Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 01:50 AM EST

PDB ID	:	3IXW
EMDB ID	:	EMD-5101
Title	:	Scorpion Hemocyanin activated state pseudo atomic model built based on cryo-EM density map
Authors	:	Cong, Y.; Zhang, Q.; Woolford, D.; Schweikardt, T.; Khant, H.; Ludtke, S.; Chiu, W.; Decker, H.
Deposited on	:	2009-02-13
Resolution	:	8.00 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *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.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

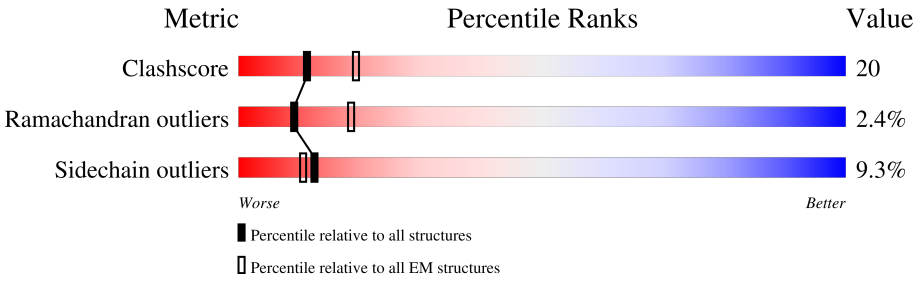
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 8.00 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	626	78% 54% 36% 8% •
1	C	626	82% 59% 33% 7% •
1	D	626	76% 58% 34% 8% •
1	E	626	77% 58% 34% 6% •
1	F	626	81% 58% 32% 8% •
1	G	626	90% 59% 33% 7% •
1	H	626	81% 60% 32% 7% •
1	I	626	77% 58% 34% 8% •

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Mol	Chain	Length	Quality of chain
1	J	626	79% 57% 35% 7%
1	K	626	93% 58% 34% 7%
1	L	626	89% 59% 33% 8%
1	M	626	94% 55% 36% 8%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 74208 atoms, of which 13476 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 Hemocyanin AA6 chain.

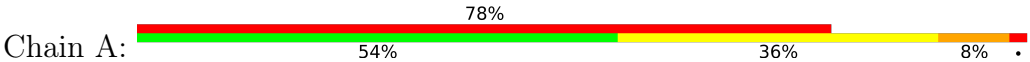
Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	626	Total	C	H	N	O	S	0	0
			6184	3199	1123	877	961	24		
1	C	626	Total	C	H	N	O	S	0	0
			6184	3199	1123	877	961	24		
1	D	626	Total	C	H	N	O	S	0	0
			6184	3199	1123	877	961	24		
1	E	626	Total	C	H	N	O	S	0	0
			6184	3199	1123	877	961	24		
1	F	626	Total	C	H	N	O	S	0	0
			6184	3199	1123	877	961	24		
1	G	626	Total	C	H	N	O	S	0	0
			6184	3199	1123	877	961	24		
1	H	626	Total	C	H	N	O	S	0	0
			6184	3199	1123	877	961	24		
1	I	626	Total	C	H	N	O	S	0	0
			6184	3199	1123	877	961	24		
1	J	626	Total	C	H	N	O	S	0	0
			6184	3199	1123	877	961	24		
1	K	626	Total	C	H	N	O	S	0	0
			6184	3199	1123	877	961	24		
1	L	626	Total	C	H	N	O	S	0	0
			6184	3199	1123	877	961	24		
1	M	626	Total	C	H	N	O	S	0	0
			6184	3199	1123	877	961	24		

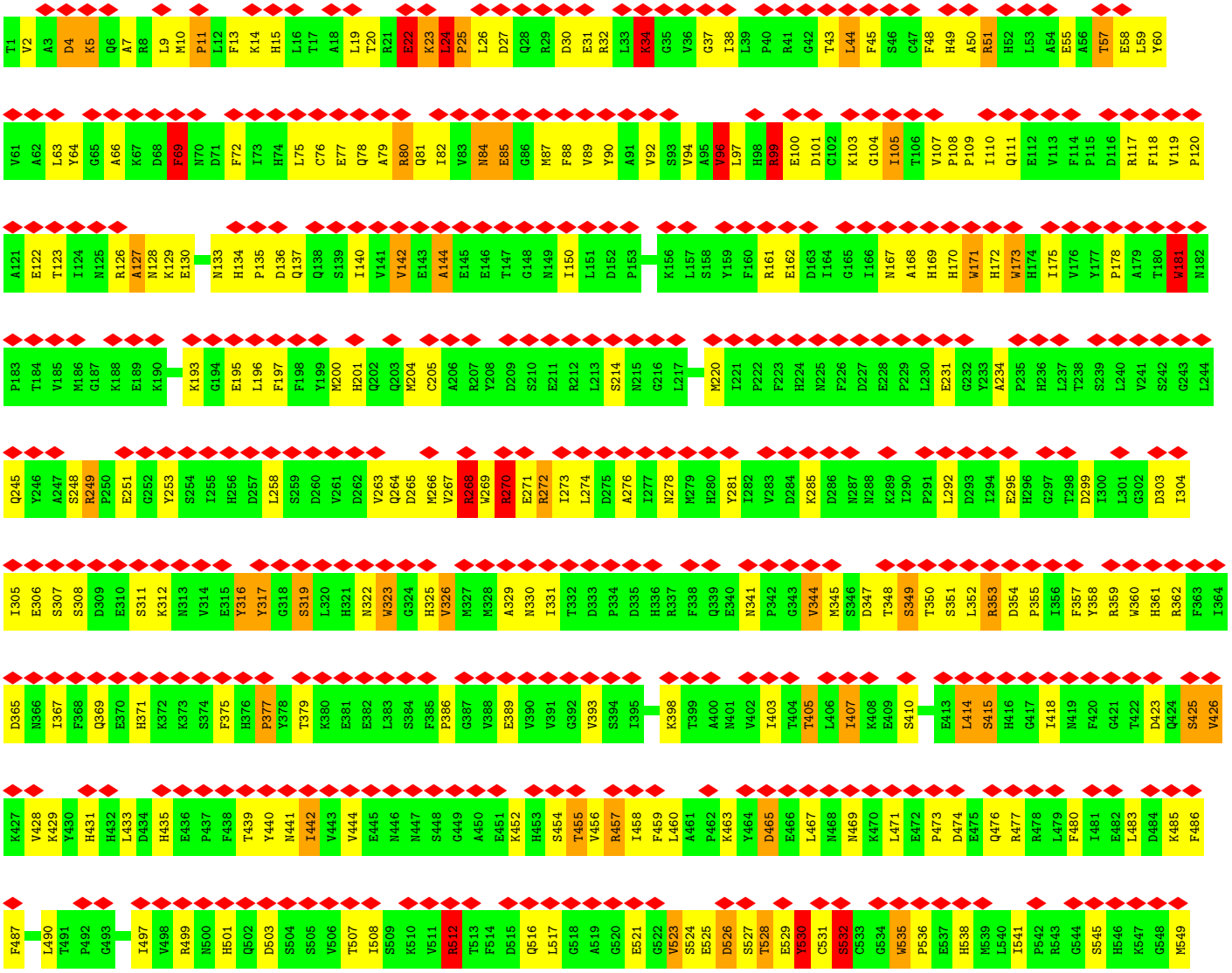
3 Residue-property plots (i)

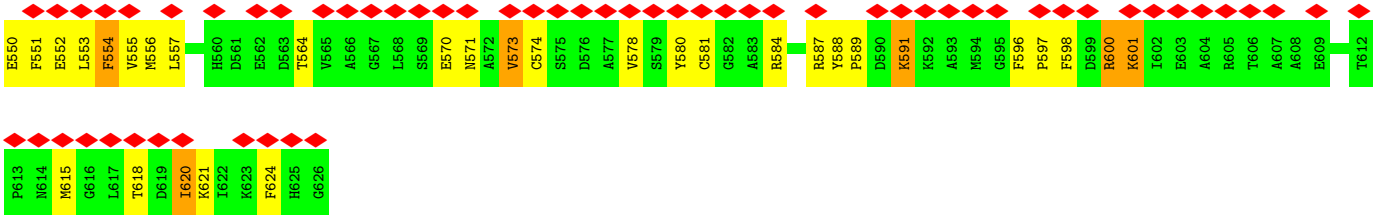
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: Hemocyanin AA6 chain

Chain A:

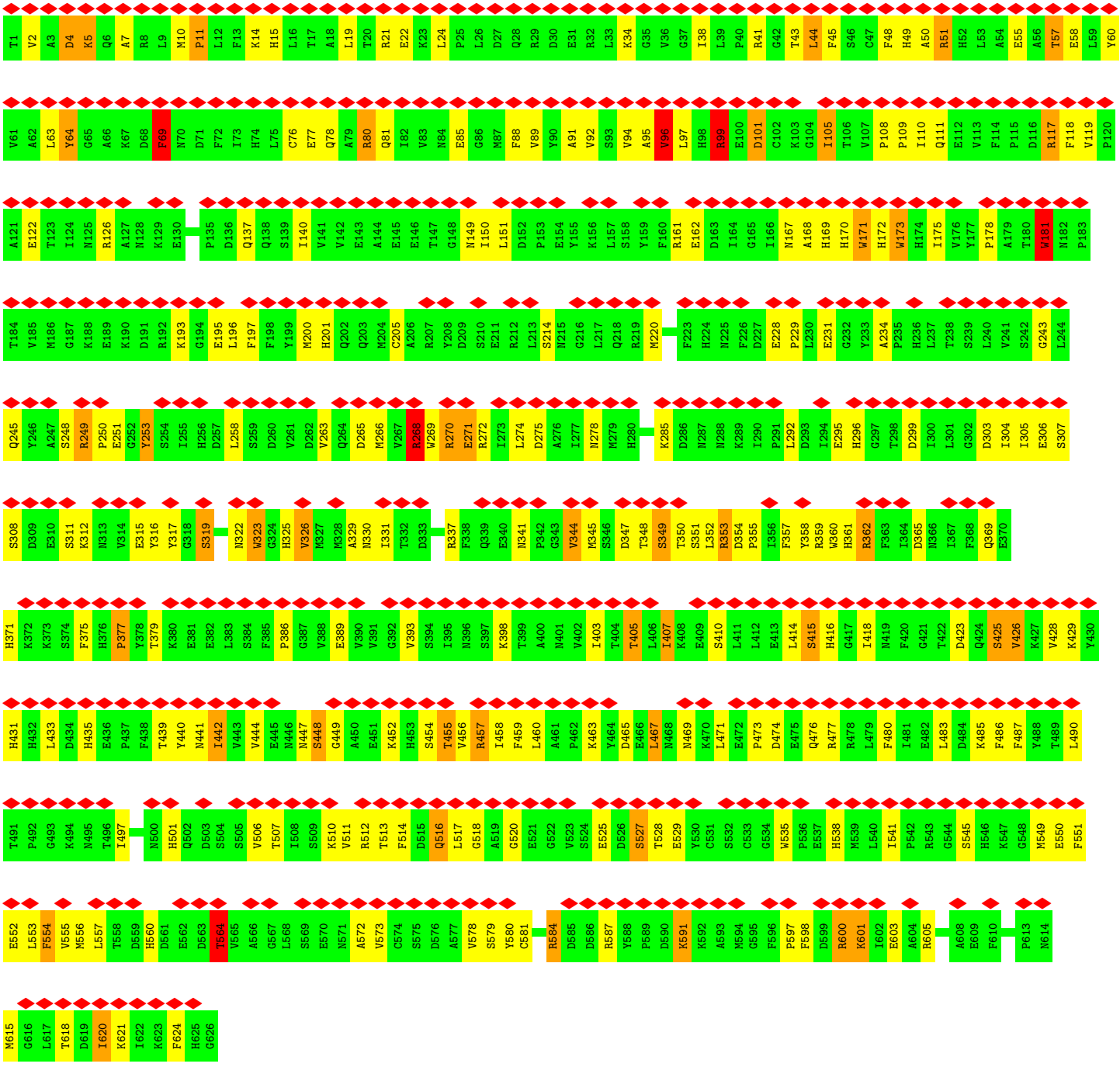






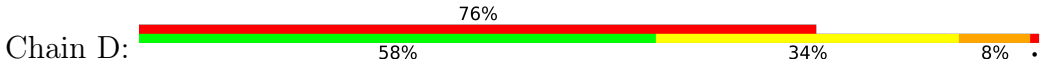
• Molecule 1: Hemocyanin AA6 chain

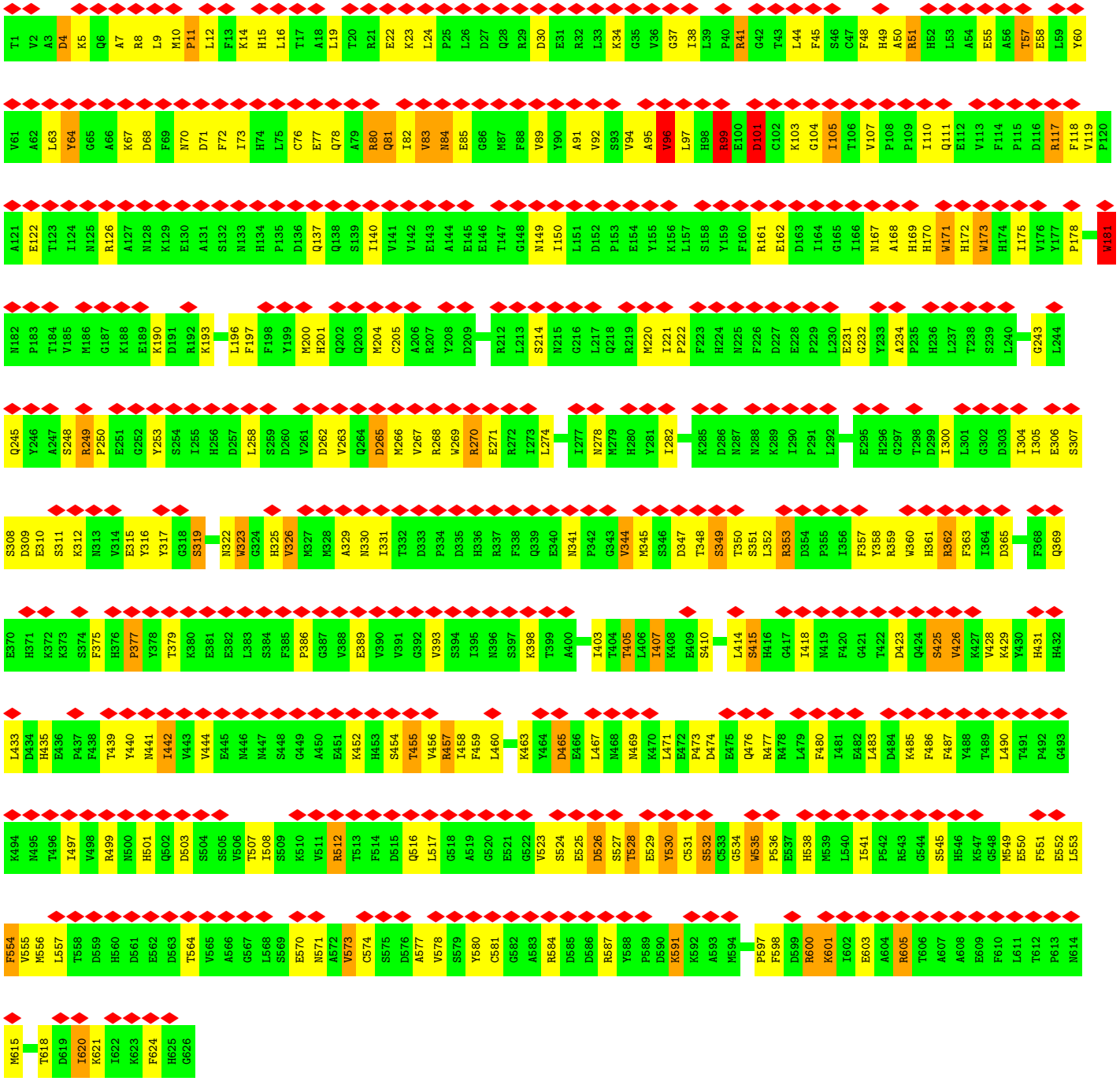
Chain C:



• Molecule 1: Hemocyanin AA6 chain

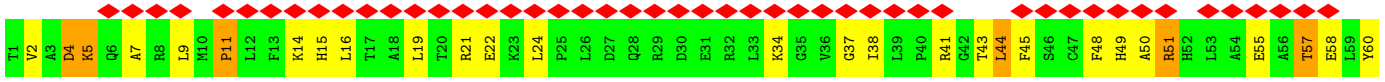
Chain D:

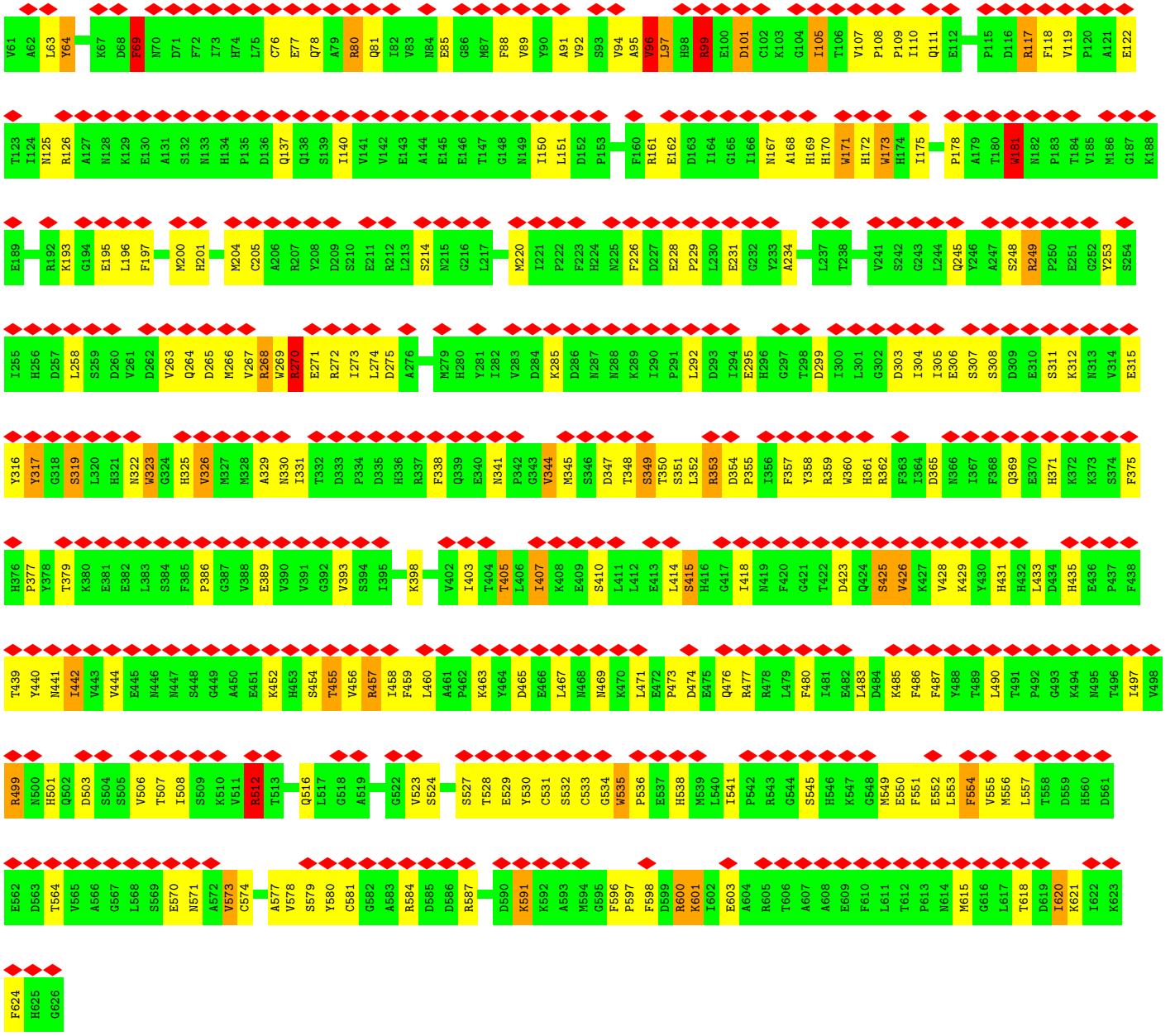




• Molecule 1: Hemocyanin AA6 chain

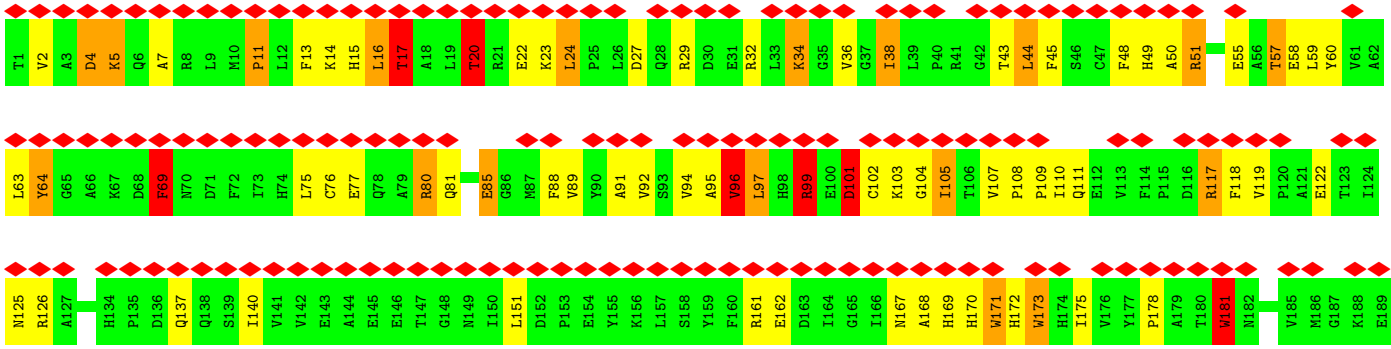
Chain E:

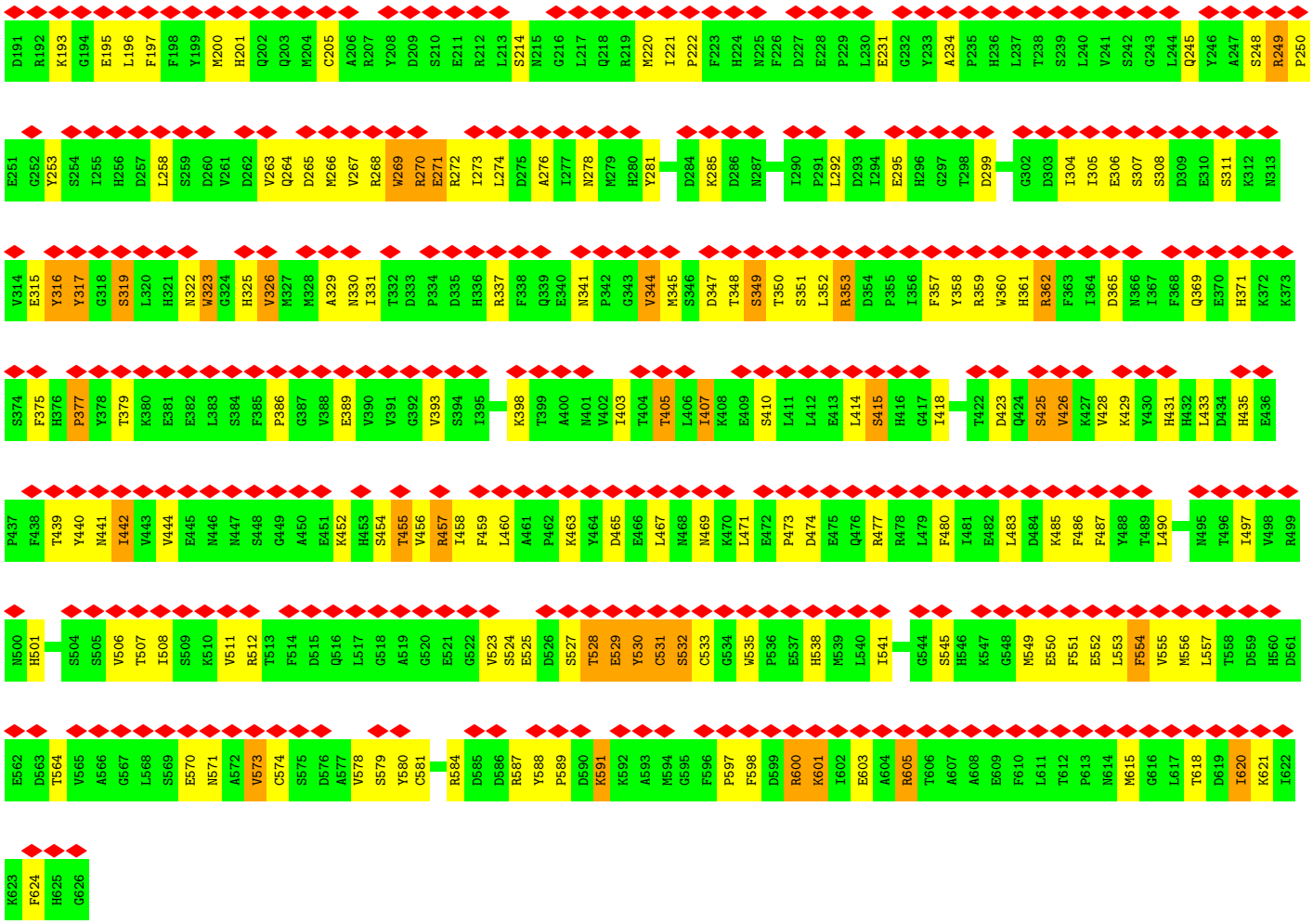




• Molecule 1: Hemocyanin AA6 chain

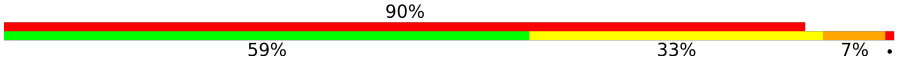
Chain F:

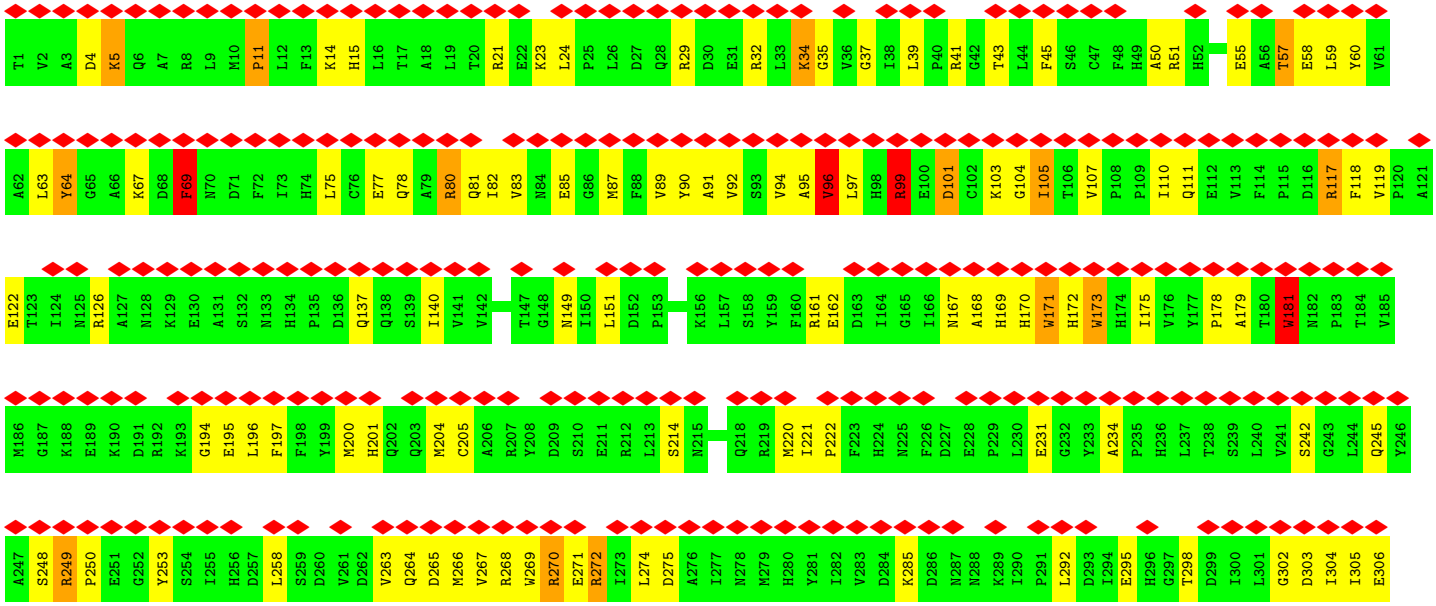


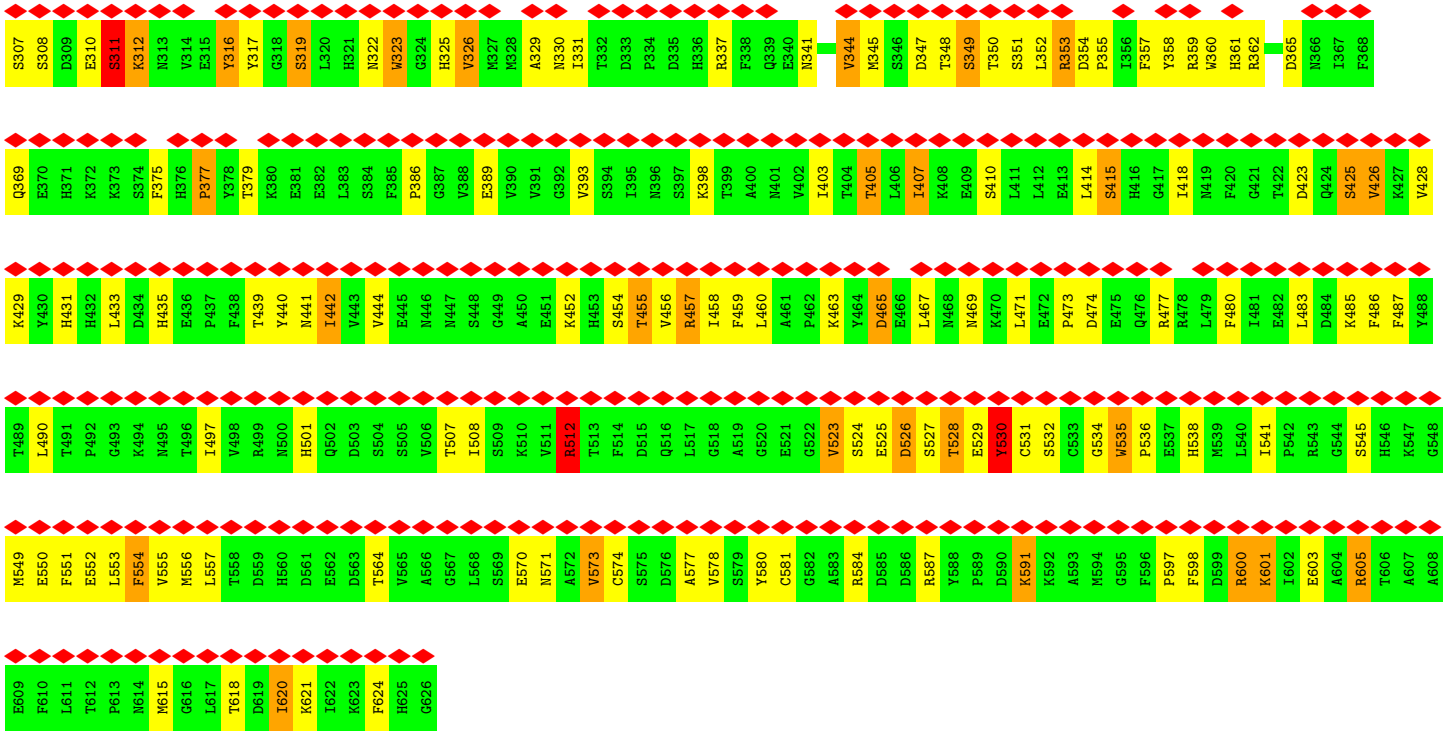


• Molecule 1: Hemocyanin AA6 chain

Chain G:

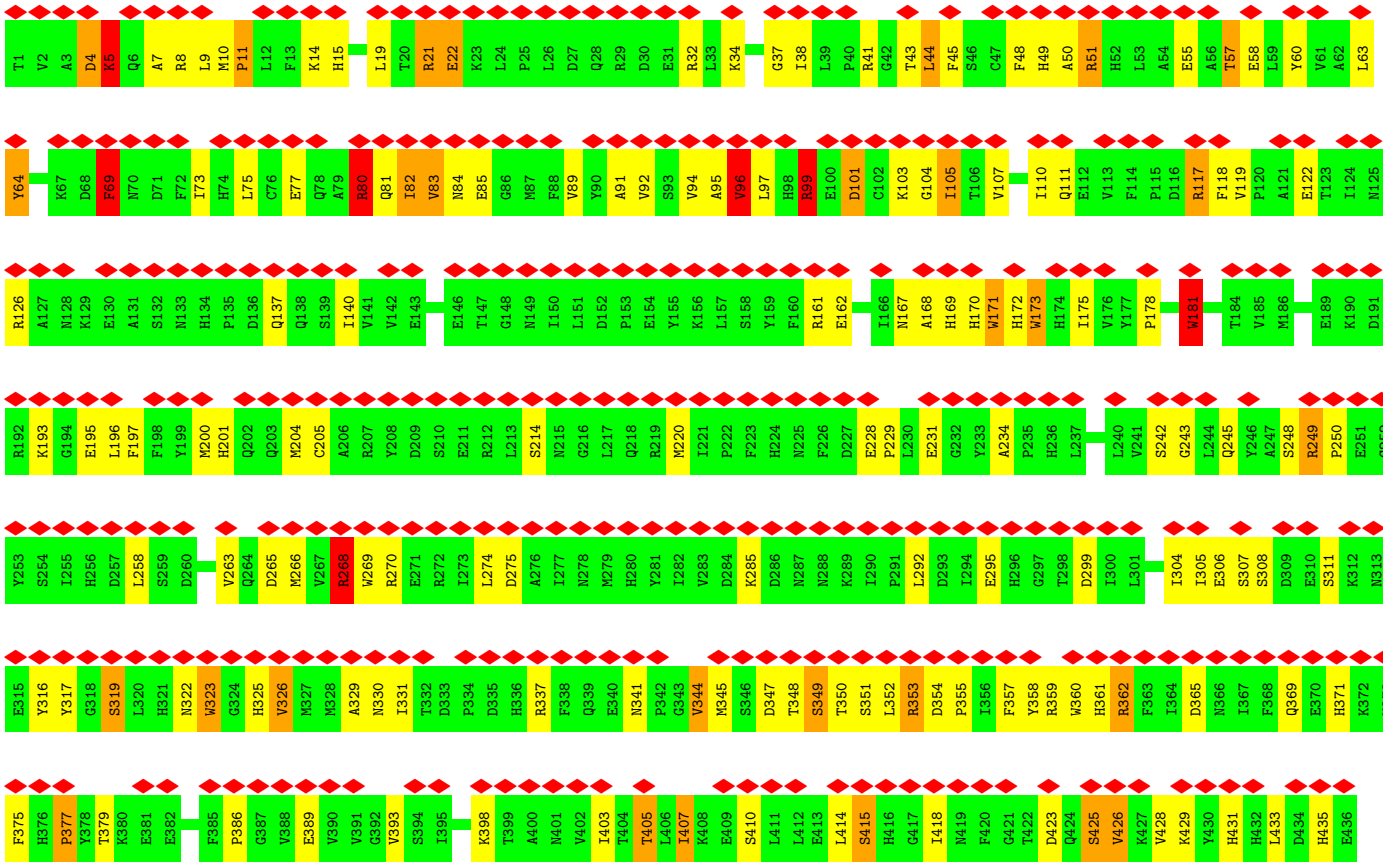






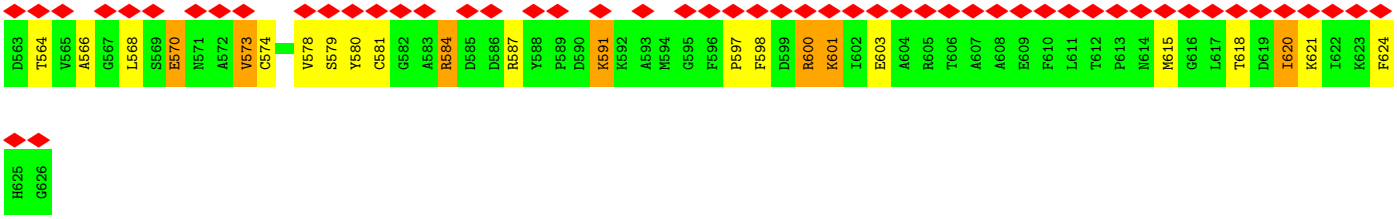
• Molecule 1: Hemocyanin AA6 chain

Chain H:



