



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

Feb 7, 2019 – 01:37 PM EST

PDB ID : 6MID  
EMDB ID: : EMD-9131  
Title : Cryo-EM structure of the ZIKV virion in complex with Fab fragments of the  
potently neutralizing human monoclonal antibody ZIKV-195  
Authors : Long, F.; Rossmann, M.G.  
Deposited on : 2018-09-19  
Resolution : 4.00 Å(reported)  
Based on PDB ID : 6CO8

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20031633

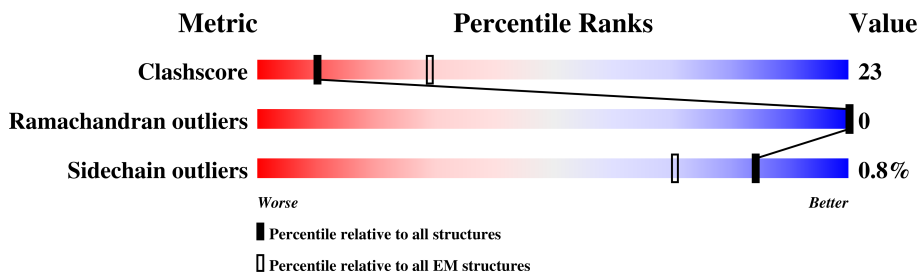
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.00 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	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

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

Mol	Chain	Length	Quality of chain	
1	A	504	61%	38% ..
1	C	504	54%	45% ..
1	E	504	60%	38% ..
2	B	75	63%	37%
2	D	75	52%	47% .
2	F	75	52%	48%
3	H	128	50%	49% .
4	L	110	59%	41%

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 15055 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 E protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	501	3787	2381	657	718	31	0	0
1	C	501	3787	2381	657	718	31	0	0
1	E	501	3790	2384	657	718	31	0	0

- Molecule 2 is a protein called M protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	75	599	391	104	103	1	0	0
2	D	75	600	391	105	103	1	0	0
2	F	75	601	391	105	104	1	0	0

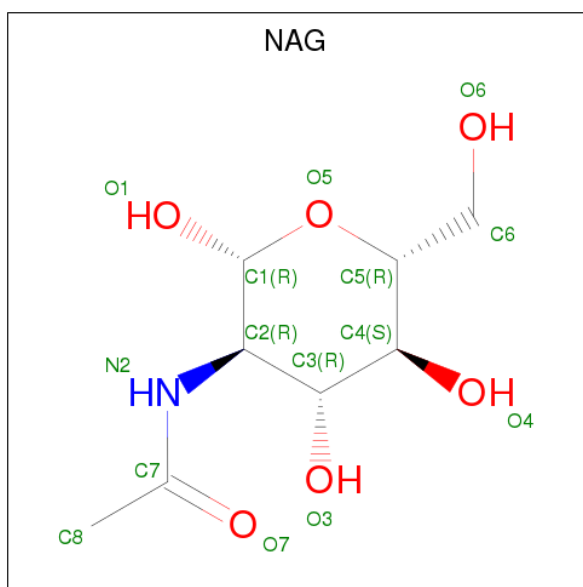
- Molecule 3 is a protein called monoclonal antibody ZIKV-195 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	H	127	981	622	169	185	5	0	0

- Molecule 4 is a protein called monoclonal antibody ZIKV-195 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	L	110	826	515	138	171	2	0	0

- Molecule 5 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).

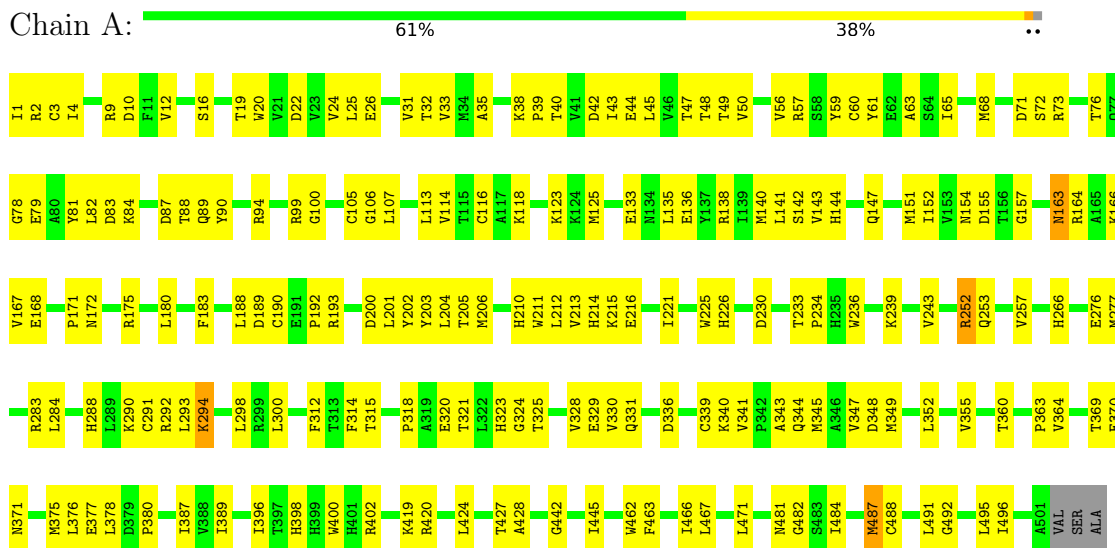


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
5	A	1	Total	C	N	O	0
			28	16	2	10	
5	A	1	Total	C	N	O	0
			28	16	2	10	
5	E	1	Total	C	N	O	0
			28	16	2	10	
5	E	1	Total	C	N	O	0
			28	16	2	10	
5	L	1	Total	C	N	O	0
			28	16	2	10	
5	L	1	Total	C	N	O	0
			28	16	2	10	

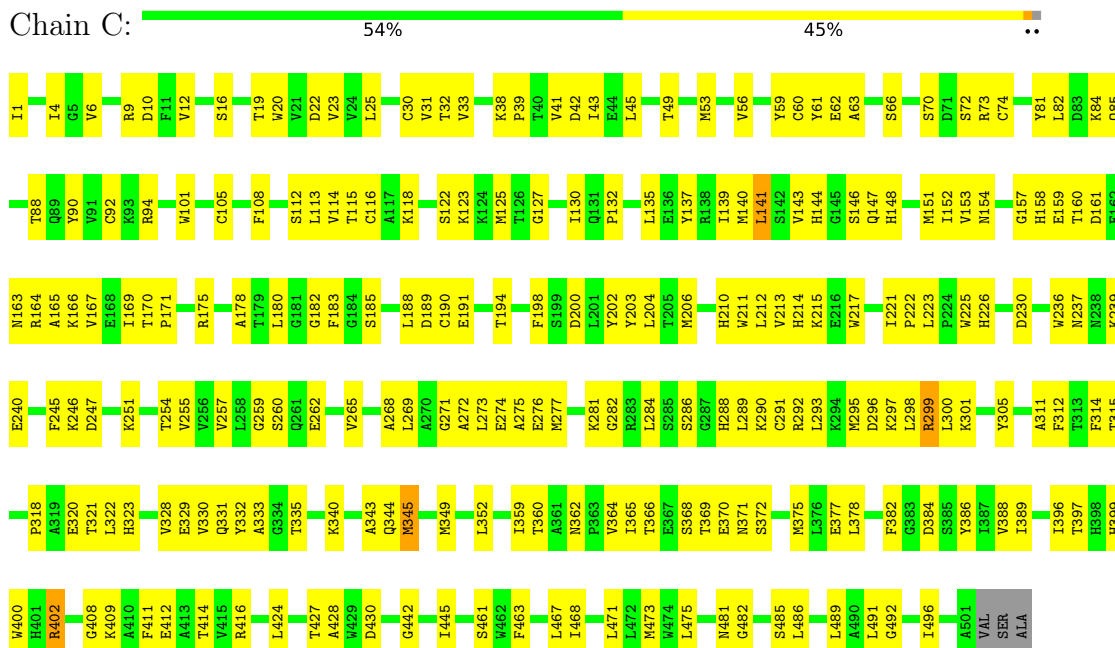
### 3 Residue-property plots

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.

