	209	LYS
5	Q	7	SER
5	Q	19	VAL
5	Q	50	ARG
5	Q	61	ARG
5	Q	78	LEU
5	Q	93	THR
5	Q	108	ARG
5	Q	123	GLU
5	Q	146	VAL
5	Q	181	LEU
6	R	50	GLN
6	R	66	ARG
6	R	92	CYS

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Mol	Chain	Res	Type
6	R	107	THR
6	R	116	THR
6	R	161	SER
6	R	207	VAL
6	R	209	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	ASN
1	A	94	ASN
1	A	114	GLN
1	A	246	GLN
1	A	279	ASN
1	A	340	ASN
1	A	355	ASN
1	A	362	ASN
1	A	478	ASN
2	B	33	GLN
2	B	73	ASN
2	B	103	ASN
2	B	110	GLN
2	B	165	GLN
3	C	100	GLN
3	C	147	GLN
3	C	198	HIS
3	C	199	GLN
4	D	82(B)	ASN
4	D	199	ASN
4	D	200	HIS
1	E	92	ASN
1	E	94	ASN
1	E	114	GLN
1	E	246	GLN
1	E	279	ASN
1	E	340	ASN
1	E	355	ASN
1	E	362	ASN
1	E	478	ASN
2	F	33	GLN
2	F	73	ASN
2	F	103	ASN

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Mol	Chain	Res	Type
2	F	110	GLN
2	F	165	GLN
3	G	100	GLN
3	G	198	HIS
3	G	199	GLN
4	H	82(B)	ASN
4	H	199	ASN
4	H	200	HIS
1	I	92	ASN
1	I	94	ASN
1	I	114	GLN
1	I	246	GLN
1	I	279	ASN
1	I	340	ASN
1	I	355	ASN
1	I	362	ASN
1	I	478	ASN
2	J	33	GLN
2	J	73	ASN
2	J	103	ASN
2	J	110	GLN
2	J	165	GLN
3	K	100	GLN
3	K	147	GLN
3	K	198	HIS
3	K	199	GLN
4	L	82(B)	ASN
4	L	199	ASN
4	L	200	HIS
5	M	79	GLN
5	M	155	GLN
6	N	62	HIS
5	O	155	GLN
6	P	62	HIS
5	Q	155	GLN
6	R	62	HIS

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 ⓘ

45 ligands are modelled in this entry.