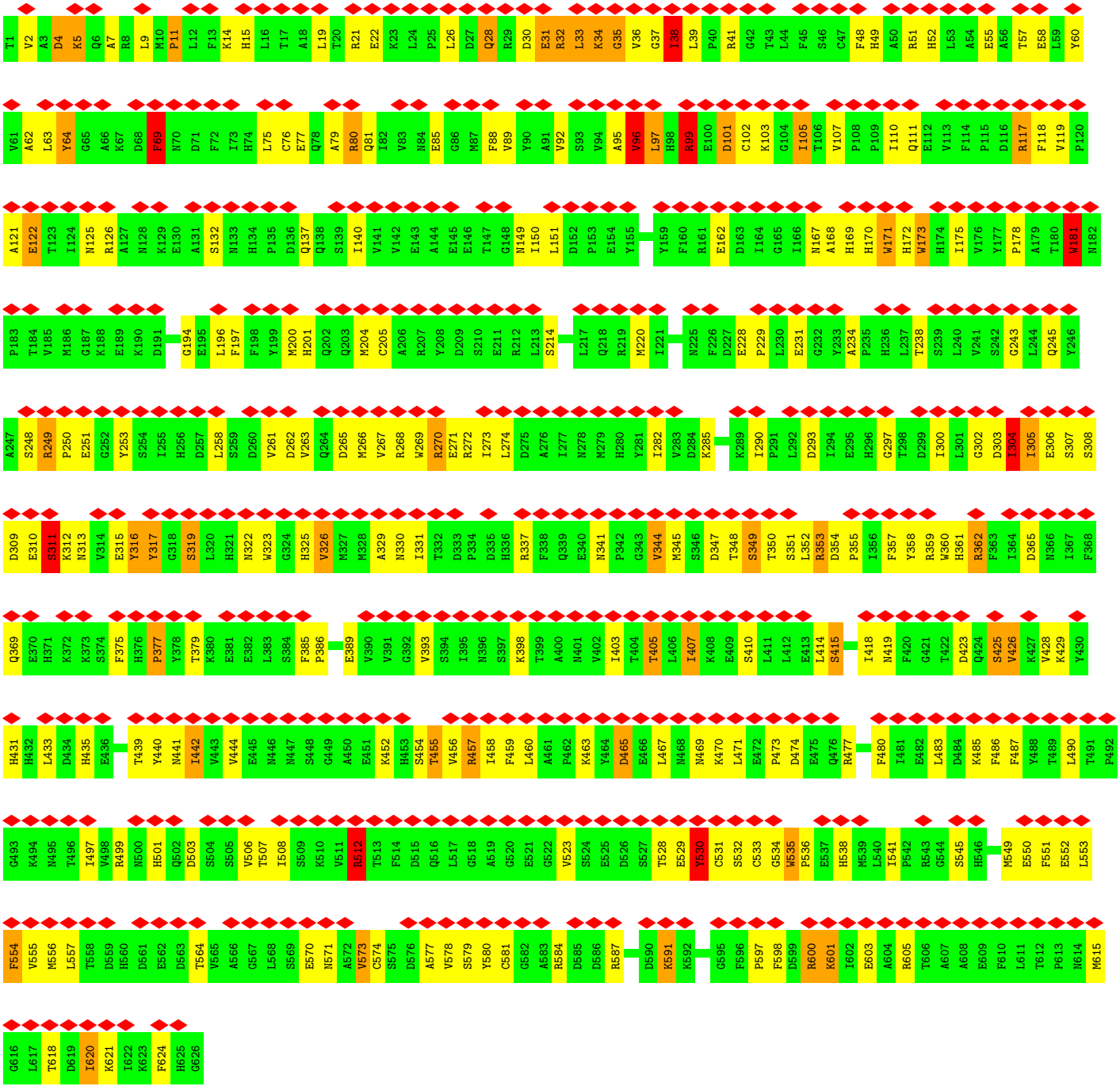
• Molecule 1: Hemocyanin AA6 chain

Chain I:



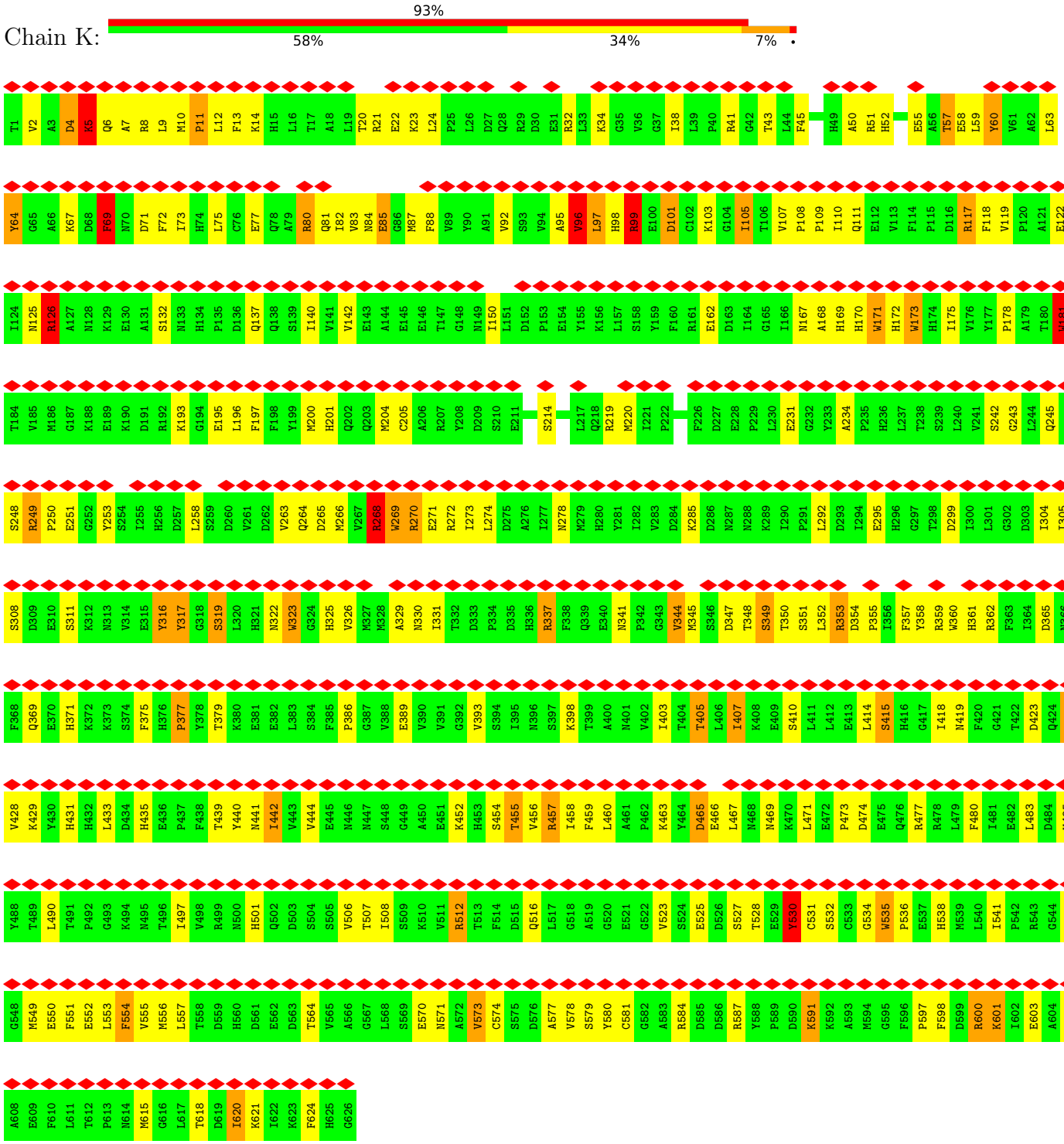
• Molecule 1: Hemocyanin AA6 chain

Chain J:



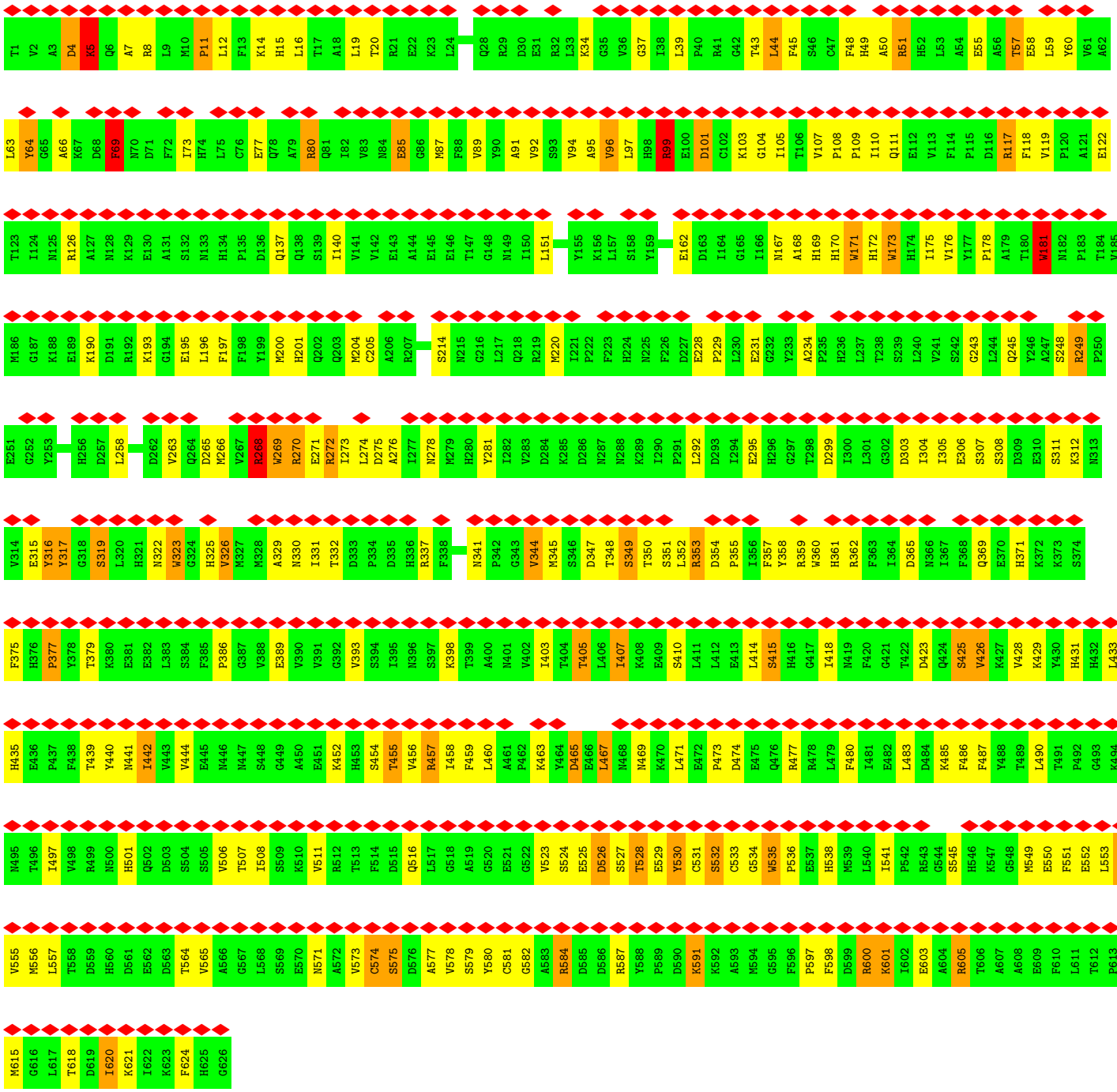
• Molecule 1: Hemocyanin AA6 chain

Chain K:



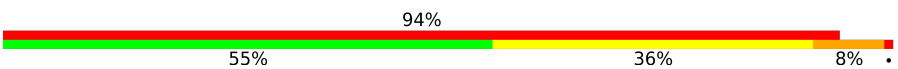
• Molecule 1: Hemocyanin AA6 chain

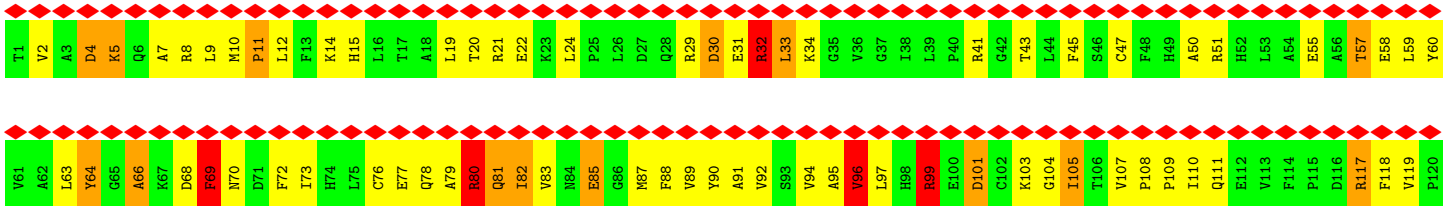
Chain L:

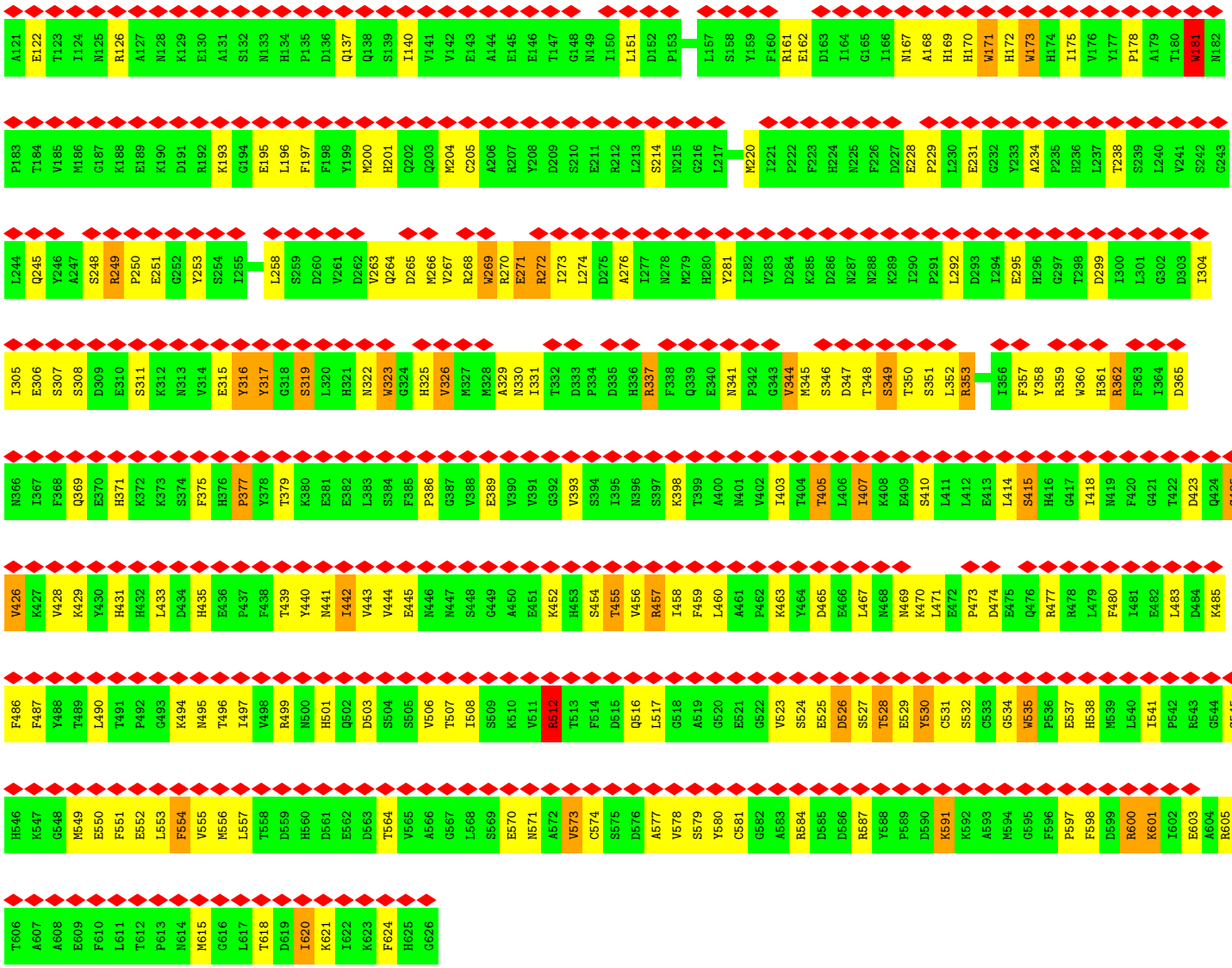


• Molecule 1: Hemocyanin AA6 chain

Chain M:






A121 E122 T123 I124 N125 R126 A127 N128 K129 E130 A131 S132 N133 H134 P135 D136 Q137 Q138 S139 I140 V141 V142 E143 A144 E145 E146 T147 G148 N149 I150 L151 D152 P153 L157 S158 Y159 F160 R161 E162 D163 I164 G165 I166 N167 A168 H169 H170 W171 H172 W173 H174 I175 V176 Y177 P178 A179 T180 W181 N182
P183 T184 V185 M186 G187 K188 E189 K190 D191 R192 K193 G194 E195 L196 F197 F198 Y199 M200 H201 Q202 Q203 M204 C205 A206 R207 Y208 D209 S210 E211 R212 L213 S214 N215 G216 L217 M220 I221 P222 F223 H224 N225 F226 D227 E228 P229 L230 E231 G232 Y233 A234 P235 H236 L237 T238 S239 L240 V241 S242 G243
L244 Q245 Y246 A247 S248 R249 P250 E251 G252 Y253 S254 I255 L258 S259 D260 V261 D262 V263 Q264 D265 M266 V267 R268 W269 R270 E271 R272 I273 L274 D275 A276 I277 N278 M279 H280 Y281 I282 V283 D284 K285 D286 N287 N288 K289 I290 P291 L292 D293 I294 E295 H296 G297 T298 D299 I300 L301 G302 D303 I304
I305 E306 S307 S308 D309 E310 S311 K312 N313 V314 E315 Y316 Y317 G318 S319 L320 H321 N322 W323 G324 H325 V326 M327 M328 A329 N330 I331 T332 D333 P334 D335 H336 R337 F338 Q339 E340 N341 P342 G343 V344 M345 S346 D347 T348 S349 T350 S351 L352 R353 I356 F357 Y358 R359 W360 H361 R362 F363 I364 D365
N366 I367 F368 Q369 E370 H371 K372 K373 S374 F375 H376 P377 Y378 T379 K380 E381 E382 L383 S384 F385 P386 G387 V388 E389 V390 V391 G392 V393 S394 I395 N396 S397 K398 T399 A400 N401 V402 I403 T404 T405 L406 I407 K408 E409 S410 L411 L412 E413 L414 S415 H416 G417 I418 N419 F420 G421 T422 D423 Q424 S425
Y426 K427 V428 K429 Y430 H431 H432 L433 D434 H435 E436 P437 F438 T439 Y440 N441 I442 V443 V444 E445 N446 N447 S448 G449 A450 E451 K452 H453 S454 T455 V456 R457 I458 F459 L460 A461 P462 K463 Y464 D465 E466 L467 N468 N469 K470 L471 E472 P473 D474 E475 Q476 R477 R478 L479 F480 I481 E482 L483 D484 K485
F486 F487 Y488 T489 L490 T491 P492 G493 K494 N495 T496 I497 V498 R499 N500 H501 Q502 D503 S504 S505 V506 T507 I508 S509 K510 V511 R512 T513 F514 D515 Q516 L517 G518 A519 G520 E521 G522 V523 S524 E525 D526 S527 T528 E529 Y530 C531 S532 C533 G534 W535 P536 E537 H538 M539 L540 I541 P542 R543 G544 S545
H546 K547 G548 M549 E550 F551 E552 L553 F554 V555 M556 L557 T558 D559 H560 D561 E562 D563 T564 V565 A566 G567 L568 S569 E570 N571 A572 V573 C574 S575 D576 A577 V578 S579 Y580 C581 G582 A583 R584 D585 D586 R587 Y588 P589 D590 K591 K592 A593 M594 G595 F596 P597 F598 D599 R600 K601 I602 E603 A604 R605
T606 A607 A608 E609 F610 L611 T612 P613 N614 M615 G616 L617 T618 D619 I620 K621 I622 K623 F624 H625 G626

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	13400	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	each micrograph	Depositor
Microscope	JEOL 3200FSC	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	18	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	50000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	1.663	Depositor
Minimum map value	-0.473	Depositor
Average map value	0.074	Depositor
Map value standard deviation	0.264	Depositor
Recommended contour level	1.16	Depositor
Map size (Å)	374.4, 374.4, 374.4	wwPDB
Map dimensions	208, 208, 208	wwPDB
Map angles (°)	90, 90, 90	wwPDB
Pixel spacing (Å)	1.8, 1.8, 1.8	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.55	11/5191 (0.2%)	1.55	54/7033 (0.8%)
1	C	1.54	8/5190 (0.2%)	1.48	38/7030 (0.5%)
1	D	0.73	1/5191 (0.0%)	1.39	46/7033 (0.7%)
1	E	1.55	9/5191 (0.2%)	1.49	44/7033 (0.6%)
1	F	1.54	8/5191 (0.2%)	1.50	46/7033 (0.7%)
1	G	1.52	8/5191 (0.2%)	1.40	47/7033 (0.7%)
1	H	1.53	9/5191 (0.2%)	1.51	49/7033 (0.7%)
1	I	1.54	8/5190 (0.2%)	1.51	46/7030 (0.7%)
1	J	1.53	8/5191 (0.2%)	1.38	40/7033 (0.6%)
1	K	1.51	8/5191 (0.2%)	1.39	42/7033 (0.6%)
1	L	1.53	9/5191 (0.2%)	1.49	43/7033 (0.6%)
1	M	1.52	8/5191 (0.2%)	1.40	47/7033 (0.7%)
All	All	1.48	95/62290 (0.2%)	1.46	542/84390 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	20
1	C	0	15
1	D	0	13
1	E	0	15
1	F	0	16
1	G	0	16
1	H	0	16
1	I	0	15
1	J	0	14
1	K	0	18
1	L	0	18
1	M	0	19
All	All	0	195

All (95) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	5	LYS	CE-NZ	50.53	2.75	1.49
1	G	5	LYS	CE-NZ	50.45	2.75	1.49
1	H	5	LYS	CE-NZ	50.33	2.74	1.49
1	L	5	LYS	CE-NZ	50.29	2.74	1.49
1	I	5	LYS	CE-NZ	50.17	2.74	1.49
1	E	5	LYS	CE-NZ	47.09	2.66	1.49
1	A	5	LYS	CE-NZ	47.06	2.66	1.49
1	J	5	LYS	CE-NZ	47.05	2.66	1.49
1	C	5	LYS	CE-NZ	47.05	2.66	1.49
1	F	5	LYS	CE-NZ	47.02	2.66	1.49
1	M	5	LYS	CE-NZ	47.01	2.66	1.49
1	J	69	PHE	CG-CD2	40.64	1.99	1.38
1	E	69	PHE	CG-CD2	40.59	1.99	1.38
1	F	69	PHE	CG-CD2	40.58	1.99	1.38
1	C	69	PHE	CG-CD2	40.55	1.99	1.38
1	A	69	PHE	CG-CD2	40.51	1.99	1.38
1	M	69	PHE	CG-CD2	40.11	1.99	1.38
1	C	69	PHE	CG-CD1	40.09	1.98	1.38
1	A	69	PHE	CG-CD1	40.08	1.98	1.38
1	J	69	PHE	CG-CD1	40.06	1.98	1.38
1	E	69	PHE	CG-CD1	40.06	1.98	1.38
1	F	69	PHE	CG-CD1	40.03	1.98	1.38
1	I	69	PHE	CG-CD2	39.30	1.97	1.38
1	G	69	PHE	CG-CD2	39.07	1.97	1.38
1	L	69	PHE	CG-CD2	39.01	1.97	1.38
1	K	69	PHE	CG-CD1	39.00	1.97	1.38
1	H	69	PHE	CG-CD2	38.93	1.97	1.38
1	L	69	PHE	CG-CD1	38.89	1.97	1.38
1	K	69	PHE	CG-CD2	38.84	1.97	1.38
1	H	69	PHE	CG-CD1	38.84	1.97	1.38
1	G	69	PHE	CG-CD1	38.69	1.96	1.38
1	I	69	PHE	CG-CD1	38.68	1.96	1.38
1	M	69	PHE	CG-CD1	38.63	1.96	1.38
1	M	69	PHE	CE1-CZ	33.79	2.01	1.37
1	M	69	PHE	CE2-CZ	33.17	2.00	1.37
1	E	69	PHE	CE2-CZ	32.79	1.99	1.37
1	J	69	PHE	CE2-CZ	32.77	1.99	1.37
1	A	69	PHE	CE2-CZ	32.70	1.99	1.37
1	C	69	PHE	CE2-CZ	32.70	1.99	1.37
1	F	69	PHE	CE2-CZ	32.66	1.99	1.37
1	J	69	PHE	CE1-CZ	32.19	1.98	1.37
1	A	69	PHE	CE1-CZ	32.19	1.98	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	69	PHE	CE1-CZ	32.18	1.98	1.37
1	F	69	PHE	CE1-CZ	32.17	1.98	1.37
1	C	69	PHE	CE1-CZ	32.15	1.98	1.37
1	I	69	PHE	CE2-CZ	31.50	1.97	1.37
1	G	69	PHE	CE2-CZ	31.38	1.97	1.37
1	L	69	PHE	CE2-CZ	31.36	1.97	1.37
1	H	69	PHE	CE2-CZ	31.33	1.96	1.37
1	L	69	PHE	CE1-CZ	31.29	1.96	1.37
1	I	69	PHE	CE1-CZ	31.22	1.96	1.37
1	H	69	PHE	CE1-CZ	31.21	1.96	1.37
1	G	69	PHE	CE1-CZ	31.13	1.96	1.37
1	K	69	PHE	CE2-CZ	30.91	1.96	1.37
1	K	69	PHE	CE1-CZ	30.29	1.95	1.37
1	A	69	PHE	CD1-CE1	30.06	1.99	1.39
1	C	69	PHE	CD1-CE1	30.05	1.99	1.39
1	F	69	PHE	CD1-CE1	30.04	1.99	1.39
1	E	69	PHE	CD1-CE1	30.02	1.99	1.39
1	J	69	PHE	CD1-CE1	29.95	1.99	1.39
1	A	69	PHE	CD2-CE2	29.74	1.98	1.39
1	F	69	PHE	CD2-CE2	29.70	1.98	1.39
1	C	69	PHE	CD2-CE2	29.65	1.98	1.39
1	E	69	PHE	CD2-CE2	29.63	1.98	1.39
1	J	69	PHE	CD2-CE2	29.62	1.98	1.39
1	M	69	PHE	CD1-CE1	28.87	1.97	1.39
1	L	69	PHE	CD1-CE1	28.82	1.96	1.39
1	I	69	PHE	CD1-CE1	28.80	1.96	1.39
1	K	69	PHE	CD1-CE1	28.80	1.96	1.39
1	M	69	PHE	CD2-CE2	28.77	1.96	1.39
1	I	69	PHE	CD2-CE2	28.76	1.96	1.39
1	H	69	PHE	CD1-CE1	28.73	1.96	1.39
1	G	69	PHE	CD1-CE1	28.63	1.96	1.39
1	H	69	PHE	CD2-CE2	28.55	1.96	1.39
1	G	69	PHE	CD2-CE2	28.52	1.96	1.39
1	L	69	PHE	CD2-CE2	28.47	1.96	1.39
1	K	69	PHE	CD2-CE2	28.24	1.95	1.39
1	I	44	LEU	C-N	16.37	1.71	1.34
1	L	44	LEU	C-N	16.37	1.71	1.34
1	H	44	LEU	C-N	16.36	1.71	1.34
1	A	44	LEU	C-N	16.35	1.71	1.34
1	C	44	LEU	C-N	16.33	1.71	1.34
1	F	44	LEU	C-N	16.32	1.71	1.34
1	E	44	LEU	C-N	16.32	1.71	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	537	GLU	C-N	9.74	1.56	1.34
1	A	24	LEU	CB-CG	8.07	1.75	1.52
1	J	536	PRO	C-N	8.06	1.52	1.34
1	A	536	PRO	C-N	8.01	1.52	1.34
1	E	536	PRO	C-N	7.91	1.52	1.34
1	A	24	LEU	CA-CB	7.89	1.71	1.53
1	K	536	PRO	C-N	7.82	1.52	1.34
1	D	536	PRO	C-N	7.20	1.50	1.34
1	H	536	PRO	C-N	6.99	1.50	1.34
1	G	536	PRO	C-N	6.99	1.50	1.34
1	L	536	PRO	C-N	6.75	1.49	1.34