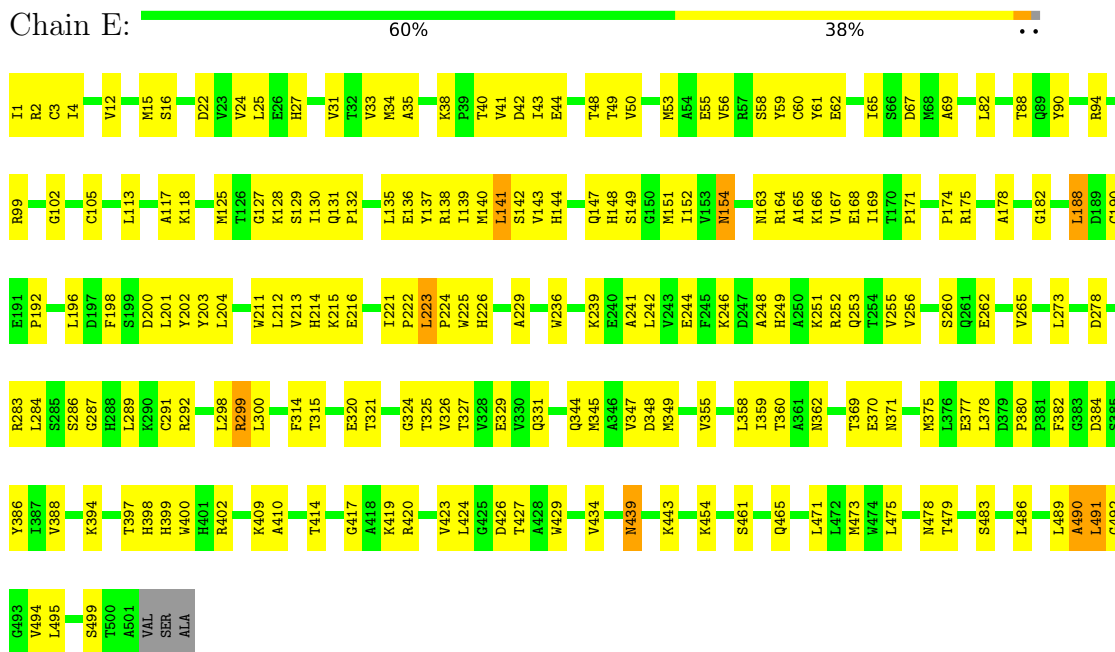
- Molecule 1: E protein



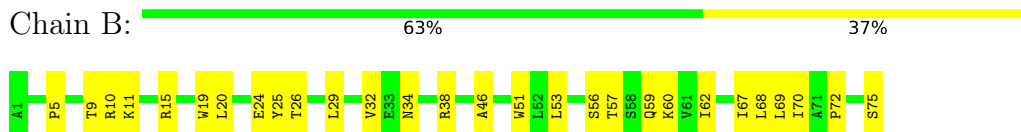
- Molecule 1: E protein



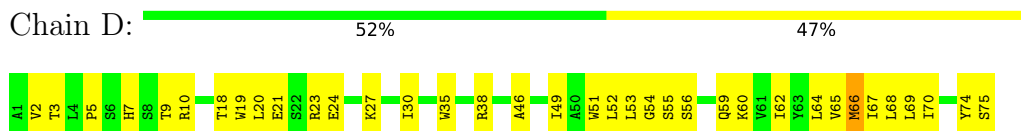
• Molecule 1: E protein



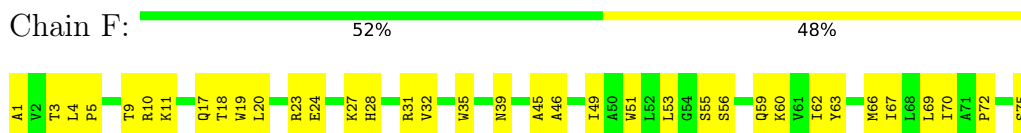
• Molecule 2: M protein



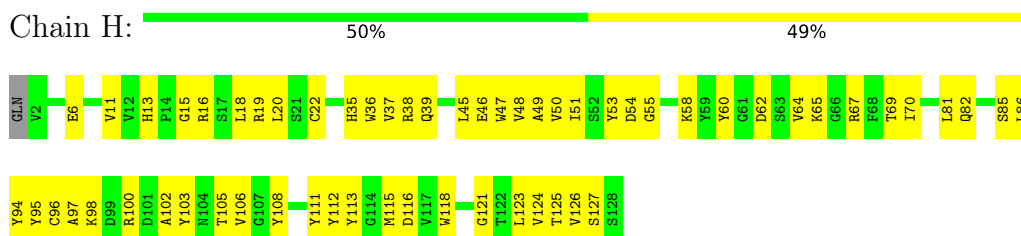
• Molecule 2: M protein



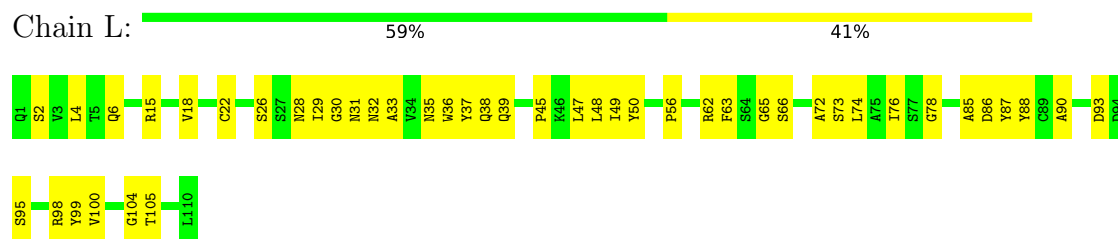
• Molecule 2: M protein



• Molecule 3: monoclonal antibody ZIKV-195 heavy chain



## ● Molecule 4: monoclonal antibody ZIKV-195 light chain



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	10687	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	30	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.37	0/3866	0.60	0/5232
1	C	0.38	0/3866	0.64	1/5232 (0.0%)
1	E	0.38	0/3869	0.67	4/5236 (0.1%)
2	B	0.32	0/614	0.63	0/836
2	D	0.37	0/615	0.68	1/838 (0.1%)
2	F	0.33	0/616	0.69	0/838
3	H	0.33	0/1006	0.54	0/1363
4	L	0.30	0/843	0.58	0/1149
All	All	0.36	0/15295	0.63	6/20724 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	491	LEU	CA-CB-CG	6.55	130.38	115.30
1	E	141	LEU	CA-CB-CG	6.45	130.13	115.30
1	C	141	LEU	CA-CB-CG	6.09	129.30	115.30
1	E	223	LEU	CA-CB-CG	5.80	128.65	115.30
1	E	188	LEU	CA-CB-CG	5.57	128.10	115.30
2	D	66	MET	CA-CB-CG	5.41	122.50	113.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	490	ALA	Mainchain

## 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	3787	0	3742	165	0
1	C	3787	0	3744	217	0
1	E	3790	0	3753	172	0
2	B	599	0	617	24	0
2	D	600	0	624	47	0
2	F	601	0	624	41	0
3	H	981	0	929	61	0
4	L	826	0	800	44	0
5	A	28	0	25	1	0
5	E	28	0	25	1	0
5	L	28	0	25	2	0
All	All	15055	0	14908	696	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 23.