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	$\# Z > 2$
7	NAG	A	588	1	14,14,15	0.63	0	15,19,21	0.88	0
7	NAG	A	697	1	14,14,15	0.65	0	15,19,21	0.67	0
7	NAG	A	734	1	14,14,15	0.61	0	15,19,21	0.55	0
7	NAG	A	741	1	14,14,15	0.56	0	15,19,21	0.66	0
7	NAG	A	762	1	14,14,15	0.61	0	15,19,21	0.77	1 (6%)
7	NAG	A	776	1	14,14,15	0.59	0	15,19,21	0.85	0
7	NAG	A	789	1	14,14,15	0.65	0	15,19,21	0.93	0
7	NAG	A	795	1	14,14,15	0.52	0	15,19,21	0.77	0
7	NAG	A	856	1	14,14,15	0.77	0	15,19,21	0.75	0
7	NAG	A	886	1	14,14,15	0.67	0	15,19,21	1.09	2 (13%)
7	NAG	A	894	1	14,14,15	0.65	0	15,19,21	0.80	1 (6%)
7	NAG	A	908	1	14,14,15	0.63	0	15,19,21	0.67	0
7	NAG	A	948	1	14,14,15	0.89	1 (7%)	15,19,21	1.00	0
7	NAG	A	963	1	14,14,15	0.75	0	15,19,21	0.69	0
7	NAG	E	588	1	14,14,15	0.62	0	15,19,21	0.88	0
7	NAG	E	697	1	14,14,15	0.65	0	15,19,21	0.68	0
7	NAG	E	734	1	14,14,15	0.62	0	15,19,21	0.56	0
7	NAG	E	741	1	14,14,15	0.56	0	15,19,21	0.66	0
7	NAG	E	762	1	14,14,15	0.61	0	15,19,21	0.77	1 (6%)
7	NAG	E	776	1	14,14,15	0.58	0	15,19,21	0.85	0
7	NAG	E	789	1	14,14,15	0.65	0	15,19,21	0.93	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	E	795	1	14,14,15	0.51	0	15,19,21	0.77	0
7	NAG	E	856	1	14,14,15	0.75	0	15,19,21	0.76	0
7	NAG	E	886	1	14,14,15	0.66	0	15,19,21	1.08	2 (13%)
7	NAG	E	894	1	14,14,15	0.67	0	15,19,21	0.79	1 (6%)
7	NAG	E	908	1	14,14,15	0.62	0	15,19,21	0.67	0
7	NAG	E	948	1	14,14,15	0.91	1 (7%)	15,19,21	1.00	1 (6%)
7	NAG	E	963	1	14,14,15	0.74	0	15,19,21	0.70	0
7	NAG	I	588	1	14,14,15	0.61	0	15,19,21	0.88	0
7	NAG	I	697	1	14,14,15	0.65	0	15,19,21	0.67	0
7	NAG	I	734	1	14,14,15	0.61	0	15,19,21	0.56	0
7	NAG	I	741	1	14,14,15	0.56	0	15,19,21	0.66	0
7	NAG	I	762	1	14,14,15	0.60	0	15,19,21	0.76	1 (6%)
7	NAG	I	776	1	14,14,15	0.58	0	15,19,21	0.86	0
7	NAG	I	789	1	14,14,15	0.65	0	15,19,21	0.94	0
7	NAG	I	795	1	14,14,15	0.51	0	15,19,21	0.78	0
7	NAG	I	856	1	14,14,15	0.77	0	15,19,21	0.77	0
7	NAG	I	886	1	14,14,15	0.67	0	15,19,21	1.09	2 (13%)
7	NAG	I	894	1	14,14,15	0.65	0	15,19,21	0.80	1 (6%)
7	NAG	I	908	1	14,14,15	0.60	0	15,19,21	0.67	0
7	NAG	I	948	1	14,14,15	0.90	1 (7%)	15,19,21	1.00	1 (6%)
7	NAG	I	963	1	14,14,15	0.75	0	15,19,21	0.69	0
7	NAG	N	1000	6	14,14,15	1.63	1 (7%)	15,19,21	1.43	1 (6%)
7	NAG	P	1000	6	14,14,15	1.64	1 (7%)	15,19,21	1.43	1 (6%)
7	NAG	R	1000	6	14,14,15	1.63	1 (7%)	15,19,21	1.42	1 (6%)