All (542) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	44	LEU	O-C-N	-41.48	56.33	122.70
1	A	44	LEU	O-C-N	-41.46	56.37	122.70
1	F	44	LEU	O-C-N	-41.45	56.38	122.70
1	C	44	LEU	O-C-N	-41.43	56.41	122.70
1	I	44	LEU	O-C-N	-41.43	56.41	122.70
1	H	44	LEU	O-C-N	-41.42	56.43	122.70
1	E	44	LEU	O-C-N	-41.40	56.46	122.70
1	A	44	LEU	CA-C-N	18.92	158.82	117.20
1	C	44	LEU	CA-C-N	18.91	158.81	117.20
1	E	44	LEU	CA-C-N	18.91	158.79	117.20
1	H	44	LEU	CA-C-N	18.88	158.74	117.20
1	L	44	LEU	CA-C-N	18.88	158.73	117.20
1	F	44	LEU	CA-C-N	18.88	158.72	117.20
1	I	44	LEU	CA-C-N	18.87	158.71	117.20
1	C	44	LEU	C-N-CA	14.27	157.36	121.70
1	H	44	LEU	C-N-CA	14.26	157.35	121.70
1	A	44	LEU	C-N-CA	14.26	157.34	121.70
1	F	44	LEU	C-N-CA	14.25	157.32	121.70
1	I	44	LEU	C-N-CA	14.24	157.31	121.70
1	E	44	LEU	C-N-CA	14.24	157.30	121.70
1	L	44	LEU	C-N-CA	14.22	157.24	121.70
1	A	24	LEU	CD1-CG-CD2	-12.59	72.74	110.50
1	F	5	LYS	CD-CE-NZ	12.17	139.69	111.70
1	J	5	LYS	CD-CE-NZ	12.15	139.66	111.70
1	M	5	LYS	CD-CE-NZ	12.15	139.64	111.70
1	E	5	LYS	CD-CE-NZ	12.14	139.62	111.70
1	C	5	LYS	CD-CE-NZ	12.13	139.61	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	5	LYS	CD-CE-NZ	12.13	139.59	111.70
1	K	5	LYS	CD-CE-NZ	12.09	139.51	111.70
1	L	272	ARG	NE-CZ-NH2	12.01	126.31	120.30
1	A	362	ARG	NE-CZ-NH2	-11.99	114.30	120.30
1	J	362	ARG	NE-CZ-NH2	-11.99	114.31	120.30
1	D	362	ARG	NE-CZ-NH2	-11.97	114.32	120.30
1	H	362	ARG	NE-CZ-NH2	-11.93	114.34	120.30
1	K	362	ARG	NE-CZ-NH2	-11.91	114.35	120.30
1	E	362	ARG	NE-CZ-NH2	-11.91	114.35	120.30
1	F	362	ARG	NE-CZ-NH2	-11.91	114.35	120.30
1	M	362	ARG	NE-CZ-NH2	-11.86	114.37	120.30
1	I	362	ARG	NE-CZ-NH2	-11.84	114.38	120.30
1	H	5	LYS	CD-CE-NZ	11.81	138.86	111.70
1	G	362	ARG	NE-CZ-NH2	-11.80	114.40	120.30
1	C	362	ARG	NE-CZ-NH2	-11.80	114.40	120.30
1	L	362	ARG	NE-CZ-NH2	-11.75	114.43	120.30
1	L	5	LYS	CD-CE-NZ	11.55	138.27	111.70
1	G	5	LYS	CD-CE-NZ	11.54	138.25	111.70
1	I	5	LYS	CD-CE-NZ	11.52	138.19	111.70
1	H	80	ARG	NE-CZ-NH2	-10.53	115.03	120.30
1	A	268	ARG	NE-CZ-NH2	-10.42	115.09	120.30
1	K	126	ARG	NE-CZ-NH2	-10.38	115.11	120.30
1	A	24	LEU	CA-CB-CG	9.96	138.21	115.30
1	A	24	LEU	CB-CG-CD2	9.92	127.86	111.00
1	D	81	GLN	N-CA-CB	-9.91	92.77	110.60
1	M	535	TRP	CD1-CG-CD2	8.81	113.35	106.30
1	A	24	LEU	CB-CG-CD1	8.78	125.92	111.00
1	L	535	TRP	CD1-CG-CD2	8.74	113.29	106.30
1	D	535	TRP	CD1-CG-CD2	8.74	113.29	106.30
1	H	535	TRP	CD1-CG-CD2	8.71	113.27	106.30
1	K	535	TRP	CD1-CG-CD2	8.65	113.22	106.30
1	J	535	TRP	CD1-CG-CD2	8.65	113.22	106.30
1	A	535	TRP	CD1-CG-CD2	8.65	113.22	106.30
1	L	532	SER	N-CA-CB	-8.64	97.53	110.50
1	E	535	TRP	CD1-CG-CD2	8.64	113.21	106.30
1	G	535	TRP	CD1-CG-CD2	8.63	113.20	106.30
1	F	535	TRP	CD1-CG-CD2	8.53	113.12	106.30
1	A	268	ARG	NE-CZ-NH1	8.53	124.56	120.30
1	J	181	TRP	CD1-CG-CD2	8.51	113.11	106.30
1	A	24	LEU	N-CA-CB	8.50	127.41	110.40
1	H	181	TRP	CD1-CG-CD2	8.49	113.09	106.30
1	E	181	TRP	CD1-CG-CD2	8.48	113.09	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	181	TRP	CD1-CG-CD2	8.47	113.08	106.30
1	C	181	TRP	CD1-CG-CD2	8.46	113.07	106.30
1	I	181	TRP	CD1-CG-CD2	8.45	113.06	106.30
1	F	181	TRP	CD1-CG-CD2	8.45	113.06	106.30
1	D	181	TRP	CD1-CG-CD2	8.45	113.06	106.30
1	K	181	TRP	CD1-CG-CD2	8.43	113.05	106.30
1	L	181	TRP	CD1-CG-CD2	8.39	113.01	106.30
1	A	181	TRP	CD1-CG-CD2	8.36	112.99	106.30
1	A	126	ARG	NE-CZ-NH2	-8.36	116.12	120.30
1	G	181	TRP	CD1-CG-CD2	8.31	112.95	106.30
1	D	173	TRP	CD1-CG-CD2	8.29	112.94	106.30
1	L	173	TRP	CD1-CG-CD2	8.29	112.93	106.30
1	F	173	TRP	CD1-CG-CD2	8.27	112.92	106.30
1	C	173	TRP	CD1-CG-CD2	8.24	112.89	106.30
1	A	173	TRP	CD1-CG-CD2	8.23	112.89	106.30
1	G	173	TRP	CD1-CG-CD2	8.23	112.89	106.30
1	K	173	TRP	CD1-CG-CD2	8.22	112.88	106.30
1	E	173	TRP	CD1-CG-CD2	8.22	112.87	106.30
1	M	173	TRP	CD1-CG-CD2	8.19	112.85	106.30
1	H	173	TRP	CD1-CG-CD2	8.17	112.83	106.30
1	I	173	TRP	CD1-CG-CD2	8.16	112.83	106.30
1	J	173	TRP	CD1-CG-CD2	8.16	112.83	106.30
1	L	269	TRP	CD1-CG-CD2	8.15	112.82	106.30
1	J	360	TRP	CD1-CG-CD2	8.11	112.79	106.30
1	F	360	TRP	CD1-CG-CD2	8.10	112.78	106.30
1	J	269	TRP	CD1-CG-CD2	8.10	112.78	106.30
1	I	360	TRP	CD1-CG-CD2	8.07	112.76	106.30
1	G	360	TRP	CD1-CG-CD2	8.07	112.76	106.30
1	L	360	TRP	CD1-CG-CD2	8.06	112.75	106.30
1	H	360	TRP	CD1-CG-CD2	8.04	112.73	106.30
1	M	360	TRP	CD1-CG-CD2	8.01	112.71	106.30
1	E	360	TRP	CD1-CG-CD2	8.00	112.70	106.30
1	D	527	SER	O-C-N	-8.00	109.91	122.70
1	K	360	TRP	CD1-CG-CD2	8.00	112.70	106.30
1	D	360	TRP	CD1-CG-CD2	7.96	112.67	106.30
1	A	360	TRP	CD1-CG-CD2	7.96	112.67	106.30
1	L	269	TRP	CE2-CD2-CG	-7.94	100.95	107.30
1	H	269	TRP	CD1-CG-CD2	7.93	112.64	106.30
1	C	535	TRP	CD1-CG-CD2	7.92	112.64	106.30
1	H	181	TRP	CE2-CD2-CG	-7.92	100.97	107.30
1	M	527	SER	O-C-N	-7.92	110.03	122.70
1	I	269	TRP	CD1-CG-CD2	7.92	112.63	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	360	TRP	CD1-CG-CD2	7.91	112.63	106.30
1	M	181	TRP	CE2-CD2-CG	-7.91	100.97	107.30
1	C	181	TRP	CE2-CD2-CG	-7.91	100.97	107.30
1	F	360	TRP	CE2-CD2-CG	-7.89	100.99	107.30
1	M	535	TRP	CE2-CD2-CG	-7.89	100.99	107.30
1	G	360	TRP	CE2-CD2-CG	-7.88	101.00	107.30
1	I	360	TRP	CE2-CD2-CG	-7.88	101.00	107.30
1	L	181	TRP	CE2-CD2-CG	-7.87	101.01	107.30
1	I	535	TRP	CD1-CG-CD2	7.86	112.59	106.30
1	M	126	ARG	NE-CZ-NH2	-7.86	116.37	120.30
1	E	360	TRP	CE2-CD2-CG	-7.86	101.01	107.30
1	A	269	TRP	CD1-CG-CD2	7.85	112.58	106.30
1	L	535	TRP	CE2-CD2-CG	-7.85	101.02	107.30
1	K	269	TRP	CD1-CG-CD2	7.85	112.58	106.30
1	J	269	TRP	CE2-CD2-CG	-7.84	101.03	107.30
1	M	360	TRP	CE2-CD2-CG	-7.84	101.02	107.30
1	D	126	ARG	NE-CZ-NH2	-7.83	116.38	120.30
1	D	535	TRP	CE2-CD2-CG	-7.83	101.03	107.30
1	F	126	ARG	NE-CZ-NH2	-7.83	116.38	120.30
1	J	360	TRP	CE2-CD2-CG	-7.83	101.03	107.30
1	J	181	TRP	CE2-CD2-CG	-7.83	101.04	107.30
1	E	126	ARG	NE-CZ-NH2	-7.82	116.39	120.30
1	D	181	TRP	CE2-CD2-CG	-7.82	101.05	107.30
1	E	535	TRP	CE2-CD2-CG	-7.82	101.05	107.30
1	H	535	TRP	CE2-CD2-CG	-7.81	101.05	107.30
1	F	181	TRP	CE2-CD2-CG	-7.81	101.05	107.30
1	F	269	TRP	CD1-CG-CD2	7.81	112.55	106.30
1	E	181	TRP	CE2-CD2-CG	-7.81	101.05	107.30
1	K	181	TRP	CE2-CD2-CG	-7.81	101.05	107.30
1	L	360	TRP	CE2-CD2-CG	-7.81	101.05	107.30
1	I	181	TRP	CE2-CD2-CG	-7.81	101.05	107.30
1	A	535	TRP	CE2-CD2-CG	-7.80	101.06	107.30
1	J	535	TRP	CE2-CD2-CG	-7.80	101.06	107.30
1	F	535	TRP	CE2-CD2-CG	-7.79	101.07	107.30
1	H	360	TRP	CE2-CD2-CG	-7.79	101.07	107.30
1	D	360	TRP	CE2-CD2-CG	-7.79	101.07	107.30
1	A	360	TRP	CE2-CD2-CG	-7.78	101.08	107.30
1	C	360	TRP	CE2-CD2-CG	-7.77	101.08	107.30
1	G	535	TRP	CE2-CD2-CG	-7.77	101.08	107.30
1	D	81	GLN	CB-CA-C	7.77	125.94	110.40
1	H	512	ARG	NE-CZ-NH2	-7.77	116.42	120.30
1	I	126	ARG	NE-CZ-NH2	-7.76	116.42	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	360	TRP	CE2-CD2-CG	-7.76	101.09	107.30
1	G	269	TRP	CD1-CG-CD2	7.76	112.50	106.30
1	G	181	TRP	CE2-CD2-CG	-7.75	101.10	107.30
1	A	173	TRP	CE2-CD2-CG	-7.74	101.11	107.30
1	E	173	TRP	CE2-CD2-CG	-7.73	101.12	107.30
1	A	181	TRP	CE2-CD2-CG	-7.73	101.12	107.30
1	G	527	SER	O-C-N	-7.71	110.36	122.70
1	H	126	ARG	NE-CZ-NH2	-7.70	116.45	120.30
1	M	269	TRP	CD1-CG-CD2	7.70	112.46	106.30
1	C	173	TRP	CE2-CD2-CG	-7.70	101.14	107.30
1	K	535	TRP	CE2-CD2-CG	-7.70	101.14	107.30
1	D	269	TRP	CD1-CG-CD2	7.70	112.46	106.30
1	F	173	TRP	CE2-CD2-CG	-7.69	101.15	107.30
1	K	173	TRP	CE2-CD2-CG	-7.69	101.15	107.30
1	H	269	TRP	CE2-CD2-CG	-7.68	101.15	107.30
1	E	269	TRP	CD1-CG-CD2	7.68	112.44	106.30
1	M	171	TRP	CE2-CD2-CG	-7.68	101.16	107.30
1	H	527	SER	O-C-N	-7.67	110.42	122.70
1	D	173	TRP	CE2-CD2-CG	-7.67	101.17	107.30
1	E	171	TRP	CE2-CD2-CG	-7.67	101.17	107.30
1	J	173	TRP	CE2-CD2-CG	-7.66	101.17	107.30
1	L	173	TRP	CE2-CD2-CG	-7.66	101.17	107.30
1	A	171	TRP	CE2-CD2-CG	-7.66	101.17	107.30
1	H	173	TRP	CE2-CD2-CG	-7.66	101.17	107.30
1	I	173	TRP	CE2-CD2-CG	-7.66	101.17	107.30
1	E	362	ARG	NE-CZ-NH1	7.65	124.13	120.30
1	C	269	TRP	CD1-CG-CD2	7.64	112.41	106.30
1	G	171	TRP	CE2-CD2-CG	-7.63	101.19	107.30
1	G	173	TRP	CE2-CD2-CG	-7.63	101.20	107.30
1	M	173	TRP	CE2-CD2-CG	-7.63	101.20	107.30
1	C	126	ARG	NE-CZ-NH2	-7.62	116.49	120.30
1	F	171	TRP	CE2-CD2-CG	-7.62	101.21	107.30
1	M	526	ASP	CA-C-N	7.62	133.96	117.20
1	H	171	TRP	CE2-CD2-CG	-7.61	101.21	107.30
1	D	526	ASP	CA-C-N	7.61	133.93	117.20
1	I	171	TRP	CE2-CD2-CG	-7.61	101.22	107.30
1	K	171	TRP	CE2-CD2-CG	-7.61	101.22	107.30
1	H	526	ASP	CA-C-N	7.60	133.93	117.20
1	G	526	ASP	CA-C-N	7.60	133.91	117.20
1	J	171	TRP	CE2-CD2-CG	-7.59	101.22	107.30
1	J	126	ARG	NE-CZ-NH2	-7.59	116.51	120.30
1	L	171	TRP	CE2-CD2-CG	-7.58	101.23	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	526	ASP	CA-C-N	7.57	133.86	117.20
1	K	269	TRP	CE2-CD2-CG	-7.57	101.24	107.30
1	A	269	TRP	CE2-CD2-CG	-7.57	101.25	107.30
1	J	362	ARG	NE-CZ-NH1	7.57	124.08	120.30
1	D	171	TRP	CE2-CD2-CG	-7.56	101.25	107.30
1	F	269	TRP	CE2-CD2-CG	-7.56	101.25	107.30
1	L	362	ARG	NE-CZ-NH1	7.56	124.08	120.30
1	C	171	TRP	CE2-CD2-CG	-7.56	101.25	107.30
1	A	270	ARG	NE-CZ-NH2	7.55	124.08	120.30
1	J	249	ARG	NE-CZ-NH2	-7.55	116.53	120.30
1	E	269	TRP	CE2-CD2-CG	-7.54	101.27	107.30
1	M	362	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	H	362	ARG	NE-CZ-NH1	7.53	124.07	120.30
1	D	362	ARG	NE-CZ-NH1	7.52	124.06	120.30
1	F	362	ARG	NE-CZ-NH1	7.52	124.06	120.30
1	A	362	ARG	NE-CZ-NH1	7.51	124.06	120.30
1	C	269	TRP	CE2-CD2-CG	-7.50	101.30	107.30
1	G	269	TRP	CE2-CD2-CG	-7.49	101.31	107.30
1	K	362	ARG	NE-CZ-NH1	7.49	124.04	120.30
1	I	269	TRP	CE2-CD2-CG	-7.48	101.31	107.30
1	I	362	ARG	NE-CZ-NH1	7.47	124.03	120.30
1	A	25	PRO	N-CA-C	-7.44	92.76	112.10
1	C	362	ARG	NE-CZ-NH1	7.42	124.01	120.30
1	M	269	TRP	CE2-CD2-CG	-7.41	101.38	107.30
1	G	323	TRP	CD1-CG-CD2	7.40	112.22	106.30
1	K	323	TRP	CD1-CG-CD2	7.40	112.22	106.30
1	C	323	TRP	CD1-CG-CD2	7.38	112.21	106.30
1	H	323	TRP	CD1-CG-CD2	7.38	112.20	106.30
1	C	535	TRP	CE2-CD2-CG	-7.38	101.40	107.30
1	A	323	TRP	CD1-CG-CD2	7.37	112.20	106.30
1	G	362	ARG	NE-CZ-NH1	7.37	123.98	120.30
1	D	269	TRP	CE2-CD2-CG	-7.36	101.41	107.30
1	F	323	TRP	CD1-CG-CD2	7.36	112.19	106.30
1	J	323	TRP	CD1-CG-CD2	7.36	112.19	106.30
1	D	323	TRP	CE2-CD2-CG	-7.35	101.42	107.30
1	M	171	TRP	CD1-CG-CD2	7.35	112.18	106.30
1	I	323	TRP	CD1-CG-CD2	7.34	112.17	106.30
1	K	323	TRP	CE2-CD2-CG	-7.33	101.43	107.30
1	A	171	TRP	CD1-CG-CD2	7.33	112.17	106.30
1	D	323	TRP	CD1-CG-CD2	7.33	112.17	106.30
1	M	323	TRP	CE2-CD2-CG	-7.33	101.44	107.30
1	I	535	TRP	CE2-CD2-CG	-7.31	101.45	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	323	TRP	CD1-CG-CD2	7.30	112.14	106.30
1	L	323	TRP	CD1-CG-CD2	7.30	112.14	106.30
1	L	323	TRP	CE2-CD2-CG	-7.30	101.46	107.30
1	E	323	TRP	CD1-CG-CD2	7.30	112.14	106.30
1	C	323	TRP	CE2-CD2-CG	-7.28	101.47	107.30
1	F	323	TRP	CE2-CD2-CG	-7.28	101.48	107.30
1	H	323	TRP	CE2-CD2-CG	-7.27	101.48	107.30
1	A	323	TRP	CE2-CD2-CG	-7.27	101.49	107.30
1	H	171	TRP	CD1-CG-CD2	7.26	112.11	106.30
1	G	171	TRP	CD1-CG-CD2	7.26	112.11	106.30
1	G	323	TRP	CE2-CD2-CG	-7.25	101.50	107.30
1	J	323	TRP	CE2-CD2-CG	-7.25	101.50	107.30
1	I	323	TRP	CE2-CD2-CG	-7.24	101.51	107.30
1	E	171	TRP	CD1-CG-CD2	7.24	112.09	106.30
1	K	171	TRP	CD1-CG-CD2	7.24	112.09	106.30
1	I	171	TRP	CD1-CG-CD2	7.23	112.09	106.30
1	J	171	TRP	CD1-CG-CD2	7.22	112.08	106.30
1	L	171	TRP	CD1-CG-CD2	7.22	112.08	106.30
1	F	171	TRP	CD1-CG-CD2	7.22	112.08	106.30
1	K	126	ARG	NE-CZ-NH1	7.22	123.91	120.30
1	K	60	TYR	CB-CG-CD2	-7.21	116.67	121.00
1	D	171	TRP	CD1-CG-CD2	7.21	112.06	106.30
1	M	512	ARG	NE-CZ-NH2	-7.15	116.72	120.30
1	C	171	TRP	CD1-CG-CD2	7.13	112.00	106.30
1	E	323	TRP	CE2-CD2-CG	-7.11	101.61	107.30
1	L	249	ARG	NE-CZ-NH2	-7.10	116.75	120.30
1	I	519	ALA	CA-C-N	7.00	130.21	116.20
1	H	21	ARG	O-C-N	-6.99	111.52	122.70
1	G	605	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	I	530	TYR	CA-CB-CG	-6.92	100.24	113.40
1	G	457	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	G	249	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	H	249	ARG	NE-CZ-NH2	-6.87	116.87	120.30
1	L	457	ARG	NE-CZ-NH1	6.85	123.73	120.30
1	E	249	ARG	NE-CZ-NH2	-6.85	116.88	120.30
1	K	457	ARG	NE-CZ-NH1	6.85	123.72	120.30
1	D	249	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	C	457	ARG	NE-CZ-NH1	6.83	123.72	120.30
1	F	532	SER	N-CA-CB	-6.83	100.25	110.50
1	E	457	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	A	249	ARG	NE-CZ-NH2	-6.81	116.89	120.30
1	A	457	ARG	NE-CZ-NH1	6.81	123.71	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	457	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	F	457	ARG	NE-CZ-NH1	6.79	123.70	120.30
1	A	34	LYS	N-CA-C	6.79	129.33	111.00
1	D	457	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	K	249	ARG	NE-CZ-NH2	-6.75	116.92	120.30
1	G	80	ARG	NE-CZ-NH2	-6.75	116.92	120.30
1	E	512	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	H	457	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	J	457	ARG	NE-CZ-NH1	6.71	123.66	120.30
1	D	83	VAL	N-CA-C	6.71	129.11	111.00
1	M	457	ARG	NE-CZ-NH1	6.71	123.65	120.30
1	A	80	ARG	NE-CZ-NH2	-6.71	116.95	120.30
1	I	249	ARG	NE-CZ-NH2	-6.69	116.96	120.30
1	F	80	ARG	NE-CZ-NH2	-6.65	116.97	120.30
1	L	80	ARG	NE-CZ-NH2	-6.65	116.97	120.30
1	E	80	ARG	NE-CZ-NH2	-6.65	116.98	120.30
1	M	171	TRP	CG-CD2-CE3	6.64	139.88	133.90
1	G	171	TRP	CG-CD2-CE3	6.64	139.87	133.90
1	I	171	TRP	CG-CD2-CE3	6.62	139.86	133.90
1	H	171	TRP	CG-CD2-CE3	6.62	139.85	133.90
1	K	171	TRP	CG-CD2-CE3	6.60	139.84	133.90
1	A	171	TRP	CG-CD2-CE3	6.58	139.82	133.90
1	L	171	TRP	CG-CD2-CE3	6.58	139.82	133.90
1	E	171	TRP	CG-CD2-CE3	6.57	139.81	133.90
1	D	171	TRP	CG-CD2-CE3	6.57	139.81	133.90
1	J	171	TRP	CG-CD2-CE3	6.55	139.80	133.90
1	I	80	ARG	NE-CZ-NH2	-6.55	117.03	120.30
1	C	80	ARG	NE-CZ-NH2	-6.55	117.03	120.30
1	G	337	ARG	NE-CZ-NH2	-6.55	117.03	120.30
1	F	171	TRP	CG-CD2-CE3	6.54	139.79	133.90
1	A	24	LEU	N-CA-C	-6.54	93.35	111.00
1	C	171	TRP	CG-CD2-CE3	6.53	139.78	133.90
1	D	80	ARG	NE-CZ-NH2	-6.51	117.04	120.30
1	E	270	ARG	NE-CZ-NH2	6.49	123.55	120.30
1	K	80	ARG	NE-CZ-NH2	-6.49	117.05	120.30
1	F	34	LYS	N-CA-C	6.46	128.44	111.00
1	M	80	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	A	512	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	J	80	ARG	NE-CZ-NH2	-6.41	117.10	120.30
1	M	80	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	G	512	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	G	605	ARG	NE-CZ-NH1	6.29	123.45	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	117	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	M	337	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	F	249	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	I	117	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	M	69	PHE	CB-CG-CD1	-6.21	116.45	120.80
1	M	249	ARG	NE-CZ-NH2	-6.19	117.20	120.30
1	J	117	ARG	NE-CZ-NH2	-6.19	117.21	120.30
1	M	117	ARG	NE-CZ-NH2	-6.19	117.21	120.30
1	E	117	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	F	117	ARG	NE-CZ-NH2	-6.17	117.21	120.30
1	C	268	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	A	135	PRO	N-CA-C	6.16	128.11	112.10
1	D	527	SER	CA-C-N	6.15	130.73	117.20
1	D	587	ARG	NE-CZ-NH2	6.15	123.37	120.30
1	M	527	SER	CA-C-N	6.09	130.60	117.20
1	L	117	ARG	NE-CZ-NH2	-6.09	117.26	120.30
1	C	117	ARG	NE-CZ-NH2	-6.09	117.26	120.30
1	L	268	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	H	587	ARG	NE-CZ-NH2	6.07	123.34	120.30
1	L	587	ARG	NE-CZ-NH2	6.07	123.34	120.30
1	I	587	ARG	NE-CZ-NH2	6.05	123.33	120.30
1	K	117	ARG	NE-CZ-NH2	-6.05	117.27	120.30
1	M	69	PHE	CA-CB-CG	-6.02	99.45	113.90
1	M	587	ARG	NE-CZ-NH2	6.01	123.31	120.30
1	D	44	LEU	N-CA-C	6.00	127.20	111.00
1	H	117	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	G	587	ARG	NE-CZ-NH2	5.99	123.29	120.30
1	C	249	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	E	587	ARG	NE-CZ-NH2	5.98	123.29	120.30
1	F	587	ARG	NE-CZ-NH2	5.98	123.29	120.30
1	K	587	ARG	NE-CZ-NH2	5.97	123.28	120.30
1	A	587	ARG	NE-CZ-NH2	5.97	123.28	120.30
1	G	126	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	J	312	LYS	CA-CB-CG	-5.94	100.33	113.40
1	H	83	VAL	N-CA-C	5.93	127.01	111.00
1	J	587	ARG	NE-CZ-NH2	5.92	123.26	120.30
1	A	22	GLU	CB-CA-C	5.92	122.24	110.40
1	D	117	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	G	527	SER	CA-C-N	5.91	130.20	117.20
1	H	337	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	J	51	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	M	51	ARG	NE-CZ-NH1	5.82	123.21	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	527	SER	CA-C-N	5.82	130.00	117.20
1	E	126	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	K	51	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	M	32	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	M	306	GLU	CA-C-N	5.76	129.87	117.20
1	K	306	GLU	CA-C-N	5.75	129.85	117.20
1	M	126	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	I	126	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	I	25	PRO	N-CA-C	5.73	127.00	112.10
1	A	306	GLU	CA-C-N	5.73	129.80	117.20
1	L	306	GLU	CA-C-N	5.73	129.80	117.20
1	F	306	GLU	CA-C-N	5.72	129.79	117.20
1	I	306	GLU	CA-C-N	5.72	129.79	117.20
1	C	306	GLU	CA-C-N	5.72	129.78	117.20
1	G	312	LYS	CA-C-N	5.72	129.78	117.20
1	F	126	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	C	51	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	E	306	GLU	CA-C-N	5.69	129.72	117.20
1	H	126	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	E	51	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	A	51	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	D	51	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	I	51	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	H	306	GLU	CA-C-N	5.66	129.66	117.20
1	L	51	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	F	531	CYS	C-N-CA	5.61	135.73	121.70
1	D	306	GLU	CA-C-N	5.61	129.54	117.20
1	C	605	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	G	51	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	D	126	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	F	51	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	G	311	SER	CA-C-N	-5.60	104.89	117.20
1	J	512	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	G	337	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	J	126	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	C	126	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	K	268	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	L	269	TRP	CG-CD2-CE3	5.54	138.89	133.90
1	M	33	LEU	N-CA-C	5.53	125.94	111.00
1	H	51	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	J	38	ILE	CA-CB-CG1	5.50	121.46	111.00
1	F	20	THR	CA-CB-CG2	5.46	120.05	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	292	LEU	CA-C-N	-5.46	105.18	117.20
1	K	530	TYR	N-CA-C	5.45	125.73	111.00
1	C	527	SER	CB-CA-C	-5.43	99.78	110.10
1	I	530	TYR	N-CA-C	5.43	125.67	111.00
1	C	564	THR	CA-CB-CG2	5.43	120.00	112.40
1	G	126	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	J	360	TRP	CG-CD2-CE3	5.41	138.77	133.90
1	I	360	TRP	CG-CD2-CE3	5.41	138.76	133.90
1	D	605	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	J	269	TRP	CG-CD2-CE3	5.39	138.75	133.90
1	H	82	ILE	O-C-N	-5.38	114.10	122.70
1	J	35	GLY	O-C-N	-5.37	114.11	122.70
1	M	30	ASP	CB-CA-C	5.36	121.12	110.40
1	G	360	TRP	CG-CD2-CE3	5.36	138.72	133.90
1	M	535	TRP	CG-CD1-NE1	-5.35	104.75	110.10
1	F	605	ARG	NE-CZ-NH2	-5.35	117.63	120.30
1	M	360	TRP	CG-CD2-CE3	5.35	138.71	133.90
1	A	360	TRP	CG-CD2-CE3	5.34	138.71	133.90
1	E	527	SER	O-C-N	-5.34	114.16	122.70
1	L	360	TRP	CG-CD2-CE3	5.34	138.70	133.90
1	L	535	TRP	CG-CD1-NE1	-5.34	104.76	110.10
1	I	530	TYR	CB-CG-CD2	-5.33	117.80	121.00
1	D	535	TRP	CG-CD1-NE1	-5.33	104.77	110.10
1	G	535	TRP	CG-CD1-NE1	-5.32	104.78	110.10
1	K	360	TRP	CG-CD2-CE3	5.32	138.69	133.90
1	K	535	TRP	CG-CD1-NE1	-5.32	104.78	110.10
1	A	535	TRP	CG-CD1-NE1	-5.32	104.78	110.10
1	H	360	TRP	CG-CD2-CE3	5.32	138.69	133.90
1	H	535	TRP	CG-CD1-NE1	-5.31	104.79	110.10
1	M	535	TRP	CG-CD2-CE3	5.31	138.68	133.90
1	E	360	TRP	CG-CD2-CE3	5.31	138.68	133.90
1	M	151	LEU	CA-CB-CG	5.31	127.50	115.30
1	H	323	TRP	CB-CG-CD1	-5.29	120.12	127.00
1	G	323	TRP	CB-CG-CD1	-5.29	120.13	127.00
1	I	521	GLU	N-CA-C	5.29	125.28	111.00
1	H	181	TRP	CG-CD2-CE3	5.28	138.65	133.90
1	E	323	TRP	CB-CG-CD1	-5.28	120.14	127.00
1	E	535	TRP	CG-CD1-NE1	-5.27	104.83	110.10
1	M	527	SER	N-CA-C	5.27	125.23	111.00
1	F	360	TRP	CG-CD2-CE3	5.26	138.64	133.90
1	L	535	TRP	CG-CD2-CE3	5.26	138.63	133.90
1	D	360	TRP	CG-CD2-CE3	5.26	138.63	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	323	TRP	CB-CG-CD1	-5.26	120.16	127.00
1	C	323	TRP	CB-CG-CD1	-5.25	120.17	127.00
1	D	527	SER	N-CA-C	5.25	125.18	111.00
1	G	535	TRP	CG-CD2-CE3	5.25	138.63	133.90
1	H	527	SER	N-CA-C	5.25	125.18	111.00
1	H	535	TRP	CG-CD2-CE3	5.25	138.63	133.90
1	I	265	ASP	CB-CG-OD2	5.25	123.03	118.30
1	D	535	TRP	CG-CD2-CE3	5.25	138.62	133.90
1	I	22	GLU	O-C-N	-5.25	114.30	122.70
1	F	323	TRP	CB-CG-CD1	-5.25	120.18	127.00
1	A	527	SER	N-CA-C	5.25	125.17	111.00
1	H	80	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	E	535	TRP	CG-CD2-CE3	5.24	138.62	133.90
1	F	605	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	C	360	TRP	CG-CD2-CE3	5.24	138.61	133.90
1	D	311	SER	CA-C-N	-5.23	105.69	117.20
1	K	69	PHE	CA-CB-CG	-5.23	101.34	113.90
1	L	181	TRP	CG-CD2-CE3	5.23	138.61	133.90
1	A	323	TRP	CB-CG-CD1	-5.23	120.20	127.00
1	M	181	TRP	CG-CD2-CE3	5.23	138.60	133.90
1	G	527	SER	N-CA-C	5.23	125.11	111.00
1	M	323	TRP	CB-CG-CD1	-5.22	120.21	127.00
1	J	535	TRP	CG-CD2-CE3	5.22	138.60	133.90
1	L	323	TRP	CB-CG-CD1	-5.22	120.22	127.00
1	M	295	GLU	CA-CB-CG	5.22	124.88	113.40
1	J	535	TRP	CG-CD1-NE1	-5.21	104.89	110.10
1	K	323	TRP	CB-CG-CD1	-5.21	120.22	127.00
1	I	264	GLN	CA-CB-CG	5.21	124.86	113.40
1	E	295	GLU	CA-CB-CG	5.21	124.86	113.40
1	H	295	GLU	CA-CB-CG	5.20	124.85	113.40
1	I	295	GLU	CA-CB-CG	5.20	124.83	113.40
1	J	323	TRP	CB-CG-CD1	-5.20	120.24	127.00
1	D	323	TRP	CB-CG-CD1	-5.19	120.25	127.00
1	E	181	TRP	CG-CD2-CE3	5.18	138.56	133.90
1	K	535	TRP	CG-CD2-CE3	5.18	138.56	133.90
1	A	295	GLU	CA-CB-CG	5.18	124.79	113.40
1	G	312	LYS	CA-C-O	-5.18	109.22	120.10
1	K	82	ILE	O-C-N	-5.18	114.41	122.70
1	L	39	LEU	N-CA-C	-5.18	97.01	111.00
1	A	126	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	J	181	TRP	CG-CD2-CE3	5.18	138.56	133.90
1	K	295	GLU	CA-CB-CG	5.17	124.78	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	295	GLU	CA-CB-CG	5.17	124.78	113.40
1	F	535	TRP	CG-CD2-CE3	5.17	138.56	133.90
1	C	181	TRP	CG-CD2-CE3	5.17	138.55	133.90
1	E	457	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	F	295	GLU	CA-CB-CG	5.16	124.76	113.40
1	L	295	GLU	CA-CB-CG	5.16	124.76	113.40
1	K	337	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	I	181	TRP	CG-CD2-CE3	5.16	138.54	133.90
1	G	457	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	A	181	TRP	CG-CD2-CE3	5.15	138.53	133.90
1	K	527	SER	N-CA-C	5.15	124.90	111.00
1	A	323	TRP	CG-CD2-CE3	5.14	138.53	133.90
1	J	323	TRP	CG-CD2-CE3	5.14	138.53	133.90
1	A	535	TRP	CG-CD2-CE3	5.14	138.52	133.90
1	F	535	TRP	CG-CD1-NE1	-5.14	104.96	110.10
1	J	33	LEU	N-CA-C	5.13	124.85	111.00
1	C	295	GLU	CA-CB-CG	5.12	124.67	113.40
1	C	323	TRP	CG-CD2-CE3	5.12	138.51	133.90
1	F	181	TRP	CG-CD1-NE1	-5.12	104.98	110.10
1	K	323	TRP	CG-CD2-CE3	5.12	138.51	133.90
1	L	457	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	L	126	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	D	181	TRP	CG-CD2-CE3	5.11	138.50	133.90
1	D	323	TRP	CG-CD2-CE3	5.11	138.50	133.90
1	I	323	TRP	CG-CD2-CE3	5.11	138.50	133.90
1	K	181	TRP	CG-CD2-CE3	5.11	138.50	133.90
1	I	337	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	L	526	ASP	CA-C-N	5.08	128.37	117.20
1	A	530	TYR	N-CA-C	5.07	124.69	111.00
1	K	181	TRP	CG-CD1-NE1	-5.07	105.03	110.10
1	F	181	TRP	CG-CD2-CE3	5.07	138.46	133.90
1	G	323	TRP	CG-CD2-CE3	5.06	138.45	133.90
1	E	181	TRP	CG-CD1-NE1	-5.05	105.05	110.10
1	G	181	TRP	CG-CD2-CE3	5.05	138.45	133.90
1	I	181	TRP	CG-CD1-NE1	-5.05	105.05	110.10
1	D	101	ASP	CB-CG-OD2	5.04	122.84	118.30
1	H	181	TRP	CG-CD1-NE1	-5.04	105.06	110.10
1	H	323	TRP	CG-CD2-CE3	5.04	138.44	133.90
1	F	323	TRP	CG-CD2-CE3	5.04	138.44	133.90
1	H	269	TRP	CG-CD2-CE3	5.04	138.44	133.90
1	J	181	TRP	CG-CD1-NE1	-5.04	105.06	110.10
1	A	25	PRO	C-N-CA	-5.04	109.11	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	311	SER	N-CA-C	5.03	124.58	111.00
1	D	265	ASP	CB-CG-OD2	5.02	122.82	118.30
1	E	268	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	F	457	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	M	323	TRP	CG-CD2-CE3	5.02	138.41	133.90
1	D	457	ARG	NE-CZ-NH2	-5.01	117.79	120.30
1	E	323	TRP	CG-CD2-CE3	5.01	138.41	133.90
1	L	323	TRP	CG-CD2-CE3	5.01	138.41	133.90
1	D	181	TRP	CG-CD1-NE1	-5.01	105.09	110.10
1	E	499	ARG	NE-CZ-NH2	-5.01	117.80	120.30
1	F	101	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

All (195) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	117	ARG	Sidechain
1	A	127	ALA	Peptide
1	A	22	GLU	Peptide
1	A	23	LYS	Peptide
1	A	24	LEU	Peptide
1	A	253	TYR	Sidechain
1	A	270	ARG	Sidechain
1	A	272	ARG	Sidechain
1	A	316	TYR	Sidechain
1	A	317	TYR	Sidechain
1	A	359	ARG	Sidechain
1	A	43	THR	Peptide
1	A	440	TYR	Sidechain
1	A	457	ARG	Sidechain
1	A	523	VAL	Peptide
1	A	530	TYR	Sidechain
1	A	600	ARG	Sidechain
1	A	69	PHE	Sidechain
1	A	96	VAL	Peptide
1	A	99	ARG	Peptide
1	C	253	TYR	Sidechain
1	C	270	ARG	Sidechain
1	C	316	TYR	Sidechain
1	C	317	TYR	Sidechain
1	C	337	ARG	Sidechain
1	C	359	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	C	43	THR	Peptide
1	C	440	TYR	Sidechain
1	C	457	ARG	Sidechain
1	C	518	GLY	Mainchain
1	C	600	ARG	Sidechain
1	C	64	TYR	Sidechain
1	C	69	PHE	Sidechain
1	C	96	VAL	Peptide
1	C	99	ARG	Peptide
1	D	270	ARG	Sidechain
1	D	316	TYR	Sidechain
1	D	317	TYR	Sidechain
1	D	359	ARG	Sidechain
1	D	440	TYR	Sidechain
1	D	457	ARG	Sidechain
1	D	523	VAL	Peptide
1	D	530	TYR	Sidechain
1	D	600	ARG	Sidechain
1	D	64	TYR	Sidechain
1	D	84	ASN	Peptide
1	D	96	VAL	Peptide
1	D	99	ARG	Peptide
1	E	253	TYR	Sidechain
1	E	270	ARG	Sidechain
1	E	316	TYR	Sidechain
1	E	317	TYR	Sidechain
1	E	359	ARG	Sidechain
1	E	43	THR	Peptide
1	E	440	TYR	Sidechain
1	E	457	ARG	Sidechain
1	E	523	VAL	Peptide
1	E	530	TYR	Sidechain
1	E	600	ARG	Sidechain
1	E	64	TYR	Sidechain
1	E	69	PHE	Sidechain
1	E	96	VAL	Peptide
1	E	99	ARG	Peptide
1	F	23	LYS	Peptide
1	F	270	ARG	Sidechain
1	F	316	TYR	Sidechain
1	F	317	TYR	Sidechain
1	F	359	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	F	43	THR	Peptide
1	F	440	TYR	Sidechain
1	F	457	ARG	Sidechain
1	F	512	ARG	Sidechain
1	F	523	VAL	Peptide
1	F	530	TYR	Sidechain
1	F	600	ARG	Sidechain
1	F	64	TYR	Sidechain
1	F	69	PHE	Sidechain
1	F	96	VAL	Peptide
1	F	99	ARG	Peptide
1	G	253	TYR	Sidechain
1	G	270	ARG	Sidechain
1	G	272	ARG	Sidechain
1	G	316	TYR	Sidechain
1	G	317	TYR	Sidechain
1	G	359	ARG	Sidechain
1	G	43	THR	Peptide
1	G	440	TYR	Sidechain
1	G	457	ARG	Sidechain
1	G	523	VAL	Peptide
1	G	530	TYR	Sidechain
1	G	600	ARG	Sidechain
1	G	64	TYR	Sidechain
1	G	69	PHE	Sidechain
1	G	96	VAL	Peptide
1	G	99	ARG	Peptide
1	H	268	ARG	Sidechain
1	H	316	TYR	Sidechain
1	H	317	TYR	Sidechain
1	H	359	ARG	Sidechain
1	H	43	THR	Peptide
1	H	440	TYR	Sidechain
1	H	457	ARG	Sidechain
1	H	523	VAL	Peptide
1	H	530	TYR	Sidechain
1	H	600	ARG	Sidechain
1	H	64	TYR	Sidechain
1	H	69	PHE	Sidechain
1	H	80	ARG	Sidechain
1	H	84	ASN	Peptide
1	H	96	VAL	Peptide

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Mol	Chain	Res	Type	Group
1	H	99	ARG	Peptide
1	I	253	TYR	Sidechain
1	I	281	TYR	Sidechain
1	I	316	TYR	Sidechain
1	I	317	TYR	Sidechain
1	I	359	ARG	Sidechain
1	I	43	THR	Peptide
1	I	440	TYR	Sidechain
1	I	457	ARG	Sidechain
1	I	518	GLY	Mainchain
1	I	530	TYR	Sidechain
1	I	600	ARG	Sidechain
1	I	64	TYR	Sidechain
1	I	69	PHE	Sidechain
1	I	96	VAL	Peptide
1	I	99	ARG	Peptide
1	J	270	ARG	Sidechain
1	J	31	GLU	Peptide
1	J	316	TYR	Sidechain
1	J	317	TYR	Sidechain
1	J	359	ARG	Sidechain
1	J	440	TYR	Sidechain
1	J	457	ARG	Sidechain
1	J	49	HIS	Sidechain
1	J	530	TYR	Sidechain
1	J	600	ARG	Sidechain
1	J	64	TYR	Sidechain
1	J	69	PHE	Sidechain
1	J	96	VAL	Peptide
1	J	99	ARG	Peptide
1	K	126	ARG	Sidechain
1	K	253	TYR	Sidechain
1	K	270	ARG	Sidechain
1	K	316	TYR	Sidechain
1	K	317	TYR	Sidechain
1	K	337	ARG	Sidechain
1	K	359	ARG	Sidechain
1	K	43	THR	Peptide
1	K	440	TYR	Sidechain
1	K	457	ARG	Sidechain
1	K	523	VAL	Peptide
1	K	530	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	K	600	ARG	Sidechain
1	K	605	ARG	Sidechain
1	K	64	TYR	Sidechain
1	K	69	PHE	Sidechain
1	K	96	VAL	Peptide
1	K	99	ARG	Peptide
1	L	268	ARG	Sidechain
1	L	270	ARG	Sidechain
1	L	316	TYR	Sidechain
1	L	317	TYR	Sidechain
1	L	337	ARG	Sidechain
1	L	359	ARG	Sidechain
1	L	43	THR	Peptide
1	L	440	TYR	Sidechain
1	L	457	ARG	Sidechain
1	L	523	VAL	Peptide
1	L	530	TYR	Sidechain
1	L	575	SER	Peptide
1	L	600	ARG	Sidechain
1	L	605	ARG	Sidechain
1	L	64	TYR	Sidechain
1	L	69	PHE	Sidechain
1	L	96	VAL	Peptide
1	L	99	ARG	Peptide
1	M	272	ARG	Sidechain
1	M	31	GLU	Peptide
1	M	316	TYR	Sidechain
1	M	317	TYR	Sidechain
1	M	32	ARG	Sidechain
1	M	337	ARG	Sidechain
1	M	359	ARG	Sidechain
1	M	43	THR	Peptide
1	M	440	TYR	Sidechain
1	M	457	ARG	Sidechain
1	M	523	VAL	Peptide
1	M	530	TYR	Sidechain
1	M	600	ARG	Sidechain
1	M	64	TYR	Sidechain
1	M	66	ALA	Mainchain
1	M	69	PHE	Sidechain
1	M	80	ARG	Sidechain
1	M	96	VAL	Peptide

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Mol	Chain	Res	Type	Group
1	M	99	ARG	Peptide

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	5061	1123	4864	260	0
1	C	5061	1123	4863	199	0
1	D	5061	1123	4865	181	0
1	E	5061	1123	4864	190	0
1	F	5061	1123	4864	193	0
1	G	5061	1123	4865	214	0
1	H	5061	1123	4864	205	0
1	I	5061	1123	4863	207	0
1	J	5061	1123	4865	242	0
1	K	5061	1123	4865	225	0
1	L	5061	1123	4864	210	0
1	M	5061	1123	4865	230	0
All	All	60732	13476	58371	2404	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 20.