All (696) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:ILE:HD12	1:C:198:PHE:CZ	1.37	1.54
1:C:130:ILE:HD12	1:C:198:PHE:CE2	1.46	1.51
1:E:41:VAL:CG2	1:E:143:VAL:HG12	1.59	1.30
1:C:130:ILE:CD1	1:C:198:PHE:CZ	2.18	1.25
1:E:41:VAL:HG22	1:E:143:VAL:CG1	1.77	1.15
1:C:169:ILE:CD1	1:C:190:CYS:SG	2.37	1.12
1:C:169:ILE:HD13	1:C:190:CYS:SG	1.90	1.11
1:C:130:ILE:CD1	1:C:198:PHE:CE2	2.38	1.05
1:E:88:THR:O	1:E:239:LYS:NZ	1.95	0.98
1:C:170:THR:HG22	1:C:171:PRO:HD2	1.45	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:ARG:NH1	1:E:349:MET:SD	2.38	0.95
1:A:71:ASP:O	1:A:113:LEU:HD12	1.68	0.94
1:E:139:ILE:HG23	1:E:167:VAL:HG23	1.49	0.91
1:C:210:HIS:HB2	1:C:275:ALA:O	1.74	0.86
1:A:193:ARG:HH21	1:E:398:HIS:HE1	1.21	0.85
1:E:41:VAL:HG22	1:E:143:VAL:HG12	0.86	0.85
1:E:138:ARG:HG2	1:E:168:GLU:HG2	1.60	0.83
1:A:138:ARG:HD2	1:A:166:LYS:HD2	1.60	0.83
2:B:32:VAL:HG23	2:B:72:PRO:HG3	1.63	0.81
1:E:24:VAL:HG11	1:E:424:LEU:HD21	1.63	0.81
2:F:56:SER:H	2:F:59:GLN:HE21	1.27	0.81
1:E:182:GLY:O	1:E:299:ARG:NH1	2.13	0.80
1:E:139:ILE:HD13	1:E:188:LEU:HD21	1.66	0.78
1:A:72:SER:OG	1:A:99:ARG:NH1	2.18	0.77
1:A:193:ARG:HH21	1:E:398:HIS:CE1	2.02	0.76
1:A:151:MET:SD	1:A:154:ASN:ND2	2.58	0.76
1:A:1:ILE:HD13	1:A:147:GLN:HB3	1.68	0.76
1:C:169:ILE:HD13	1:C:190:CYS:CB	2.16	0.75
1:C:212:LEU:HD11	1:C:284:LEU:HD23	1.67	0.75
1:C:200:ASP:OD2	1:C:214:HIS:NE2	2.20	0.74
1:E:154:ASN:O	1:E:164:ARG:NH1	2.21	0.74
1:C:41:VAL:HG22	1:C:143:VAL:HG12	1.69	0.73
1:C:473:MET:HG3	1:C:491:LEU:HD11	1.69	0.73
1:C:152:ILE:HG21	1:E:102:GLY:HA2	1.69	0.73
1:E:321:THR:OG1	1:E:325:THR:OG1	2.07	0.72
1:C:331:GLN:HE21	1:C:371:ASN:HB3	1.54	0.72
3:H:64:VAL:HG13	3:H:67:ARG:HH21	1.54	0.72
1:A:56:VAL:HG12	1:A:57:ARG:H	1.53	0.71
1:A:48:THR:HG23	1:A:284:LEU:HB2	1.72	0.71
1:C:382:PHE:HA	1:C:402:ARG:HD2	1.73	0.71
1:A:105:CYS:SG	1:A:106:GLY:N	2.63	0.71
2:D:51:TRP:HA	2:D:60:LYS:HD2	1.73	0.71
1:C:330:VAL:HG11	1:C:389:ILE:HG21	1.73	0.70
1:E:314:PHE:HE2	1:E:398:HIS:HB2	1.55	0.70
1:E:49:THR:HG22	1:E:283:ARG:HG3	1.73	0.70
1:C:62:GLU:OE2	1:C:122:SER:OG	2.08	0.70
1:C:139:ILE:HB	1:C:167:VAL:HG23	1.72	0.70
1:E:221:ILE:HG22	2:F:5:PRO:HD2	1.74	0.70
1:A:340:LYS:HA	1:A:364:VAL:HG12	1.75	0.69
1:C:169:ILE:HD11	1:C:190:CYS:SG	2.30	0.69
1:E:236:TRP:O	1:E:239:LYS:HG2	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:ASP:HA	1:A:164:ARG:HH12	1.56	0.69
1:A:331:GLN:HE21	1:A:371:ASN:HB3	1.57	0.69
2:B:26:THR:HA	2:B:29:LEU:HD21	1.73	0.69
1:A:320:GLU:HB3	1:A:400:TRP:HZ2	1.58	0.68
2:B:51:TRP:HA	2:B:60:LYS:HD2	1.76	0.68
1:C:247:ASP:O	2:F:17:GLN:NE2	2.26	0.68
1:C:88:THR:O	1:C:239:LYS:NZ	2.24	0.68
1:C:170:THR:HG22	1:C:171:PRO:CD	2.20	0.68
4:L:36:TRP:CG	4:L:74:LEU:HD13	2.28	0.68
1:C:305:TYR:O	1:C:340:LYS:NZ	2.27	0.68
1:C:408:GLY:HA2	1:C:411:PHE:CE1	2.30	0.67
2:D:75:SER:OG	2:F:28:HIS:ND1	2.27	0.67
2:D:30:ILE:HD11	2:F:3:THR:HB	1.77	0.67
1:A:78:GLY:HA2	1:C:56:VAL:HG12	1.77	0.67
1:E:67:ASP:OD1	3:H:100:ARG:NH2	2.27	0.67
1:A:10:ASP:OD2	1:A:420:ARG:NH2	2.28	0.67
1:A:314:PHE:HE2	1:A:398:HIS:HB2	1.60	0.66
1:A:1:ILE:HG23	1:A:2:ARG:H	1.59	0.66
1:C:66:SER:HB3	1:C:118:LYS:HB3	1.75	0.66
4:L:37:TYR:HH	4:L:99:TYR:HH	1.44	0.66
1:E:130:ILE:HD11	1:E:201:LEU:HB2	1.77	0.66
1:E:300:LEU:HB3	1:E:362:ASN:HD21	1.60	0.66
1:E:58:SER:OG	1:E:226:HIS:NE2	2.28	0.66
1:E:41:VAL:CG2	1:E:143:VAL:CG1	2.55	0.66
1:A:65:ILE:HD11	1:A:243:VAL:HG12	1.76	0.66
1:A:133:GLU:CD	1:A:193:ARG:HH22	1.99	0.66
1:A:330:VAL:HG11	1:A:389:ILE:HD13	1.78	0.66
1:E:249:HIS:O	3:H:111:TYR:OH	2.12	0.65
1:C:240:GLU:O	2:F:23:ARG:NH2	2.28	0.65
1:A:143:VAL:O	1:A:163:ASN:ND2	2.19	0.65
1:E:141:LEU:HD23	1:E:165:ALA:O	1.96	0.65
4:L:37:TYR:HB2	4:L:88:TYR:HB2	1.78	0.65
1:C:140:MET:SD	1:C:166:LYS:HG2	2.36	0.65
4:L:15:ARG:HA	4:L:78:GLY:HA2	1.78	0.65
1:C:222:PRO:HG3	2:D:3:THR:HG23	1.77	0.65
1:E:200:ASP:OD2	1:E:214:HIS:NE2	2.29	0.65
1:A:20:TRP:HA	1:A:293:LEU:O	1.97	0.65
1:A:369:THR:HG22	1:A:370:GLU:H	1.61	0.65
1:E:38:LYS:NZ	1:E:298:LEU:O	2.29	0.65
3:H:53:TYR:CD1	3:H:102:ALA:HB1	2.32	0.65
1:C:226:HIS:ND1	1:C:230:ASP:OD1	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:VAL:HG13	1:A:355:VAL:HG11	1.78	0.64
4:L:18:VAL:HB	4:L:76:ILE:HG23	1.77	0.64
1:A:201:LEU:HD23	1:A:212:LEU:HG	1.80	0.64
1:C:169:ILE:HD13	1:C:190:CYS:HB2	1.80	0.64
1:A:2:ARG:HA	1:A:152:ILE:HG23	1.80	0.63
4:L:39:GLN:HG3	4:L:86:ASP:HB3	1.79	0.63
1:A:348:ASP:OD1	1:A:349:MET:N	2.32	0.63
1:C:158:HIS:HA	1:C:161:ASP:HB2	1.79	0.63
3:H:11:VAL:HG22	3:H:125:THR:HB	1.80	0.63
3:H:69:THR:HG23	3:H:82:GLN:HB3	1.80	0.63
1:C:42:ASP:OD2	1:C:144:HIS:NE2	2.31	0.63
1:A:138:ARG:HG2	1:A:168:GLU:HG3	1.80	0.63
1:C:473:MET:HG2	1:C:491:LEU:HD21	1.80	0.63
1:A:35:ALA:HB3	1:A:38:LYS:HB2	1.81	0.63
1:E:2:ARG:NH2	1:E:44:GLU:OE2	2.31	0.63
1:C:188:LEU:HD22	1:C:291:CYS:SG	2.39	0.62
1:E:491:LEU:HD12	1:E:492:GLY:H	1.62	0.62
1:C:19:THR:HG23	1:C:20:TRP:CD1	2.33	0.62
1:A:155:ASP:HA	1:A:164:ARG:NH1	2.14	0.62
1:C:158:HIS:CE1	1:C:166:LYS:HE2	2.34	0.62
1:E:495:LEU:O	1:E:499:SER:N	2.23	0.62
4:L:62:ARG:NH1	4:L:78:GLY:O	2.32	0.62
1:E:4:ILE:HD11	1:E:152:ILE:HD13	1.82	0.62
1:A:26:GLU:HA	1:A:288:HIS:HA	1.82	0.62
1:C:154:ASN:OD1	4:L:95:SER:OG	2.17	0.62
1:A:189:ASP:HB2	1:A:294:LYS:HE2	1.82	0.62
1:C:59:TYR:CD1	1:C:225:TRP:HB3	2.35	0.61
3:H:51:ILE:HG13	3:H:70:ILE:HD12	1.83	0.61
1:A:236:TRP:HB2	1:A:239:LYS:HE2	1.83	0.61
1:C:475:LEU:HD11	2:F:53:LEU:HG	1.83	0.61
1:A:389:ILE:HG23	1:A:396:ILE:HG13	1.82	0.61
2:D:49:ILE:HD12	2:D:52:LEU:HD21	1.83	0.61
1:E:331:GLN:HE21	1:E:371:ASN:HB3	1.64	0.61
1:E:491:LEU:HD12	1:E:492:GLY:N	2.16	0.61
1:C:203:TYR:OH	1:C:276:GLU:O	2.18	0.60
1:E:137:TYR:HD2	1:E:289:LEU:HD22	1.64	0.60
1:C:272:ALA:O	2:D:18:THR:OG1	2.14	0.60
1:C:236:TRP:O	1:C:239:LYS:HG3	2.01	0.60
1:E:59:TYR:CD1	1:E:225:TRP:HB3	2.36	0.60
1:A:47:THR:HG23	1:A:283:ARG:HG3	1.84	0.60
1:C:320:GLU:HB2	1:C:400:TRP:HZ2	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:465:GLN:HG2	1:E:494:VAL:HG13	1.82	0.60
1:C:217:TRP:NE1	2:D:5:PRO:O	2.25	0.60
1:A:172:ASN:HA	1:E:398:HIS:CD2	2.35	0.60
1:A:60:CYS:HB2	1:A:236:TRP:CZ3	2.36	0.59
1:C:25:LEU:HB3	1:C:45:LEU:HD22	1.84	0.59
2:D:19:TRP:CD1	2:D:20:LEU:HD13	2.37	0.59