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
7	NAG	A	588	1	1/1/5/7	0/6/23/26	0/1/1/1
7	NAG	A	697	1	-	1/6/23/26	0/1/1/1
7	NAG	A	734	1	-	0/6/23/26	0/1/1/1
7	NAG	A	741	1	1/1/5/7	0/6/23/26	0/1/1/1
7	NAG	A	762	1	-	0/6/23/26	0/1/1/1
7	NAG	A	776	1	-	0/6/23/26	0/1/1/1
7	NAG	A	789	1	-	1/6/23/26	0/1/1/1
7	NAG	A	795	1	-	0/6/23/26	0/1/1/1
7	NAG	A	856	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	A	886	1	-	0/6/23/26	0/1/1/1
7	NAG	A	894	1	-	0/6/23/26	0/1/1/1
7	NAG	A	908	1	-	0/6/23/26	0/1/1/1
7	NAG	A	948	1	-	0/6/23/26	0/1/1/1
7	NAG	A	963	1	-	1/6/23/26	0/1/1/1
7	NAG	E	588	1	1/1/5/7	0/6/23/26	0/1/1/1
7	NAG	E	697	1	-	1/6/23/26	0/1/1/1
7	NAG	E	734	1	-	0/6/23/26	0/1/1/1
7	NAG	E	741	1	1/1/5/7	0/6/23/26	0/1/1/1
7	NAG	E	762	1	-	0/6/23/26	0/1/1/1
7	NAG	E	776	1	-	0/6/23/26	0/1/1/1
7	NAG	E	789	1	-	1/6/23/26	0/1/1/1
7	NAG	E	795	1	-	0/6/23/26	0/1/1/1
7	NAG	E	856	1	-	0/6/23/26	0/1/1/1
7	NAG	E	886	1	-	0/6/23/26	0/1/1/1
7	NAG	E	894	1	-	0/6/23/26	0/1/1/1
7	NAG	E	908	1	-	0/6/23/26	0/1/1/1
7	NAG	E	948	1	-	0/6/23/26	0/1/1/1
7	NAG	E	963	1	-	1/6/23/26	0/1/1/1
7	NAG	I	588	1	1/1/5/7	0/6/23/26	0/1/1/1
7	NAG	I	697	1	-	1/6/23/26	0/1/1/1
7	NAG	I	734	1	-	0/6/23/26	0/1/1/1
7	NAG	I	741	1	1/1/5/7	0/6/23/26	0/1/1/1
7	NAG	I	762	1	-	0/6/23/26	0/1/1/1
7	NAG	I	776	1	-	0/6/23/26	0/1/1/1
7	NAG	I	789	1	-	1/6/23/26	0/1/1/1
7	NAG	I	795	1	-	0/6/23/26	0/1/1/1
7	NAG	I	856	1	-	0/6/23/26	0/1/1/1
7	NAG	I	886	1	-	0/6/23/26	0/1/1/1
7	NAG	I	894	1	-	0/6/23/26	0/1/1/1
7	NAG	I	908	1	-	0/6/23/26	0/1/1/1
7	NAG	I	948	1	-	0/6/23/26	0/1/1/1
7	NAG	I	963	1	-	1/6/23/26	0/1/1/1
7	NAG	N	1000	6	-	0/6/23/26	0/1/1/1
7	NAG	P	1000	6	-	0/6/23/26	0/1/1/1
7	NAG	R	1000	6	-	0/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	P	1000	NAG	O5-C1	-5.76	1.34	1.43
7	N	1000	NAG	O5-C1	-5.75	1.34	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	R	1000	NAG	O5-C1	-5.73	1.34	1.43
7	A	948	NAG	C1-C2	2.64	1.56	1.52
7	E	948	NAG	C1-C2	2.66	1.56	1.52
7	I	948	NAG	C1-C2	2.68	1.56	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	P	1000	NAG	C1-O5-C5	-4.63	105.78	112.17
7	N	1000	NAG	C1-O5-C5	-4.61	105.81	112.17
7	R	1000	NAG	C1-O5-C5	-4.61	105.82	112.17
7	I	886	NAG	C2-N2-C7	-2.65	119.08	122.94
7	A	886	NAG	C2-N2-C7	-2.62	119.12	122.94
7	E	886	NAG	C2-N2-C7	-2.61	119.13	122.94
7	A	762	NAG	C2-N2-C7	-2.21	119.71	122.94
7	E	762	NAG	C2-N2-C7	-2.17	119.78	122.94
7	I	762	NAG	C2-N2-C7	-2.15	119.80	122.94
7	A	894	NAG	C2-N2-C7	-2.12	119.85	122.94
7	I	894	NAG	C2-N2-C7	-2.11	119.87	122.94
7	A	886	NAG	C4-C3-C2	-2.09	107.95	111.02
7	I	886	NAG	C4-C3-C2	-2.08	107.97	111.02
7	E	894	NAG	C2-N2-C7	-2.07	119.93	122.94
7	E	886	NAG	C4-C3-C2	-2.04	108.02	111.02
7	I	948	NAG	C2-N2-C7	-2.04	119.97	122.94
7	E	948	NAG	C2-N2-C7	-2.01	120.02	122.94

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	E	588	NAG	C1
7	A	588	NAG	C1
7	I	588	NAG	C1
7	E	741	NAG	C1
7	I	741	NAG	C1
7	A	741	NAG	C1

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	I	963	NAG	O7-C7-N2-C2
7	E	963	NAG	O7-C7-N2-C2
7	A	963	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
7	A	697	NAG	O7-C7-N2-C2
7	I	697	NAG	O7-C7-N2-C2
7	E	697	NAG	O7-C7-N2-C2
7	E	789	NAG	O7-C7-N2-C2
7	I	789	NAG	O7-C7-N2-C2
7	A	789	NAG	O7-C7-N2-C2

There are no ring outliers.

27 monomers are involved in 59 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	741	NAG	1	0
7	A	762	NAG	1	0
7	A	776	NAG	1	0
7	A	789	NAG	5	0
7	A	856	NAG	1	0
7	A	894	NAG	3	0
7	A	908	NAG	3	0
7	A	948	NAG	3	0
7	A	963	NAG	2	0
7	E	741	NAG	1	0
7	E	762	NAG	1	0
7	E	776	NAG	1	0
7	E	789	NAG	5	0
7	E	856	NAG	1	0
7	E	894	NAG	3	0
7	E	908	NAG	3	0
7	E	948	NAG	3	0
7	E	963	NAG	1	0
7	I	741	NAG	1	0
7	I	762	NAG	1	0
7	I	776	NAG	1	0
7	I	789	NAG	5	0
7	I	856	NAG	1	0
7	I	894	NAG	3	0
7	I	908	NAG	4	0
7	I	948	NAG	3	0
7	I	963	NAG	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.