All (2404) 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:A:24:LEU:CB	1:A:24:LEU:CG	1.76	1.56
1:K:69:PHE:CE1	1:K:69:PHE:CZ	1.94	1.55
1:G:69:PHE:CD2	1:G:69:PHE:CE2	1.96	1.54
1:G:69:PHE:CD1	1:G:69:PHE:CE1	1.96	1.54
1:H:69:PHE:CD2	1:H:69:PHE:CE2	1.96	1.53
1:H:69:PHE:CE2	1:H:69:PHE:CZ	1.96	1.53
1:H:69:PHE:CD1	1:H:69:PHE:CE1	1.96	1.53
1:K:69:PHE:CG	1:K:69:PHE:CD2	1.97	1.53
1:H:69:PHE:CD2	1:H:69:PHE:CG	1.97	1.53
1:H:69:PHE:CE1	1:H:69:PHE:CZ	1.96	1.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:69:PHE:CD2	1:K:69:PHE:CE2	1.95	1.52
1:L:69:PHE:CE2	1:L:69:PHE:CZ	1.96	1.52
1:H:69:PHE:CD1	1:H:69:PHE:CG	1.97	1.52
1:E:69:PHE:CE1	1:E:69:PHE:CZ	1.98	1.52
1:C:69:PHE:CE2	1:C:69:PHE:CD2	1.98	1.52
1:L:69:PHE:CD1	1:L:69:PHE:CG	1.97	1.52
1:M:69:PHE:CG	1:M:69:PHE:CD1	1.96	1.52
1:E:69:PHE:CG	1:E:69:PHE:CD1	1.98	1.51
1:J:69:PHE:CG	1:J:69:PHE:CD1	1.98	1.51
1:M:69:PHE:CD1	1:M:69:PHE:CE1	1.97	1.51
1:C:69:PHE:CD1	1:C:69:PHE:CG	1.98	1.51
1:A:69:PHE:CD2	1:A:69:PHE:CE2	1.98	1.51
1:C:69:PHE:CD1	1:C:69:PHE:CE1	1.99	1.51
1:E:69:PHE:CG	1:E:69:PHE:CD2	1.99	1.51
1:G:69:PHE:CD1	1:G:69:PHE:CG	1.96	1.51
1:J:69:PHE:CZ	1:J:69:PHE:CE2	1.99	1.51
1:A:69:PHE:CE2	1:A:69:PHE:CZ	1.99	1.51
1:A:69:PHE:CD1	1:A:69:PHE:CG	1.98	1.51
1:J:69:PHE:CE2	1:J:69:PHE:CD2	1.98	1.51
1:K:69:PHE:CE1	1:K:69:PHE:CD1	1.96	1.51
1:C:69:PHE:CE2	1:C:69:PHE:CZ	1.99	1.50
1:E:69:PHE:CD2	1:E:69:PHE:CE2	1.98	1.50
1:I:69:PHE:CD1	1:I:69:PHE:CG	1.96	1.50
1:A:69:PHE:CD1	1:A:69:PHE:CE1	1.99	1.50
1:J:69:PHE:CD1	1:J:69:PHE:CE1	1.99	1.50
1:K:69:PHE:CZ	1:K:69:PHE:CE2	1.96	1.50
1:M:69:PHE:CD2	1:M:69:PHE:CE2	1.96	1.50
1:E:69:PHE:CZ	1:E:69:PHE:CE2	1.99	1.50
1:G:69:PHE:CE1	1:G:69:PHE:CZ	1.96	1.50
1:F:69:PHE:CE2	1:F:69:PHE:CD2	1.98	1.50
1:I:69:PHE:CE1	1:I:69:PHE:CZ	1.96	1.50
1:L:69:PHE:CE2	1:L:69:PHE:CD2	1.96	1.50
1:E:69:PHE:CE1	1:E:69:PHE:CD1	1.99	1.50
1:I:69:PHE:CD1	1:I:69:PHE:CE1	1.96	1.50
1:L:69:PHE:CD1	1:L:69:PHE:CE1	1.96	1.50
1:M:69:PHE:CG	1:M:69:PHE:CD2	1.98	1.50
1:A:79:ALA:HB3	1:A:88:PHE:CE1	1.45	1.49
1:G:69:PHE:CE2	1:G:69:PHE:CZ	1.97	1.49
1:I:69:PHE:CD2	1:I:69:PHE:CE2	1.96	1.49
1:F:69:PHE:CD1	1:F:69:PHE:CE1	1.99	1.49
1:I:69:PHE:CZ	1:I:69:PHE:CE2	1.97	1.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:69:PHE:CG	1:L:69:PHE:CD2	1.97	1.49
1:A:69:PHE:CD2	1:A:69:PHE:CG	1.99	1.49
1:A:69:PHE:CZ	1:A:69:PHE:CE1	1.98	1.49
1:K:69:PHE:CG	1:K:69:PHE:CD1	1.97	1.49
1:L:69:PHE:CZ	1:L:69:PHE:CE1	1.96	1.49
1:M:69:PHE:CE2	1:M:69:PHE:CZ	2.00	1.49
1:F:69:PHE:CD1	1:F:69:PHE:CG	1.98	1.48
1:F:69:PHE:CE1	1:F:69:PHE:CZ	1.98	1.48
1:C:69:PHE:CD2	1:C:69:PHE:CG	1.99	1.48
1:F:69:PHE:CD2	1:F:69:PHE:CG	1.99	1.48
1:I:69:PHE:CG	1:I:69:PHE:CD2	1.97	1.48
1:F:69:PHE:CE2	1:F:69:PHE:CZ	1.99	1.48
1:L:104:GLY:CA	1:L:525:GLU:HB3	1.39	1.48
1:G:69:PHE:CD2	1:G:69:PHE:CG	1.97	1.48
1:J:69:PHE:CZ	1:J:69:PHE:CE1	1.98	1.48
1:C:69:PHE:CE1	1:C:69:PHE:CZ	1.98	1.48
1:J:69:PHE:CG	1:J:69:PHE:CD2	1.99	1.47
1:D:104:GLY:CA	1:D:525:GLU:HB3	1.41	1.46
1:M:104:GLY:CA	1:M:525:GLU:HB3	1.41	1.46
1:H:104:GLY:CA	1:H:525:GLU:HB3	1.41	1.46
1:M:69:PHE:CE1	1:M:69:PHE:CZ	2.01	1.46
1:G:104:GLY:CA	1:G:525:GLU:HB3	1.43	1.43
1:K:175:ILE:CG2	1:K:528:THR:HG21	1.47	1.42
1:E:175:ILE:CG2	1:E:528:THR:HG21	1.47	1.42
1:J:175:ILE:CG2	1:J:528:THR:HG21	1.48	1.41
1:L:63:LEU:CD2	1:L:91:ALA:HB1	1.47	1.39
1:C:151:LEU:CD1	1:G:467:LEU:HD11	1.54	1.37
1:F:104:GLY:CA	1:F:525:GLU:HB3	1.54	1.35
1:H:467:LEU:CD1	1:J:151:LEU:HD13	1.55	1.35
1:C:151:LEU:HD13	1:G:467:LEU:CD1	1.56	1.33
1:H:467:LEU:HD11	1:J:151:LEU:CD1	1.57	1.32
1:H:467:LEU:CD1	1:J:151:LEU:HA	1.59	1.30
1:K:8:ARG:NE	1:K:73:ILE:HG21	1.48	1.26
1:E:175:ILE:HG23	1:E:528:THR:HG21	1.25	1.19
1:D:104:GLY:HA2	1:D:525:GLU:HB3	1.20	1.19
1:M:104:GLY:HA2	1:M:525:GLU:HB3	1.19	1.18
1:L:104:GLY:CA	1:L:525:GLU:CB	2.23	1.16
1:G:104:GLY:HA2	1:G:525:GLU:HB3	1.22	1.16
1:C:151:LEU:HA	1:G:467:LEU:CD1	1.75	1.15
1:G:63:LEU:CD2	1:G:91:ALA:HB1	1.75	1.15
1:M:104:GLY:CA	1:M:525:GLU:CB	2.25	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:104:GLY:HA2	1:L:525:GLU:HB3	1.20	1.15
1:E:97:LEU:HD11	1:E:528:THR:HB	1.19	1.15
1:A:66:ALA:CB	1:A:99:ARG:HH21	1.60	1.14
1:A:104:GLY:HA2	1:A:525:GLU:CB	1.76	1.14
1:J:175:ILE:HG23	1:J:528:THR:HG21	1.26	1.13
1:D:104:GLY:CA	1:D:525:GLU:CB	2.25	1.13
1:A:72:PHE:CZ	1:A:96:VAL:HB	1.83	1.13
1:F:104:GLY:HA3	1:F:525:GLU:HB3	1.21	1.13
1:J:175:ILE:HG21	1:J:528:THR:HG21	1.24	1.13
1:H:104:GLY:CA	1:H:525:GLU:CB	2.25	1.12
1:H:104:GLY:HA2	1:H:525:GLU:HB3	1.20	1.12
1:J:97:LEU:HD11	1:J:528:THR:HB	1.20	1.12
1:G:104:GLY:CA	1:G:525:GLU:CB	2.27	1.12
1:J:290:ILE:CD1	1:J:300:ILE:HD12	1.80	1.11
1:K:175:ILE:HG23	1:K:528:THR:HG21	1.25	1.11
1:K:175:ILE:HG21	1:K:528:THR:HG21	1.25	1.11
1:E:175:ILE:HG21	1:E:528:THR:HG21	1.24	1.10
1:A:72:PHE:HZ	1:A:96:VAL:HB	1.12	1.10
1:J:204:MET:HG2	1:J:535:TRP:CH2	1.86	1.10
1:K:97:LEU:HD11	1:K:528:THR:HB	1.19	1.10
1:E:204:MET:HG2	1:E:535:TRP:CH2	1.87	1.10
1:K:204:MET:HG2	1:K:535:TRP:CH2	1.87	1.10
1:M:204:MET:HG2	1:M:535:TRP:CH2	1.87	1.10
1:A:204:MET:HG2	1:A:535:TRP:CH2	1.87	1.09
1:K:59:LEU:HD11	1:K:87:MET:CE	1.83	1.09
1:H:104:GLY:HA3	1:H:525:GLU:HB3	1.09	1.08
1:E:175:ILE:CG2	1:E:528:THR:CG2	2.32	1.08
1:G:104:GLY:HA3	1:G:525:GLU:HB3	1.10	1.08
1:I:272:ARG:HB3	1:I:316:TYR:CZ	1.88	1.08
1:H:467:LEU:HD13	1:J:151:LEU:HA	1.31	1.08
1:L:63:LEU:HD23	1:L:91:ALA:HB1	1.25	1.08
1:A:104:GLY:CA	1:A:525:GLU:HB3	1.84	1.08
1:G:204:MET:HG2	1:G:535:TRP:CH2	1.88	1.08
1:J:132:SER:HB2	1:K:419:ASN:ND2	1.69	1.08
1:L:204:MET:HG2	1:L:535:TRP:CH2	1.89	1.08
1:G:24:LEU:HD13	1:G:81:GLN:NE2	1.68	1.07
1:H:467:LEU:CD1	1:J:151:LEU:CA	2.32	1.07
1:A:24:LEU:CB	1:A:24:LEU:HG	1.84	1.07
1:J:5:LYS:NZ	1:J:69:PHE:CZ	2.23	1.07
1:J:175:ILE:CG2	1:J:528:THR:CG2	2.33	1.07
1:D:204:MET:HG2	1:D:535:TRP:CH2	1.88	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5:LYS:NZ	1:E:69:PHE:CZ	2.23	1.07
1:K:175:ILE:CG2	1:K:528:THR:CG2	2.32	1.07
1:C:5:LYS:NZ	1:C:69:PHE:CG	2.23	1.07
1:D:9:LEU:HD21	1:D:72:PHE:CZ	1.90	1.07
1:K:59:LEU:HD11	1:K:87:MET:HE3	1.08	1.07
1:H:5:LYS:NZ	1:H:69:PHE:CZ	2.23	1.07
1:J:5:LYS:NZ	1:J:69:PHE:CG	2.23	1.07
1:A:72:PHE:CE2	1:A:96:VAL:HG23	1.89	1.06
1:C:5:LYS:NZ	1:C:69:PHE:CE1	2.23	1.06
1:E:5:LYS:NZ	1:E:69:PHE:CE1	2.23	1.06
1:E:5:LYS:NZ	1:E:69:PHE:CE2	2.23	1.06
1:E:5:LYS:NZ	1:E:69:PHE:CD1	2.24	1.06
1:F:5:LYS:NZ	1:F:69:PHE:CZ	2.23	1.06
1:F:104:GLY:HA2	1:F:525:GLU:HB3	1.27	1.06
1:H:204:MET:HG2	1:H:535:TRP:CH2	1.89	1.06
1:J:5:LYS:NZ	1:J:69:PHE:CD1	2.24	1.06
1:C:5:LYS:NZ	1:C:69:PHE:CD1	2.24	1.06
1:F:5:LYS:NZ	1:F:69:PHE:CD1	2.24	1.06
1:G:5:LYS:NZ	1:G:69:PHE:CZ	2.23	1.06
1:I:5:LYS:NZ	1:I:69:PHE:CZ	2.23	1.06
1:K:5:LYS:NZ	1:K:69:PHE:CG	2.24	1.06
1:M:64:TYR:OH	1:M:94:VAL:HG12	1.54	1.06
1:A:5:LYS:NZ	1:A:69:PHE:CZ	2.23	1.06
1:A:5:LYS:NZ	1:A:69:PHE:CE2	2.23	1.06
1:C:5:LYS:NZ	1:C:69:PHE:CZ	2.23	1.06
1:K:5:LYS:NZ	1:K:69:PHE:CE1	2.24	1.06
1:M:5:LYS:NZ	1:M:69:PHE:CE2	2.24	1.06
1:A:5:LYS:NZ	1:A:69:PHE:CG	2.23	1.06
1:G:5:LYS:NZ	1:G:69:PHE:CE1	2.24	1.06
1:H:5:LYS:NZ	1:H:69:PHE:CG	2.24	1.06
1:H:5:LYS:NZ	1:H:69:PHE:CE1	2.24	1.06
1:I:5:LYS:NZ	1:I:69:PHE:CE1	2.24	1.06
1:E:5:LYS:NZ	1:E:69:PHE:CG	2.23	1.06
1:F:5:LYS:NZ	1:F:69:PHE:CE1	2.23	1.06
1:H:5:LYS:NZ	1:H:69:PHE:CE2	2.24	1.06
1:J:5:LYS:NZ	1:J:69:PHE:CE2	2.23	1.06
1:C:5:LYS:NZ	1:C:69:PHE:CD2	2.24	1.05
1:C:5:LYS:NZ	1:C:69:PHE:CE2	2.23	1.05
1:D:104:GLY:HA3	1:D:525:GLU:HB3	1.09	1.05
1:F:5:LYS:NZ	1:F:69:PHE:CD2	2.24	1.05
1:I:5:LYS:NZ	1:I:69:PHE:CG	2.24	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:5:LYS:NZ	1:I:69:PHE:CD2	2.24	1.05
1:I:5:LYS:NZ	1:I:69:PHE:CE2	2.24	1.05
1:K:5:LYS:NZ	1:K:69:PHE:CD1	2.24	1.05
1:K:5:LYS:NZ	1:K:69:PHE:CE2	2.24	1.05
1:M:104:GLY:HA3	1:M:525:GLU:HB3	1.10	1.05
1:G:5:LYS:NZ	1:G:69:PHE:CG	2.24	1.05
1:I:5:LYS:NZ	1:I:69:PHE:CD1	2.24	1.05
1:J:5:LYS:NZ	1:J:69:PHE:CD2	2.24	1.05
1:K:5:LYS:NZ	1:K:69:PHE:CZ	2.24	1.05
1:L:5:LYS:NZ	1:L:69:PHE:CE2	2.24	1.05
1:M:5:LYS:NZ	1:M:69:PHE:CZ	2.23	1.05
1:A:5:LYS:NZ	1:A:69:PHE:CE1	2.23	1.05
1:A:5:LYS:NZ	1:A:69:PHE:CD1	2.24	1.05
1:A:76:CYS:HA	1:A:88:PHE:CZ	1.91	1.05
1:E:5:LYS:NZ	1:E:69:PHE:CD2	2.24	1.05
1:G:5:LYS:NZ	1:G:69:PHE:CD1	2.24	1.05
1:H:5:LYS:NZ	1:H:69:PHE:CD2	2.24	1.05
1:K:5:LYS:NZ	1:K:69:PHE:CD2	2.25	1.05
1:L:5:LYS:NZ	1:L:69:PHE:CD1	2.24	1.05
1:L:5:LYS:NZ	1:L:69:PHE:CE1	2.24	1.05
1:L:5:LYS:NZ	1:L:69:PHE:CZ	2.24	1.05
1:A:5:LYS:NZ	1:A:69:PHE:CD2	2.24	1.05
1:F:5:LYS:NZ	1:F:69:PHE:CE2	2.23	1.05
1:G:5:LYS:NZ	1:G:69:PHE:CE2	2.24	1.05
1:M:5:LYS:NZ	1:M:69:PHE:CD1	2.25	1.05
1:J:5:LYS:NZ	1:J:69:PHE:CE1	2.23	1.05
1:L:5:LYS:NZ	1:L:69:PHE:CG	2.23	1.05
1:A:79:ALA:CB	1:A:88:PHE:CE1	2.39	1.04
1:G:5:LYS:NZ	1:G:69:PHE:CD2	2.24	1.04
1:L:104:GLY:HA3	1:L:525:GLU:CB	1.83	1.04
1:M:5:LYS:NZ	1:M:69:PHE:CG	2.25	1.04
1:H:5:LYS:NZ	1:H:69:PHE:CD1	2.24	1.04
1:M:5:LYS:NZ	1:M:69:PHE:CE1	2.25	1.04
1:M:9:LEU:CD1	1:M:73:ILE:HD11	1.85	1.04
1:D:104:GLY:HA3	1:D:525:GLU:CB	1.86	1.04
1:F:5:LYS:NZ	1:F:69:PHE:CG	2.23	1.04
1:L:63:LEU:CD2	1:L:91:ALA:CB	2.35	1.04
1:A:72:PHE:CE2	1:A:96:VAL:CG2	2.40	1.04
1:D:9:LEU:HD11	1:D:72:PHE:CE2	1.92	1.04
1:L:5:LYS:NZ	1:L:69:PHE:CD2	2.25	1.03
1:M:5:LYS:NZ	1:M:69:PHE:CD2	2.25	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:9:LEU:HD11	1:M:73:ILE:HD11	1.37	1.03
1:A:66:ALA:HB1	1:A:99:ARG:HH21	1.20	1.03
1:G:64:TYR:OH	1:G:94:VAL:HG12	1.57	1.02
1:H:104:GLY:HA3	1:H:525:GLU:CB	1.87	1.02
1:K:24:LEU:HD13	1:K:81:GLN:NE2	1.74	1.02
1:A:104:GLY:HA2	1:A:525:GLU:HB3	1.04	1.02
1:M:104:GLY:HA2	1:M:525:GLU:CB	1.90	1.01
1:I:10:MET:HE1	1:I:517:LEU:O	1.60	1.01
1:D:9:LEU:HD11	1:D:72:PHE:HE2	1.24	1.00
1:D:9:LEU:CD1	1:D:72:PHE:HE2	1.74	1.00
1:F:104:GLY:CA	1:F:525:GLU:CB	2.37	1.00
1:L:104:GLY:HA3	1:L:525:GLU:HB3	1.06	1.00
1:M:104:GLY:HA3	1:M:525:GLU:CB	1.86	1.00
1:J:290:ILE:HD12	1:J:300:ILE:HD12	1.43	1.00
1:G:63:LEU:HD22	1:G:91:ALA:HB1	1.41	1.00
1:G:104:GLY:HA3	1:G:525:GLU:CB	1.87	1.00
1:M:79:ALA:HB3	1:M:88:PHE:CE1	1.96	0.99
1:H:104:GLY:HA2	1:H:525:GLU:CB	1.92	0.99
1:J:175:ILE:HG21	1:J:528:THR:CG2	1.92	0.99
1:F:172:HIS:CD2	1:F:532:SER:HB3	1.98	0.98
1:E:175:ILE:HG21	1:E:528:THR:CG2	1.92	0.98
1:E:97:LEU:CD1	1:E:528:THR:HB	1.95	0.97
1:K:97:LEU:CD1	1:K:528:THR:HB	1.95	0.96
1:C:278:ASN:HB3	1:F:315:GLU:HG3	1.48	0.96
1:L:104:GLY:HA2	1:L:525:GLU:CB	1.90	0.96
1:K:175:ILE:HG21	1:K:528:THR:CG2	1.93	0.96
1:J:97:LEU:CD1	1:J:528:THR:HB	1.95	0.95
1:H:103:LYS:HG2	1:H:525:GLU:O	1.64	0.95
1:K:97:LEU:HD11	1:K:528:THR:CB	1.96	0.95
1:D:104:GLY:HA2	1:D:525:GLU:CB	1.91	0.95
1:E:97:LEU:HD11	1:E:528:THR:CB	1.96	0.95
1:A:24:LEU:HD11	1:A:27:ASP:HA	1.47	0.95
1:I:272:ARG:HD3	1:I:316:TYR:CD1	2.02	0.94
1:C:448:SER:HA	1:I:286:ASP:HB3	1.49	0.94
1:K:59:LEU:CD1	1:K:87:MET:HE3	1.97	0.94
1:H:467:LEU:HD11	1:J:151:LEU:HA	1.45	0.94
1:J:63:LEU:HA	1:J:75:LEU:HD21	1.49	0.94
1:J:97:LEU:HD11	1:J:528:THR:CB	1.97	0.94
1:G:104:GLY:HA2	1:G:525:GLU:CB	1.93	0.94
1:L:8:ARG:CZ	1:L:73:ILE:HG21	1.99	0.94
1:D:103:LYS:HG2	1:D:525:GLU:O	1.66	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:8:ARG:CZ	1:K:73:ILE:HG21	1.99	0.93
1:H:274:LEU:HB2	1:K:268:ARG:HH12	1.31	0.93
1:M:9:LEU:CD1	1:M:73:ILE:CD1	2.46	0.93
1:J:238:THR:HG21	1:K:243:GLY:O	1.69	0.93
1:G:103:LYS:HG2	1:G:525:GLU:O	1.68	0.92
1:L:19:LEU:HB3	1:L:80:ARG:CD	1.98	0.92
1:H:467:LEU:HD12	1:J:150:ILE:C	1.90	0.92
1:A:72:PHE:HE2	1:A:96:VAL:CG2	1.81	0.92
1:I:272:ARG:HD3	1:I:316:TYR:CE1	2.04	0.91
1:F:104:GLY:HA3	1:F:525:GLU:CB	1.98	0.91
1:G:32:ARG:NH2	1:G:75:LEU:HD22	1.85	0.91
1:M:103:LYS:HG2	1:M:525:GLU:O	1.69	0.91
1:I:10:MET:SD	1:I:517:LEU:CB	2.59	0.91
1:M:5:LYS:CE	1:M:69:PHE:CE2	2.54	0.91
1:A:79:ALA:CB	1:A:88:PHE:HE1	1.79	0.91
1:M:5:LYS:CE	1:M:69:PHE:CE1	2.54	0.90
1:H:8:ARG:CZ	1:H:73:ILE:HG21	2.02	0.90
1:H:467:LEU:CG	1:J:151:LEU:HD13	2.01	0.90
1:M:5:LYS:CE	1:M:69:PHE:CD2	2.55	0.90
1:M:5:LYS:CE	1:M:69:PHE:CZ	2.55	0.89
1:A:24:LEU:HD13	1:A:81:GLN:NE2	1.87	0.89
1:D:24:LEU:HB2	1:D:81:GLN:HB3	1.54	0.89
1:J:107:VAL:HG21	1:J:528:THR:OG1	1.73	0.89
1:M:5:LYS:CE	1:M:69:PHE:CD1	2.56	0.89
1:K:50:ALA:HB2	1:K:323:TRP:CH2	2.07	0.89
1:K:107:VAL:HG21	1:K:528:THR:OG1	1.73	0.89
1:D:8:ARG:CZ	1:D:73:ILE:HG21	2.02	0.89
1:M:5:LYS:CE	1:M:69:PHE:CG	2.55	0.89
1:K:5:LYS:CE	1:K:69:PHE:CD2	2.56	0.88
1:H:5:LYS:CE	1:H:69:PHE:CD2	2.57	0.88
1:K:24:LEU:HD13	1:K:81:GLN:HE21	1.37	0.88
1:F:5:LYS:CE	1:F:69:PHE:CD1	2.57	0.88
1:K:5:LYS:CE	1:K:69:PHE:CD1	2.56	0.88
1:C:5:LYS:CE	1:C:69:PHE:CD1	2.57	0.88
1:I:5:LYS:CE	1:I:69:PHE:CD1	2.57	0.88
1:G:5:LYS:CE	1:G:69:PHE:CD1	2.57	0.88
1:G:24:LEU:HD13	1:G:81:GLN:HE22	1.39	0.88
1:G:5:LYS:CE	1:G:69:PHE:CD2	2.57	0.88
1:A:76:CYS:HA	1:A:88:PHE:HZ	1.33	0.88
1:C:5:LYS:CE	1:C:69:PHE:CD2	2.56	0.88
1:E:5:LYS:CE	1:E:69:PHE:CD2	2.57	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:5:LYS:CE	1:J:69:PHE:CD2	2.56	0.88
1:J:290:ILE:HD12	1:J:300:ILE:CD1	2.03	0.88
1:L:5:LYS:CE	1:L:69:PHE:CG	2.57	0.88
1:L:63:LEU:HD22	1:L:91:ALA:HB1	1.52	0.88
1:H:5:LYS:CE	1:H:69:PHE:CG	2.57	0.87
1:I:5:LYS:CE	1:I:69:PHE:CD2	2.56	0.87
1:K:5:LYS:CE	1:K:69:PHE:CG	2.56	0.87
1:L:5:LYS:CE	1:L:69:PHE:CD1	2.57	0.87
1:M:9:LEU:HD11	1:M:73:ILE:CD1	2.03	0.87
1:G:63:LEU:CD2	1:G:91:ALA:CB	2.52	0.87
1:J:5:LYS:CE	1:J:69:PHE:CD1	2.57	0.87
1:L:5:LYS:CE	1:L:69:PHE:CD2	2.57	0.87
1:A:5:LYS:CE	1:A:69:PHE:CG	2.58	0.87
1:C:5:LYS:CE	1:C:69:PHE:CG	2.58	0.87
1:H:5:LYS:CE	1:H:69:PHE:CE2	2.57	0.87
1:E:5:LYS:CE	1:E:69:PHE:CG	2.58	0.87
1:H:5:LYS:CE	1:H:69:PHE:CD1	2.57	0.87
1:J:5:LYS:CE	1:J:69:PHE:CG	2.58	0.87
1:E:5:LYS:CE	1:E:69:PHE:CE2	2.58	0.87
1:F:5:LYS:CE	1:F:69:PHE:CD2	2.56	0.87
1:F:5:LYS:CE	1:F:69:PHE:CE1	2.58	0.87
1:M:5:LYS:HE2	1:M:69:PHE:CD2	2.10	0.87
1:A:5:LYS:CE	1:A:69:PHE:CD1	2.57	0.87
1:A:5:LYS:CE	1:A:69:PHE:CE2	2.58	0.87
1:C:5:LYS:CE	1:C:69:PHE:CE1	2.58	0.87
1:C:5:LYS:CE	1:C:69:PHE:CE2	2.58	0.87
1:F:104:GLY:HA2	1:F:525:GLU:CB	2.00	0.87
1:A:5:LYS:CE	1:A:69:PHE:CE1	2.58	0.87
1:F:5:LYS:CE	1:F:69:PHE:CE2	2.57	0.87
1:I:272:ARG:HB3	1:I:316:TYR:CE2	2.10	0.87
1:A:5:LYS:CE	1:A:69:PHE:CD2	2.57	0.87
1:H:467:LEU:HD12	1:J:151:LEU:N	1.90	0.87
1:I:5:LYS:CE	1:I:69:PHE:CE2	2.57	0.87
1:L:5:LYS:CE	1:L:69:PHE:CE2	2.57	0.87
1:E:5:LYS:CE	1:E:69:PHE:CD1	2.57	0.87
1:E:5:LYS:CE	1:E:69:PHE:CE1	2.58	0.87
1:J:5:LYS:CE	1:J:69:PHE:CE2	2.58	0.87
1:K:59:LEU:CD1	1:K:87:MET:CE	2.51	0.87
1:G:5:LYS:CE	1:G:69:PHE:CE2	2.57	0.86
1:H:19:LEU:HB3	1:H:80:ARG:HD3	1.56	0.86
1:I:10:MET:SD	1:I:517:LEU:HB3	2.14	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:5:LYS:CE	1:L:69:PHE:CE1	2.59	0.86
1:C:151:LEU:HA	1:G:467:LEU:HD13	1.54	0.86
1:E:107:VAL:HG21	1:E:528:THR:OG1	1.75	0.86
1:H:5:LYS:CE	1:H:69:PHE:CE1	2.58	0.86
1:K:5:LYS:CE	1:K:69:PHE:CE2	2.58	0.86
1:L:19:LEU:HB3	1:L:80:ARG:HD2	1.56	0.86
1:I:5:LYS:CE	1:I:69:PHE:CG	2.58	0.86
1:J:5:LYS:CE	1:J:69:PHE:CE1	2.58	0.86
1:K:5:LYS:CE	1:K:69:PHE:CZ	2.59	0.86
1:G:5:LYS:CE	1:G:69:PHE:CE1	2.58	0.86
1:G:5:LYS:CE	1:G:69:PHE:CG	2.58	0.86
1:H:8:ARG:NH2	1:H:73:ILE:HG13	1.90	0.86
1:F:5:LYS:CE	1:F:69:PHE:CG	2.58	0.86
1:G:32:ARG:HH21	1:G:75:LEU:HD13	1.41	0.86
1:K:5:LYS:CE	1:K:69:PHE:CE1	2.58	0.86
1:L:172:HIS:CD2	1:L:532:SER:HB3	2.09	0.86
1:A:24:LEU:HD23	1:A:82:ILE:HG22	1.56	0.86
1:H:243:GLY:N	1:I:125:ASN:ND2	2.24	0.86
1:I:5:LYS:CE	1:I:69:PHE:CE1	2.58	0.86
1:A:66:ALA:CB	1:A:99:ARG:NH2	2.38	0.86
1:A:5:LYS:CE	1:A:69:PHE:CZ	2.59	0.85
1:D:9:LEU:CG	1:D:72:PHE:HE2	1.88	0.85
1:C:5:LYS:CE	1:C:69:PHE:CZ	2.59	0.85
1:F:5:LYS:CE	1:F:69:PHE:CZ	2.59	0.85
1:G:5:LYS:CE	1:G:69:PHE:CZ	2.59	0.85
1:E:5:LYS:CE	1:E:69:PHE:CZ	2.59	0.85
1:I:5:LYS:CE	1:I:69:PHE:CZ	2.59	0.85
1:L:5:LYS:CE	1:L:69:PHE:CZ	2.59	0.85
1:L:64:TYR:OH	1:L:94:VAL:HG12	1.75	0.85
1:C:14:LYS:HE2	1:C:514:PHE:CZ	2.11	0.85
1:F:5:LYS:HE2	1:F:69:PHE:CD2	2.12	0.85
1:H:5:LYS:CE	1:H:69:PHE:CZ	2.59	0.85
1:J:5:LYS:HE2	1:J:69:PHE:CD2	2.12	0.85
1:F:103:LYS:HG2	1:F:525:GLU:O	1.77	0.85
1:J:5:LYS:CE	1:J:69:PHE:CZ	2.59	0.84
1:E:5:LYS:HE2	1:E:69:PHE:CD2	2.12	0.84
1:A:204:MET:HG2	1:A:535:TRP:CZ3	2.12	0.84
1:C:5:LYS:HE2	1:C:69:PHE:CD2	2.12	0.84
1:H:467:LEU:HG	1:J:149:ASN:OD1	1.77	0.84
1:A:5:LYS:HE2	1:A:69:PHE:CD2	2.12	0.83
1:H:467:LEU:HD11	1:J:151:LEU:HD13	0.87	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:63:LEU:CD2	1:M:91:ALA:HB1	2.07	0.83
1:H:275:ASP:OD1	1:K:316:TYR:HE1	1.61	0.83
1:E:204:MET:HG2	1:E:535:TRP:CZ3	2.13	0.83
1:M:204:MET:HG2	1:M:535:TRP:CZ3	2.12	0.83
1:K:57:THR:HA	1:K:60:TYR:HD2	1.43	0.83
1:J:204:MET:HG2	1:J:535:TRP:CZ3	2.13	0.82
1:K:204:MET:HG2	1:K:535:TRP:CZ3	2.13	0.82
1:I:268:ARG:HH12	1:J:274:LEU:HB2	1.42	0.82
1:L:5:LYS:HE3	1:L:69:PHE:CG	2.15	0.82
1:A:72:PHE:CZ	1:A:96:VAL:CB	2.62	0.82
1:A:66:ALA:HB3	1:A:99:ARG:HH21	1.45	0.81
1:C:151:LEU:HA	1:G:467:LEU:HD11	1.61	0.81
1:H:467:LEU:HD11	1:J:151:LEU:CA	2.04	0.81
1:E:97:LEU:CD1	1:E:528:THR:CB	2.57	0.81
1:D:9:LEU:CD2	1:D:72:PHE:CZ	2.63	0.81
1:G:5:LYS:HE2	1:G:69:PHE:CD2	2.15	0.81
1:L:204:MET:HG2	1:L:535:TRP:CZ3	2.15	0.81
1:D:204:MET:HG2	1:D:535:TRP:CZ3	2.14	0.81
1:H:204:MET:HG2	1:H:535:TRP:CZ3	2.14	0.81
1:G:204:MET:HG2	1:G:535:TRP:CZ3	2.15	0.81
1:A:24:LEU:CD1	1:A:27:ASP:HA	2.09	0.81
1:I:10:MET:SD	1:I:517:LEU:HB2	2.20	0.81
1:L:8:ARG:HH21	1:L:73:ILE:HG13	1.45	0.81
1:J:268:ARG:HH22	1:L:274:LEU:HD12	1.46	0.81
1:M:5:LYS:HE3	1:M:69:PHE:CD1	2.14	0.81
1:D:78:GLN:O	1:D:81:GLN:HB2	1.81	0.81
1:I:5:LYS:HE2	1:I:69:PHE:CD2	2.16	0.80
1:J:132:SER:CB	1:K:419:ASN:HD22	1.95	0.80
1:J:132:SER:CB	1:K:419:ASN:ND2	2.43	0.80
1:F:5:LYS:HE3	1:F:69:PHE:CD1	2.17	0.80
1:A:5:LYS:HE3	1:A:69:PHE:CD1	2.17	0.80
1:F:529:GLU:HG3	1:F:574:CYS:SG	2.21	0.80
1:M:22:GLU:HB2	1:M:81:GLN:HB3	1.61	0.80
1:K:97:LEU:CD1	1:K:528:THR:CB	2.57	0.80
1:G:50:ALA:HB2	1:G:323:TRP:CH2	2.17	0.80
1:L:8:ARG:NH2	1:L:73:ILE:HG13	1.97	0.80
1:K:5:LYS:HE2	1:K:69:PHE:CD2	2.16	0.79
1:J:5:LYS:HE3	1:J:69:PHE:CD1	2.17	0.79
1:C:151:LEU:CA	1:G:467:LEU:CD1	2.58	0.79
1:D:9:LEU:HD21	1:D:72:PHE:CE2	2.17	0.79
1:E:5:LYS:HE3	1:E:69:PHE:CD1	2.17	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:8:ARG:HH21	1:H:73:ILE:HG13	1.44	0.79
1:I:272:ARG:HH11	1:I:316:TYR:HA	1.47	0.79
1:L:508:ILE:HD11	1:L:531:CYS:HA	1.63	0.79
1:D:9:LEU:CG	1:D:72:PHE:CE2	2.65	0.79
1:H:5:LYS:HE2	1:H:69:PHE:CD2	2.17	0.79
1:D:8:ARG:NE	1:D:73:ILE:HG13	1.97	0.79
1:M:63:LEU:HD22	1:M:91:ALA:HB1	1.65	0.79
1:M:5:LYS:HZ2	1:M:72:PHE:HD2	1.28	0.79
1:A:66:ALA:HB3	1:A:99:ARG:NH2	1.97	0.78
1:C:151:LEU:HD13	1:G:467:LEU:HD11	0.82	0.78
1:A:129:LYS:HZ1	1:C:243:GLY:HA3	1.47	0.78
1:G:63:LEU:HD23	1:G:91:ALA:HB1	1.66	0.78
1:L:5:LYS:HE2	1:L:69:PHE:CE2	2.19	0.78
1:C:5:LYS:HE3	1:C:69:PHE:CD1	2.17	0.78
1:M:8:ARG:NE	1:M:73:ILE:HG21	1.98	0.78
1:I:273:ILE:HG12	1:I:317:TYR:HD1	1.48	0.78
1:K:10:MET:HG2	1:K:108:PRO:HG3	1.65	0.78
1:L:19:LEU:HD22	1:L:80:ARG:HH11	1.47	0.78
1:L:104:GLY:HA2	1:L:525:GLU:CA	2.14	0.77
1:M:9:LEU:HD12	1:M:73:ILE:HD11	1.66	0.77
1:A:129:LYS:NZ	1:C:243:GLY:HA3	1.99	0.77
1:G:50:ALA:HB2	1:G:323:TRP:HH2	1.49	0.77
1:M:9:LEU:HD12	1:M:73:ILE:CD1	2.14	0.77
1:H:467:LEU:CD1	1:J:151:LEU:N	2.46	0.77
1:K:32:ARG:HH21	1:K:75:LEU:HD13	1.50	0.77
1:A:268:ARG:HH12	1:G:274:LEU:HB2	1.49	0.77
1:K:274:LEU:HD12	1:M:268:ARG:HH22	1.50	0.77
1:G:5:LYS:HE3	1:G:69:PHE:CD1	2.20	0.76
1:H:242:SER:C	1:I:125:ASN:HD21	1.88	0.76
1:G:194:GLY:HA3	1:G:302:GLY:HA3	1.67	0.76
1:D:12:LEU:HD13	1:D:76:CYS:SG	2.25	0.76
1:G:24:LEU:HB2	1:G:81:GLN:NE2	2.00	0.76
1:L:63:LEU:HD21	1:L:91:ALA:HB1	1.65	0.76
1:F:17:THR:HG23	1:F:85:GLU:HG3	1.67	0.76
1:J:97:LEU:CD1	1:J:528:THR:CB	2.58	0.76
1:J:32:ARG:HB3	1:J:62:ALA:HB1	1.66	0.76
1:J:132:SER:HB2	1:K:419:ASN:HD22	1.47	0.76
1:J:290:ILE:HD11	1:J:300:ILE:HD12	1.68	0.76
1:A:24:LEU:HD13	1:A:81:GLN:HE21	1.51	0.75
1:A:72:PHE:HE2	1:A:96:VAL:HG21	1.49	0.75
1:E:96:VAL:HG22	1:E:105:ILE:HG21	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:304:ILE:HD11	1:G:312:LYS:HB2	1.69	0.75
1:M:104:GLY:HA2	1:M:525:GLU:CA	2.16	0.74
1:A:20:THR:OG1	1:A:85:GLU:HB3	1.87	0.74
1:A:204:MET:HG2	1:A:535:TRP:HH2	1.50	0.74
1:D:104:GLY:HA2	1:D:525:GLU:CA	2.17	0.74
1:A:76:CYS:O	1:A:88:PHE:HE2	1.70	0.74
1:K:2:VAL:O	1:K:5:LYS:HB3	1.88	0.74
1:M:69:PHE:CE1	1:M:72:PHE:CD2	2.76	0.74
1:C:315:GLU:HG3	1:D:278:ASN:HB3	1.70	0.74
1:G:204:MET:HG2	1:G:535:TRP:HH2	1.51	0.74
1:E:204:MET:HG2	1:E:535:TRP:HH2	1.50	0.73
1:M:79:ALA:CB	1:M:88:PHE:CE1	2.70	0.73
1:A:80:ARG:HB2	1:A:88:PHE:CE2	2.23	0.73
1:K:5:LYS:HE3	1:K:69:PHE:CD1	2.22	0.73