1:E:315:THR:OG1	1:E:329:GLU:OE1	2.19	0.59
4:L:6:GLN:OE1	4:L:105:THR:OG1	2.20	0.59
1:C:170:THR:CG2	1:C:171:PRO:HD2	2.25	0.59
1:E:2:ARG:HG2	1:E:152:ILE:O	2.03	0.59
1:C:141:LEU:HD23	1:C:165:ALA:O	2.01	0.59
1:A:352:LEU:HG	1:A:352:LEU:O	2.03	0.59
4:L:28:ASN:OD1	4:L:29:ILE:N	2.34	0.59
1:A:26:GLU:OE2	2:B:15:ARG:NE	2.34	0.59
2:D:54:GLY:HA3	2:D:60:LYS:HG2	1.84	0.59
1:C:61:TYR:CZ	1:C:123:LYS:HB3	2.37	0.59
1:C:225:TRP:O	1:C:237:ASN:N	2.36	0.59
1:E:62:GLU:HG3	1:E:260:SER:HB2	1.84	0.59
1:E:314:PHE:CE2	1:E:398:HIS:HB2	2.38	0.58
1:E:358:LEU:HG	1:E:378:LEU:HD13	1.85	0.58
1:A:467:LEU:HD11	2:B:69:LEU:HD21	1.85	0.58
1:C:139:ILE:HB	1:C:167:VAL:CG2	2.33	0.58
1:C:147:GLN:OE1	1:C:163:ASN:ND2	2.35	0.58
2:F:45:ALA:O	2:F:49:ILE:HD12	2.04	0.58
2:F:59:GLN:O	2:F:62:ILE:HG22	2.03	0.58
4:L:22:CYS:HB3	4:L:72:ALA:HB3	1.85	0.58
1:C:274:GLU:OE1	1:E:246:LYS:NZ	2.30	0.58
1:E:137:TYR:HE2	1:E:289:LEU:HD13	1.69	0.58
1:A:462:TRP:O	1:A:466:ILE:HD12	2.04	0.58
1:C:39:PRO:HG3	1:C:183:PHE:CD1	2.38	0.58
1:E:345:MET:HE2	1:E:378:LEU:HB3	1.86	0.58
3:H:49:ALA:HB1	3:H:70:ILE:HD13	1.86	0.58
4:L:28:ASN:HB3	4:L:93:ASP:HB3	1.86	0.58
1:A:31:VAL:HG13	1:A:43:ILE:HB	1.86	0.57
1:A:88:THR:O	1:A:239:LYS:NZ	2.37	0.57
1:C:19:THR:HA	1:C:296:ASP:HB3	1.86	0.57
1:A:157:GLY:O	1:A:164:ARG:NH2	2.37	0.57
2:F:51:TRP:HA	2:F:60:LYS:HD2	1.85	0.57
1:A:320:GLU:HB3	1:A:400:TRP:CZ2	2.39	0.57
1:A:81:TYR:CD2	1:C:230:ASP:HB3	2.40	0.57
1:C:492:GLY:O	1:C:496:ILE:HG12	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:343:ALA:HA	1:C:388:VAL:O	2.04	0.57
3:H:113:TYR:OH	4:L:33:ALA:O	2.21	0.57
1:A:39:PRO:HD3	1:A:300:LEU:HB3	1.86	0.57
1:C:135:LEU:HD21	1:C:198:PHE:CD2	2.40	0.57
1:C:485:SER:O	1:C:489:LEU:N	2.31	0.57
1:E:386:TYR:HE1	1:E:399:HIS:CD2	2.23	0.57
1:A:147:GLN:NE2	1:A:163:ASN:OD1	2.38	0.57
1:A:89:GLN:OE1	1:A:118:LYS:NZ	2.37	0.57
1:C:157:GLY:O	1:C:164:ARG:NH2	2.36	0.57
1:E:216:GLU:HG3	2:F:10:ARG:NH1	2.20	0.57
4:L:62:ARG:HH11	4:L:78:GLY:HA3	1.69	0.57
1:A:204:LEU:HD13	1:A:213:VAL:HG11	1.86	0.56
1:C:72:SER:HA	1:C:112:SER:O	2.04	0.56
1:E:48:THR:HG23	1:E:137:TYR:CE1	2.40	0.56
3:H:15:GLY:H	3:H:86:LEU:HD23	1.71	0.56
1:C:144:HIS:HB3	1:C:360:THR:HG23	1.88	0.56
1:A:59:TYR:O	1:A:125:MET:N	2.36	0.56
1:C:212:LEU:HB2	1:C:273:LEU:HB2	1.87	0.56
1:A:140:MET:SD	1:A:166:LYS:HB2	2.46	0.56
1:A:321:THR:O	1:A:323:HIS:N	2.39	0.56
4:L:37:TYR:OH	4:L:99:TYR:OH	2.16	0.56
1:A:328:VAL:HG21	1:A:387:ILE:HD13	1.86	0.56
1:C:141:LEU:HD11	1:C:180:LEU:HD11	1.86	0.56
1:C:178:ALA:O	1:C:185:SER:HA	2.05	0.56
3:H:35:HIS:HE1	3:H:115:MET:HB3	1.69	0.56
3:H:64:VAL:HG12	3:H:67:ARG:HB2	1.88	0.56
1:C:214:HIS:CE1	2:D:10:ARG:HE	2.25	0.55
1:A:90:TYR:HB3	1:A:116:CYS:SG	2.47	0.55
1:C:185:SER:OG	1:C:297:LYS:HE3	2.07	0.55
2:F:55:SER:H	2:F:59:GLN:NE2	2.04	0.55
1:C:202:TYR:CE2	1:C:215:LYS:HG3	2.41	0.55
1:C:22:ASP:OD1	1:C:292:ARG:HG2	2.06	0.55
2:F:23:ARG:O	2:F:27:LYS:HB2	2.06	0.55
1:E:347:VAL:HG13	1:E:355:VAL:HG21	1.88	0.55
1:C:468:ILE:HD11	2:F:67:ILE:HD11	1.87	0.55
1:C:74:CYS:SG	1:C:105:CYS:HB2	2.47	0.55
1:C:19:THR:O	1:C:295:MET:N	2.39	0.55
1:E:251:LYS:HD3	4:L:32:ASN:HB3	1.88	0.55
1:C:49:THR:HG21	1:C:281:LYS:HD3	1.89	0.55
3:H:13:HIS:HB2	3:H:16:ARG:HH12	1.71	0.55
2:D:23:ARG:NH1	1:E:244:GLU:OE2	2.26	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:320:GLU:HB2	1:E:400:TRP:HZ2	1.71	0.54
1:E:248:ALA:HB2	1:E:253:GLN:OE1	2.07	0.54
3:H:62:ASP:HA	3:H:65:LYS:HG3	1.89	0.54
1:C:70:SER:HA	1:C:114:VAL:O	2.06	0.54
2:D:67:ILE:HG23	2:D:68:LEU:HD12	1.88	0.54
1:C:59:TYR:HD1	1:C:225:TRP:HB3	1.73	0.54
4:L:39:GLN:O	4:L:85:ALA:HB1	2.07	0.54
1:A:154:ASN:HD21	5:A:600:NAG:C1	2.20	0.54
1:C:141:LEU:HD21	1:C:165:ALA:HB3	1.89	0.54
3:H:38:ARG:NH1	3:H:46:GLU:OE1	2.41	0.54
3:H:45:LEU:HD13	4:L:88:TYR:CE2	2.43	0.54
2:D:66:MET:HG2	2:F:66:MET:HG2	1.89	0.54
1:E:137:TYR:CE2	1:E:289:LEU:HD13	2.43	0.54
1:E:167:VAL:CG1	1:E:178:ALA:HB2	2.38	0.54
4:L:6:GLN:NE2	4:L:104:GLY:H	2.05	0.54
1:C:53:MET:HG2	1:C:130:ILE:HG22	1.90	0.54
1:C:148:HIS:HA	1:C:375:MET:HG3	1.90	0.54
3:H:115:MET:HG2	3:H:118:TRP:HE1	1.73	0.54
1:C:152:ILE:HG23	1:C:153:VAL:H	1.73	0.54
1:C:84:LYS:HB3	1:C:90:TYR:CD2	2.43	0.54
1:A:133:GLU:OE1	1:A:193:ARG:NH2	2.41	0.53
1:A:206:MET:HB3	1:A:211:TRP:HZ3	1.73	0.53
1:E:214:HIS:CD2	1:E:215:LYS:H	2.26	0.53
1:C:245:PHE:CD1	1:C:255:VAL:HG12	2.42	0.53
1:E:248:ALA:HB1	3:H:111:TYR:OH	2.08	0.53
4:L:65:GLY:HA2	4:L:74:LEU:HD23	1.90	0.53
2:B:11:LYS:NZ	2:B:24:GLU:OE2	2.34	0.53
1:E:249:HIS:HB2	1:E:252:ARG:HG2	1.91	0.53
1:C:62:GLU:HG3	1:C:123:LYS:HB2	1.90	0.53
1:E:167:VAL:HG11	1:E:178:ALA:HB2	1.91	0.53
1:E:212:LEU:HD13	1:E:284:LEU:HD13	1.91	0.53
2:F:63:TYR:O	2:F:67:ILE:HG22	2.09	0.53
1:A:221:ILE:HG22	2:B:5:PRO:HD2	1.91	0.53
1:C:296:ASP:OD1	1:C:297:LYS:N	2.42	0.53
1:E:1:ILE:HG22	1:E:144:HIS:CD2	2.43	0.53
1:E:140:MET:SD	1:E:166:LYS:HB3	2.49	0.53
3:H:97:ALA:HB1	3:H:115:MET:HG3	1.91	0.52
1:E:465:GLN:HG2	1:E:494:VAL:CG1	2.39	0.52
2:D:27:LYS:HG2	2:F:3:THR:HG22	1.92	0.52
3:H:62:ASP:H	4:L:98:ARG:HE	1.56	0.52
1:A:180:LEU:HB3	1:A:183:PHE:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:THR:HG23	1:A:210:HIS:CE1	2.44	0.52
2:B:46:ALA:CB	2:B:67:ILE:HD11	2.39	0.52
1:C:388:VAL:HA	1:C:396:ILE:O	2.10	0.52
1:E:384:ASP:OD2	1:E:399:HIS:NE2	2.42	0.52
4:L:36:TRP:CD1	4:L:74:LEU:HD13	2.44	0.52
1:A:276:GLU:HG3	1:A:277:MET:H	1.75	0.52
2:B:9:THR:HG23	2:B:10:ARG:HG2	1.90	0.52
1:C:369:THR:HG22	1:C:370:GLU:H	1.74	0.52
1:C:82:LEU:H	1:C:85:GLN:HE22	1.55	0.52
1:E:358:LEU:HD23	1:E:360:THR:H	1.73	0.52
3:H:47:TRP:CZ2	3:H:50:VAL:HG13	2.45	0.52
1:A:144:HIS:HB3	1:A:360:THR:HG23	1.92	0.52
1:A:90:TYR:CE1	1:A:118:LYS:HB2	2.45	0.52
2:D:23:ARG:NH1	1:E:241:ALA:O	2.38	0.52
1:C:39:PRO:HG3	1:C:183:PHE:HD1	1.75	0.51
1:E:359:ILE:HG22	1:E:377:GLU:O	2.11	0.51
1:E:369:THR:HG22	1:E:370:GLU:H	1.74	0.51
2:F:46:ALA:HB1	2:F:67:ILE:HG23	1.92	0.51
1:C:189:ASP:HB2	1:C:292:ARG:HB2	1.92	0.51
1:C:276:GLU:HG3	1:C:277:MET:H	1.74	0.51
1:E:154:ASN:HD21	5:E:600:NAG:C1	2.23	0.51
3:H:35:HIS:CE1	3:H:97:ALA:HB3	2.45	0.51
1:C:72:SER:OG	1:C:113:LEU:HD13	2.10	0.51
1:A:203:TYR:OH	1:A:276:GLU:O	2.28	0.51
1:A:345:MET:CE	1:A:378:LEU:HB3	2.40	0.51
1:C:152:ILE:HG12	1:C:153:VAL:HG13	1.92	0.51
2:D:70:ILE:HG13	2:F:66:MET:HG3	1.91	0.51
1:A:189:ASP:HB3	1:A:292:ARG:HB2	1.93	0.51
1:E:284:LEU:HG	1:E:286:SER:H	1.75	0.51
1:C:290:LYS:HE3	1:C:430:ASP:HB3	1.91	0.51
1:E:65:ILE:HG23	1:E:117:ALA:HB1	1.92	0.51
1:A:87:ASP:HB3	1:A:90:TYR:HD2	1.76	0.51
1:C:411:PHE:HA	1:C:414:THR:HG22	1.93	0.51
1:A:9:ARG:HH21	1:A:32:THR:HG21	1.76	0.51
1:C:384:ASP:OD2	1:C:399:HIS:HE1	1.94	0.51
2:D:19:TRP:NE1	2:D:20:LEU:HD13	2.25	0.51
1:E:4:ILE:HD11	1:E:152:ILE:HG21	1.93	0.51
1:A:419:LYS:HE2	2:B:15:ARG:NH1	2.26	0.51
1:E:204:LEU:HD13	1:E:213:VAL:HG11	1.91	0.51
3:H:93:VAL:HG22	3:H:123:LEU:HB3	1.93	0.51
1:A:19:THR:HG23	1:A:20:TRP:CD1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:ALA:HB3	1:C:257:VAL:HG21	1.93	0.51
1:E:386:TYR:HE1	1:E:399:HIS:HD2	1.58	0.51
1:C:175:ARG:HG3	1:C:189:ASP:OD1	2.10	0.50
1:C:60:CYS:HB2	1:C:236:TRP:CZ3	2.46	0.50
1:E:2:ARG:H	1:E:152:ILE:HG23	1.75	0.50
1:A:491:LEU:O	1:A:495:LEU:HD23	2.11	0.50
2:D:46:ALA:O	2:D:49:ILE:HG22	2.11	0.50
2:D:38:ARG:NH1	1:E:216:GLU:OE1	2.44	0.50
4:L:49:ILE:HD11	4:L:63:PHE:HB3	1.94	0.50
1:C:1:ILE:HG22	1:C:144:HIS:HD2	1.76	0.50
1:E:324:GLY:HA3	1:E:402:ARG:HH21	1.77	0.50
1:E:59:TYR:HE2	1:E:221:ILE:CG1	2.24	0.50
1:C:154:ASN:HD21	5:L:600:NAG:C1	2.25	0.50
1:C:259:GLY:HA3	1:E:262:GLU:HG3	1.92	0.50
1:C:349:MET:HB2	1:C:386:TYR:CD2	2.47	0.50
1:C:70:SER:HB3	1:C:113:LEU:HD11	1.94	0.50
2:D:19:TRP:HH2	1:E:256:VAL:HG11	1.77	0.50
1:E:216:GLU:HG3	2:F:10:ARG:CZ	2.42	0.50
1:C:301:LYS:O	1:C:362:ASN:ND2	2.44	0.50
3:H:47:TRP:HZ2	3:H:50:VAL:HG13	1.76	0.50
1:A:39:PRO:HD2	1:A:298:LEU:HB3	1.94	0.50
1:A:266:HIS:O	2:B:19:TRP:HZ3	1.95	0.49
4:L:38:GLN:HB2	4:L:48:LEU:HD11	1.94	0.49
2:B:29:LEU:HA	2:B:32:VAL:HG12	1.94	0.49
1:C:158:HIS:HE1	1:C:166:LYS:HE2	1.75	0.49
1:C:331:GLN:NE2	1:C:371:ASN:HB3	2.23	0.49
1:E:423:VAL:HG23	1:E:424:LEU:HD13	1.93	0.49
3:H:37:VAL:HB	3:H:95:TYR:HB2	1.94	0.49
3:H:67:ARG:HH12	3:H:87:ARG:N	2.10	0.49
1:C:9:ARG:NH2	1:C:32:THR:OG1	2.46	0.49
1:E:31:VAL:HB	1:E:43:ILE:HG13	1.93	0.49
1:A:344:GLN:HE21	1:A:352:LEU:HD11	1.77	0.49
1:C:349:MET:HB2	1:C:386:TYR:HD2	1.76	0.49
1:A:167:VAL:HG21	1:A:188:LEU:HD12	1.94	0.49
1:A:10:ASP:CG	1:A:420:ARG:HH22	2.15	0.49
1:A:424:LEU:HB2	1:A:428:ALA:HB2	1.93	0.49
1:C:16:SER:O	1:C:19:THR:HG22	2.13	0.49
1:E:3:CYS:HB2	1:E:42:ASP:HB2	1.92	0.49
2:F:27:LYS:HE2	2:F:31:ARG:HH21	1.77	0.49
1:C:333:ALA:HA	1:C:370:GLU:O	2.12	0.49
1:C:461:SER:OG	2:D:24:GLU:OE2	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:331:GLN:NE2	1:E:371:ASN:HB3	2.27	0.49
1:A:57:ARG:HG3	1:A:225:TRP:HB2	1.95	0.49
1:C:159:GLU:HG2	1:C:160:THR:HG23	1.93	0.49
1:C:320:GLU:HB2	1:C:400:TRP:CZ2	2.47	0.49
1:E:169:ILE:HD11	1:E:174:PRO:O	2.13	0.49
1:A:135:LEU:O	1:A:171:PRO:HD3	2.13	0.49
1:A:369:THR:HG22	1:A:370:GLU:N	2.27	0.49
1:E:344:GLN:HG3	1:E:388:VAL:HG23	1.95	0.49
3:H:64:VAL:HG13	3:H:67:ARG:NH2	2.27	0.49
1:C:82:LEU:HD22	1:C:116:CYS:SG	2.53	0.48
1:C:322:LEU:HD13	1:C:322:LEU:O	2.14	0.48
3:H:94:TYR:HE2	3:H:124:VAL:HG22	1.78	0.48
1:E:129:SER:HA	1:E:202:TYR:HD1	1.78	0.48
4:L:39:GLN:HA	4:L:45:PRO:HA	1.95	0.48
2:B:59:GLN:HA	2:B:62:ILE:HG22	1.93	0.48
1:C:84:LYS:HB3	1:C:90:TYR:HD2	1.77	0.48
3:H:105:THR:OG1	3:H:108:TYR:O	2.26	0.48
3:H:6:GLU:HG3	3:H:96:CYS:SG	2.54	0.48
1:A:94:ARG:HG2	1:A:114:VAL:HG12	1.94	0.48
1:C:135:LEU:HD21	1:C:198:PHE:CE2	2.49	0.48
1:C:442:GLY:HA2	1:C:445:ILE:HG12	1.95	0.48
1:E:56:VAL:HG22	1:E:127:GLY:O	2.14	0.48
1:E:151:MET:HA	1:E:154:ASN:HB3	1.94	0.48
1:E:15:MET:HE1	1:E:34:MET:O	2.13	0.48
1:E:429:TRP:HB2	1:E:443:LYS:HB3	1.96	0.48
1:E:25:LEU:HD12	1:E:43:ILE:HD12	1.96	0.48
3:H:91:THR:HB	3:H:126:VAL:H	1.78	0.48
1:A:202:TYR:CZ	1:A:215:LYS:HG2	2.49	0.48
1:C:471:LEU:HD11	2:F:49:ILE:HG21	1.95	0.48
2:D:62:ILE:HA	2:D:65:VAL:HG22	1.95	0.48
1:E:473:MET:HG2	1:E:491:LEU:HD22	1.94	0.48
2:F:11:LYS:HD2	2:F:18:THR:HG21	1.96	0.48
2:F:32:VAL:HG12	2:F:72:PRO:HB2	1.95	0.48
1:A:343:ALA:HB2	1:A:389:ILE:HG13	1.96	0.48
1:C:151:MET:SD	1:C:154:ASN:ND2	2.84	0.48
1:C:167:VAL:HG11	1:C:178:ALA:HB2	1.95	0.48
1:C:191:GLU:HG3	1:C:194:THR:HG22	1.95	0.48
1:E:461:SER:O	1:E:465:GLN:HB2	2.13	0.48
1:A:175:ARG:HH21	1:E:397:THR:HG21	1.79	0.48
1:E:55:GLU:HB2	1:E:229:ALA:HB2	1.94	0.48
1:E:326:VAL:HG23	1:E:378:LEU:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:35:TRP:HE1	2:F:9:THR:HG23	1.78	0.48
2:D:62:ILE:O	2:D:65:VAL:HG22	2.13	0.48
3:H:20:LEU:HD22	3:H:36:TRP:HZ2	1.79	0.48
1:A:492:GLY:O	1:A:496:ILE:HG22	2.13	0.47
1:E:16:SER:HB2	1:E:434:VAL:HB	1.96	0.47
1:E:410:ALA:O	1:E:414:THR:HG23	2.14	0.47
4:L:6:GLN:HE21	4:L:104:GLY:H	1.62	0.47
1:A:63:ALA:HB3	1:A:257:VAL:HG21	1.96	0.47
1:A:3:CYS:O	1:A:9:ARG:HD3	2.14	0.47
1:C:81:TYR:HA	1:C:85:GLN:HE22	1.78	0.47
1:C:170:THR:CG2	1:C:171:PRO:CD	2.88	0.47
2:D:9:THR:HG23	2:D:10:ARG:HG2	1.96	0.47
1:E:12:VAL:HG23	1:E:33:VAL:HG12	1.96	0.47
3:H:13:HIS:ND1	3:H:127:SER:O	2.46	0.47
3:H:36:TRP:O	3:H:48:VAL:HB	2.14	0.47
1:A:100:GLY:O	1:A:105:CYS:HB3	2.15	0.47
1:C:265:VAL:HA	1:C:268:ALA:HB3	1.97	0.47
4:L:26:SER:HA	4:L:30:GLY:HA3	1.97	0.47
4:L:50:TYR:CD1	4:L:56:PRO:HG3	2.50	0.47
1:A:200:ASP:C	1:A:201:LEU:HD12	2.35	0.47
1:A:42:ASP:OD1	1:A:142:SER:HB2	2.14	0.47
3:H:51:ILE:CG1	3:H:70:ILE:HD12	2.44	0.47
1:A:87:ASP:HB3	1:A:90:TYR:CD2	2.50	0.47
1:C:182:GLY:O	1:C:299:ARG:NE	2.30	0.47
1:E:94:ARG:HA	1:E:113:LEU:O	2.15	0.47
1:C:137:TYR:CD2	1:C:289:LEU:HD11	2.49	0.47
1:A:387:ILE:CG2	1:A:398:HIS:HB3	2.43	0.47
1:C:386:TYR:HB3	1:C:397:THR:HG23	1.97	0.47
1:E:439:ASN:O	1:E:439:ASN:ND2	2.48	0.47
1:A:487:MET:SD	1:A:488:CYS:N	2.88	0.47
2:B:19:TRP:CE3	2:B:20:LEU:HD13	2.49	0.47
1:C:20:TRP:HA	1:C:293:LEU:O	2.15	0.47
1:C:315:THR:HB	1:C:329:GLU:OE1	2.15	0.47
3:H:118:TRP:N	3:H:118:TRP:CD1	2.83	0.47
1:C:135:LEU:O	1:C:170:THR:HG23	2.15	0.46
1:C:365:ILE:HD11	1:C:372:SER:HB3	1.96	0.46
1:C:31:VAL:HG23	1:C:43:ILE:HB	1.98	0.46
1:E:12:VAL:CG2	1:E:33:VAL:HG12	2.45	0.46
1:E:324:GLY:O	1:E:380:PRO:HD2	2.15	0.46
1:E:478:ASN:O	1:E:479:THR:OG1	2.24	0.46
3:H:15:GLY:HA2	3:H:85:SER:HA	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:13:HIS:HB2	3:H:16:ARG:NH1	2.29	0.46
1:A:190:CYS:HA	1:A:291:CYS:HA	1.96	0.46