1:A:76:CYS:O	1:A:88:PHE:CE2	2.41	0.73
1:A:129:LYS:NZ	1:C:243:GLY:CA	2.52	0.73
1:E:512:ARG:HB2	1:E:531:CYS:SG	2.28	0.73
1:I:272:ARG:CB	1:I:316:TYR:CZ	2.70	0.73
1:G:24:LEU:CD1	1:G:81:GLN:NE2	2.48	0.73
1:G:104:GLY:HA2	1:G:525:GLU:CA	2.17	0.73
1:A:249:ARG:HE	1:A:331:ILE:HG21	1.53	0.73
1:D:315:GLU:HG3	1:F:278:ASN:HB3	1.69	0.73
1:H:104:GLY:HA2	1:H:525:GLU:CA	2.18	0.73
1:D:30:ASP:OD1	1:D:78:GLN:NE2	2.21	0.73
1:I:9:LEU:HD22	1:I:105:ILE:HD11	1.71	0.73
1:I:5:LYS:HE3	1:I:69:PHE:CD1	2.23	0.72
1:J:204:MET:HG2	1:J:535:TRP:HH2	1.50	0.72
1:L:63:LEU:HD21	1:L:91:ALA:CB	2.19	0.72
1:L:103:LYS:HG2	1:L:525:GLU:O	1.88	0.72
1:K:5:LYS:HE3	1:K:69:PHE:CG	2.23	0.72
1:A:128:ASN:ND2	1:A:414:LEU:HD12	2.04	0.72
1:C:448:SER:HA	1:I:286:ASP:CB	2.18	0.71
1:H:5:LYS:HE3	1:H:69:PHE:CD1	2.23	0.71
1:I:249:ARG:HE	1:I:331:ILE:HG21	1.56	0.71
1:K:8:ARG:CD	1:K:73:ILE:HG21	2.19	0.71
1:F:24:LEU:HD11	1:F:29:ARG:HG3	1.72	0.71
1:H:5:LYS:HE3	1:H:69:PHE:CG	2.24	0.71
1:K:249:ARG:HE	1:K:331:ILE:HG21	1.56	0.71
1:M:204:MET:HG2	1:M:535:TRP:HH2	1.51	0.71
1:A:24:LEU:HD22	1:A:81:GLN:HE21	1.56	0.71
1:D:204:MET:HG2	1:D:535:TRP:HH2	1.51	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:467:LEU:CD1	1:J:150:ILE:C	2.59	0.71
1:J:194:GLY:HA3	1:J:302:GLY:HA3	1.73	0.71
1:G:249:ARG:HE	1:G:331:ILE:HG21	1.56	0.70
1:H:204:MET:HG2	1:H:535:TRP:HH2	1.52	0.70
1:A:129:LYS:HZ2	1:C:243:GLY:CA	2.04	0.70
1:C:249:ARG:HE	1:C:331:ILE:HG21	1.55	0.70
1:E:249:ARG:HE	1:E:331:ILE:HG21	1.56	0.70
1:F:249:ARG:HE	1:F:331:ILE:HG21	1.55	0.70
1:H:467:LEU:CD1	1:J:150:ILE:O	2.39	0.70
1:I:5:LYS:HE3	1:I:69:PHE:CG	2.26	0.70
1:M:33:LEU:HA	1:M:58:GLU:OE2	1.90	0.70
1:M:249:ARG:HE	1:M:331:ILE:HG21	1.57	0.70
1:C:63:LEU:CD2	1:C:91:ALA:HB1	2.22	0.70
1:E:63:LEU:CD2	1:E:91:ALA:HB1	2.22	0.70
1:F:511:VAL:HA	1:F:531:CYS:HB2	1.72	0.70
1:J:304:ILE:HG12	1:J:313:ASN:H	1.57	0.70
1:D:249:ARG:HE	1:D:331:ILE:HG21	1.56	0.70
1:D:63:LEU:CD2	1:D:91:ALA:HB1	2.22	0.70
1:H:375:PHE:HB2	1:H:600:ARG:HD3	1.74	0.70
1:J:375:PHE:HB2	1:J:600:ARG:HD3	1.74	0.70
1:M:5:LYS:HE3	1:M:69:PHE:CG	2.27	0.70
1:E:21:ARG:HD3	1:E:41:ARG:CD	2.22	0.70
1:G:307:SER:H	1:G:319:SER:HB3	1.56	0.70
1:I:63:LEU:CD2	1:I:91:ALA:HB1	2.22	0.70
1:L:64:TYR:OH	1:L:94:VAL:CG1	2.40	0.70
1:J:26:LEU:HB3	1:J:28:GLN:HG3	1.74	0.69
1:K:8:ARG:CZ	1:K:73:ILE:CG2	2.69	0.69
1:C:21:ARG:HD3	1:C:41:ARG:CD	2.22	0.69
1:A:274:LEU:HD12	1:E:268:ARG:HH22	1.56	0.69
1:D:19:LEU:HD22	1:D:80:ARG:HD3	1.74	0.69
1:H:21:ARG:HD3	1:H:41:ARG:CD	2.22	0.69
1:J:307:SER:H	1:J:319:SER:HB3	1.56	0.69
1:L:249:ARG:HE	1:L:331:ILE:HG21	1.57	0.69
1:A:24:LEU:HD23	1:A:82:ILE:CG2	2.21	0.69
1:A:24:LEU:CD1	1:A:81:GLN:NE2	2.55	0.69
1:G:194:GLY:CA	1:G:302:GLY:HA3	2.21	0.69
1:M:21:ARG:HD3	1:M:41:ARG:CD	2.22	0.69
1:A:175:ILE:HG21	1:A:528:THR:HG21	1.75	0.69
1:H:169:HIS:HE1	1:H:581:CYS:SG	2.16	0.69
1:L:344:VAL:HB	1:L:350:THR:HB	1.75	0.69
1:A:344:VAL:HB	1:A:350:THR:HB	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:169:HIS:HE1	1:I:581:CYS:SG	2.16	0.69
1:A:375:PHE:HB2	1:A:600:ARG:HD3	1.74	0.69
1:E:169:HIS:HE1	1:E:581:CYS:SG	2.16	0.69
1:G:375:PHE:HB2	1:G:600:ARG:HD3	1.74	0.69
1:I:10:MET:CE	1:I:517:LEU:O	2.39	0.69
1:K:375:PHE:HB2	1:K:600:ARG:HD3	1.74	0.69
1:G:32:ARG:NH2	1:G:75:LEU:HD13	2.07	0.69
1:H:96:VAL:HG22	1:H:105:ILE:HG21	1.75	0.69
1:H:344:VAL:HB	1:H:350:THR:HB	1.75	0.69
1:I:21:ARG:HD3	1:I:41:ARG:CD	2.22	0.69
1:K:344:VAL:HB	1:K:350:THR:HB	1.75	0.69
1:F:63:LEU:CD2	1:F:91:ALA:HB1	2.22	0.69
1:J:21:ARG:HD3	1:J:41:ARG:CD	2.22	0.69
1:J:122:GLU:HG2	1:K:242:SER:OG	1.92	0.69
1:K:204:MET:HG2	1:K:535:TRP:HH2	1.50	0.69
1:F:169:HIS:HE1	1:F:581:CYS:SG	2.16	0.68
1:G:169:HIS:HE1	1:G:581:CYS:SG	2.16	0.68
1:G:344:VAL:HB	1:G:350:THR:HB	1.75	0.68
1:I:96:VAL:HG22	1:I:105:ILE:HG21	1.76	0.68
1:I:375:PHE:HB2	1:I:600:ARG:HD3	1.74	0.68
1:M:96:VAL:HG22	1:M:105:ILE:HG21	1.75	0.68
1:A:129:LYS:HZ2	1:C:243:GLY:HA2	1.56	0.68
1:C:169:HIS:HE1	1:C:581:CYS:SG	2.16	0.68
1:C:375:PHE:HB2	1:C:600:ARG:HD3	1.74	0.68
1:D:169:HIS:HE1	1:D:581:CYS:SG	2.16	0.68
1:E:375:PHE:HB2	1:E:600:ARG:HD3	1.74	0.68
1:H:63:LEU:CD2	1:H:91:ALA:HB1	2.22	0.68
1:J:169:HIS:HE1	1:J:581:CYS:SG	2.16	0.68
1:M:375:PHE:HB2	1:M:600:ARG:HD3	1.74	0.68
1:G:96:VAL:HG22	1:G:105:ILE:HG21	1.75	0.68
1:D:96:VAL:HG22	1:D:105:ILE:HG21	1.75	0.68
1:J:308:SER:O	1:J:311:SER:HB2	1.93	0.68
1:K:169:HIS:HE1	1:K:581:CYS:SG	2.16	0.68
1:A:24:LEU:HD12	1:A:26:LEU:O	1.94	0.68
1:E:344:VAL:HB	1:E:350:THR:HB	1.75	0.68
1:H:249:ARG:HE	1:H:331:ILE:HG21	1.57	0.68
1:K:512:ARG:HB2	1:K:531:CYS:SG	2.34	0.68
1:D:300:ILE:HG22	1:D:312:LYS:HE2	1.76	0.68
1:A:59:LEU:HD11	1:A:87:MET:HE3	1.74	0.68
1:D:344:VAL:HB	1:D:350:THR:HB	1.75	0.68
1:F:375:PHE:HB2	1:F:600:ARG:HD3	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:512:ARG:HB2	1:J:531:CYS:SG	2.34	0.68
1:L:169:HIS:HE1	1:L:581:CYS:SG	2.16	0.68
1:A:24:LEU:HA	1:A:81:GLN:NE2	2.08	0.68
1:F:344:VAL:HB	1:F:350:THR:HB	1.75	0.68
1:H:467:LEU:HD13	1:J:150:ILE:O	1.94	0.68
1:L:103:LYS:CG	1:L:525:GLU:O	2.42	0.68
1:M:169:HIS:HE1	1:M:581:CYS:SG	2.16	0.68
1:A:169:HIS:HE1	1:A:581:CYS:SG	2.16	0.67
1:C:344:VAL:HB	1:C:350:THR:HB	1.75	0.67
1:F:125:ASN:ND2	1:G:242:SER:O	2.28	0.67
1:L:63:LEU:HD23	1:L:91:ALA:CB	2.12	0.67
1:L:375:PHE:HB2	1:L:600:ARG:HD3	1.74	0.67
1:M:79:ALA:HB3	1:M:88:PHE:CZ	2.29	0.67
1:A:80:ARG:HB2	1:A:88:PHE:CD2	2.29	0.67
1:D:375:PHE:HB2	1:D:600:ARG:HD3	1.74	0.67
1:K:5:LYS:HA	1:K:69:PHE:CE2	2.29	0.67
1:J:162:GLU:HG2	1:J:353:ARG:HB3	1.76	0.67
1:J:249:ARG:HE	1:J:331:ILE:HG21	1.58	0.67
1:L:162:GLU:HG2	1:L:353:ARG:HB3	1.77	0.67
1:M:405:THR:HA	1:M:435:HIS:HA	1.77	0.67
1:M:442:ILE:HG23	1:M:497:ILE:HB	1.75	0.67
1:F:97:LEU:CD1	1:F:528:THR:OG1	2.43	0.67
1:F:405:THR:HA	1:F:435:HIS:HA	1.76	0.67
1:G:24:LEU:CD1	1:G:81:GLN:HE22	2.07	0.67
1:G:405:THR:HA	1:G:435:HIS:HA	1.76	0.67
1:I:19:LEU:HD13	1:I:80:ARG:HH11	1.60	0.67
1:J:5:LYS:HE3	1:J:69:PHE:CG	2.29	0.67
1:J:344:VAL:HB	1:J:350:THR:HB	1.75	0.67
1:M:344:VAL:HB	1:M:350:THR:HB	1.75	0.67
1:C:151:LEU:HD13	1:G:467:LEU:CG	2.23	0.67
1:G:5:LYS:HE3	1:G:69:PHE:CG	2.30	0.67
1:F:96:VAL:HG22	1:F:105:ILE:HG21	1.75	0.67
1:I:264:GLN:HE22	1:J:270:ARG:HH12	1.43	0.67
1:I:344:VAL:HB	1:I:350:THR:HB	1.75	0.67
1:J:405:THR:HA	1:J:435:HIS:HA	1.77	0.67
1:M:19:LEU:O	1:M:81:GLN:HA	1.93	0.67
1:I:405:THR:HA	1:I:435:HIS:HA	1.77	0.67
1:A:512:ARG:HB2	1:A:531:CYS:SG	2.35	0.67
1:C:162:GLU:HG2	1:C:353:ARG:HB3	1.77	0.67
1:E:19:LEU:HD13	1:E:80:ARG:HH11	1.60	0.67
1:H:405:THR:HA	1:H:435:HIS:HA	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:5:LYS:HE3	1:F:69:PHE:CG	2.29	0.67
1:H:467:LEU:CG	1:J:149:ASN:OD1	2.43	0.67
1:A:5:LYS:HE3	1:A:69:PHE:CG	2.29	0.67
1:C:96:VAL:HG22	1:C:105:ILE:HG21	1.75	0.67
1:D:162:GLU:HG2	1:D:353:ARG:HB3	1.77	0.67
1:E:5:LYS:HE3	1:E:69:PHE:CG	2.30	0.67
1:L:5:LYS:HE2	1:L:69:PHE:CD2	2.30	0.67
1:L:204:MET:HG2	1:L:535:TRP:HH2	1.52	0.67
1:A:19:LEU:HD13	1:A:80:ARG:HH11	1.59	0.66
1:J:19:LEU:HD13	1:J:80:ARG:HH11	1.60	0.66
1:C:405:THR:HA	1:C:435:HIS:HA	1.77	0.66
1:G:162:GLU:HG2	1:G:353:ARG:HB3	1.77	0.66
1:H:162:GLU:HG2	1:H:353:ARG:HB3	1.76	0.66
1:H:467:LEU:HD11	1:J:151:LEU:CG	2.22	0.66
1:I:162:GLU:HG2	1:I:353:ARG:HB3	1.77	0.66
1:K:8:ARG:NH2	1:K:73:ILE:HB	2.10	0.66
1:A:24:LEU:CD1	1:A:81:GLN:HE21	2.07	0.66
1:F:162:GLU:HG2	1:F:353:ARG:HB3	1.76	0.66
1:G:512:ARG:HB2	1:G:531:CYS:SG	2.35	0.66
1:D:22:GLU:HB2	1:D:80:ARG:O	1.96	0.66
1:C:5:LYS:HE3	1:C:69:PHE:CG	2.29	0.66
1:E:162:GLU:HG2	1:E:353:ARG:HB3	1.77	0.66
1:F:268:ARG:HD2	1:F:272:ARG:HE	1.61	0.66
1:G:24:LEU:HB2	1:G:81:GLN:HE21	1.58	0.66
1:L:405:THR:HA	1:L:435:HIS:HA	1.77	0.66
1:M:162:GLU:HG2	1:M:353:ARG:HB3	1.77	0.66
1:G:64:TYR:HH	1:G:181:TRP:HZ3	1.44	0.66
1:M:69:PHE:O	1:M:72:PHE:HB3	1.94	0.66
1:A:162:GLU:HG2	1:A:353:ARG:HB3	1.77	0.65
1:K:22:GLU:HB2	1:K:81:GLN:HA	1.78	0.65
1:E:405:THR:HA	1:E:435:HIS:HA	1.77	0.65
1:F:169:HIS:CE1	1:F:533:CYS:SG	2.89	0.65
1:H:405:THR:HG23	1:H:624:PHE:HA	1.78	0.65
1:K:162:GLU:HG2	1:K:353:ARG:HB3	1.77	0.65
1:H:205:CYS:HG	1:H:358:TYR:HD1	1.45	0.65
1:I:278:ASN:HB3	1:L:315:GLU:HG3	1.79	0.65
1:I:405:THR:HG23	1:I:624:PHE:HA	1.78	0.65
1:D:8:ARG:CZ	1:D:73:ILE:HG13	2.26	0.65
1:D:405:THR:HA	1:D:435:HIS:HA	1.77	0.65
1:D:9:LEU:CD2	1:D:72:PHE:CE2	2.80	0.65
1:F:32:ARG:HH21	1:F:75:LEU:HD13	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:405:THR:HG23	1:L:624:PHE:HA	1.78	0.65
1:A:59:LEU:HD21	1:A:87:MET:CE	2.27	0.65
1:C:19:LEU:HD13	1:C:80:ARG:HH11	1.60	0.65
1:E:175:ILE:HG23	1:E:528:THR:CG2	2.14	0.65
1:G:405:THR:HG23	1:G:624:PHE:HA	1.78	0.65
1:L:564:THR:HG22	1:L:565:VAL:O	1.97	0.65
1:A:405:THR:HA	1:A:435:HIS:HA	1.77	0.65
1:E:19:LEU:HD13	1:E:80:ARG:NH1	2.12	0.65
1:M:30:ASP:HB2	1:M:33:LEU:HB2	1.79	0.65
1:G:64:TYR:OH	1:G:94:VAL:CG1	2.39	0.65
1:J:405:THR:HG23	1:J:624:PHE:HA	1.78	0.65
1:K:405:THR:HA	1:K:435:HIS:HA	1.77	0.65
1:D:405:THR:HG23	1:D:624:PHE:HA	1.79	0.64
1:E:270:ARG:NH1	1:G:264:GLN:OE1	2.30	0.64
1:M:273:ILE:HG12	1:M:317:TYR:HD1	1.63	0.64
1:J:245:GLN:HG2	1:K:245:GLN:HG2	1.79	0.64
1:C:21:ARG:HD3	1:C:41:ARG:HD2	1.80	0.64
1:H:21:ARG:HD3	1:H:41:ARG:HD2	1.80	0.64
1:K:57:THR:HA	1:K:60:TYR:CD2	2.30	0.64
1:A:24:LEU:CG	1:A:81:GLN:HE21	2.10	0.64
1:F:405:THR:HG23	1:F:624:PHE:HA	1.79	0.64
1:K:405:THR:HG23	1:K:624:PHE:HA	1.78	0.64
1:M:405:THR:HG23	1:M:624:PHE:HA	1.78	0.64
1:J:19:LEU:HD13	1:J:80:ARG:NH1	2.12	0.64
1:F:32:ARG:NH2	1:F:75:LEU:HD13	2.11	0.64
1:A:19:LEU:HD13	1:A:80:ARG:NH1	2.12	0.64
1:A:405:THR:HG23	1:A:624:PHE:HA	1.78	0.64
1:L:19:LEU:HB3	1:L:80:ARG:HD3	1.75	0.64
1:C:150:ILE:C	1:G:467:LEU:HD12	2.18	0.64
1:D:9:LEU:CD2	1:D:72:PHE:HZ	2.09	0.64
1:H:467:LEU:HD21	1:J:151:LEU:CD1	2.28	0.64
1:H:242:SER:C	1:I:125:ASN:ND2	2.52	0.64
1:C:268:ARG:NE	1:C:272:ARG:HH21	1.96	0.64
1:E:405:THR:HG23	1:E:624:PHE:HA	1.79	0.64
1:F:97:LEU:HD11	1:F:528:THR:HB	1.80	0.64
1:F:104:GLY:HA2	1:F:525:GLU:CA	2.28	0.64
1:I:5:LYS:HE2	1:I:69:PHE:CE2	2.33	0.64
1:I:19:LEU:HD13	1:I:80:ARG:NH1	2.12	0.64
1:M:512:ARG:HB2	1:M:531:CYS:SG	2.37	0.64
1:C:19:LEU:HD13	1:C:80:ARG:NH1	2.12	0.63
1:C:405:THR:HG23	1:C:624:PHE:HA	1.78	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:416:HIS:CE1	1:C:514:PHE:CB	2.81	0.63
1:K:5:LYS:HE2	1:K:69:PHE:CE2	2.33	0.63
1:K:32:ARG:NH2	1:K:75:LEU:HD13	2.12	0.63
1:G:59:LEU:HD11	1:G:87:MET:HE1	1.81	0.63
1:J:175:ILE:HG23	1:J:528:THR:CG2	2.15	0.63
1:A:76:CYS:CA	1:A:88:PHE:HZ	2.10	0.63
1:I:442:ILE:HG23	1:I:497:ILE:HB	1.81	0.63
1:A:270:ARG:O	1:A:274:LEU:HG	1.99	0.63
1:D:107:VAL:HG21	1:D:528:THR:OG1	1.98	0.63
1:H:377:PRO:HG3	1:H:601:LYS:HB3	1.81	0.63
1:J:442:ILE:HG23	1:J:497:ILE:HB	1.81	0.63
1:F:97:LEU:HG	1:F:528:THR:OG1	1.99	0.63
1:H:5:LYS:HE2	1:H:69:PHE:CE2	2.32	0.63
1:I:13:PHE:HD2	1:I:113:VAL:HG11	1.63	0.63
1:M:63:LEU:CD2	1:M:91:ALA:CB	2.77	0.63
1:C:270:ARG:HH12	1:F:264:GLN:NE2	1.97	0.63
1:F:97:LEU:HD23	1:F:527:SER:HB2	1.81	0.63
1:I:21:ARG:HD3	1:I:41:ARG:HD2	1.80	0.63
1:A:104:GLY:CA	1:A:525:GLU:CB	2.59	0.63
1:M:21:ARG:HD3	1:M:41:ARG:HD2	1.80	0.63
1:C:377:PRO:HG3	1:C:601:LYS:HB3	1.81	0.63
1:D:8:ARG:HE	1:D:73:ILE:HG13	1.62	0.63
1:E:21:ARG:HD3	1:E:41:ARG:HD2	1.80	0.63
1:I:377:PRO:HG3	1:I:601:LYS:HB3	1.81	0.63
1:A:377:PRO:HG3	1:A:601:LYS:HB3	1.81	0.62
1:K:377:PRO:HG3	1:K:601:LYS:HB3	1.81	0.62
1:M:107:VAL:HG21	1:M:528:THR:OG1	1.98	0.62
1:A:24:LEU:CD2	1:A:81:GLN:HE21	2.12	0.62
1:C:442:ILE:HG23	1:C:497:ILE:HB	1.81	0.62
1:C:525:GLU:HA	1:C:572:ALA:HB1	1.79	0.62
1:H:107:VAL:HG21	1:H:528:THR:OG1	1.99	0.62
1:K:8:ARG:O	1:K:12:LEU:HG	1.99	0.62
1:L:329:ALA:HB2	1:L:345:MET:HB3	1.82	0.62
1:A:268:ARG:NE	1:A:272:ARG:HH21	1.98	0.62
1:C:63:LEU:HD23	1:C:91:ALA:HB1	1.81	0.62
1:H:329:ALA:HB2	1:H:345:MET:HB3	1.82	0.62
1:I:273:ILE:HA	1:I:317:TYR:HE1	1.62	0.62
1:M:20:THR:HA	1:M:80:ARG:O	1.99	0.62
1:M:377:PRO:HG3	1:M:601:LYS:HB3	1.81	0.62
1:C:416:HIS:HE1	1:C:514:PHE:HB3	1.63	0.62
1:D:329:ALA:HB2	1:D:345:MET:HB3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:329:ALA:HB2	1:F:345:MET:HB3	1.81	0.62
1:E:377:PRO:HG3	1:E:601:LYS:HB3	1.81	0.62
1:F:442:ILE:HG23	1:F:497:ILE:HB	1.81	0.62
1:L:377:PRO:HG3	1:L:601:LYS:HB3	1.81	0.62
1:D:4:ASP:HA	1:D:7:ALA:HB3	1.82	0.62
1:H:63:LEU:HD23	1:H:91:ALA:HB1	1.81	0.62
1:I:63:LEU:HD23	1:I:91:ALA:HB1	1.81	0.62
1:M:205:CYS:HG	1:M:358:TYR:HD1	1.46	0.62
1:G:377:PRO:HG3	1:G:601:LYS:HB3	1.81	0.62
1:J:205:CYS:HG	1:J:358:TYR:HD1	1.48	0.62
1:G:442:ILE:HG23	1:G:497:ILE:HB	1.81	0.62
1:I:329:ALA:HB2	1:I:345:MET:HB3	1.82	0.61
1:J:110:ILE:HD11	1:J:168:ALA:HA	1.82	0.61
1:A:329:ALA:HB2	1:A:345:MET:HB3	1.82	0.61
1:F:110:ILE:HD11	1:F:168:ALA:HA	1.82	0.61
1:G:329:ALA:HB2	1:G:345:MET:HB3	1.81	0.61
1:H:32:ARG:NH2	1:H:75:LEU:HD22	2.15	0.61
1:H:442:ILE:HG23	1:H:497:ILE:HB	1.81	0.61
1:J:329:ALA:HB2	1:J:345:MET:HB3	1.81	0.61
1:M:59:LEU:HD11	1:M:87:MET:HE1	1.81	0.61
1:M:329:ALA:HB2	1:M:345:MET:HB3	1.82	0.61
1:F:377:PRO:HG3	1:F:601:LYS:HB3	1.81	0.61
1:J:407:ILE:HD11	1:J:431:HIS:HD2	1.65	0.61
1:M:19:LEU:HB2	1:M:80:ARG:HD2	1.81	0.61
1:D:442:ILE:HG23	1:D:497:ILE:HB	1.81	0.61
1:E:110:ILE:HD11	1:E:168:ALA:HA	1.82	0.61
1:G:107:VAL:HG21	1:G:528:THR:OG1	1.99	0.61
1:J:21:ARG:HD3	1:J:41:ARG:HD2	1.80	0.61
1:A:407:ILE:HD11	1:A:431:HIS:HD2	1.65	0.61
1:E:63:LEU:HD23	1:E:91:ALA:HB1	1.81	0.61
1:F:407:ILE:HD11	1:F:431:HIS:HD2	1.66	0.61
1:K:442:ILE:HG23	1:K:497:ILE:HB	1.81	0.61
1:L:110:ILE:HD11	1:L:168:ALA:HA	1.82	0.61
1:M:5:LYS:HE2	1:M:69:PHE:CE2	2.35	0.61
1:M:110:ILE:HD11	1:M:168:ALA:HA	1.82	0.61
1:D:23:LYS:O	1:D:81:GLN:HB3	1.99	0.61
1:H:110:ILE:HD11	1:H:168:ALA:HA	1.82	0.61
1:L:442:ILE:HG23	1:L:497:ILE:HB	1.81	0.61
1:D:9:LEU:HG	1:D:72:PHE:CE2	2.34	0.61
1:D:103:LYS:HD2	1:D:526:ASP:OD1	2.01	0.61
1:D:307:SER:H	1:D:319:SER:HB3	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:377:PRO:HG3	1:D:601:LYS:HB3	1.81	0.61
1:E:442:ILE:HG23	1:E:497:ILE:HB	1.81	0.61
1:G:110:ILE:HD11	1:G:168:ALA:HA	1.82	0.61
1:H:80:ARG:HA	1:H:83:VAL:HG22	1.83	0.61
1:H:103:LYS:HD2	1:H:526:ASP:OD1	2.01	0.61
1:C:416:HIS:CE1	1:C:514:PHE:HB2	2.36	0.61
1:D:205:CYS:HG	1:D:358:TYR:HD1	1.49	0.61
1:E:329:ALA:HB2	1:E:345:MET:HB3	1.81	0.61
1:F:63:LEU:HD23	1:F:91:ALA:HB1	1.81	0.61
1:J:377:PRO:HG3	1:J:601:LYS:HB3	1.81	0.61
1:D:512:ARG:HB2	1:D:531:CYS:SG	2.41	0.61
1:K:110:ILE:HD11	1:K:168:ALA:HA	1.83	0.61
1:C:407:ILE:HD11	1:C:431:HIS:HD2	1.66	0.61
1:D:407:ILE:HD11	1:D:431:HIS:HD2	1.66	0.61
1:A:64:TYR:OH	1:A:94:VAL:HG12	2.01	0.60
1:A:77:GLU:HA	1:A:80:ARG:NH2	2.16	0.60
1:K:268:ARG:NE	1:K:272:ARG:HH21	1.98	0.60
1:M:407:ILE:HD11	1:M:431:HIS:HD2	1.65	0.60
1:A:442:ILE:HG23	1:A:497:ILE:HB	1.81	0.60
1:L:268:ARG:CZ	1:L:272:ARG:HH21	2.15	0.60
1:L:407:ILE:HD11	1:L:431:HIS:HD2	1.66	0.60
1:I:110:ILE:HD11	1:I:168:ALA:HA	1.82	0.60
1:A:24:LEU:HG	1:A:24:LEU:HB3	1.80	0.60
1:A:110:ILE:HD11	1:A:168:ALA:HA	1.83	0.60
1:A:205:CYS:HG	1:A:358:TYR:HD1	1.47	0.60
1:C:329:ALA:HB2	1:C:345:MET:HB3	1.81	0.60
1:E:275:ASP:N	1:G:268:ARG:HH12	1.97	0.60
1:D:110:ILE:HD11	1:D:168:ALA:HA	1.82	0.60
1:E:407:ILE:HD11	1:E:431:HIS:HD2	1.66	0.60
1:G:407:ILE:HD11	1:G:431:HIS:HD2	1.66	0.60
1:I:407:ILE:HD11	1:I:431:HIS:HD2	1.66	0.60
1:K:10:MET:HG2	1:K:108:PRO:CG	2.32	0.60
1:K:278:ASN:HB3	1:M:315:GLU:HG3	1.83	0.60
1:L:273:ILE:HG12	1:L:317:TYR:HD1	1.66	0.60
1:C:89:VAL:HA	1:C:92:VAL:HG22	1.84	0.60
1:D:63:LEU:HD23	1:D:91:ALA:HB1	1.81	0.60
1:I:4:ASP:HA	1:I:7:ALA:HB3	1.84	0.60
1:I:307:SER:H	1:I:319:SER:HB3	1.67	0.60
1:K:59:LEU:HD13	1:K:87:MET:SD	2.41	0.60
1:L:89:VAL:HA	1:L:92:VAL:HG22	1.84	0.60
1:L:272:ARG:HB3	1:L:316:TYR:CE2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:307:SER:H	1:E:319:SER:HB3	1.67	0.60
1:G:103:LYS:HD2	1:G:526:ASP:OD1	2.02	0.60
1:G:554:PHE:HE1	1:G:615:MET:HB3	1.67	0.60
1:H:407:ILE:HD11	1:H:431:HIS:HD2	1.65	0.60
1:I:76:CYS:HA	1:I:88:PHE:HZ	1.67	0.60
1:C:110:ILE:HD11	1:C:168:ALA:HA	1.83	0.60
1:F:97:LEU:HD11	1:F:528:THR:CB	2.31	0.60
1:F:307:SER:H	1:F:319:SER:HB3	1.67	0.60
1:J:270:ARG:O	1:J:274:LEU:HG	2.02	0.60
1:L:554:PHE:HE1	1:L:615:MET:HB3	1.67	0.60
1:D:89:VAL:HA	1:D:92:VAL:HG22	1.84	0.60
1:E:89:VAL:HA	1:E:92:VAL:HG22	1.84	0.60
1:I:89:VAL:HA	1:I:92:VAL:HG22	1.84	0.60
1:I:273:ILE:HA	1:I:317:TYR:CE1	2.36	0.60
1:K:329:ALA:HB2	1:K:345:MET:HB3	1.82	0.60
1:A:76:CYS:HA	1:A:88:PHE:CE2	2.37	0.59
1:C:76:CYS:HA	1:C:88:PHE:HZ	1.67	0.59
1:H:89:VAL:HA	1:H:92:VAL:HG22	1.84	0.59
1:I:10:MET:CE	1:I:517:LEU:C	2.70	0.59
1:A:307:SER:H	1:A:319:SER:HB3	1.67	0.59
1:H:554:PHE:HE1	1:H:615:MET:HB3	1.67	0.59
1:I:10:MET:HE1	1:I:517:LEU:C	2.21	0.59
1:M:72:PHE:CZ	1:M:96:VAL:CG2	2.85	0.59
1:A:64:TYR:HH	1:A:181:TRP:HZ3	1.49	0.59
1:E:554:PHE:HE1	1:E:615:MET:HB3	1.67	0.59
1:F:89:VAL:HA	1:F:92:VAL:HG22	1.84	0.59
1:I:10:MET:HB3	1:I:514:PHE:CE1	2.37	0.59
1:I:554:PHE:HE1	1:I:615:MET:HB3	1.67	0.59
1:M:554:PHE:HE1	1:M:615:MET:HB3	1.67	0.59
1:G:89:VAL:HA	1:G:92:VAL:HG22	1.84	0.59
1:G:205:CYS:HG	1:G:358:TYR:HD1	1.50	0.59
1:I:205:CYS:HG	1:I:358:TYR:HD1	1.50	0.59
1:K:407:ILE:HD11	1:K:431:HIS:HD2	1.66	0.59
1:C:416:HIS:CE1	1:C:514:PHE:HB3	2.38	0.59
1:D:554:PHE:HE1	1:D:615:MET:HB3	1.67	0.59
1:H:307:SER:H	1:H:319:SER:HB3	1.67	0.59
1:J:76:CYS:HA	1:J:88:PHE:HZ	1.67	0.59
1:M:307:SER:H	1:M:319:SER:HB3	1.67	0.59
1:F:5:LYS:HE2	1:F:69:PHE:CE2	2.38	0.59
1:F:175:ILE:HG21	1:F:528:THR:HG21	1.85	0.59
1:J:554:PHE:HE1	1:J:615:MET:HB3	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:103:LYS:HD2	1:M:526:ASP:OD1	2.03	0.59
1:D:8:ARG:NH2	1:D:73:ILE:HG13	2.17	0.59
1:E:205:CYS:HG	1:E:358:TYR:HD1	1.50	0.59
1:M:64:TYR:HH	1:M:94:VAL:HG12	1.68	0.59
1:A:304:ILE:HA	1:A:311:SER:OG	2.03	0.59
1:G:5:LYS:HE2	1:G:69:PHE:CE2	2.37	0.59
1:J:307:SER:N	1:J:319:SER:HB3	2.17	0.59
1:L:169:HIS:CE1	1:L:533:CYS:SG	2.96	0.59
1:C:304:ILE:HA	1:C:311:SER:OG	2.03	0.58
1:E:5:LYS:NZ	1:E:5:LYS:CE	2.66	0.58
1:F:554:PHE:HE1	1:F:615:MET:HB3	1.67	0.58
1:K:307:SER:H	1:K:319:SER:HB3	1.67	0.58
1:L:8:ARG:NH2	1:L:73:ILE:CG1	2.65	0.58
1:L:304:ILE:HA	1:L:311:SER:OG	2.03	0.58
1:M:304:ILE:HA	1:M:311:SER:OG	2.03	0.58
1:C:5:LYS:NZ	1:C:5:LYS:CE	2.66	0.58
1:J:5:LYS:NZ	1:J:5:LYS:CE	2.66	0.58
1:J:529:GLU:HG3	1:J:574:CYS:SG	2.42	0.58
1:M:24:LEU:HD22	1:M:82:ILE:HG21	1.84	0.58
1:M:29:ARG:HG3	1:M:78:GLN:HE22	1.69	0.58
1:A:69:PHE:HE1	1:A:96:VAL:CG2	2.16	0.58
1:A:79:ALA:HB3	1:A:88:PHE:HE1	0.89	0.58
1:A:508:ILE:HD11	1:A:531:CYS:HA	1.84	0.58
1:H:304:ILE:HA	1:H:311:SER:OG	2.03	0.58
1:J:125:ASN:ND2	1:K:242:SER:O	2.37	0.58
1:K:32:ARG:NH2	1:K:75:LEU:HD22	2.18	0.58
1:M:5:LYS:NZ	1:M:5:LYS:CE	2.66	0.58
1:A:554:PHE:HE1	1:A:615:MET:HB3	1.67	0.58
1:I:272:ARG:CD	1:I:316:TYR:CE1	2.84	0.58
1:J:89:VAL:HA	1:J:92:VAL:HG22	1.84	0.58
1:K:304:ILE:HA	1:K:311:SER:OG	2.03	0.58
1:L:307:SER:H	1:L:319:SER:HB3	1.67	0.58
1:A:5:LYS:NZ	1:A:5:LYS:CE	2.66	0.58
1:A:214:SER:HA	1:A:549:MET:SD	2.44	0.58
1:C:307:SER:H	1:C:319:SER:HB3	1.67	0.58
1:G:32:ARG:CZ	1:G:75:LEU:HD22	2.33	0.58
1:M:89:VAL:HA	1:M:92:VAL:HG22	1.84	0.58
1:H:512:ARG:HB2	1:H:531:CYS:SG	2.43	0.58
1:K:214:SER:HA	1:K:549:MET:SD	2.44	0.58
1:L:214:SER:HA	1:L:549:MET:SD	2.44	0.58
1:A:59:LEU:CD1	1:A:87:MET:SD	2.91	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:VAL:HG11	1:A:428:VAL:HG11	1.85	0.58
1:E:76:CYS:HA	1:E:88:PHE:HZ	1.67	0.58
1:E:214:SER:HA	1:E:549:MET:SD	2.44	0.58
1:H:467:LEU:HD11	1:J:151:LEU:CB	2.33	0.58
1:I:304:ILE:HA	1:I:311:SER:OG	2.03	0.58
1:K:97:LEU:HG	1:K:528:THR:OG1	2.04	0.58
1:C:77:GLU:HA	1:C:80:ARG:NH2	2.19	0.58
1:C:214:SER:HA	1:C:549:MET:SD	2.44	0.58
1:D:8:ARG:NH1	1:D:73:ILE:HG21	2.18	0.58
1:F:304:ILE:HA	1:F:311:SER:OG	2.03	0.58
1:I:271:GLU:HA	1:L:268:ARG:NH1	2.18	0.58
1:K:24:LEU:CD1	1:K:81:GLN:NE2	2.58	0.58
1:E:304:ILE:HA	1:E:311:SER:OG	2.03	0.58
1:F:5:LYS:NZ	1:F:5:LYS:CE	2.66	0.58
1:F:76:CYS:HA	1:F:88:PHE:HZ	1.67	0.58
1:G:77:GLU:HA	1:G:80:ARG:NH2	2.19	0.58
1:G:214:SER:HA	1:G:549:MET:SD	2.44	0.58
1:H:270:ARG:O	1:H:274:LEU:HG	2.04	0.58
1:I:214:SER:HA	1:I:549:MET:SD	2.44	0.58
1:K:77:GLU:HA	1:K:80:ARG:NH2	2.19	0.58
1:K:554:PHE:HE1	1:K:615:MET:HB3	1.68	0.58
1:A:5:LYS:HE2	1:A:69:PHE:CE2	2.38	0.57
1:J:77:GLU:HA	1:J:80:ARG:NH2	2.19	0.57
1:L:77:GLU:HA	1:L:80:ARG:NH2	2.19	0.57
1:L:529:GLU:HB2	1:L:574:CYS:HB3	1.85	0.57
1:D:24:LEU:HB2	1:D:81:GLN:CB	2.31	0.57
1:H:243:GLY:CA	1:I:125:ASN:ND2	2.67	0.57
1:A:59:LEU:HD13	1:A:87:MET:SD	2.44	0.57
1:C:554:PHE:HE1	1:C:615:MET:HB3	1.67	0.57
1:I:33:LEU:HG	1:I:58:GLU:HG2	1.85	0.57