1:E:27:HIS:HB2	1:E:287:GLY:O	2.16	0.46
2:B:68:LEU:HD23	2:B:68:LEU:O	2.14	0.46
1:C:25:LEU:O	1:C:288:HIS:HA	2.16	0.46
1:C:273:LEU:HD13	1:C:286:SER:OG	2.16	0.46
3:H:86:LEU:HD23	3:H:86:LEU:H	1.80	0.46
1:A:56:VAL:HG12	1:A:57:ARG:N	2.25	0.46
1:E:252:ARG:N	3:H:111:TYR:HE1	2.13	0.46
1:C:132:PRO:O	1:C:171:PRO:HG2	2.15	0.46
1:C:214:HIS:ND1	2:D:10:ARG:HB3	2.29	0.46
1:C:335:THR:HG23	1:C:368:SER:O	2.15	0.46
1:A:22:ASP:OD1	1:A:292:ARG:HD2	2.16	0.46
1:E:419:LYS:O	1:E:423:VAL:HG22	2.16	0.46
1:C:269:LEU:O	1:C:271:GLY:N	2.49	0.46
2:D:53:LEU:HD12	1:E:475:LEU:HD11	1.97	0.46
2:D:2:VAL:O	2:F:27:LYS:HE3	2.15	0.46
3:H:62:ASP:OD1	3:H:65:LYS:HE2	2.16	0.46
1:A:463:PHE:CE2	1:A:467:LEU:HD12	2.50	0.46
1:C:1:ILE:N	1:C:4:ILE:HG23	2.30	0.46
1:C:59:TYR:HB2	1:C:125:MET:HB2	1.98	0.46
1:C:1:ILE:N	1:C:42:ASP:OD2	2.46	0.46
1:E:50:VAL:HG11	1:E:130:ILE:HG22	1.97	0.46
1:C:130:ILE:CD1	1:C:198:PHE:CE1	2.91	0.46
1:C:312:PHE:CE1	1:C:332:TYR:HB2	2.50	0.46
1:C:60:CYS:O	1:C:223:LEU:HG	2.16	0.46
1:A:24:VAL:HG22	1:A:290:LYS:HG2	1.98	0.45
1:A:345:MET:HE3	1:A:378:LEU:HB3	1.98	0.45
2:D:53:LEU:HD11	1:E:471:LEU:HD11	1.97	0.45
3:H:115:MET:CG	3:H:118:TRP:HE1	2.29	0.45
4:L:2:SER:HA	4:L:100:VAL:HG11	1.99	0.45
1:A:31:VAL:CG1	1:A:43:ILE:HB	2.46	0.45
1:E:90:TYR:CE1	1:E:118:LYS:HB2	2.51	0.45
3:H:35:HIS:CB	3:H:50:VAL:HG12	2.47	0.45
1:A:72:SER:HB2	1:A:113:LEU:HD13	1.98	0.45
1:A:25:LEU:O	1:A:25:LEU:HD12	2.17	0.45
1:A:47:THR:CG2	1:A:283:ARG:HG3	2.46	0.45
1:A:50:VAL:HG22	1:A:135:LEU:HD23	1.98	0.45
1:C:62:GLU:HB3	1:C:260:SER:HA	1.98	0.45
4:L:39:GLN:CG	4:L:86:ASP:HB3	2.45	0.45
1:A:1:ILE:O	1:A:4:ILE:HB	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:LYS:HD2	1:C:295:MET:HG3	1.97	0.45
1:C:82:LEU:N	1:C:85:GLN:HE22	2.15	0.45
2:D:66:MET:HG3	2:F:70:ILE:CD1	2.45	0.45
3:H:49:ALA:HB2	3:H:60:TYR:CD1	2.52	0.45
1:C:202:TYR:HE2	1:C:215:LYS:HG3	1.81	0.45
1:C:276:GLU:HG3	1:C:277:MET:N	2.32	0.45
1:C:377:GLU:C	1:C:378:LEU:HD12	2.37	0.45
1:C:345:MET:HE1	1:C:378:LEU:HG	1.98	0.45
4:L:31:ASN:OD1	4:L:32:ASN:N	2.49	0.45
1:A:336:ASP:HB3	1:A:339:CYS:SG	2.56	0.45
1:C:318:PRO:HB3	1:C:328:VAL:HG22	1.99	0.45
1:E:196:LEU:HB3	1:E:198:PHE:CZ	2.51	0.45
2:D:55:SER:HB2	2:D:59:GLN:OE1	2.16	0.45
1:E:265:VAL:HG22	2:F:4:LEU:HD21	1.97	0.45
1:C:402:ARG:HD3	1:C:402:ARG:O	2.17	0.45
2:B:53:LEU:O	2:B:60:LYS:HG2	2.17	0.45
1:C:1:ILE:H2	1:C:4:ILE:HG23	1.82	0.45
1:C:225:TRP:CE2	1:C:237:ASN:HB2	2.52	0.45
1:C:183:PHE:O	1:C:298:LEU:HD12	2.17	0.45
1:A:252:ARG:HG2	1:A:253:GLN:N	2.31	0.45
1:C:137:TYR:CG	1:C:289:LEU:HD11	2.52	0.44
1:E:417:GLY:HA2	1:E:420:ARG:HE	1.82	0.44
4:L:35:ASN:ND2	4:L:37:TYR:OH	2.49	0.44
1:A:324:GLY:HA2	1:A:402:ARG:HD2	2.00	0.44
1:A:40:THR:HG21	1:A:360:THR:HA	2.00	0.44
1:C:321:THR:O	1:C:323:HIS:N	2.50	0.44
1:C:362:ASN:O	1:C:364:VAL:HG23	2.17	0.44
2:D:30:ILE:HD11	2:F:3:THR:CB	2.46	0.44
1:E:33:VAL:O	1:E:40:THR:HA	2.17	0.44
1:E:35:ALA:HB3	1:E:38:LYS:HB2	1.99	0.44
1:A:81:TYR:CE2	1:A:83:ASP:HA	2.52	0.44
1:C:167:VAL:CG1	1:C:178:ALA:HB2	2.48	0.44
1:C:411:PHE:O	1:C:414:THR:HG22	2.17	0.44
1:E:148:HIS:HA	1:E:375:MET:HG3	1.99	0.44
1:E:203:TYR:HA	1:E:211:TRP:O	2.17	0.44
1:E:60:CYS:HB2	1:E:236:TRP:CZ3	2.53	0.44
3:H:70:ILE:HG22	3:H:81:LEU:HD23	1.99	0.44
1:A:43:ILE:HG12	1:A:141:LEU:HD22	2.00	0.44
1:A:90:TYR:HE1	1:A:118:LYS:HB2	1.83	0.44
1:C:203:TYR:HA	1:C:211:TRP:O	2.17	0.44
1:E:475:LEU:HD23	1:E:475:LEU:HA	1.74	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:47:LEU:HG	4:L:56:PRO:HG2	1.98	0.44
1:A:324:GLY:CA	1:A:402:ARG:HD2	2.47	0.44
2:B:34:ASN:O	2:B:38:ARG:HG2	2.17	0.44
1:E:255:VAL:HG22	1:E:255:VAL:O	2.18	0.44
1:C:108:PHE:CG	1:E:321:THR:HG22	2.52	0.44
1:E:60:CYS:HB2	1:E:236:TRP:CH2	2.52	0.44
1:A:49:THR:HA	1:A:283:ARG:HA	2.00	0.44
1:A:2:ARG:NH2	1:A:44:GLU:OE2	2.51	0.44
1:A:321:THR:HB	1:A:325:THR:HB	1.98	0.44
2:D:56:SER:O	2:D:60:LYS:HG3	2.17	0.44
1:C:152:ILE:HD13	1:E:102:GLY:HA3	1.99	0.44
1:E:171:PRO:HB3	1:E:192:PRO:HG2	2.00	0.44
4:L:87:TYR:HB2	4:L:105:THR:HB	2.00	0.44
1:A:40:THR:HG23	1:A:144:HIS:HB2	2.00	0.44
1:A:467:LEU:HD11	2:B:69:LEU:CD2	2.48	0.44
1:C:369:THR:HG22	1:C:370:GLU:N	2.32	0.44
1:C:221:ILE:HG22	2:D:5:PRO:HD2	1.99	0.44
1:E:394:LYS:O	1:E:394:LYS:HG3	2.18	0.44
2:D:70:ILE:HD12	2:F:69:LEU:HD23	2.00	0.44
1:A:47:THR:HG22	1:A:48:THR:N	2.33	0.44
2:B:70:ILE:HD11	2:B:75:SER:HB3	1.99	0.44
1:C:166:LYS:HB2	1:C:166:LYS:HE3	1.75	0.44
1:C:23:VAL:HG22	1:C:293:LEU:HD11	1.99	0.44
1:E:1:ILE:HG12	1:E:147:GLN:OE1	2.18	0.44
1:E:169:ILE:HD13	1:E:190:CYS:SG	2.58	0.44
1:E:2:ARG:HH12	1:E:44:GLU:HG2	1.82	0.44
1:E:69:ALA:HA	3:H:112:TYR:HD2	1.83	0.44
2:F:24:GLU:N	2:F:24:GLU:OE1	2.51	0.44
1:C:312:PHE:O	1:C:396:ILE:HD11	2.18	0.43
1:E:149:SER:HA	1:E:375:MET:SD	2.58	0.43
1:E:53:MET:HB3	1:E:128:LYS:HB3	1.99	0.43
1:E:59:TYR:HB3	1:E:223:LEU:CD2	2.48	0.43
1:E:59:TYR:O	1:E:125:MET:N	2.51	0.43
1:E:490:ALA:O	1:E:494:VAL:HG23	2.19	0.43
1:E:69:ALA:HB3	1:E:82:LEU:HD21	2.00	0.43
1:A:481:ASN:OD1	1:A:482:GLY:N	2.49	0.43
1:C:424:LEU:HB3	1:C:427:THR:OG1	2.17	0.43
1:C:213:VAL:HA	2:D:7:HIS:CE1	2.53	0.43
1:E:42:ASP:OD1	1:E:142:SER:HB3	2.18	0.43
1:C:314:PHE:HE1	1:C:328:VAL:HG13	1.84	0.43
4:L:90:ALA:HA	4:L:100:VAL:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:63:PHE:CE1	4:L:76:ILE:HD12	2.53	0.43
1:C:94:ARG:HD3	1:C:114:VAL:HB	2.00	0.43
1:C:340:LYS:HG2	1:C:364:VAL:HG22	2.00	0.43
1:C:463:PHE:O	1:C:467:LEU:HD23	2.18	0.43
1:E:131:GLN:HA	1:E:132:PRO:HD3	1.89	0.43
1:E:190:CYS:HA	1:E:291:CYS:HA	2.01	0.43
4:L:66:SER:OG	4:L:73:SER:O	2.33	0.43
1:A:314:PHE:CE2	1:A:398:HIS:HB2	2.48	0.43
1:C:251:LYS:O	1:C:251:LYS:HD3	2.19	0.43
3:H:58:LYS:HE2	3:H:58:LYS:HB3	1.89	0.43
1:A:39:PRO:HB2	1:A:143:VAL:HG21	2.00	0.43
1:C:12:VAL:CG2	1:C:33:VAL:HG12	2.49	0.43
1:C:486:LEU:HA	1:C:489:LEU:HG	2.01	0.43
3:H:47:TRP:CD2	4:L:99:TYR:HB3	2.54	0.43
1:A:12:VAL:CG2	1:A:33:VAL:HG22	2.48	0.42
3:H:103:TYR:HD1	3:H:106:VAL:HA	1.83	0.42
1:A:76:THR:OG1	1:A:107:LEU:HD11	2.18	0.42
1:A:276:GLU:HG3	1:A:277:MET:N	2.34	0.42
1:A:290:LYS:HD2	1:A:427:THR:HG23	2.01	0.42
1:A:94:ARG:HG2	1:A:114:VAL:CG1	2.48	0.42
1:C:206:MET:HE3	1:C:206:MET:HB2	1.78	0.42
1:C:409:LYS:O	1:C:412:GLU:HG3	2.19	0.42
1:C:424:LEU:HB2	1:C:428:ALA:HB2	2.00	0.42
1:C:73:ARG:HA	1:C:73:ARG:HD3	1.75	0.42
1:E:278:ASP:HB2	1:E:283:ARG:NE	2.35	0.42
3:H:39:GLN:C	3:H:92:ALA:HB1	2.39	0.42
1:A:136:GLU:OE2	1:A:168:GLU:HG2	2.19	0.42
1:A:315:THR:HG23	1:A:329:GLU:OE1	2.20	0.42
1:A:39:PRO:HB2	1:A:143:VAL:CG2	2.49	0.42
1:C:246:LYS:HG2	1:C:254:THR:HG22	2.01	0.42
1:C:471:LEU:O	1:C:475:LEU:HD23	2.18	0.42
1:A:2:ARG:HG2	1:A:152:ILE:O	2.18	0.42
1:A:378:LEU:O	1:A:380:PRO:HD3	2.19	0.42
1:A:442:GLY:HA2	1:A:445:ILE:HG22	2.00	0.42
1:A:484:ILE:HB	1:A:487:MET:HE2	2.01	0.42
1:E:61:TYR:CE2	1:E:262:GLU:HB3	2.54	0.42
2:D:69:LEU:HD23	2:F:70:ILE:HD13	2.00	0.42
4:L:50:TYR:HD1	4:L:56:PRO:HG3	1.84	0.42
1:A:4:ILE:HG13	1:A:377:GLU:OE2	2.20	0.42
1:C:161:ASP:OD1	1:C:164:ARG:NH2	2.49	0.42
1:C:59:TYR:CD2	1:C:221:ILE:HD11	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:9:THR:HG23	2:D:10:ARG:N	2.33	0.42
1:E:320:GLU:HB2	1:E:400:TRP:CZ2	2.52	0.42
1:C:101:TRP:CZ3	1:E:327:THR:HG22	2.55	0.42
1:E:345:MET:CE	1:E:380:PRO:HG3	2.49	0.42
1:E:382:PHE:HZ	1:E:409:LYS:HG3	1.84	0.42
3:H:91:THR:OG1	3:H:125:THR:HA	2.19	0.42
1:A:344:GLN:NE2	1:A:352:LEU:CD1	2.83	0.42
2:B:46:ALA:HB1	2:B:67:ILE:HD11	2.01	0.42
1:C:148:HIS:CE1	1:C:151:MET:HG2	2.55	0.42
1:C:269:LEU:C	1:C:271:GLY:H	2.23	0.42
2:D:49:ILE:HD12	2:D:49:ILE:HA	1.84	0.42
1:E:135:LEU:O	1:E:171:PRO:HD2	2.20	0.42
1:E:59:TYR:HE2	1:E:221:ILE:HG13	1.84	0.42
3:H:6:GLU:HA	3:H:22:CYS:HB3	2.00	0.42
1:A:318:PRO:HB3	1:A:328:VAL:HG22	2.02	0.42
2:D:74:TYR:OH	2:F:9:THR:HA	2.19	0.42
1:A:12:VAL:HG23	1:A:33:VAL:HA	2.02	0.42
1:A:230:ASP:OD2	1:A:234:PRO:HA	2.20	0.42
1:A:312:PHE:CZ	1:A:341:VAL:HG13	2.55	0.42
1:A:73:ARG:HD3	1:A:73:ARG:HA	1.89	0.42
2:B:26:THR:HA	2:B:29:LEU:CD2	2.46	0.42
1:C:282:GLY:O	1:C:284:LEU:HD12	2.20	0.42
1:C:481:ASN:OD1	1:C:482:GLY:N	2.48	0.42
1:E:224:PRO:CD	1:E:242:LEU:HD13	2.49	0.42
1:E:369:THR:HG22	1:E:370:GLU:N	2.35	0.42
1:E:454:LYS:HB3	1:E:454:LYS:HE2	1.93	0.42
1:A:59:TYR:CD1	1:A:225:TRP:HB3	2.55	0.42
1:C:146:SER:OG	1:C:366:THR:HG22	2.20	0.42
1:C:61:TYR:CE2	1:C:262:GLU:HB3	2.55	0.42
1:E:426:ASP:OD1	1:E:427:THR:N	2.53	0.42
2:D:10:ARG:HH11	2:F:39:ASN:HD21	1.68	0.42
2:F:53:LEU:HD22	2:F:63:TYR:CZ	2.55	0.42
1:C:463:PHE:HE2	2:F:75:SER:HB3	1.84	0.42
1:C:10:ASP:OD1	1:C:416:ARG:NH1	2.52	0.42
1:C:130:ILE:CG1	1:C:198:PHE:CE2	3.02	0.42
2:D:66:MET:HG3	2:F:70:ILE:HD11	2.02	0.42
1:A:4:ILE:HG22	1:A:152:ILE:HG21	2.01	0.41
1:A:363:PRO:HG3	1:A:376:LEU:HG	2.00	0.41
1:A:89:GLN:NE2	1:A:233:THR:HG21	2.35	0.41
2:B:56:SER:O	2:B:57:THR:OG1	2.35	0.41
4:L:86:ASP:OD1	4:L:87:TYR:N	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:204:LEU:HD12	1:C:213:VAL:HG11	2.02	0.41
1:C:273:LEU:HD23	2:D:18:THR:HA	2.01	0.41
1:E:40:THR:HG23	1:E:144:HIS:ND1	2.35	0.41
1:E:347:VAL:HG23	1:E:348:ASP:H	1.85	0.41
1:A:226:HIS:CD2	1:A:234:PRO:HB3	2.55	0.41
1:C:212:LEU:HD11	1:C:284:LEU:CD2	2.44	0.41
2:D:64:LEU:O	2:D:68:LEU:HD13	2.19	0.41
1:A:171:PRO:HA	1:A:192:PRO:HG3	2.03	0.41
1:A:147:GLN:O	1:A:375:MET:N	2.53	0.41
1:A:79:GLU:OE2	1:A:94:ARG:HD2	2.21	0.41
1:C:188:LEU:HA	1:C:188:LEU:HD23	1.88	0.41
1:E:344:GLN:CG	1:E:388:VAL:HG23	2.51	0.41
1:A:226:HIS:HB3	1:A:236:TRP:H	1.86	0.41
1:A:25:LEU:CD1	1:A:45:LEU:HB2	2.50	0.41
1:C:56:VAL:HG22	1:C:127:GLY:O	2.21	0.41
1:A:81:TYR:CE2	1:C:230:ASP:HB3	2.55	0.41
1:E:130:ILE:HD13	1:E:198:PHE:HD1	1.85	0.41
1:E:143:VAL:HG22	1:E:163:ASN:O	2.20	0.41
2:F:35:TRP:CE3	2:F:72:PRO:HG3	2.55	0.41
1:A:99:ARG:HG3	1:A:105:CYS:HB2	2.02	0.41
1:C:214:HIS:HE1	2:D:10:ARG:HE	1.68	0.41
1:E:25:LEU:N	1:E:289:LEU:O	2.50	0.41
3:H:98:LYS:O	3:H:115:MET:HA	2.21	0.41
1:A:471:LEU:CD1	2:B:62:ILE:HD11	2.51	0.41
1:C:300:LEU:HD21	1:C:362:ASN:HB3	2.03	0.41
1:E:22:ASP:OD1	1:E:292:ARG:HG2	2.20	0.41
3:H:18:LEU:HD21	3:H:124:VAL:HG11	2.02	0.41
3:H:35:HIS:HB2	3:H:49:ALA:O	2.19	0.41
1:C:202:TYR:CD2	1:C:215:LYS:HA	2.56	0.41
1:E:130:ILE:HD12	1:E:130:ILE:O	2.20	0.41
1:E:139:ILE:HD13	1:E:188:LEU:CD2	2.44	0.41
1:A:133:GLU:OE2	1:A:193:ARG:NH1	2.49	0.41
1:C:92:CYS:HA	1:C:115:THR:O	2.20	0.41
2:D:9:THR:HG23	2:D:10:ARG:H	1.86	0.41
1:E:236:TRP:O	1:E:239:LYS:HE2	2.21	0.41
3:H:19:ARG:NH2	3:H:82:GLN:HB2	2.36	0.41
1:A:82:LEU:HG	1:A:84:LYS:HG2	2.02	0.41
1:E:222:PRO:HG2	2:F:1:ALA:HB3	2.02	0.41
3:H:54:ASP:OD1	3:H:55:GLY:N	2.54	0.41
3:H:6:GLU:HB2	3:H:121:GLY:HA2	2.02	0.41
2:F:19:TRP:CD1	2:F:20:LEU:HG	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:103:TYR:CD1	3:H:106:VAL:HG23	2.56	0.41
1:A:61:TYR:CZ	1:A:123:LYS:HG3	2.56	0.40
1:C:311:ALA:HB1	1:C:333:ALA:HB3	2.03	0.40
1:E:1:ILE:HD12	1:E:152:ILE:HG12	2.02	0.40
1:A:16:SER:O	1:A:19:THR:HG22	2.21	0.40
1:A:344:GLN:HE21	1:A:352:LEU:CD1	2.34	0.40
1:E:201:LEU:HD23	1:E:214:HIS:HA	2.03	0.40
3:H:37:VAL:HG11	3:H:45:LEU:HD23	2.02	0.40
4:L:36:TRP:CD2	4:L:74:LEU:HD13	2.56	0.40
1:C:246:LYS:HG2	1:C:254:THR:CG2	2.52	0.40
1:C:344:GLN:HE21	1:C:352:LEU:HD21	1.86	0.40
4:L:4:LEU:O	4:L:4:LEU:HD23	2.21	0.40
1:A:2:ARG:NH1	1:A:140:MET:HB3	2.36	0.40
1:A:1:ILE:N	1:A:144:HIS:CD2	2.89	0.40
1:A:214:HIS:CD2	1:A:216:GLU:H	2.40	0.40
1:C:6:VAL:HG21	1:C:30:CYS:SG	2.61	0.40
1:E:273:LEU:HA	1:E:273:LEU:HD23	1.84	0.40
1:E:483:SER:O	1:E:486:LEU:HB2	2.21	0.40
1:E:265:VAL:HG22	2:F:4:LEU:CD2	2.50	0.40
2:B:25:TYR:O	2:B:29:LEU:HD21	2.22	0.40
1:C:45:LEU:HD13	1:C:289:LEU:HD13	2.03	0.40
1:C:297:LYS:HB3	1:C:297:LYS:HE2	1.89	0.40
1:C:352:LEU:HD23	1:C:352:LEU:O	2.21	0.40
1:C:359:ILE:HB	1:C:377:GLU:CB	2.51	0.40
1:C:467:LEU:O	1:C:471:LEU:HB2	2.22	0.40
2:D:18:THR:CG2	2:D:21:GLU:HG3	2.51	0.40
1:E:49:THR:OG1	1:E:136:GLU:HG3	2.22	0.40
1:E:99:ARG:HB3	1:E:105:CYS:SG	2.62	0.40
3:H:116:ASP:HA	4:L:47:LEU:HD22	2.03	0.40
4:L:95:SER:HA	5:L:600:NAG:H82	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	499/504 (99%)	459 (92%)	40 (8%)	0	100	100
1	C	499/504 (99%)	442 (89%)	57 (11%)	0	100	100
1	E	499/504 (99%)	458 (92%)	41 (8%)	0	100	100
2	B	73/75 (97%)	65 (89%)	8 (11%)	0	100	100
2	D	73/75 (97%)	68 (93%)	5 (7%)	0	100	100
2	F	73/75 (97%)	69 (94%)	4 (6%)	0	100	100
3	H	125/128 (98%)	113 (90%)	12 (10%)	0	100	100
4	L	108/110 (98%)	101 (94%)	7 (6%)	0	100	100
All	All	1949/1975 (99%)	1775 (91%)	174 (9%)	0	100	100