1:M:59:LEU:CD1	1:M:87:MET:CE	2.82	0.57
1:A:128:ASN:OD1	1:A:426:VAL:HB	2.04	0.57
1:K:13:PHE:HD1	1:K:108:PRO:HG2	1.69	0.57
1:L:5:LYS:HE3	1:L:69:PHE:CD1	2.40	0.57
1:L:19:LEU:HD13	1:L:80:ARG:HD3	1.86	0.57
1:F:77:GLU:HA	1:F:80:ARG:NH2	2.19	0.57
1:G:512:ARG:HH22	1:G:523:VAL:HG21	1.70	0.57
1:D:214:SER:HA	1:D:549:MET:SD	2.44	0.57
1:F:97:LEU:HG	1:F:528:THR:H	1.70	0.57
1:G:529:GLU:HG3	1:G:574:CYS:SG	2.45	0.57
1:H:214:SER:HA	1:H:549:MET:SD	2.44	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:214:SER:HA	1:M:549:MET:SD	2.44	0.57
1:C:296:HIS:HE1	1:I:566:ALA:O	1.87	0.57
1:E:77:GLU:HA	1:E:80:ARG:NH2	2.19	0.57
1:F:214:SER:HA	1:F:549:MET:SD	2.44	0.57
1:G:270:ARG:O	1:G:274:LEU:HG	2.05	0.57
1:K:50:ALA:HB2	1:K:323:TRP:HH2	1.66	0.57
1:K:64:TYR:OH	1:K:181:TRP:HZ3	1.88	0.57
1:G:553:LEU:HB2	1:G:620:ILE:HD12	1.87	0.57
1:J:5:LYS:HE2	1:J:69:PHE:CE2	2.38	0.57
1:J:214:SER:HA	1:J:549:MET:SD	2.44	0.57
1:D:77:GLU:HA	1:D:80:ARG:NH2	2.19	0.56
1:M:69:PHE:CE2	1:M:73:ILE:HG12	2.40	0.56
1:A:79:ALA:HB3	1:A:88:PHE:CD1	2.29	0.56
1:D:553:LEU:HB2	1:D:620:ILE:HD12	1.87	0.56
1:J:553:LEU:HB2	1:J:620:ILE:HD12	1.87	0.56
1:M:444:VAL:HG11	1:M:490:LEU:HD23	1.87	0.56
1:A:389:GLU:O	1:A:444:VAL:HA	2.05	0.56
1:D:9:LEU:CD1	1:D:72:PHE:CE2	2.61	0.56
1:F:4:ASP:HA	1:F:7:ALA:HB3	1.87	0.56
1:H:4:ASP:HA	1:H:7:ALA:HB3	1.87	0.56
1:I:77:GLU:HA	1:I:80:ARG:NH2	2.19	0.56
1:I:183:PRO:HB3	1:I:189:GLU:HB3	1.88	0.56
1:J:273:ILE:HG12	1:J:317:TYR:HD1	1.71	0.56
1:K:553:LEU:HB2	1:K:620:ILE:HD12	1.87	0.56
1:A:553:LEU:HB2	1:A:620:ILE:HD12	1.87	0.56
1:C:172:HIS:HA	1:C:175:ILE:HG22	1.88	0.56
1:H:389:GLU:O	1:H:444:VAL:HA	2.05	0.56
1:J:306:GLU:N	1:J:307:SER:HA	2.20	0.56
1:K:389:GLU:O	1:K:444:VAL:HA	2.05	0.56
1:C:389:GLU:O	1:C:444:VAL:HA	2.05	0.56
1:C:553:LEU:HB2	1:C:620:ILE:HD12	1.87	0.56
1:K:9:LEU:CD1	1:K:73:ILE:HD11	2.35	0.56
1:L:389:GLU:O	1:L:444:VAL:HA	2.05	0.56
1:M:4:ASP:HA	1:M:7:ALA:HB3	1.87	0.56
1:M:389:GLU:O	1:M:444:VAL:HA	2.05	0.56
1:D:268:ARG:NH1	1:F:271:GLU:HA	2.21	0.56
1:E:4:ASP:HA	1:E:7:ALA:HB3	1.87	0.56
1:E:553:LEU:HB2	1:E:620:ILE:HD12	1.87	0.56
1:F:205:CYS:HG	1:F:358:TYR:HD1	1.51	0.56
1:F:389:GLU:O	1:F:444:VAL:HA	2.05	0.56
1:H:172:HIS:HA	1:H:175:ILE:HG22	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:238:THR:CG2	1:K:243:GLY:O	2.46	0.56
1:J:389:GLU:O	1:J:444:VAL:HA	2.05	0.56
1:K:172:HIS:HA	1:K:175:ILE:HG22	1.88	0.56
1:A:172:HIS:HA	1:A:175:ILE:HG22	1.88	0.56
1:C:151:LEU:CA	1:G:467:LEU:HD11	2.31	0.56
1:F:22:GLU:HB2	1:F:81:GLN:HB3	1.87	0.56
1:H:410:SER:O	1:H:429:LYS:HA	2.06	0.56
1:K:508:ILE:HD11	1:K:531:CYS:HA	1.87	0.56
1:L:410:SER:O	1:L:429:LYS:HA	2.06	0.56
1:C:5:LYS:HE2	1:C:69:PHE:CE2	2.38	0.56
1:D:389:GLU:O	1:D:444:VAL:HA	2.05	0.56
1:D:410:SER:O	1:D:429:LYS:HA	2.06	0.56
1:G:172:HIS:HA	1:G:175:ILE:HG22	1.88	0.56
1:F:553:LEU:HB2	1:F:620:ILE:HD12	1.87	0.56
1:G:389:GLU:O	1:G:444:VAL:HA	2.05	0.56
1:G:410:SER:O	1:G:429:LYS:HA	2.06	0.56
1:K:8:ARG:HE	1:K:73:ILE:HG21	1.61	0.56
1:L:553:LEU:HB2	1:L:620:ILE:HD12	1.87	0.56
1:A:118:PHE:HA	1:A:353:ARG:HH12	1.71	0.56
1:H:553:LEU:HB2	1:H:620:ILE:HD12	1.87	0.56
1:K:96:VAL:HG22	1:K:105:ILE:HG21	1.88	0.56
1:K:268:ARG:CZ	1:K:272:ARG:HH21	2.19	0.56
1:L:19:LEU:CB	1:L:80:ARG:HD3	2.36	0.56
1:M:95:ALA:HB1	1:M:99:ARG:HD2	1.88	0.56
1:A:410:SER:O	1:A:429:LYS:HA	2.06	0.55
1:E:97:LEU:HG	1:E:528:THR:OG1	2.05	0.55
1:E:172:HIS:HA	1:E:175:ILE:HG22	1.88	0.55
1:E:389:GLU:O	1:E:444:VAL:HA	2.05	0.55
1:A:4:ASP:HA	1:A:7:ALA:HB3	1.87	0.55
1:J:167:ASN:HB3	1:J:349:SER:O	2.07	0.55
1:K:410:SER:O	1:K:429:LYS:HA	2.06	0.55
1:M:172:HIS:HA	1:M:175:ILE:HG22	1.88	0.55
1:C:14:LYS:HG3	1:C:514:PHE:CE2	2.41	0.55
1:C:95:ALA:HB1	1:C:99:ARG:HD2	1.88	0.55
1:C:274:LEU:HD12	1:F:268:ARG:NH2	2.22	0.55
1:D:95:ALA:HB1	1:D:99:ARG:HD2	1.88	0.55
1:E:95:ALA:HB1	1:E:99:ARG:HD2	1.88	0.55
1:F:107:VAL:HG21	1:F:528:THR:OG1	2.05	0.55
1:H:167:ASN:HB3	1:H:349:SER:O	2.07	0.55
1:I:389:GLU:O	1:I:444:VAL:HA	2.05	0.55
1:J:97:LEU:HG	1:J:528:THR:OG1	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:573:VAL:CG1	1:L:584:ARG:HB2	2.36	0.55
1:A:59:LEU:HD21	1:A:87:MET:HE3	1.88	0.55
1:A:167:ASN:HB3	1:A:349:SER:O	2.07	0.55
1:C:560:HIS:O	1:C:564:THR:HB	2.05	0.55
1:E:226:PHE:CE1	1:E:270:ARG:NH2	2.75	0.55
1:E:263:VAL:O	1:E:266:MET:HB2	2.07	0.55
1:F:167:ASN:HB3	1:F:349:SER:O	2.07	0.55
1:G:24:LEU:CB	1:G:81:GLN:NE2	2.70	0.55
1:G:508:ILE:HD11	1:G:531:CYS:HA	1.88	0.55
1:I:553:LEU:HB2	1:I:620:ILE:HD12	1.87	0.55
1:L:5:LYS:HA	1:L:69:PHE:CE2	2.42	0.55
1:A:127:ALA:HB2	1:A:142:VAL:HG21	1.86	0.55
1:C:167:ASN:HB3	1:C:349:SER:O	2.07	0.55
1:D:172:HIS:HA	1:D:175:ILE:HG22	1.88	0.55
1:F:410:SER:O	1:F:429:LYS:HA	2.06	0.55
1:I:172:HIS:HA	1:I:175:ILE:HG22	1.88	0.55
1:K:2:VAL:HG11	1:K:103:LYS:O	2.07	0.55
1:C:4:ASP:HA	1:C:7:ALA:HB3	1.88	0.55
1:C:410:SER:O	1:C:429:LYS:HA	2.06	0.55
1:H:95:ALA:HB1	1:H:99:ARG:HD2	1.89	0.55
1:I:167:ASN:HB3	1:I:349:SER:O	2.07	0.55
1:J:95:ALA:HB1	1:J:99:ARG:HD2	1.88	0.55
1:M:69:PHE:CZ	1:M:72:PHE:HD2	2.25	0.55
1:F:95:ALA:HB1	1:F:99:ARG:HD2	1.88	0.55
1:I:410:SER:O	1:I:429:LYS:HA	2.06	0.55
1:J:172:HIS:HA	1:J:175:ILE:HG22	1.88	0.55
1:L:172:HIS:HA	1:L:175:ILE:HG22	1.88	0.55
1:H:508:ILE:HD11	1:H:531:CYS:HA	1.89	0.55
1:F:234:ALA:HA	1:F:248:SER:HB2	1.89	0.55
1:H:234:ALA:HA	1:H:248:SER:HB2	1.89	0.55
1:K:167:ASN:HB3	1:K:349:SER:O	2.07	0.55
1:K:234:ALA:HA	1:K:248:SER:HB2	1.89	0.55
1:L:50:ALA:HB2	1:L:323:TRP:HH2	1.72	0.55
1:M:410:SER:O	1:M:429:LYS:HA	2.06	0.55
1:M:553:LEU:HB2	1:M:620:ILE:HD12	1.87	0.55
1:F:172:HIS:HA	1:F:175:ILE:HG22	1.88	0.55
1:I:234:ALA:HA	1:I:248:SER:HB2	1.89	0.55
1:J:4:ASP:HA	1:J:7:ALA:HB3	1.88	0.55
1:L:234:ALA:HA	1:L:248:SER:HB2	1.89	0.55
1:E:234:ALA:HA	1:E:248:SER:HB2	1.89	0.54
1:G:234:ALA:HA	1:G:248:SER:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:456:VAL:HG22	1:L:557:LEU:HG	1.90	0.54
1:A:234:ALA:HA	1:A:248:SER:HB2	1.89	0.54
1:I:10:MET:HE3	1:I:518:GLY:HA2	1.89	0.54
1:K:4:ASP:HA	1:K:7:ALA:HB3	1.88	0.54
1:K:205:CYS:HG	1:K:358:TYR:HD1	1.54	0.54
1:C:173:TRP:HZ2	1:C:196:LEU:HG	1.73	0.54
1:E:167:ASN:HB3	1:E:349:SER:O	2.07	0.54
1:F:173:TRP:HZ2	1:F:196:LEU:HG	1.73	0.54
1:I:173:TRP:HZ2	1:I:196:LEU:HG	1.73	0.54
1:J:245:GLN:CG	1:K:245:GLN:HG2	2.36	0.54
1:K:456:VAL:HG22	1:K:557:LEU:HG	1.89	0.54
1:L:167:ASN:HB3	1:L:349:SER:O	2.07	0.54
1:M:167:ASN:HB3	1:M:349:SER:O	2.07	0.54
1:D:234:ALA:HA	1:D:248:SER:HB2	1.89	0.54
1:F:50:ALA:HB2	1:F:323:TRP:HH2	1.73	0.54
1:G:167:ASN:HB3	1:G:349:SER:O	2.07	0.54
1:G:307:SER:N	1:G:319:SER:HB3	2.22	0.54
1:I:456:VAL:HG22	1:I:557:LEU:HG	1.90	0.54
1:J:48:PHE:HB3	1:J:326:VAL:HG22	1.89	0.54
1:J:322:ASN:O	1:J:325:HIS:HB2	2.08	0.54
1:K:95:ALA:HB1	1:K:99:ARG:HD2	1.89	0.54
1:L:322:ASN:O	1:L:325:HIS:HB2	2.08	0.54
1:A:322:ASN:O	1:A:325:HIS:HB2	2.08	0.54
1:D:167:ASN:HB3	1:D:349:SER:O	2.07	0.54
1:E:5:LYS:HE2	1:E:69:PHE:CE2	2.38	0.54
1:E:456:VAL:HG22	1:E:557:LEU:HG	1.89	0.54
1:H:50:ALA:HB2	1:H:323:TRP:HH2	1.73	0.54
1:H:322:ASN:O	1:H:325:HIS:HB2	2.08	0.54
1:L:511:VAL:HA	1:L:531:CYS:HB2	1.89	0.54
1:F:270:ARG:O	1:F:274:LEU:HG	2.08	0.54
1:I:322:ASN:O	1:I:325:HIS:HB2	2.08	0.54
1:K:322:ASN:O	1:K:325:HIS:HB2	2.08	0.54
1:E:410:SER:O	1:E:429:LYS:HA	2.06	0.54
1:H:268:ARG:NH1	1:M:274:LEU:HB2	2.23	0.54
1:I:50:ALA:HB2	1:I:323:TRP:HH2	1.72	0.54
1:J:410:SER:O	1:J:429:LYS:HA	2.06	0.54
1:K:175:ILE:HG23	1:K:528:THR:CG2	2.15	0.54
1:M:72:PHE:HZ	1:M:96:VAL:HB	1.72	0.54
1:M:82:ILE:HG23	1:M:83:VAL:HG13	1.88	0.54
1:A:173:TRP:HZ2	1:A:196:LEU:HG	1.73	0.54
1:A:456:VAL:HG22	1:A:557:LEU:HG	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:234:ALA:HA	1:C:248:SER:HB2	1.89	0.54
1:G:173:TRP:HZ2	1:G:196:LEU:HG	1.73	0.54
1:J:173:TRP:HZ2	1:J:196:LEU:HG	1.73	0.54
1:L:173:TRP:HZ2	1:L:196:LEU:HG	1.73	0.54
1:L:176:VAL:HG11	1:L:529:GLU:HB3	1.89	0.54
1:M:234:ALA:HA	1:M:248:SER:HB2	1.89	0.54
1:A:50:ALA:HB2	1:A:323:TRP:HH2	1.72	0.54
1:A:107:VAL:HG21	1:A:528:THR:OG1	2.08	0.54
1:D:249:ARG:HG2	1:D:250:PRO:O	2.07	0.54
1:H:77:GLU:HA	1:H:80:ARG:NH2	2.23	0.54
1:J:263:VAL:O	1:J:266:MET:HB2	2.08	0.54
1:A:59:LEU:HD21	1:A:87:MET:HE2	1.90	0.54
1:D:48:PHE:CB	1:D:326:VAL:HG22	2.38	0.54
1:D:529:GLU:HG3	1:D:574:CYS:SG	2.48	0.54
1:E:50:ALA:HB2	1:E:323:TRP:HH2	1.72	0.54
1:E:97:LEU:CD1	1:E:528:THR:OG1	2.56	0.54
1:F:322:ASN:O	1:F:325:HIS:HB2	2.08	0.54
1:I:48:PHE:CB	1:I:326:VAL:HG22	2.38	0.54
1:A:136:ASP:O	1:A:423:ASP:HB3	2.08	0.53
1:C:50:ALA:HB2	1:C:323:TRP:HH2	1.72	0.53
1:F:172:HIS:HD2	1:F:532:SER:HB3	1.70	0.53
1:H:529:GLU:HG3	1:H:574:CYS:SG	2.48	0.53
1:I:95:ALA:HB1	1:I:99:ARG:HD2	1.88	0.53
1:L:444:VAL:HG11	1:L:490:LEU:HD23	1.90	0.53
1:C:38:ILE:HD13	1:D:605:ARG:HH12	1.73	0.53
1:C:274:LEU:HB2	1:F:268:ARG:HH22	1.74	0.53
1:C:444:VAL:HG11	1:C:490:LEU:HD23	1.91	0.53
1:E:322:ASN:O	1:E:325:HIS:HB2	2.08	0.53
1:E:529:GLU:HG3	1:E:574:CYS:SG	2.48	0.53
1:G:456:VAL:HG22	1:G:557:LEU:HG	1.89	0.53
1:J:456:VAL:HG22	1:J:557:LEU:HG	1.89	0.53
1:K:59:LEU:CD1	1:K:87:MET:SD	2.96	0.53
1:M:69:PHE:CE2	1:M:73:ILE:CG1	2.90	0.53
1:M:456:VAL:HG22	1:M:557:LEU:HG	1.90	0.53
1:C:322:ASN:O	1:C:325:HIS:HB2	2.08	0.53
1:D:173:TRP:HZ2	1:D:196:LEU:HG	1.73	0.53
1:D:456:VAL:HG22	1:D:557:LEU:HG	1.90	0.53
1:E:118:PHE:HA	1:E:353:ARG:HH12	1.74	0.53
1:I:444:VAL:HG11	1:I:490:LEU:HD23	1.91	0.53
1:J:121:ALA:HB1	1:K:243:GLY:HA3	1.90	0.53
1:J:444:VAL:HG11	1:J:490:LEU:HD23	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:21:ARG:HD3	1:K:41:ARG:HD2	1.89	0.53
1:A:69:PHE:CE1	1:A:96:VAL:CG2	2.92	0.53
1:F:444:VAL:HG11	1:F:490:LEU:HD23	1.91	0.53
1:K:270:ARG:O	1:K:274:LEU:HG	2.09	0.53
1:A:76:CYS:CA	1:A:88:PHE:CZ	2.79	0.53
1:A:84:ASN:HD22	1:A:84:ASN:N	2.07	0.53
1:A:268:ARG:HD2	1:A:272:ARG:HE	1.73	0.53
1:A:444:VAL:HG11	1:A:490:LEU:HD23	1.91	0.53
1:D:50:ALA:HB2	1:D:323:TRP:HH2	1.72	0.53
1:F:117:ARG:HB2	1:F:350:THR:HG23	1.91	0.53
1:G:95:ALA:HB1	1:G:99:ARG:HD2	1.88	0.53
1:G:322:ASN:O	1:G:325:HIS:HB2	2.08	0.53
1:J:573:VAL:HG22	1:J:574:CYS:H	1.74	0.53
1:L:465:ASP:HB3	1:L:467:LEU:H	1.74	0.53
1:M:269:TRP:O	1:M:273:ILE:HG13	2.08	0.53
1:A:48:PHE:CB	1:A:326:VAL:HG22	2.38	0.53
1:C:48:PHE:CB	1:C:326:VAL:HG22	2.38	0.53
1:C:270:ARG:O	1:C:274:LEU:HG	2.08	0.53
1:D:322:ASN:O	1:D:325:HIS:HB2	2.08	0.53
1:H:8:ARG:NH2	1:H:73:ILE:CG1	2.66	0.53
1:K:97:LEU:CD1	1:K:528:THR:OG1	2.56	0.53
1:K:444:VAL:HG11	1:K:490:LEU:HD23	1.91	0.53
1:M:72:PHE:CE2	1:M:96:VAL:CG2	2.91	0.53
1:C:14:LYS:HG3	1:C:514:PHE:CZ	2.44	0.53
1:D:118:PHE:HA	1:D:353:ARG:HH12	1.74	0.53
1:D:444:VAL:HG11	1:D:490:LEU:HD23	1.91	0.53
1:G:118:PHE:HA	1:G:353:ARG:HH12	1.74	0.53
1:I:268:ARG:NH1	1:J:271:GLU:HA	2.24	0.53
1:M:9:LEU:HD12	1:M:73:ILE:HD12	1.89	0.53
1:C:118:PHE:HA	1:C:353:ARG:HH12	1.74	0.53
1:E:173:TRP:HZ2	1:E:196:LEU:HG	1.73	0.53
1:F:573:VAL:HG22	1:F:574:CYS:H	1.74	0.53
1:H:118:PHE:HA	1:H:353:ARG:HH12	1.74	0.53
1:J:30:ASP:O	1:J:33:LEU:N	2.42	0.53
1:K:173:TRP:HZ2	1:K:196:LEU:HG	1.73	0.53
1:L:460:LEU:HA	1:L:552:GLU:O	2.09	0.53
1:A:23:LYS:O	1:A:25:PRO:HD3	2.09	0.53
1:C:456:VAL:HG22	1:C:557:LEU:HG	1.89	0.53
1:E:444:VAL:HG11	1:E:490:LEU:HD23	1.90	0.53
1:F:118:PHE:HA	1:F:353:ARG:HH12	1.74	0.53
1:F:456:VAL:HG22	1:F:557:LEU:HG	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:444:VAL:HG11	1:H:490:LEU:HD23	1.91	0.53
1:H:456:VAL:HG22	1:H:557:LEU:HG	1.89	0.53
1:I:117:ARG:HB2	1:I:350:THR:HG23	1.91	0.53
1:J:118:PHE:HA	1:J:353:ARG:HH12	1.74	0.53
1:L:48:PHE:CB	1:L:326:VAL:HG22	2.38	0.53
1:C:460:LEU:HA	1:C:552:GLU:O	2.09	0.53
1:D:117:ARG:HB2	1:D:350:THR:HG23	1.91	0.53
1:E:48:PHE:CB	1:E:326:VAL:HG22	2.38	0.53
1:F:456:VAL:O	1:F:485:LYS:HA	2.10	0.53
1:G:444:VAL:HG11	1:G:490:LEU:HD23	1.91	0.53
1:M:117:ARG:HB2	1:M:350:THR:HG23	1.91	0.53
1:M:508:ILE:HD11	1:M:531:CYS:HA	1.90	0.53
1:C:510:LYS:HE2	1:C:511:VAL:O	2.08	0.52
1:D:270:ARG:O	1:D:274:LEU:HG	2.09	0.52
1:E:270:ARG:O	1:E:274:LEU:HG	2.10	0.52
1:F:337:ARG:HA	1:G:151:LEU:HD23	1.91	0.52
1:F:460:LEU:HA	1:F:552:GLU:O	2.09	0.52
1:H:64:TYR:OH	1:H:94:VAL:HG12	2.09	0.52
1:J:117:ARG:HB2	1:J:350:THR:HG23	1.91	0.52
1:K:573:VAL:HG22	1:K:574:CYS:H	1.74	0.52
1:L:95:ALA:HB1	1:L:99:ARG:HD2	1.91	0.52
1:M:460:LEU:HA	1:M:552:GLU:O	2.09	0.52
1:H:173:TRP:HZ2	1:H:196:LEU:HG	1.73	0.52
1:H:460:LEU:HA	1:H:552:GLU:O	2.09	0.52
1:J:456:VAL:O	1:J:485:LYS:HA	2.10	0.52
1:L:118:PHE:HA	1:L:353:ARG:HH12	1.74	0.52
1:L:172:HIS:HD2	1:L:532:SER:O	1.93	0.52
1:M:433:LEU:O	1:M:538:HIS:HB2	2.10	0.52
1:M:456:VAL:O	1:M:485:LYS:HA	2.10	0.52
1:A:89:VAL:HA	1:A:92:VAL:HG22	1.91	0.52
1:A:433:LEU:O	1:A:538:HIS:HB2	2.10	0.52
1:C:117:ARG:HB2	1:C:350:THR:HG23	1.91	0.52
1:C:433:LEU:O	1:C:538:HIS:HB2	2.10	0.52
1:D:23:LYS:O	1:D:81:GLN:CB	2.56	0.52
1:D:433:LEU:O	1:D:538:HIS:HB2	2.10	0.52
1:D:456:VAL:O	1:D:485:LYS:HA	2.10	0.52
1:E:433:LEU:O	1:E:538:HIS:HB2	2.10	0.52
1:F:48:PHE:CB	1:F:326:VAL:HG22	2.38	0.52
1:G:117:ARG:HB2	1:G:350:THR:HG23	1.91	0.52
1:H:456:VAL:O	1:H:485:LYS:HA	2.10	0.52
1:M:173:TRP:HZ2	1:M:196:LEU:HG	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:322:ASN:O	1:M:325:HIS:HB2	2.08	0.52
1:A:59:LEU:HD11	1:A:87:MET:CE	2.40	0.52
1:C:64:TYR:OH	1:C:94:VAL:HG12	2.09	0.52
1:E:107:VAL:HG21	1:E:528:THR:HG1	1.72	0.52
1:G:23:LYS:O	1:G:81:GLN:CD	2.48	0.52
1:I:13:PHE:HB2	1:I:514:PHE:HZ	1.74	0.52
1:I:30:ASP:HB3	1:I:33:LEU:HD13	1.90	0.52
1:C:473:PRO:O	1:C:477:ARG:HG3	2.10	0.52
1:G:460:LEU:HA	1:G:552:GLU:O	2.09	0.52
1:I:38:ILE:HD12	1:J:605:ARG:HH22	1.75	0.52
1:I:64:TYR:OH	1:I:94:VAL:HG12	2.09	0.52
1:J:459:PHE:O	1:J:553:LEU:HA	2.10	0.52
1:K:117:ARG:HB2	1:K:350:THR:HG23	1.91	0.52
1:M:60:TYR:HH	1:M:90:TYR:HD2	1.54	0.52
1:M:178:PRO:HG2	1:M:181:TRP:HB2	1.92	0.52
1:E:178:PRO:HG2	1:E:181:TRP:HB2	1.92	0.52
1:F:433:LEU:O	1:F:538:HIS:HB2	2.10	0.52
1:H:48:PHE:CB	1:H:326:VAL:HG22	2.38	0.52
1:I:178:PRO:HG2	1:I:181:TRP:HB2	1.92	0.52
1:J:460:LEU:HA	1:J:552:GLU:O	2.09	0.52
1:L:433:LEU:O	1:L:538:HIS:HB2	2.09	0.52
1:A:170:HIS:CG	1:A:352:LEU:HD11	2.45	0.52
1:A:178:PRO:HG2	1:A:181:TRP:HB2	1.91	0.52
1:A:473:PRO:O	1:A:477:ARG:HG3	2.10	0.52
1:D:170:HIS:CG	1:D:352:LEU:HD11	2.45	0.52
1:F:178:PRO:HG2	1:F:181:TRP:HB2	1.92	0.52
1:F:459:PHE:O	1:F:553:LEU:HA	2.10	0.52
1:G:433:LEU:O	1:G:538:HIS:HB2	2.10	0.52
1:H:170:HIS:CG	1:H:352:LEU:HD11	2.45	0.52
1:I:118:PHE:HA	1:I:353:ARG:HH12	1.74	0.52
1:I:433:LEU:O	1:I:538:HIS:HB2	2.09	0.52
1:J:508:ILE:HD11	1:J:531:CYS:HA	1.91	0.52
1:L:117:ARG:HB2	1:L:350:THR:HG23	1.91	0.52
1:L:456:VAL:O	1:L:485:LYS:HA	2.10	0.52
1:M:72:PHE:CZ	1:M:96:VAL:HG23	2.45	0.52
1:M:118:PHE:HA	1:M:353:ARG:HH12	1.74	0.52
1:M:253:TYR:HD2	1:M:331:ILE:HG13	1.75	0.52
1:C:456:VAL:O	1:C:485:LYS:HA	2.10	0.52
1:E:573:VAL:HG22	1:E:574:CYS:H	1.74	0.52
1:G:64:TYR:OH	1:G:181:TRP:HZ3	1.92	0.52
1:H:573:VAL:HG22	1:H:574:CYS:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:268:ARG:HH11	1:J:271:GLU:HA	1.74	0.52
1:J:178:PRO:HG2	1:J:181:TRP:HB2	1.92	0.52
1:J:473:PRO:O	1:J:477:ARG:HG3	2.10	0.52
1:K:263:VAL:O	1:K:266:MET:HB2	2.09	0.52
1:K:456:VAL:O	1:K:485:LYS:HA	2.10	0.52
1:A:456:VAL:O	1:A:485:LYS:HA	2.10	0.52
1:C:14:LYS:HE2	1:C:514:PHE:CE1	2.44	0.52
1:C:151:LEU:N	1:G:467:LEU:HD12	2.25	0.52
1:D:573:VAL:HG22	1:D:574:CYS:H	1.74	0.52
1:E:64:TYR:OH	1:E:94:VAL:HG12	2.09	0.52
1:E:459:PHE:O	1:E:553:LEU:HA	2.10	0.52
1:F:170:HIS:CG	1:F:352:LEU:HD11	2.45	0.52
1:G:456:VAL:O	1:G:485:LYS:HA	2.09	0.52
1:G:473:PRO:O	1:G:477:ARG:HG3	2.10	0.52
1:H:433:LEU:O	1:H:538:HIS:HB2	2.10	0.52
1:I:473:PRO:O	1:I:477:ARG:HG3	2.10	0.52
1:J:97:LEU:CG	1:J:528:THR:HB	2.40	0.52
1:K:460:LEU:HA	1:K:552:GLU:O	2.09	0.52
1:M:66:ALA:HB3	1:M:99:ARG:HH21	1.74	0.52
1:M:69:PHE:CZ	1:M:72:PHE:CD2	2.98	0.52
1:M:170:HIS:CG	1:M:352:LEU:HD11	2.45	0.52
1:A:104:GLY:HA2	1:A:525:GLU:HB2	1.85	0.52
1:A:460:LEU:HA	1:A:552:GLU:O	2.09	0.52
1:C:205:CYS:HG	1:C:358:TYR:HD1	1.57	0.52
1:C:278:ASN:O	1:F:315:GLU:OE2	2.28	0.52
1:D:473:PRO:O	1:D:477:ARG:HG3	2.10	0.52
1:E:97:LEU:CG	1:E:528:THR:HB	2.40	0.52
1:E:170:HIS:CG	1:E:352:LEU:HD11	2.45	0.52
1:F:64:TYR:OH	1:F:94:VAL:HG12	2.09	0.52
1:F:263:VAL:O	1:F:266:MET:HB2	2.09	0.52
1:I:456:VAL:O	1:I:485:LYS:HA	2.10	0.52
1:J:107:VAL:HG21	1:J:528:THR:HG1	1.71	0.52
1:J:419:ASN:HD22	1:K:132:SER:HB2	1.74	0.52
1:J:433:LEU:O	1:J:538:HIS:HB2	2.10	0.52
1:L:8:ARG:NE	1:L:73:ILE:HG21	2.24	0.52
1:L:170:HIS:CG	1:L:352:LEU:HD11	2.45	0.52
1:M:59:LEU:HD13	1:M:87:MET:CE	2.39	0.52
1:M:573:VAL:HG22	1:M:574:CYS:H	1.74	0.52
1:A:130:GLU:HA	1:A:133:ASN:HB2	1.91	0.51
1:A:137:GLN:HA	1:A:423:ASP:HA	1.92	0.51
1:A:573:VAL:HG22	1:A:574:CYS:H	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:178:PRO:HG2	1:D:181:TRP:HB2	1.92	0.51
1:G:170:HIS:CG	1:G:352:LEU:HD11	2.45	0.51
1:H:178:PRO:HG2	1:H:181:TRP:HB2	1.92	0.51
1:I:11:PRO:HA	1:I:14:LYS:HE3	1.92	0.51
1:I:455:THR:HA	1:I:486:PHE:O	2.11	0.51
1:I:573:VAL:HG22	1:I:574:CYS:H	1.74	0.51
1:K:459:PHE:O	1:K:553:LEU:HA	2.10	0.51
1:A:24:LEU:CG	1:A:24:LEU:HB2	2.18	0.51
1:E:455:THR:HA	1:E:486:PHE:O	2.11	0.51
1:F:455:THR:HA	1:F:486:PHE:O	2.11	0.51
1:F:508:ILE:HG12	1:F:531:CYS:O	2.10	0.51
1:G:178:PRO:HG2	1:G:181:TRP:HB2	1.92	0.51
1:H:117:ARG:HB2	1:H:350:THR:HG23	1.91	0.51
1:H:459:PHE:O	1:H:553:LEU:HA	2.10	0.51
1:J:97:LEU:CD1	1:J:528:THR:OG1	2.58	0.51
1:K:473:PRO:O	1:K:477:ARG:HG3	2.10	0.51
1:L:205:CYS:HG	1:L:358:TYR:HD1	1.57	0.51
1:A:459:PHE:O	1:A:553:LEU:HA	2.10	0.51
1:D:64:TYR:OH	1:D:94:VAL:HG12	2.09	0.51
1:E:460:LEU:HA	1:E:552:GLU:O	2.09	0.51
1:G:459:PHE:O	1:G:553:LEU:HA	2.10	0.51
1:I:459:PHE:O	1:I:553:LEU:HA	2.10	0.51
1:K:433:LEU:O	1:K:538:HIS:HB2	2.10	0.51
1:L:270:ARG:O	1:L:274:LEU:HG	2.11	0.51
1:M:455:THR:HA	1:M:486:PHE:O	2.11	0.51
1:M:459:PHE:O	1:M:553:LEU:HA	2.10	0.51
1:C:170:HIS:CG	1:C:352:LEU:HD11	2.45	0.51
1:C:528:THR:OG1	1:C:584:ARG:HB3	2.11	0.51
1:I:170:HIS:CG	1:I:352:LEU:HD11	2.45	0.51
1:M:63:LEU:HD23	1:M:91:ALA:HB1	1.89	0.51
1:M:473:PRO:O	1:M:477:ARG:HG3	2.10	0.51
1:A:55:GLU:O	1:A:58:GLU:HB3	2.11	0.51
1:D:459:PHE:O	1:D:553:LEU:HA	2.10	0.51
1:G:573:VAL:HG22	1:G:574:CYS:H	1.74	0.51
1:H:407:ILE:HD11	1:H:431:HIS:CD2	2.46	0.51
1:H:473:PRO:O	1:H:477:ARG:HG3	2.10	0.51
1:I:271:GLU:HB3	1:L:268:ARG:HD3	1.93	0.51
1:J:38:ILE:HD12	1:L:605:ARG:NH1	2.25	0.51
1:K:178:PRO:HG2	1:K:181:TRP:HB2	1.92	0.51
1:K:249:ARG:NE	1:K:331:ILE:HG21	2.25	0.51
1:L:55:GLU:O	1:L:58:GLU:HB3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:THR:HA	1:A:486:PHE:O	2.11	0.51
1:E:9:LEU:HD22	1:E:105:ILE:HD11	1.91	0.51
1:E:249:ARG:NE	1:E:331:ILE:HG21	2.25	0.51
1:J:132:SER:HB3	1:K:419:ASN:HD22	1.74	0.51
1:J:303:ASP:HB2	1:J:310:GLU:HB3	1.93	0.51
1:K:118:PHE:HA	1:K:353:ARG:HH12	1.74	0.51
1:K:455:THR:HA	1:K:486:PHE:O	2.11	0.51
1:L:455:THR:HA	1:L:486:PHE:O	2.11	0.51
1:M:55:GLU:O	1:M:58:GLU:HB3	2.11	0.51
1:C:178:PRO:HG2	1:C:181:TRP:HB2	1.92	0.51
1:D:460:LEU:HA	1:D:552:GLU:O	2.09	0.51
1:E:55:GLU:O	1:E:58:GLU:HB3	2.11	0.51
1:E:473:PRO:O	1:E:477:ARG:HG3	2.10	0.51
1:H:55:GLU:O	1:H:58:GLU:HB3	2.11	0.51
1:H:275:ASP:OD1	1:K:316:TYR:CE1	2.52	0.51
1:H:455:THR:HA	1:H:486:PHE:O	2.11	0.51
1:K:9:LEU:HD12	1:K:73:ILE:HD11	1.92	0.51
1:K:170:HIS:CG	1:K:352:LEU:HD11	2.45	0.51
1:C:459:PHE:O	1:C:553:LEU:HA	2.10	0.51
1:J:36:VAL:HG23	1:J:55:GLU:HB3	1.91	0.51
1:J:55:GLU:HG2	1:L:605:ARG:HH22	1.75	0.51
1:M:407:ILE:HD11	1:M:431:HIS:CD2	2.46	0.51
1:C:55:GLU:O	1:C:58:GLU:HB3	2.11	0.51
1:E:117:ARG:HB2	1:E:350:THR:HG23	1.91	0.51
1:F:11:PRO:HA	1:F:14:LYS:HE3	1.92	0.51
1:F:473:PRO:O	1:F:477:ARG:HG3	2.10	0.51
1:A:123:THR:HG21	1:A:144:ALA:HA	1.93	0.51
1:E:456:VAL:O	1:E:485:LYS:HA	2.10	0.51
1:H:5:LYS:NZ	1:H:5:LYS:CE	2.74	0.51
1:K:97:LEU:CG	1:K:528:THR:HB	2.40	0.51
1:L:459:PHE:O	1:L:553:LEU:HA	2.10	0.51
1:C:150:ILE:O	1:G:467:LEU:CD1	2.59	0.50
1:F:477:ARG:HG2	1:F:598:PHE:HB3	1.93	0.50
1:G:455:THR:HA	1:G:486:PHE:O	2.11	0.50
1:I:5:LYS:NZ	1:I:5:LYS:CE	2.74	0.50
1:I:467:LEU:HD22	1:I:470:LYS:HE3	1.94	0.50
1:J:170:HIS:CG	1:J:352:LEU:HD11	2.45	0.50
1:K:126:ARG:HD3	1:K:142:VAL:HG11	1.93	0.50
1:L:103:LYS:HD2	1:L:526:ASP:OD1	2.11	0.50
1:C:268:ARG:HD2	1:C:272:ARG:HE	1.76	0.50
1:C:477:ARG:HG2	1:C:598:PHE:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:48:PHE:HB3	1:D:326:VAL:HG22	1.94	0.50
1:F:125:ASN:ND2	1:G:242:SER:C	2.65	0.50
1:G:5:LYS:NZ	1:G:5:LYS:CE	2.75	0.50
1:I:460:LEU:HA	1:I:552:GLU:O	2.09	0.50
1:L:5:LYS:NZ	1:L:5:LYS:CE	2.74	0.50
1:L:477:ARG:HG2	1:L:598:PHE:HB3	1.94	0.50
1:G:32:ARG:HH22	1:G:75:LEU:HD22	1.70	0.50