There are no Ramachandran outliers to report.

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	407/410 (99%)	402 (99%)	5 (1%)	74	87
1	C	407/410 (99%)	404 (99%)	3 (1%)	85	93
1	E	408/410 (100%)	403 (99%)	5 (1%)	74	87
2	B	64/64 (100%)	64 (100%)	0	100	100
2	D	64/64 (100%)	64 (100%)	0	100	100
2	F	64/64 (100%)	64 (100%)	0	100	100
3	H	101/104 (97%)	101 (100%)	0	100	100
4	L	93/93 (100%)	93 (100%)	0	100	100
All	All	1608/1619 (99%)	1595 (99%)	13 (1%)	84	92

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	MET
1	A	163	ASN
1	A	252	ARG
1	A	294	LYS
1	A	487	MET
1	C	299	ARG
1	C	345	MET
1	C	402	ARG
1	E	154	ASN
1	E	175	ARG
1	E	299	ARG
1	E	439	ASN
1	E	489	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	214	HIS
1	A	235	HIS
1	A	331	GLN
1	C	134	ASN
1	C	158	HIS
1	C	331	GLN
1	C	399	HIS
2	D	28	HIS
1	E	154	ASN
1	E	331	GLN
1	E	362	ASN
1	E	398	HIS
1	E	439	ASN
1	E	446	HIS
2	F	17	GLN
2	F	39	ASN
2	F	59	GLN
3	H	35	HIS
4	L	6	GLN
4	L	80	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

6 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
5	NAG	A	600	5	14,14,15	0.27	0	17,19,21	0.48	0
5	NAG	A	601	5	14,14,15	0.22	0	17,19,21	0.50	0
5	NAG	E	600	5	14,14,15	0.56	1 (7%)	17,19,21	0.50	0
5	NAG	E	601	5	14,14,15	0.25	0	17,19,21	0.51	0
5	NAG	L	600	5	14,14,15	0.39	0	17,19,21	0.63	1 (5%)
5	NAG	L	601	5	14,14,15	0.15	0	17,19,21	0.60	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	600	5	-	0/6/23/26	0/1/1/1
5	NAG	A	601	5	-	0/6/23/26	0/1/1/1
5	NAG	E	600	5	-	0/6/23/26	0/1/1/1
5	NAG	E	601	5	-	0/6/23/26	0/1/1/1
5	NAG	L	600	5	-	0/6/23/26	0/1/1/1
5	NAG	L	601	5	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	600	NAG	O5-C1	-2.02	1.40	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	600	NAG	C1-O5-C5	2.09	115.07	112.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	600	NAG	1	0
5	E	600	NAG	1	0
5	L	600	NAG	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.