1:J:19:LEU:HB3	1:J:80:ARG:HD2	1.94	0.50
1:L:178:PRO:HG2	1:L:181:TRP:HB2	1.92	0.50
1:L:473:PRO:O	1:L:477:ARG:HG3	2.10	0.50
1:M:477:ARG:HG2	1:M:598:PHE:HB3	1.94	0.50
1:C:275:ASP:HB2	1:F:268:ARG:HH11	1.77	0.50
1:C:455:THR:HA	1:C:486:PHE:O	2.11	0.50
1:D:68:ASP:CG	1:D:70:ASN:HB2	2.31	0.50
1:G:55:GLU:O	1:G:58:GLU:HB3	2.11	0.50
1:H:268:ARG:HH12	1:M:274:LEU:HB2	1.77	0.50
1:J:107:VAL:CG2	1:J:528:THR:OG1	2.54	0.50
1:K:477:ARG:HG2	1:K:598:PHE:HB3	1.94	0.50
1:A:24:LEU:HD12	1:A:26:LEU:C	2.31	0.50
1:D:263:VAL:O	1:D:266:MET:HB2	2.10	0.50
1:D:455:THR:HA	1:D:486:PHE:O	2.11	0.50
1:E:477:ARG:HG2	1:E:598:PHE:HB3	1.94	0.50
1:A:407:ILE:HD11	1:A:431:HIS:CD2	2.46	0.50
1:D:9:LEU:HD21	1:D:72:PHE:HZ	1.59	0.50
1:F:55:GLU:O	1:F:58:GLU:HB3	2.11	0.50
1:H:477:ARG:HA	1:H:480:PHE:HD2	1.77	0.50
1:J:477:ARG:HA	1:J:480:PHE:HD2	1.77	0.50
1:K:55:GLU:O	1:K:58:GLU:HB3	2.11	0.50
1:L:12:LEU:HD22	1:L:80:ARG:NH1	2.26	0.50
1:M:20:THR:OG1	1:M:85:GLU:HB3	2.12	0.50
1:D:477:ARG:HG2	1:D:598:PHE:HB3	1.94	0.50
1:E:508:ILE:HD11	1:E:531:CYS:HA	1.94	0.50
1:G:249:ARG:HG2	1:G:250:PRO:O	2.11	0.50
1:I:264:GLN:NE2	1:J:270:ARG:HH12	2.08	0.50
1:M:272:ARG:HH11	1:M:316:TYR:HA	1.76	0.50
1:A:19:LEU:HB3	1:A:80:ARG:HD2	1.93	0.50
1:A:477:ARG:HG2	1:A:598:PHE:HB3	1.94	0.50
1:D:477:ARG:HA	1:D:480:PHE:HD2	1.77	0.50
1:E:407:ILE:HD11	1:E:431:HIS:CD2	2.46	0.50
1:E:477:ARG:HA	1:E:480:PHE:HD2	1.77	0.50
1:F:407:ILE:HD11	1:F:431:HIS:CD2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:249:ARG:NE	1:J:331:ILE:HG21	2.26	0.50
1:J:293:ASP:HB3	1:J:297:GLY:H	1.76	0.50
1:J:315:GLU:HG3	1:L:278:ASN:HB3	1.93	0.50
1:C:19:LEU:HB3	1:C:80:ARG:HD2	1.93	0.50
1:J:39:LEU:HD13	1:J:52:HIS:NE2	2.27	0.50
1:K:5:LYS:NZ	1:K:5:LYS:CE	2.75	0.50
1:K:477:ARG:HA	1:K:480:PHE:HD2	1.77	0.50
1:L:243:GLY:O	1:M:238:THR:HG21	2.11	0.50
1:M:72:PHE:CE2	1:M:96:VAL:HG23	2.46	0.50
1:M:77:GLU:HA	1:M:80:ARG:HH22	1.75	0.50
1:E:48:PHE:HB3	1:E:326:VAL:HG22	1.94	0.49
1:I:19:LEU:HB3	1:I:80:ARG:HD2	1.93	0.49
1:I:48:PHE:HB3	1:I:326:VAL:HG22	1.94	0.49
1:M:477:ARG:HA	1:M:480:PHE:HD2	1.77	0.49
1:C:477:ARG:HA	1:C:480:PHE:HD2	1.77	0.49
1:D:55:GLU:O	1:D:58:GLU:HB3	2.11	0.49
1:D:249:ARG:NE	1:D:331:ILE:HG21	2.25	0.49
1:F:97:LEU:CG	1:F:528:THR:OG1	2.60	0.49
1:H:465:ASP:HB3	1:H:467:LEU:H	1.77	0.49
1:H:467:LEU:HA	1:J:150:ILE:O	2.11	0.49
1:I:477:ARG:HA	1:I:480:PHE:HD2	1.77	0.49
1:J:455:THR:HA	1:J:486:PHE:O	2.11	0.49
1:L:66:ALA:HB3	1:L:99:ARG:HH21	1.76	0.49
1:A:2:VAL:HA	1:A:5:LYS:HB3	1.94	0.49
1:D:68:ASP:HA	1:D:101:ASP:OD2	2.12	0.49
1:L:407:ILE:HD11	1:L:431:HIS:CD2	2.46	0.49
1:A:24:LEU:CA	1:A:81:GLN:NE2	2.73	0.49
1:A:59:LEU:HD11	1:A:87:MET:SD	2.52	0.49
1:C:14:LYS:HE2	1:C:514:PHE:HZ	1.67	0.49
1:C:150:ILE:O	1:G:467:LEU:HD12	2.12	0.49
1:D:38:ILE:HD12	1:F:605:ARG:HH21	1.78	0.49
1:E:226:PHE:HE1	1:E:270:ARG:CZ	2.26	0.49
1:I:269:TRP:O	1:I:273:ILE:HG13	2.12	0.49
1:I:272:ARG:NH1	1:I:316:TYR:HA	2.22	0.49
1:J:305:ILE:C	1:J:307:SER:HA	2.33	0.49
1:L:172:HIS:NE2	1:L:532:SER:HB3	2.27	0.49
1:A:72:PHE:CE2	1:A:96:VAL:CB	2.89	0.49
1:D:407:ILE:HD11	1:D:431:HIS:CD2	2.46	0.49
1:G:477:ARG:HA	1:G:480:PHE:HD2	1.77	0.49
1:H:249:ARG:NE	1:H:331:ILE:HG21	2.25	0.49
1:L:477:ARG:HA	1:L:480:PHE:HD2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:79:ALA:HB3	1:M:88:PHE:HE1	1.68	0.49
1:C:10:MET:HB3	1:C:514:PHE:CE2	2.48	0.49
1:F:249:ARG:NE	1:F:331:ILE:HG21	2.25	0.49
1:G:306:GLU:N	1:G:307:SER:HA	2.28	0.49
1:G:477:ARG:HG2	1:G:598:PHE:HB3	1.93	0.49
1:H:249:ARG:HG2	1:H:250:PRO:O	2.13	0.49
1:L:414:LEU:HB2	1:L:426:VAL:HG23	1.95	0.49
1:A:48:PHE:HB3	1:A:326:VAL:HG22	1.93	0.49
1:A:477:ARG:HA	1:A:480:PHE:HD2	1.77	0.49
1:C:48:PHE:HB3	1:C:326:VAL:HG22	1.94	0.49
1:C:463:LYS:HD3	1:C:550:GLU:HG2	1.95	0.49
1:D:119:VAL:HG11	1:D:428:VAL:HG11	1.95	0.49
1:D:454:SER:O	1:D:487:PHE:HA	2.13	0.49
1:F:463:LYS:HD3	1:F:550:GLU:HG2	1.95	0.49
1:J:119:VAL:HG11	1:J:428:VAL:HG11	1.95	0.49
1:M:454:SER:O	1:M:487:PHE:HA	2.13	0.49
1:A:38:ILE:HG12	1:G:605:ARG:HH22	1.78	0.49
1:F:119:VAL:HG11	1:F:428:VAL:HG11	1.95	0.49
1:I:527:SER:HA	1:I:584:ARG:HB3	1.94	0.49
1:K:12:LEU:HD13	1:K:80:ARG:NH2	2.27	0.49
1:K:59:LEU:HD13	1:K:87:MET:CE	2.42	0.49
1:K:407:ILE:HD11	1:K:431:HIS:CD2	2.46	0.49
1:L:573:VAL:HG12	1:L:584:ARG:HB2	1.95	0.49
1:E:151:LEU:HA	1:F:467:LEU:HD22	1.95	0.49
1:A:454:SER:O	1:A:487:PHE:HA	2.13	0.49
1:D:268:ARG:HH11	1:F:271:GLU:HA	1.77	0.49
1:E:2:VAL:HA	1:E:5:LYS:HB3	1.95	0.49
1:E:22:GLU:HB2	1:E:81:GLN:HB3	1.95	0.49
1:E:454:SER:O	1:E:487:PHE:HA	2.13	0.49
1:E:463:LYS:HD3	1:E:550:GLU:HG2	1.95	0.49
1:G:407:ILE:HD11	1:G:431:HIS:CD2	2.46	0.49
1:G:465:ASP:HB3	1:G:467:LEU:H	1.78	0.49
1:J:22:GLU:HB2	1:J:81:GLN:HB3	1.95	0.49
1:J:407:ILE:HD11	1:J:431:HIS:CD2	2.46	0.49
1:L:454:SER:O	1:L:487:PHE:HA	2.13	0.49
1:E:414:LEU:HB2	1:E:426:VAL:HG23	1.95	0.48
1:H:454:SER:O	1:H:487:PHE:HA	2.13	0.48
1:I:38:ILE:HD11	1:I:55:GLU:HG2	1.94	0.48
1:L:48:PHE:HB3	1:L:326:VAL:HG22	1.93	0.48
1:M:119:VAL:HG11	1:M:428:VAL:HG11	1.95	0.48
1:A:59:LEU:HD22	1:A:87:MET:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:407:ILE:HD11	1:C:431:HIS:CD2	2.46	0.48
1:C:414:LEU:HB2	1:C:426:VAL:HG23	1.95	0.48
1:D:232:GLY:HA3	1:E:338:PHE:HZ	1.78	0.48
1:E:19:LEU:HB3	1:E:80:ARG:HD2	1.94	0.48
1:F:36:VAL:HG11	1:F:59:LEU:HD11	1.94	0.48
1:F:477:ARG:HA	1:F:480:PHE:HD2	1.77	0.48
1:G:463:LYS:HD3	1:G:550:GLU:HG2	1.95	0.48
1:H:32:ARG:HH22	1:H:75:LEU:HD22	1.78	0.48
1:H:119:VAL:HG11	1:H:428:VAL:HG11	1.95	0.48
1:J:414:LEU:HB2	1:J:426:VAL:HG23	1.95	0.48
1:M:2:VAL:HA	1:M:5:LYS:HB3	1.95	0.48
1:M:463:LYS:HD3	1:M:550:GLU:HG2	1.95	0.48
1:C:151:LEU:HD12	1:G:467:LEU:HD11	1.76	0.48
1:E:267:VAL:HA	1:E:270:ARG:HH21	1.79	0.48
1:F:414:LEU:HB2	1:F:426:VAL:HG23	1.95	0.48
1:H:48:PHE:HB3	1:H:326:VAL:HG22	1.94	0.48
1:I:119:VAL:HG11	1:I:428:VAL:HG11	1.95	0.48
1:I:275:ASP:HA	1:I:278:ASN:ND2	2.28	0.48
1:I:477:ARG:HG2	1:I:598:PHE:HB3	1.94	0.48
1:K:119:VAL:HG11	1:K:428:VAL:HG11	1.95	0.48
1:M:10:MET:SD	1:M:517:LEU:HB3	2.54	0.48
1:M:249:ARG:HG2	1:M:250:PRO:O	2.13	0.48
1:A:463:LYS:HD3	1:A:550:GLU:HG2	1.95	0.48
1:H:463:LYS:HD3	1:H:550:GLU:HG2	1.95	0.48
1:K:45:PHE:HE1	1:K:52:HIS:HB3	1.78	0.48
1:K:271:GLU:HA	1:M:268:ARG:HH11	1.77	0.48
1:M:245:GLN:O	1:M:341:ASN:HB2	2.14	0.48
1:A:24:LEU:CD2	1:A:81:GLN:HB2	2.44	0.48
1:C:2:VAL:HA	1:C:5:LYS:HB3	1.94	0.48
1:C:169:HIS:CE1	1:C:581:CYS:SG	3.04	0.48
1:C:275:ASP:OD1	1:F:316:TYR:CE1	2.66	0.48
1:F:48:PHE:HB3	1:F:326:VAL:HG22	1.94	0.48
1:I:463:LYS:HD3	1:I:550:GLU:HG2	1.95	0.48
1:J:2:VAL:HA	1:J:5:LYS:HB3	1.95	0.48
1:K:463:LYS:HD3	1:K:550:GLU:HG2	1.95	0.48
1:A:66:ALA:HB1	1:A:99:ARG:NH2	2.06	0.48
1:A:365:ASP:O	1:A:369:GLN:HG2	2.14	0.48
1:D:365:ASP:O	1:D:369:GLN:HG2	2.14	0.48
1:E:169:HIS:CE1	1:E:581:CYS:SG	3.04	0.48
1:F:2:VAL:HA	1:F:5:LYS:HB3	1.95	0.48
1:G:249:ARG:NE	1:G:331:ILE:HG21	2.25	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:195:GLU:H	1:H:299:ASP:HA	1.79	0.48
1:H:365:ASP:O	1:H:369:GLN:HG2	2.14	0.48
1:H:467:LEU:HD12	1:J:150:ILE:O	2.06	0.48
1:H:477:ARG:HG2	1:H:598:PHE:HB3	1.94	0.48
1:J:477:ARG:HG2	1:J:598:PHE:HB3	1.94	0.48
1:A:249:ARG:NE	1:A:331:ILE:HG21	2.24	0.48
1:C:195:GLU:H	1:C:299:ASP:HA	1.79	0.48
1:E:195:GLU:H	1:E:299:ASP:HA	1.79	0.48
1:F:454:SER:O	1:F:487:PHE:HA	2.13	0.48
1:G:365:ASP:O	1:G:369:GLN:HG2	2.14	0.48
1:H:414:LEU:HB2	1:H:426:VAL:HG23	1.95	0.48
1:I:169:HIS:CE1	1:I:581:CYS:SG	3.04	0.48
1:I:407:ILE:HD11	1:I:431:HIS:CD2	2.46	0.48
1:K:23:LYS:O	1:K:81:GLN:HB3	2.14	0.48
1:L:463:LYS:HD3	1:L:550:GLU:HG2	1.95	0.48
1:A:24:LEU:CB	1:A:81:GLN:NE2	2.76	0.48
1:A:263:VAL:O	1:A:266:MET:HB2	2.14	0.48
1:D:169:HIS:CE1	1:D:581:CYS:SG	3.04	0.48
1:E:119:VAL:HG11	1:E:428:VAL:HG11	1.95	0.48
1:G:179:ALA:O	1:G:308:SER:HA	2.13	0.48
1:G:195:GLU:HB2	1:G:298:THR:HB	1.94	0.48
1:I:22:GLU:HB2	1:I:81:GLN:HB3	1.95	0.48
1:I:463:LYS:HG3	1:I:471:LEU:HD21	1.96	0.48
1:J:549:MET:HB3	1:J:551:PHE:HE1	1.79	0.48
1:K:454:SER:O	1:K:487:PHE:HA	2.13	0.48
1:C:454:SER:O	1:C:487:PHE:HA	2.13	0.48
1:C:463:LYS:HG3	1:C:471:LEU:HD21	1.96	0.48
1:G:24:LEU:HD13	1:G:81:GLN:HE21	1.67	0.48
1:G:60:TYR:HH	1:G:90:TYR:HE2	1.53	0.48
1:I:414:LEU:HB2	1:I:426:VAL:HG23	1.95	0.48
1:J:34:LYS:HD2	1:J:35:GLY:N	2.28	0.48
1:J:169:HIS:CE1	1:J:581:CYS:SG	3.04	0.48
1:J:365:ASP:O	1:J:369:GLN:HG2	2.14	0.48
1:K:549:MET:HB3	1:K:551:PHE:HE1	1.79	0.48
1:L:103:LYS:HG3	1:L:525:GLU:O	2.13	0.48
1:L:249:ARG:NE	1:L:331:ILE:HG21	2.26	0.48
1:M:195:GLU:H	1:M:299:ASP:HA	1.79	0.48
1:M:365:ASP:O	1:M:369:GLN:HG2	2.14	0.48
1:A:76:CYS:SG	1:A:92:VAL:HG21	2.54	0.48
1:A:274:LEU:CD2	1:A:367:ILE:HG23	2.44	0.48
1:A:467:LEU:HG	1:D:150:ILE:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:GLU:HB2	1:C:81:GLN:HB3	1.95	0.48
1:C:249:ARG:NE	1:C:331:ILE:HG21	2.26	0.48
1:G:512:ARG:NH2	1:G:523:VAL:HG21	2.29	0.48
1:H:549:MET:HB3	1:H:551:PHE:HE1	1.79	0.48
1:I:365:ASP:O	1:I:369:GLN:HG2	2.14	0.48
1:L:195:GLU:H	1:L:299:ASP:HA	1.79	0.48
1:L:365:ASP:O	1:L:369:GLN:HG2	2.14	0.48
1:L:463:LYS:HG3	1:L:471:LEU:HD21	1.96	0.48
1:M:22:GLU:HB2	1:M:81:GLN:CB	2.41	0.48
1:M:414:LEU:HB2	1:M:426:VAL:HG23	1.95	0.48
1:A:22:GLU:HB3	1:A:24:LEU:N	2.29	0.47
1:A:24:LEU:CD1	1:A:27:ASP:CA	2.87	0.47
1:F:38:ILE:HD13	1:F:38:ILE:H	1.79	0.47
1:J:454:SER:O	1:J:487:PHE:HA	2.13	0.47
1:M:72:PHE:CZ	1:M:96:VAL:HB	2.49	0.47
1:D:414:LEU:HB2	1:D:426:VAL:HG23	1.95	0.47
1:F:108:PRO:HA	1:F:109:PRO:HD3	1.81	0.47
1:H:463:LYS:HG3	1:H:471:LEU:HD21	1.96	0.47
1:I:268:ARG:NH1	1:J:274:LEU:HB2	2.18	0.47
1:I:549:MET:HB3	1:I:551:PHE:HE1	1.79	0.47
1:J:102:CYS:O	1:J:105:ILE:HG22	2.14	0.47
1:L:529:GLU:HA	1:L:533:CYS:HB3	1.96	0.47
1:L:549:MET:HB3	1:L:551:PHE:HE1	1.79	0.47
1:A:549:MET:HB3	1:A:551:PHE:HE1	1.79	0.47
1:C:119:VAL:HG11	1:C:428:VAL:HG11	1.95	0.47
1:C:365:ASP:O	1:C:369:GLN:HG2	2.14	0.47
1:D:463:LYS:HD3	1:D:550:GLU:HG2	1.95	0.47
1:E:365:ASP:O	1:E:369:GLN:HG2	2.14	0.47
1:F:463:LYS:HG3	1:F:471:LEU:HD21	1.96	0.47
1:G:463:LYS:HG3	1:G:471:LEU:HD21	1.96	0.47
1:I:454:SER:O	1:I:487:PHE:HA	2.13	0.47
1:J:463:LYS:HD3	1:J:550:GLU:HG2	1.95	0.47
1:L:119:VAL:HG11	1:L:428:VAL:HG11	1.95	0.47
1:F:549:MET:HB3	1:F:551:PHE:HE1	1.79	0.47
1:G:454:SER:O	1:G:487:PHE:HA	2.13	0.47
1:K:195:GLU:H	1:K:299:ASP:HA	1.79	0.47
1:L:4:ASP:HA	1:L:7:ALA:HB3	1.95	0.47
1:A:512:ARG:HH22	1:A:523:VAL:HG21	1.80	0.47
1:G:304:ILE:HA	1:G:311:SER:OG	2.14	0.47
1:H:467:LEU:HB3	1:J:149:ASN:OD1	2.15	0.47
1:I:24:LEU:HD12	1:I:81:GLN:HE21	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:414:LEU:HB2	1:K:426:VAL:HG23	1.95	0.47
1:C:38:ILE:HD13	1:D:605:ARG:NH1	2.30	0.47
1:G:39:LEU:HD21	1:G:45:PHE:HB2	1.97	0.47
1:G:414:LEU:HB2	1:G:426:VAL:HG23	1.95	0.47
1:H:19:LEU:HD22	1:H:80:ARG:HH11	1.79	0.47
1:K:467:LEU:HD22	1:L:151:LEU:HA	1.97	0.47
1:M:463:LYS:HG3	1:M:471:LEU:HD21	1.96	0.47
1:A:150:ILE:O	1:D:467:LEU:HG	2.15	0.47
1:A:258:LEU:HD22	1:A:330:ASN:HD21	1.80	0.47
1:C:549:MET:HB3	1:C:551:PHE:HE1	1.79	0.47
1:G:119:VAL:HG11	1:G:428:VAL:HG11	1.95	0.47
1:G:549:MET:HB3	1:G:551:PHE:HE1	1.79	0.47
1:H:38:ILE:HD12	1:M:605:ARG:NH2	2.30	0.47
1:H:258:LEU:HD22	1:H:330:ASN:HD21	1.80	0.47
1:I:32:ARG:NH2	1:I:62:ALA:HA	2.30	0.47
1:I:57:THR:HA	1:I:60:TYR:CD2	2.50	0.47
1:J:63:LEU:HA	1:J:75:LEU:CD2	2.33	0.47
1:J:267:VAL:O	1:J:271:GLU:HG2	2.15	0.47
1:K:365:ASP:O	1:K:369:GLN:HG2	2.14	0.47
1:M:64:TYR:OH	1:M:94:VAL:CG1	2.45	0.47
1:M:249:ARG:NE	1:M:331:ILE:HG21	2.26	0.47
1:A:278:ASN:HB3	1:E:315:GLU:HG3	1.96	0.47
1:C:587:ARG:NH2	1:I:568:LEU:HB2	2.30	0.47
1:E:463:LYS:HG3	1:E:471:LEU:HD21	1.96	0.47
1:F:249:ARG:HG2	1:F:250:PRO:O	2.15	0.47
1:F:365:ASP:O	1:F:369:GLN:HG2	2.14	0.47
1:L:107:VAL:HG21	1:L:528:THR:OG1	2.15	0.47
1:M:19:LEU:HD13	1:M:80:ARG:HH11	1.80	0.47
1:A:463:LYS:HG3	1:A:471:LEU:HD21	1.96	0.47
1:D:463:LYS:HG3	1:D:471:LEU:HD21	1.96	0.47
1:E:467:LEU:HD22	1:F:151:LEU:HA	1.97	0.47
1:M:30:ASP:HB3	1:M:32:ARG:HB2	1.95	0.47
1:A:169:HIS:CE1	1:A:581:CYS:SG	3.04	0.47
1:C:275:ASP:N	1:F:268:ARG:HH12	2.12	0.47
1:D:403:ILE:HG21	1:D:541:ILE:HG21	1.97	0.47
1:E:200:MET:SD	1:E:580:TYR:HB3	2.55	0.47
1:I:193:LYS:NZ	1:I:308:SER:OG	2.48	0.47
1:I:200:MET:SD	1:I:580:TYR:HB3	2.55	0.47
1:J:463:LYS:HG3	1:J:471:LEU:HD21	1.96	0.47
1:K:268:ARG:HD2	1:K:272:ARG:HE	1.79	0.47
1:K:273:ILE:HG12	1:K:317:TYR:HD1	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:20:THR:HG23	1:M:83:VAL:O	2.15	0.47
1:M:549:MET:HB3	1:M:551:PHE:HE1	1.79	0.47
1:G:169:HIS:CE1	1:G:581:CYS:SG	3.04	0.46
1:I:525:GLU:HB2	1:I:570:GLU:HG2	1.97	0.46
1:C:149:ASN:OD1	1:G:467:LEU:HG	2.15	0.46
1:D:549:MET:HB3	1:D:551:PHE:HE1	1.79	0.46
1:E:108:PRO:HA	1:E:109:PRO:HD3	1.81	0.46
1:E:549:MET:HB3	1:E:551:PHE:HE1	1.79	0.46
1:I:103:LYS:NZ	1:I:525:GLU:O	2.49	0.46
1:I:528:THR:O	1:I:574:CYS:HB2	2.15	0.46
1:M:24:LEU:HD22	1:M:82:ILE:CG2	2.45	0.46
1:M:258:LEU:HD22	1:M:330:ASN:HD21	1.80	0.46
1:F:195:GLU:H	1:F:299:ASP:HA	1.79	0.46
1:G:23:LYS:O	1:G:81:GLN:NE2	2.48	0.46
1:J:200:MET:SD	1:J:580:TYR:HB3	2.55	0.46
1:L:200:MET:SD	1:L:580:TYR:HB3	2.55	0.46
1:L:258:LEU:HD22	1:L:330:ASN:HD21	1.80	0.46
1:A:195:GLU:H	1:A:299:ASP:HA	1.79	0.46
1:D:200:MET:SD	1:D:580:TYR:HB3	2.55	0.46
1:E:226:PHE:HE1	1:E:270:ARG:NH2	2.12	0.46
1:F:13:PHE:CD2	1:F:16:LEU:HD22	2.51	0.46
1:I:195:GLU:H	1:I:299:ASP:HA	1.79	0.46
1:M:50:ALA:HB2	1:M:323:TRP:HH2	1.80	0.46
1:E:193:LYS:NZ	1:E:308:SER:OG	2.48	0.46
1:F:200:MET:SD	1:F:580:TYR:HB3	2.56	0.46
1:I:274:LEU:HB2	1:L:268:ARG:HH12	1.79	0.46
1:J:465:ASP:HB3	1:J:467:LEU:H	1.79	0.46
1:K:249:ARG:HG2	1:K:250:PRO:O	2.15	0.46
1:K:274:LEU:CD2	1:K:367:ILE:HG23	2.45	0.46
1:D:268:ARG:HH12	1:F:274:LEU:HB2	1.80	0.46
1:G:258:LEU:HD22	1:G:330:ASN:HD21	1.80	0.46
1:I:5:LYS:HG3	1:I:69:PHE:CZ	2.49	0.46
1:A:63:LEU:HA	1:A:75:LEU:HD21	1.98	0.46
1:A:120:PRO:O	1:A:123:THR:HG22	2.16	0.46
1:C:258:LEU:HD22	1:C:330:ASN:HD21	1.80	0.46
1:D:258:LEU:HD22	1:D:330:ASN:HD21	1.80	0.46
1:G:32:ARG:NH2	1:G:75:LEU:CD2	2.68	0.46
1:K:107:VAL:CG2	1:K:528:THR:OG1	2.55	0.46
1:A:386:PRO:O	1:A:452:LYS:NZ	2.49	0.46
1:C:200:MET:SD	1:C:580:TYR:HB3	2.55	0.46
1:G:24:LEU:HD11	1:G:78:GLN:HE21	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:169:HIS:CE1	1:H:581:CYS:SG	3.04	0.46
1:K:463:LYS:HG3	1:K:471:LEU:HD21	1.96	0.46
1:K:506:VAL:HG12	1:K:579:SER:HB2	1.98	0.46
1:M:200:MET:SD	1:M:580:TYR:HB3	2.56	0.46
1:M:386:PRO:O	1:M:452:LYS:NZ	2.49	0.46
1:A:245:GLN:O	1:A:341:ASN:HB2	2.16	0.46
1:I:272:ARG:CG	1:I:316:TYR:CE1	2.98	0.46
1:I:531:CYS:HB2	1:I:574:CYS:SG	2.56	0.46
1:A:80:ARG:CB	1:A:88:PHE:CD2	2.98	0.46
1:A:171:TRP:HA	1:A:348:THR:HG23	1.98	0.46
1:A:465:ASP:HB3	1:A:467:LEU:H	1.80	0.46
1:C:108:PRO:HA	1:C:109:PRO:HD3	1.81	0.46
1:D:10:MET:SD	1:D:517:LEU:HB3	2.56	0.46
1:D:245:GLN:O	1:D:341:ASN:HB2	2.16	0.46
1:H:200:MET:SD	1:H:580:TYR:HB3	2.56	0.46
1:I:245:GLN:O	1:I:341:ASN:HB2	2.16	0.46
1:L:193:LYS:NZ	1:L:308:SER:OG	2.48	0.46
1:M:529:GLU:HG3	1:M:574:CYS:SG	2.55	0.46
1:M:556:MET:SD	1:M:597:PRO:HG3	2.56	0.46
1:C:556:MET:SD	1:C:597:PRO:HG3	2.56	0.45
1:E:258:LEU:HD22	1:E:330:ASN:HD21	1.80	0.45
1:K:219:ARG:HD2	1:K:466:GLU:OE2	2.16	0.45
1:L:243:GLY:C	1:M:238:THR:HG21	2.36	0.45
1:L:245:GLN:O	1:L:341:ASN:HB2	2.16	0.45
1:L:556:MET:SD	1:L:597:PRO:HG3	2.56	0.45
1:A:24:LEU:H	1:A:81:GLN:HB3	1.80	0.45
1:A:273:ILE:HG12	1:A:317:TYR:HD1	1.81	0.45
1:C:171:TRP:HA	1:C:348:THR:HG23	1.99	0.45
1:G:171:TRP:HA	1:G:348:THR:HG23	1.99	0.45
1:G:200:MET:SD	1:G:580:TYR:HB3	2.55	0.45
1:H:171:TRP:HA	1:H:348:THR:HG23	1.98	0.45
1:H:245:GLN:O	1:H:341:ASN:HB2	2.16	0.45
1:H:556:MET:SD	1:H:597:PRO:HG3	2.57	0.45
1:I:13:PHE:HB2	1:I:514:PHE:CZ	2.50	0.45
1:K:258:LEU:HD22	1:K:330:ASN:HD21	1.80	0.45
1:L:268:ARG:NH2	1:L:272:ARG:HH21	2.15	0.45
1:L:386:PRO:O	1:L:452:LYS:NZ	2.49	0.45
1:M:19:LEU:HD22	1:M:80:ARG:NH1	2.31	0.45
1:A:200:MET:SD	1:A:580:TYR:HB3	2.55	0.45
1:F:171:TRP:HA	1:F:348:THR:HG23	1.98	0.45
1:F:258:LEU:HD22	1:F:330:ASN:HD21	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:9:LEU:HD11	1:H:69:PHE:HZ	1.81	0.45
1:J:556:MET:SD	1:J:597:PRO:HG3	2.56	0.45
1:K:5:LYS:HE2	1:K:5:LYS:HB2	1.36	0.45
1:K:99:ARG:HH12	1:K:101:ASP:CG	2.19	0.45
1:K:200:MET:SD	1:K:580:TYR:HB3	2.56	0.45
1:L:59:LEU:HD11	1:L:87:MET:HE1	1.97	0.45
1:M:5:LYS:NZ	1:M:69:PHE:O	2.50	0.45
1:A:127:ALA:HB2	1:A:142:VAL:CG2	2.45	0.45
1:A:266:MET:SD	1:A:323:TRP:HB3	2.56	0.45
1:A:556:MET:SD	1:A:597:PRO:HG3	2.57	0.45
1:C:11:PRO:HA	1:C:14:LYS:HE3	1.99	0.45
1:E:556:MET:SD	1:E:597:PRO:HG3	2.56	0.45
1:H:549:MET:O	1:H:621:LYS:HA	2.17	0.45
1:I:258:LEU:HD22	1:I:330:ASN:HD21	1.80	0.45
1:J:55:GLU:O	1:J:58:GLU:HB3	2.16	0.45
1:K:9:LEU:HD11	1:K:73:ILE:HD11	1.99	0.45
1:L:549:MET:O	1:L:621:LYS:HA	2.17	0.45
1:A:128:ASN:HD22	1:A:414:LEU:HD12	1.79	0.45
1:D:171:TRP:HA	1:D:348:THR:HG23	1.99	0.45
1:E:171:TRP:HA	1:E:348:THR:HG23	1.99	0.45
1:F:273:ILE:HG12	1:F:317:TYR:HD1	1.82	0.45
1:F:556:MET:SD	1:F:597:PRO:HG3	2.56	0.45
1:H:11:PRO:HA	1:H:14:LYS:HE3	1.99	0.45
1:I:271:GLU:HA	1:L:268:ARG:HH12	1.81	0.45
1:I:275:ASP:HA	1:I:278:ASN:HD22	1.82	0.45
1:J:245:GLN:O	1:J:341:ASN:HB2	2.16	0.45
1:J:249:ARG:HG2	1:J:250:PRO:O	2.17	0.45
1:J:258:LEU:HD22	1:J:330:ASN:HD21	1.80	0.45
1:K:20:THR:HG23	1:K:83:VAL:O	2.16	0.45
1:K:393:VAL:HB	1:K:618:THR:OG1	2.17	0.45
1:K:556:MET:SD	1:K:597:PRO:HG3	2.57	0.45
1:M:169:HIS:CE1	1:M:581:CYS:SG	3.04	0.45
1:A:24:LEU:CD2	1:A:82:ILE:CG2	2.92	0.45
1:D:556:MET:SD	1:D:597:PRO:HG3	2.56	0.45
1:G:59:LEU:HD11	1:G:87:MET:CE	2.45	0.45
1:G:245:GLN:O	1:G:341:ASN:HB2	2.16	0.45
1:H:8:ARG:NH1	1:H:73:ILE:HG21	2.30	0.45
1:H:362:ARG:HD3	1:H:362:ARG:HA	1.84	0.45
1:I:549:MET:O	1:I:621:LYS:HA	2.16	0.45
1:J:171:TRP:HA	1:J:348:THR:HG23	1.99	0.45
1:J:290:ILE:HD12	1:J:300:ILE:HD13	1.95	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:354:ASP:HA	1:J:355:PRO:HD3	1.85	0.45
1:L:8:ARG:NH2	1:L:73:ILE:CB	2.80	0.45
1:M:549:MET:O	1:M:621:LYS:HA	2.17	0.45
1:C:245:GLN:O	1:C:341:ASN:HB2	2.17	0.45
1:C:354:ASP:HA	1:C:355:PRO:HD3	1.85	0.45
1:D:393:VAL:HB	1:D:618:THR:OG1	2.17	0.45
1:E:393:VAL:HB	1:E:618:THR:OG1	2.17	0.45
1:E:549:MET:O	1:E:621:LYS:HA	2.16	0.45
1:J:393:VAL:HB	1:J:618:THR:OG1	2.17	0.45
1:K:5:LYS:NZ	1:K:72:PHE:HD2	2.15	0.45
1:K:549:MET:O	1:K:621:LYS:HA	2.17	0.45
1:L:169:HIS:CE1	1:L:581:CYS:SG	3.04	0.45
1:M:228:GLU:HA	1:M:229:PRO:HD3	1.88	0.45
1:A:393:VAL:HB	1:A:618:THR:OG1	2.17	0.45
1:C:228:GLU:HA	1:C:229:PRO:HD3	1.88	0.45
1:D:549:MET:O	1:D:621:LYS:HA	2.17	0.45
1:E:245:GLN:O	1:E:341:ASN:HB2	2.16	0.45
1:G:11:PRO:HA	1:G:14:LYS:HE3	1.99	0.45
1:G:549:MET:O	1:G:621:LYS:HA	2.17	0.45
1:H:243:GLY:N	1:I:125:ASN:HD21	2.00	0.45
1:H:270:ARG:NH1	1:K:264:GLN:OE1	2.49	0.45
1:H:386:PRO:O	1:H:452:LYS:NZ	2.49	0.45
1:I:270:ARG:HD3	1:I:320:LEU:HD21	1.98	0.45
1:J:9:LEU:HD22	1:J:105:ILE:HD11	1.99	0.45
1:J:549:MET:O	1:J:621:LYS:HA	2.17	0.45
1:K:193:LYS:NZ	1:K:308:SER:OG	2.48	0.45
1:A:528:THR:O	1:A:532:SER:HB3	2.16	0.45
1:H:10:MET:SD	1:H:517:LEU:HB3	2.57	0.45
1:I:171:TRP:HA	1:I:348:THR:HG23	1.99	0.45
1:J:467:LEU:HD22	1:J:470:LYS:HE3	1.98	0.45
1:K:108:PRO:HA	1:K:109:PRO:HD3	1.81	0.45
1:M:171:TRP:HA	1:M:348:THR:HG23	1.99	0.45
1:M:250:PRO:HB2	1:M:253:TYR:CE1	2.52	0.45
1:M:263:VAL:O	1:M:266:MET:HB2	2.17	0.45
1:E:268:ARG:O	1:E:272:ARG:HG3	2.17	0.45
1:E:273:ILE:HG12	1:E:317:TYR:HD1	1.81	0.45
1:G:304:ILE:HA	1:G:311:SER:CB	2.47	0.45
1:H:393:VAL:HB	1:H:618:THR:OG1	2.17	0.45
1:I:556:MET:SD	1:I:597:PRO:HG3	2.56	0.45
1:K:171:TRP:HA	1:K:348:THR:HG23	1.99	0.45
1:K:403:ILE:HG21	1:K:541:ILE:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:PHE:HZ	1:A:89:VAL:HG23	1.82	0.44
1:A:38:ILE:HD13	1:G:605:ARG:HH12	1.82	0.44
1:A:205:CYS:SG	1:A:358:TYR:HD1	2.40	0.44
1:A:316:TYR:HE1	1:G:275:ASP:OD1	1.99	0.44
1:F:253:TYR:OH	1:G:250:PRO:HG3	2.17	0.44
1:F:386:PRO:O	1:F:452:LYS:NZ	2.49	0.44
1:F:403:ILE:HG21	1:F:541:ILE:HG21	1.99	0.44
1:H:8:ARG:CZ	1:H:73:ILE:HG13	2.46	0.44
1:H:467:LEU:CD2	1:J:151:LEU:HD13	2.45	0.44
1:I:249:ARG:NE	1:I:331:ILE:HG21	2.25	0.44
1:I:403:ILE:HG21	1:I:541:ILE:HG21	1.99	0.44
1:K:354:ASP:HA	1:K:355:PRO:HD3	1.85	0.44
1:M:393:VAL:HB	1:M:618:THR:OG1	2.17	0.44
1:A:22:GLU:HB3	1:A:24:LEU:H	1.82	0.44
1:D:270:ARG:HD3	1:D:363:PHE:CZ	2.52	0.44
1:D:386:PRO:O	1:D:452:LYS:NZ	2.49	0.44
1:E:107:VAL:CG2	1:E:528:THR:OG1	2.56	0.44
1:F:245:GLN:O	1:F:341:ASN:HB2	2.16	0.44
1:G:29:ARG:HB3	1:G:78:GLN:HE22	1.82	0.44
1:H:605:ARG:NH2	1:K:38:ILE:HD12	2.32	0.44
1:L:20:THR:OG1	1:L:85:GLU:HB3	2.18	0.44
1:M:445:GLU:OE2	1:M:494:LYS:NZ	2.50	0.44
1:E:205:CYS:SG	1:E:358:TYR:HD1	2.40	0.44
1:E:512:ARG:CB	1:E:531:CYS:SG	3.02	0.44
1:G:393:VAL:HB	1:G:618:THR:OG1	2.17	0.44
1:I:273:ILE:HG12	1:I:317:TYR:CD1	2.40	0.44
1:I:386:PRO:O	1:I:452:LYS:NZ	2.49	0.44
1:K:386:PRO:O	1:K:452:LYS:NZ	2.49	0.44
1:L:231:GLU:O	1:L:249:ARG:HD2	2.17	0.44
1:L:354:ASP:HA	1:L:355:PRO:HD3	1.85	0.44
1:L:393:VAL:HB	1:L:618:THR:OG1	2.17	0.44
1:F:458:ILE:HG23	1:F:555:VAL:HG22	2.00	0.44
1:F:549:MET:O	1:F:621:LYS:HA	2.16	0.44
1:G:403:ILE:HG21	1:G:541:ILE:HG21	1.99	0.44
1:I:205:CYS:SG	1:I:358:TYR:HD1	2.40	0.44
1:J:11:PRO:HA	1:J:14:LYS:HE3	1.99	0.44
1:K:11:PRO:HA	1:K:14:LYS:HE3	1.99	0.44
1:L:11:PRO:HA	1:L:14:LYS:HE3	1.99	0.44
1:L:162:GLU:HG2	1:L:353:ARG:CB	2.47	0.44
1:L:403:ILE:HG21	1:L:541:ILE:HG21	1.99	0.44
1:M:403:ILE:HG21	1:M:541:ILE:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:LYS:NZ	1:A:308:SER:OG	2.48	0.44
1:A:549:MET:O	1:A:621:LYS:HA	2.17	0.44
1:C:162:GLU:HG2	1:C:353:ARG:CB	2.47	0.44
1:C:231:GLU:O	1:C:249:ARG:HD2	2.18	0.44
1:C:403:ILE:HG21	1:C:541:ILE:HG21	1.99	0.44
1:D:243:GLY:CA	1:E:125:ASN:ND2	2.80	0.44
1:E:96:VAL:HG22	1:E:105:ILE:CG2	2.45	0.44
1:F:267:VAL:O	1:F:271:GLU:HG2	2.17	0.44
1:G:556:MET:SD	1:G:597:PRO:HG3	2.57	0.44
1:K:97:LEU:CG	1:K:528:THR:CB	2.96	0.44
1:K:169:HIS:CE1	1:K:581:CYS:SG	3.04	0.44
1:L:99:ARG:HH12	1:L:101:ASP:CG	2.21	0.44
1:M:11:PRO:HA	1:M:14:LYS:HE3	1.99	0.44
1:M:467:LEU:HD22	1:M:470:LYS:HE3	1.98	0.44
1:A:59:LEU:CD2	1:A:87:MET:CE	2.96	0.44
1:C:205:CYS:SG	1:C:358:TYR:HD1	2.40	0.44
1:E:11:PRO:HA	1:E:14:LYS:HE3	1.99	0.44
1:E:403:ILE:HG21	1:E:541:ILE:HG21	1.99	0.44
1:H:458:ILE:HG23	1:H:555:VAL:HG22	2.00	0.44
1:I:393:VAL:HB	1:I:618:THR:OG1	2.17	0.44
1:K:64:TYR:OH	1:K:98:HIS:HB2	2.18	0.44
1:L:205:CYS:SG	1:L:358:TYR:HD1	2.41	0.44
1:A:50:ALA:HB2	1:A:323:TRP:CH2	2.53	0.44
1:C:447:ASN:HB2	1:I:288:ASN:HD21	1.81	0.44
1:F:162:GLU:HG2	1:F:353:ARG:CB	2.47	0.44
1:G:59:LEU:CD1	1:G:87:MET:CE	2.95	0.44
1:J:512:ARG:HH22	1:J:523:VAL:HG21	1.82	0.44
1:K:245:GLN:O	1:K:341:ASN:HB2	2.16	0.44
1:L:8:ARG:CZ	1:L:73:ILE:HG13	2.45	0.44
1:L:171:TRP:HA	1:L:348:THR:HG23	1.99	0.44
1:L:458:ILE:HG23	1:L:555:VAL:HG22	2.00	0.44
1:M:5:LYS:HG3	1:M:69:PHE:CZ	2.53	0.44
1:M:47:CYS:HB2	1:M:346:SER:O	2.17	0.44
1:A:10:MET:SD	1:A:517:LEU:HB3	2.58	0.44
1:A:103:LYS:HD2	1:A:526:ASP:OD1	2.18	0.44
1:C:467:LEU:HD11	1:G:149:ASN:OD1	2.18	0.44
1:M:231:GLU:O	1:M:249:ARG:HD2	2.18	0.44
1:M:506:VAL:HG12	1:M:579:SER:HB2	1.99	0.44
1:A:403:ILE:HG21	1:A:541:ILE:HG21	1.99	0.44
1:A:458:ILE:HG23	1:A:555:VAL:HG22	2.00	0.44
1:C:393:VAL:HB	1:C:618:THR:OG1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:458:ILE:HG23	1:E:555:VAL:HG22	2.00	0.44
1:F:97:LEU:CD2	1:F:528:THR:H	2.30	0.44
1:H:205:CYS:SG	1:H:358:TYR:HD1	2.41	0.44
1:H:263:VAL:O	1:H:266:MET:HB2	2.17	0.44
1:J:386:PRO:O	1:J:452:LYS:NZ	2.49	0.44
1:L:108:PRO:HA	1:L:109:PRO:HD3	1.81	0.44
1:A:11:PRO:HA	1:A:14:LYS:HE3	1.99	0.43
1:A:197:PHE:O	1:A:201:HIS:ND1	2.51	0.43
1:D:310:GLU:O	1:D:312:LYS:NZ	2.51	0.43
1:G:386:PRO:O	1:G:452:LYS:NZ	2.49	0.43
1:J:205:CYS:SG	1:J:358:TYR:HD1	2.40	0.43
1:K:205:CYS:SG	1:K:358:TYR:HD1	2.41	0.43
1:M:197:PHE:O	1:M:201:HIS:ND1	2.51	0.43
1:D:11:PRO:HA	1:D:14:LYS:HE3	1.99	0.43
1:F:393:VAL:HB	1:F:618:THR:OG1	2.17	0.43
1:H:534:GLY:HA2	1:H:577:ALA:CB	2.48	0.43
1:K:197:PHE:O	1:K:201:HIS:ND1	2.51	0.43
1:A:34:LYS:NZ	1:A:58:GLU:OE1	2.48	0.43
1:C:549:MET:O	1:C:621:LYS:HA	2.17	0.43
1:D:250:PRO:HG2	1:D:253:TYR:CZ	2.53	0.43
1:D:282:ILE:HD11	1:D:300:ILE:HD12	1.99	0.43
1:G:354:ASP:HA	1:G:355:PRO:HD3	1.85	0.43
1:L:197:PHE:O	1:L:201:HIS:ND1	2.51	0.43
1:M:205:CYS:SG	1:M:358:TYR:HD1	2.40	0.43
1:C:197:PHE:O	1:C:201:HIS:ND1	2.51	0.43
1:C:513:THR:HG23	1:C:516:GLN:H	1.82	0.43
1:E:386:PRO:O	1:E:452:LYS:NZ	2.49	0.43
1:F:205:CYS:SG	1:F:358:TYR:HD1	2.41	0.43
1:G:63:LEU:HD23	1:G:91:ALA:CB	2.38	0.43
1:G:197:PHE:O	1:G:201:HIS:ND1	2.51	0.43
1:G:205:CYS:SG	1:G:358:TYR:HD1	2.40	0.43
1:G:458:ILE:HG23	1:G:555:VAL:HG22	2.00	0.43
1:I:49:HIS:CE1	1:I:51:ARG:HG2	2.54	0.43
1:L:49:HIS:CE1	1:L:51:ARG:HG2	2.54	0.43
1:C:250:PRO:HG2	1:C:253:TYR:CZ	2.54	0.43
1:D:5:LYS:HE3	1:D:105:ILE:HG13	2.00	0.43
1:D:197:PHE:O	1:D:201:HIS:ND1	2.51	0.43
1:F:49:HIS:CE1	1:F:51:ARG:HG2	2.54	0.43
1:I:197:PHE:O	1:I:201:HIS:ND1	2.51	0.43
1:J:33:LEU:HD21	1:J:79:ALA:HB1	2.00	0.43
1:M:72:PHE:CE2	1:M:96:VAL:HG21	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:108:PRO:HA	1:M:109:PRO:HD3	1.81	0.43
1:M:276:ALA:HB1	1:M:281:TYR:O	2.19	0.43
1:A:25:PRO:C	1:A:26:LEU:HG	2.38	0.43
1:A:266:MET:HE3	1:A:266:MET:HB3	1.86	0.43
1:C:375:PHE:CB	1:C:600:ARG:HD3	2.48	0.43
1:D:508:ILE:HD11	1:D:531:CYS:HA	2.00	0.43
1:H:193:LYS:NZ	1:H:308:SER:OG	2.48	0.43
1:H:467:LEU:HD21	1:J:151:LEU:HD12	1.99	0.43
1:J:403:ILE:HG21	1:J:541:ILE:HG21	1.99	0.43
1:L:107:VAL:HB	1:L:528:THR:HG23	1.99	0.43
1:M:458:ILE:HG23	1:M:555:VAL:HG22	2.00	0.43
1:C:525:GLU:CD	1:C:529:GLU:HA	2.39	0.43
1:D:205:CYS:SG	1:D:358:TYR:HD1	2.41	0.43
1:E:49:HIS:CE1	1:E:51:ARG:HG2	2.54	0.43
1:G:375:PHE:CB	1:G:600:ARG:HD3	2.48	0.43
1:H:49:HIS:CE1	1:H:51:ARG:HG2	2.54	0.43
1:I:458:ILE:HG23	1:I:555:VAL:HG22	2.00	0.43
1:J:419:ASN:HD22	1:K:132:SER:CB	2.32	0.43
1:K:20:THR:OG1	1:K:85:GLU:HB3	2.18	0.43
1:L:137:GLN:HA	1:L:423:ASP:HA	2.01	0.43
1:A:49:HIS:CE1	1:A:51:ARG:HG2	2.54	0.43
1:C:49:HIS:CE1	1:C:51:ARG:HG2	2.54	0.43
1:D:362:ARG:HD3	1:D:362:ARG:HA	1.84	0.43
1:D:458:ILE:HG23	1:D:555:VAL:HG22	2.00	0.43
1:E:97:LEU:CG	1:E:528:THR:CB	2.96	0.43
1:E:197:PHE:O	1:E:201:HIS:ND1	2.52	0.43
1:F:169:HIS:CE1	1:F:581:CYS:SG	3.04	0.43
1:F:197:PHE:O	1:F:201:HIS:ND1	2.51	0.43
1:G:221:ILE:HA	1:G:222:PRO:HD2	1.92	0.43
1:H:393:VAL:HA	1:H:441:ASN:O	2.19	0.43
1:I:103:LYS:NZ	1:I:524:SER:OG	2.46	0.43
1:K:97:LEU:HG	1:K:528:THR:CB	2.49	0.43
1:K:269:TRP:O	1:K:273:ILE:HG13	2.18	0.43
1:M:12:LEU:HD22	1:M:80:ARG:HH12	1.84	0.43
1:M:267:VAL:HG22	1:M:270:ARG:NH2	2.34	0.43
1:C:263:VAL:O	1:C:266:MET:HB2	2.19	0.43
1:F:393:VAL:HA	1:F:441:ASN:O	2.19	0.43
1:H:197:PHE:O	1:H:201:HIS:ND1	2.51	0.43
1:J:250:PRO:HB2	1:J:253:TYR:CE1	2.54	0.43
1:K:393:VAL:HA	1:K:441:ASN:O	2.19	0.43
1:M:50:ALA:HB2	1:M:323:TRP:CH2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:443:VAL:HA	1:M:495:ASN:O	2.19	0.43
1:C:386:PRO:O	1:C:452:LYS:NZ	2.49	0.43
1:D:49:HIS:CE1	1:D:51:ARG:HG2	2.54	0.43
1:D:162:GLU:HG2	1:D:353:ARG:CB	2.47	0.43
1:D:193:LYS:NZ	1:D:308:SER:OG	2.47	0.43
1:I:393:VAL:HA	1:I:441:ASN:O	2.19	0.43
1:I:527:SER:HB3	1:I:573:VAL:HG21	2.01	0.43
1:J:76:CYS:HG	1:J:88:PHE:HE2	1.65	0.43
1:L:19:LEU:HD13	1:L:80:ARG:CD	2.49	0.43
1:L:228:GLU:HA	1:L:229:PRO:HD3	1.88	0.43
1:M:79:ALA:CB	1:M:88:PHE:HE1	2.26	0.43
1:A:354:ASP:HA	1:A:355:PRO:HD3	1.85	0.42
1:A:393:VAL:HA	1:A:441:ASN:O	2.19	0.42
1:C:393:VAL:HA	1:C:441:ASN:O	2.19	0.42
1:G:357:PHE:O	1:G:361:HIS:ND1	2.53	0.42
1:I:271:GLU:HB3	1:L:268:ARG:HH11	1.84	0.42
1:K:137:GLN:HA	1:K:423:ASP:HA	2.01	0.42
1:K:458:ILE:HG23	1:K:555:VAL:HG22	2.00	0.42
1:M:76:CYS:O	1:M:80:ARG:NH2	2.49	0.42
1:A:276:ALA:HB1	1:A:281:TYR:O	2.19	0.42
1:A:316:TYR:CE1	1:G:275:ASP:OD1	2.72	0.42
1:A:529:GLU:O	1:A:531:CYS:N	2.52	0.42
1:A:591:LYS:HA	1:A:591:LYS:HE3	2.02	0.42
1:C:458:ILE:HG23	1:C:555:VAL:HG22	2.00	0.42
1:C:527:SER:HB3	1:C:573:VAL:HG23	2.00	0.42
1:E:97:LEU:HG	1:E:528:THR:CB	2.49	0.42
1:E:303:ASP:OD2	1:E:312:LYS:NZ	2.52	0.42
1:G:5:LYS:HG3	1:G:69:PHE:CZ	2.54	0.42
1:G:263:VAL:O	1:G:266:MET:HB2	2.19	0.42
1:G:529:GLU:O	1:G:531:CYS:N	2.51	0.42
1:H:228:GLU:HA	1:H:229:PRO:HD3	1.88	0.42
1:J:228:GLU:HA	1:J:229:PRO:HD3	1.88	0.42
1:L:263:VAL:O	1:L:266:MET:HB2	2.19	0.42
1:M:137:GLN:HA	1:M:423:ASP:HA	2.01	0.42
1:C:357:PHE:O	1:C:361:HIS:ND1	2.53	0.42
1:D:8:ARG:HH21	1:D:73:ILE:HG13	1.83	0.42
1:D:137:GLN:HA	1:D:423:ASP:HA	2.01	0.42
1:D:231:GLU:O	1:D:249:ARG:HD2	2.19	0.42
1:D:534:GLY:HA2	1:D:577:ALA:CB	2.49	0.42
1:J:197:PHE:O	1:J:201:HIS:ND1	2.51	0.42
1:J:393:VAL:HA	1:J:441:ASN:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:TYR:O	1:A:94:VAL:HG23	2.20	0.42
1:E:266:MET:HB3	1:E:266:MET:HE3	1.91	0.42
1:F:506:VAL:HG12	1:F:579:SER:HB2	2.01	0.42
1:H:467:LEU:CD2	1:J:151:LEU:CD1	2.97	0.42
1:H:467:LEU:CB	1:J:149:ASN:OD1	2.66	0.42
1:H:529:GLU:O	1:H:531:CYS:N	2.52	0.42
1:I:50:ALA:HB2	1:I:323:TRP:CH2	2.53	0.42
1:I:137:GLN:HA	1:I:423:ASP:HA	2.01	0.42
1:J:5:LYS:HG2	1:J:105:ILE:HB	2.01	0.42
1:J:96:VAL:HG22	1:J:105:ILE:HG21	2.01	0.42
1:J:137:GLN:HA	1:J:423:ASP:HA	2.01	0.42
1:J:591:LYS:HA	1:J:591:LYS:HE3	2.02	0.42
1:L:393:VAL:HA	1:L:441:ASN:O	2.19	0.42
1:A:9:LEU:HD22	1:A:105:ILE:HD11	2.02	0.42
1:A:79:ALA:CB	1:A:88:PHE:CD1	2.97	0.42
1:A:108:PRO:HA	1:A:109:PRO:HD3	1.81	0.42
1:C:275:ASP:OD1	1:F:316:TYR:HE1	2.03	0.42
1:D:529:GLU:O	1:D:531:CYS:N	2.52	0.42
1:D:591:LYS:HA	1:D:591:LYS:HE3	2.02	0.42
1:F:357:PHE:O	1:F:361:HIS:ND1	2.53	0.42
1:G:34:LYS:HG3	1:G:35:GLY:H	1.85	0.42
1:G:303:ASP:HB2	1:G:310:GLU:HB2	2.01	0.42
1:G:393:VAL:HA	1:G:441:ASN:O	2.19	0.42
1:I:357:PHE:O	1:I:361:HIS:ND1	2.53	0.42
1:J:97:LEU:CG	1:J:528:THR:CB	2.97	0.42
1:J:303:ASP:C	1:J:311:SER:HA	2.39	0.42
1:K:24:LEU:HD13	1:K:81:GLN:HE22	1.70	0.42
1:K:231:GLU:O	1:K:249:ARG:HD2	2.19	0.42
1:L:19:LEU:CD1	1:L:80:ARG:HD3	2.49	0.42
1:M:193:LYS:NZ	1:M:308:SER:OG	2.48	0.42
1:M:357:PHE:O	1:M:361:HIS:ND1	2.52	0.42
1:A:303:ASP:OD2	1:A:312:LYS:NZ	2.52	0.42
1:A:467:LEU:HD23	1:D:149:ASN:OD1	2.19	0.42
1:D:357:PHE:O	1:D:361:HIS:ND1	2.53	0.42
1:D:393:VAL:HA	1:D:441:ASN:O	2.19	0.42
1:F:137:GLN:HA	1:F:423:ASP:HA	2.01	0.42
1:H:107:VAL:HG21	1:H:528:THR:HG1	1.85	0.42
1:H:403:ILE:HG21	1:H:541:ILE:HG21	1.99	0.42
1:H:605:ARG:NH1	1:K:38:ILE:HB	2.35	0.42
1:I:267:VAL:HG13	1:I:270:ARG:NH2	2.34	0.42
1:J:162:GLU:HG2	1:J:353:ARG:CB	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:282:ILE:HD12	1:J:304:ILE:HD12	2.01	0.42
1:J:357:PHE:O	1:J:361:HIS:ND1	2.53	0.42
1:K:465:ASP:HB3	1:K:467:LEU:H	1.84	0.42
1:M:5:LYS:CD	1:M:69:PHE:CZ	3.02	0.42
1:M:529:GLU:O	1:M:531:CYS:N	2.52	0.42
1:M:591:LYS:HA	1:M:591:LYS:HE3	2.02	0.42
1:A:267:VAL:HG13	1:A:270:ARG:NH2	2.34	0.42
1:E:50:ALA:HB2	1:E:323:TRP:CH2	2.53	0.42
1:E:357:PHE:O	1:E:361:HIS:ND1	2.52	0.42
1:F:375:PHE:CB	1:F:600:ARG:HD3	2.47	0.42
1:G:534:GLY:HA2	1:G:577:ALA:CB	2.49	0.42
1:L:357:PHE:O	1:L:361:HIS:ND1	2.52	0.42
1:M:393:VAL:HA	1:M:441:ASN:O	2.19	0.42
1:A:357:PHE:O	1:A:361:HIS:ND1	2.52	0.42
1:C:137:GLN:HA	1:C:423:ASP:HA	2.01	0.42
1:D:232:GLY:HA3	1:E:338:PHE:CZ	2.55	0.42
1:E:76:CYS:HG	1:E:88:PHE:HE2	1.66	0.42
1:F:97:LEU:HD11	1:F:528:THR:OG1	2.18	0.42
1:F:415:SER:OG	1:F:425:SER:HA	2.20	0.42
1:F:588:TYR:HA	1:F:589:PRO:HD3	1.91	0.42
1:G:591:LYS:HA	1:G:591:LYS:HE3	2.01	0.42
1:H:137:GLN:HA	1:H:423:ASP:HA	2.01	0.42
1:H:140:ILE:HB	1:H:426:VAL:HG12	2.02	0.42
1:I:48:PHE:HB2	1:I:326:VAL:HG22	2.02	0.42
1:I:162:GLU:HG2	1:I:353:ARG:CB	2.47	0.42
1:I:508:ILE:HD13	1:I:533:CYS:O	2.20	0.42
1:J:140:ILE:HB	1:J:426:VAL:HG12	2.02	0.42
1:J:534:GLY:HA2	1:J:577:ALA:CB	2.49	0.42
1:K:8:ARG:NE	1:K:73:ILE:CG2	2.43	0.42
1:K:162:GLU:HG2	1:K:353:ARG:CB	2.47	0.42
1:M:362:ARG:HD3	1:M:362:ARG:HA	1.84	0.42
1:M:415:SER:OG	1:M:425:SER:HA	2.20	0.42
1:A:231:GLU:O	1:A:249:ARG:HD2	2.20	0.42
1:C:48:PHE:HB2	1:C:326:VAL:HG22	2.02	0.42
1:C:591:LYS:HA	1:C:591:LYS:HE3	2.02	0.42
1:E:137:GLN:HA	1:E:423:ASP:HA	2.01	0.42
1:E:266:MET:SD	1:E:323:TRP:HB3	2.60	0.42
1:I:99:ARG:HH12	1:I:101:ASP:CG	2.24	0.42
1:J:458:ILE:HG23	1:J:555:VAL:HG22	2.00	0.42
1:K:357:PHE:O	1:K:361:HIS:ND1	2.53	0.42
1:D:50:ALA:HB2	1:D:323:TRP:CH2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:304:ILE:HD11	1:D:312:LYS:HB2	2.01	0.42
1:D:605:ARG:HA	1:D:605:ARG:HD3	1.90	0.42
1:E:393:VAL:HA	1:E:441:ASN:O	2.19	0.42
1:F:140:ILE:HB	1:F:426:VAL:HG12	2.02	0.42
1:F:193:LYS:NZ	1:F:308:SER:OG	2.48	0.42
1:F:221:ILE:HA	1:F:222:PRO:HD2	1.92	0.42
1:H:354:ASP:HA	1:H:355:PRO:HD3	1.85	0.42
1:J:234:ALA:HA	1:J:248:SER:HB2	2.01	0.42
1:K:292:LEU:HB3	1:K:371:HIS:CE1	2.55	0.42
1:L:269:TRP:O	1:L:273:ILE:HG13	2.19	0.42
1:L:276:ALA:HB1	1:L:281:TYR:O	2.20	0.42
1:M:69:PHE:CE1	1:M:72:PHE:HD2	2.33	0.42
1:M:107:VAL:HB	1:M:528:THR:HG23	2.02	0.42
1:A:84:ASN:N	1:A:84:ASN:ND2	2.68	0.41
1:C:416:HIS:ND1	1:C:514:PHE:HB2	2.35	0.41
1:D:415:SER:OG	1:D:425:SER:HA	2.20	0.41
1:E:5:LYS:HG3	1:E:69:PHE:CZ	2.55	0.41
1:E:354:ASP:HA	1:E:355:PRO:HD3	1.85	0.41
1:E:529:GLU:HB2	1:E:533:CYS:HB2	2.01	0.41
1:F:48:PHE:HB2	1:F:326:VAL:HG22	2.02	0.41
1:H:357:PHE:O	1:H:361:HIS:ND1	2.52	0.41
1:I:140:ILE:HB	1:I:426:VAL:HG12	2.02	0.41
1:J:60:TYR:O	1:J:64:TYR:HD2	2.04	0.41
1:J:97:LEU:HG	1:J:528:THR:CB	2.49	0.41
1:J:529:GLU:O	1:J:531:CYS:N	2.53	0.41
1:K:140:ILE:HB	1:K:426:VAL:HG12	2.02	0.41
1:A:162:GLU:HG2	1:A:353:ARG:CB	2.47	0.41
1:C:271:GLU:HB3	1:F:268:ARG:HD3	2.02	0.41
1:E:292:LEU:HB3	1:E:371:HIS:CE1	2.55	0.41
1:E:506:VAL:HG12	1:E:579:SER:HB2	2.02	0.41
1:F:591:LYS:HA	1:F:591:LYS:HE3	2.01	0.41
1:G:137:GLN:HA	1:G:423:ASP:HA	2.01	0.41
1:G:231:GLU:O	1:G:249:ARG:HD2	2.19	0.41
1:J:362:ARG:HD3	1:J:362:ARG:HA	1.84	0.41
1:L:8:ARG:HH21	1:L:73:ILE:CG1	2.20	0.41
1:M:140:ILE:HB	1:M:426:VAL:HG12	2.02	0.41
1:A:415:SER:OG	1:A:425:SER:HA	2.20	0.41
1:C:292:LEU:HB3	1:C:371:HIS:CE1	2.56	0.41
1:D:474:ASP:HA	1:D:477:ARG:HE	1.86	0.41
1:E:57:THR:HA	1:E:60:TYR:CD2	2.56	0.41
1:E:97:LEU:HG	1:E:528:THR:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:228:GLU:HA	1:E:229:PRO:HD3	1.88	0.41
1:F:76:CYS:HG	1:F:88:PHE:HE2	1.65	0.41
1:F:276:ALA:HB1	1:F:281:TYR:O	2.20	0.41
1:I:271:GLU:HG3	1:L:268:ARG:HG3	2.02	0.41
1:I:591:LYS:HA	1:I:591:LYS:HE3	2.01	0.41
1:M:99:ARG:HH12	1:M:101:ASP:CG	2.24	0.41
1:A:292:LEU:HB3	1:A:371:HIS:CE1	2.55	0.41
1:A:588:TYR:HA	1:A:589:PRO:HD3	1.92	0.41
1:D:161:ARG:HB3	1:D:353:ARG:HA	2.03	0.41
1:D:270:ARG:HD3	1:D:363:PHE:HZ	1.85	0.41
1:E:231:GLU:O	1:E:249:ARG:HD2	2.19	0.41
1:G:474:ASP:HA	1:G:477:ARG:HE	1.85	0.41
1:I:231:GLU:O	1:I:249:ARG:HD2	2.19	0.41
1:L:48:PHE:HB2	1:L:326:VAL:HG22	2.02	0.41
1:L:140:ILE:HB	1:L:426:VAL:HG12	2.02	0.41
1:M:59:LEU:CD1	1:M:87:MET:HE3	2.50	0.41
1:M:474:ASP:HA	1:M:477:ARG:HE	1.86	0.41
1:A:499:ARG:NH1	1:A:503:ASP:O	2.53	0.41
1:C:193:LYS:NZ	1:C:308:SER:OG	2.48	0.41
1:D:57:THR:HA	1:D:60:TYR:CD2	2.56	0.41
1:D:221:ILE:HA	1:D:222:PRO:HD2	1.92	0.41
1:E:161:ARG:HB3	1:E:353:ARG:HA	2.03	0.41
1:E:375:PHE:CB	1:E:600:ARG:HD3	2.48	0.41
1:E:474:ASP:HA	1:E:477:ARG:HE	1.85	0.41
1:H:591:LYS:HE3	1:H:591:LYS:HA	2.02	0.41
1:I:474:ASP:HA	1:I:477:ARG:HE	1.86	0.41
1:I:506:VAL:HG12	1:I:579:SER:HB2	2.02	0.41
1:J:415:SER:OG	1:J:425:SER:HA	2.20	0.41
1:K:24:LEU:CD1	1:K:81:GLN:HE21	2.20	0.41
1:L:12:LEU:HD22	1:L:80:ARG:CZ	2.51	0.41
1:L:272:ARG:NH1	1:L:315:GLU:O	2.53	0.41
1:L:332:THR:OG1	1:M:250:PRO:HG2	2.21	0.41
1:M:59:LEU:HD11	1:M:87:MET:CE	2.44	0.41
1:M:375:PHE:CB	1:M:600:ARG:HD3	2.48	0.41
1:M:442:ILE:O	1:M:496:THR:HA	2.21	0.41
1:M:534:GLY:HA2	1:M:577:ALA:CB	2.51	0.41
1:A:24:LEU:CG	1:A:27:ASP:N	2.83	0.41
1:A:161:ARG:HB3	1:A:353:ARG:HA	2.03	0.41
1:D:465:ASP:HB3	1:D:467:LEU:H	1.85	0.41
1:E:591:LYS:HE3	1:E:591:LYS:HA	2.02	0.41
1:F:57:THR:HA	1:F:60:TYR:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:474:ASP:HA	1:F:477:ARG:HE	1.86	0.41
1:G:99:ARG:HH12	1:G:101:ASP:CG	2.24	0.41
1:G:161:ARG:HB3	1:G:353:ARG:HA	2.03	0.41
1:G:415:SER:OG	1:G:425:SER:HA	2.20	0.41
1:I:108:PRO:HA	1:I:109:PRO:HD3	1.81	0.41
1:I:354:ASP:HA	1:I:355:PRO:HD3	1.85	0.41
1:K:80:ARG:HA	1:K:83:VAL:HG22	2.02	0.41
1:D:9:LEU:HG	1:D:72:PHE:HE2	1.68	0.41
1:D:266:MET:SD	1:D:323:TRP:HB3	2.60	0.41
1:E:60:TYR:O	1:E:64:TYR:HD2	2.04	0.41
1:E:99:ARG:HH12	1:E:101:ASP:CG	2.24	0.41
1:H:415:SER:OG	1:H:425:SER:HA	2.20	0.41
1:I:24:LEU:HG	1:I:25:PRO:HD2	2.02	0.41
1:I:292:LEU:HB3	1:I:371:HIS:CE1	2.56	0.41
1:I:415:SER:OG	1:I:425:SER:HA	2.20	0.41
1:J:48:PHE:CB	1:J:326:VAL:HG22	2.50	0.41
1:K:6:GLN:NE2	1:K:105:ILE:HA	2.35	0.41
1:K:9:LEU:HD11	1:K:69:PHE:CZ	2.56	0.41
1:K:22:GLU:O	1:K:81:GLN:O	2.38	0.41
1:K:88:PHE:O	1:K:92:VAL:HG22	2.20	0.41
1:K:415:SER:OG	1:K:425:SER:HA	2.20	0.41
1:L:591:LYS:HA	1:L:591:LYS:HE3	2.02	0.41
1:M:161:ARG:HB3	1:M:353:ARG:HA	2.03	0.41
1:M:499:ARG:NH1	1:M:503:ASP:O	2.53	0.41
1:C:275:ASP:HB2	1:F:268:ARG:NH1	2.36	0.41
1:C:474:ASP:HA	1:C:477:ARG:HE	1.86	0.41
1:D:107:VAL:HB	1:D:528:THR:HG23	2.03	0.41
1:D:140:ILE:HB	1:D:426:VAL:HG12	2.02	0.41
1:D:499:ARG:NH1	1:D:503:ASP:O	2.53	0.41
1:E:140:ILE:HB	1:E:426:VAL:HG12	2.02	0.41
1:E:534:GLY:HA2	1:E:577:ALA:CB	2.50	0.41
1:F:5:LYS:HG3	1:F:69:PHE:CZ	2.55	0.41
1:F:231:GLU:O	1:F:249:ARG:HD2	2.20	0.41
1:G:21:ARG:HD3	1:G:41:ARG:HD3	2.02	0.41
1:H:50:ALA:HB2	1:H:323:TRP:CH2	2.53	0.41
1:H:162:GLU:HG2	1:H:353:ARG:CB	2.47	0.41
1:H:292:LEU:HB3	1:H:371:HIS:CE1	2.56	0.41
1:I:161:ARG:HB3	1:I:353:ARG:HA	2.03	0.41
1:J:5:LYS:HG3	1:J:69:PHE:CZ	2.55	0.41
1:J:99:ARG:HH12	1:J:101:ASP:CG	2.24	0.41
1:J:243:GLY:HA2	1:K:125:ASN:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:591:LYS:HA	1:K:591:LYS:HE3	2.02	0.41
1:L:303:ASP:OD2	1:L:312:LYS:NZ	2.52	0.41
1:L:415:SER:OG	1:L:425:SER:HA	2.20	0.41
1:L:506:VAL:HG12	1:L:579:SER:HB2	2.02	0.41
1:L:534:GLY:HA2	1:L:577:ALA:CB	2.51	0.41
1:A:5:LYS:HG3	1:A:69:PHE:CZ	2.55	0.41
1:A:24:LEU:CG	1:A:81:GLN:NE2	2.79	0.41
1:A:24:LEU:CD2	1:A:82:ILE:HG22	2.40	0.41
1:A:474:ASP:HA	1:A:477:ARG:HE	1.86	0.41
1:A:512:ARG:CB	1:A:531:CYS:SG	3.08	0.41
1:A:596:PHE:HA	1:A:597:PRO:C	2.41	0.41
1:C:5:LYS:HG3	1:C:69:PHE:CZ	2.56	0.41
1:C:99:ARG:HH12	1:C:101:ASP:CG	2.24	0.41
1:C:473:PRO:HA	1:C:476:GLN:HB2	2.03	0.41
1:C:506:VAL:HG12	1:C:579:SER:HB2	2.02	0.41
1:C:511:VAL:HG22	1:C:512:ARG:H	1.86	0.41
1:D:48:PHE:HB2	1:D:326:VAL:HG22	2.02	0.41
1:D:67:LYS:HB3	1:D:71:ASP:HB2	2.02	0.41
1:E:48:PHE:HB2	1:E:326:VAL:HG22	2.02	0.41
1:E:596:PHE:HA	1:E:597:PRO:C	2.41	0.41
1:F:362:ARG:HD3	1:F:362:ARG:HA	1.84	0.41
1:G:107:VAL:HB	1:G:528:THR:HG23	2.03	0.41
1:H:268:ARG:HH11	1:M:271:GLU:HA	1.85	0.41
1:I:272:ARG:HB3	1:I:316:TYR:CE1	2.50	0.41
1:J:385:PHE:HA	1:J:386:PRO:HD3	1.90	0.41
1:J:499:ARG:NH1	1:J:503:ASP:O	2.53	0.41
1:K:5:LYS:HA	1:K:69:PHE:HE2	1.83	0.41
1:K:534:GLY:HA2	1:K:577:ALA:CB	2.50	0.41
1:L:60:TYR:O	1:L:64:TYR:HD2	2.04	0.41
1:L:104:GLY:HA2	1:L:525:GLU:C	2.42	0.41
1:L:575:SER:HA	1:L:582:GLY:O	2.21	0.41
1:M:82:ILE:HG23	1:M:83:VAL:N	2.36	0.41
1:C:76:CYS:HG	1:C:88:PHE:HE2	1.64	0.41
1:C:415:SER:OG	1:C:425:SER:HA	2.20	0.41
1:D:68:ASP:C	1:D:70:ASN:N	2.75	0.41
1:F:99:ARG:HH12	1:F:101:ASP:CG	2.24	0.41
1:F:292:LEU:HB3	1:F:371:HIS:CE1	2.55	0.41
1:G:60:TYR:O	1:G:64:TYR:HD2	2.04	0.41
1:G:272:ARG:HD3	1:G:316:TYR:CE1	2.56	0.41
1:G:555:VAL:O	1:G:615:MET:HA	2.21	0.41
1:H:57:THR:HA	1:H:60:TYR:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:474:ASP:HA	1:H:477:ARG:HE	1.85	0.41
1:H:596:PHE:HA	1:H:597:PRO:C	2.41	0.41
1:I:150:ILE:O	1:M:467:LEU:HG	2.21	0.41
1:I:303:ASP:OD2	1:I:312:LYS:NZ	2.52	0.41
1:J:261:VAL:HG12	1:J:262:ASP:O	2.21	0.41
1:K:474:ASP:HA	1:K:477:ARG:HE	1.86	0.41
1:M:292:LEU:HB3	1:M:371:HIS:CE1	2.55	0.41
1:A:57:THR:HA	1:A:60:TYR:CD2	2.56	0.40
1:C:57:THR:HA	1:C:60:TYR:CD2	2.56	0.40
1:C:140:ILE:HB	1:C:426:VAL:HG12	2.02	0.40
1:C:303:ASP:OD2	1:C:312:LYS:NZ	2.52	0.40
1:D:267:VAL:HG13	1:D:270:ARG:NH2	2.36	0.40
1:E:274:LEU:HB2	1:G:268:ARG:NH1	2.37	0.40
1:E:415:SER:OG	1:E:425:SER:HA	2.20	0.40
1:E:473:PRO:HA	1:E:476:GLN:HB2	2.03	0.40
1:F:69:PHE:CD1	1:F:102:CYS:SG	3.14	0.40
1:F:161:ARG:HB3	1:F:353:ARG:HA	2.02	0.40
1:G:323:TRP:O	1:G:326:VAL:HG23	2.22	0.40
1:G:530:TYR:CD2	1:G:531:CYS:SG	3.12	0.40
1:H:99:ARG:HH12	1:H:101:ASP:CG	2.24	0.40
1:H:175:ILE:HG21	1:H:528:THR:HG21	2.02	0.40
1:H:231:GLU:O	1:H:249:ARG:HD2	2.21	0.40
1:H:473:PRO:HA	1:H:476:GLN:HB2	2.03	0.40
1:H:555:VAL:O	1:H:615:MET:HA	2.21	0.40
1:I:186:MET:N	1:I:186:MET:SD	2.94	0.40
1:I:555:VAL:O	1:I:615:MET:HA	2.21	0.40
1:J:30:ASP:HB3	1:J:32:ARG:HB2	2.03	0.40
1:J:97:LEU:HG	1:J:528:THR:H	1.86	0.40
1:J:530:TYR:CD2	1:J:531:CYS:SG	3.14	0.40
1:K:2:VAL:C	1:K:5:LYS:HB3	2.41	0.40
1:L:292:LEU:HB3	1:L:371:HIS:CE1	2.55	0.40
1:L:474:ASP:HA	1:L:477:ARG:HE	1.86	0.40
1:M:104:GLY:HA2	1:M:525:GLU:C	2.42	0.40
1:A:48:PHE:HB2	1:A:326:VAL:HG22	2.02	0.40
1:A:140:ILE:HB	1:A:426:VAL:HG12	2.02	0.40
1:A:473:PRO:HA	1:A:476:GLN:HB2	2.03	0.40
1:A:555:VAL:O	1:A:615:MET:HA	2.21	0.40
1:C:24:LEU:HD11	1:C:78:GLN:HE21	1.87	0.40
1:C:517:LEU:HA	1:C:520:GLY:N	2.36	0.40
1:D:99:ARG:HH12	1:D:101:ASP:CG	2.24	0.40
1:D:172:HIS:CD2	1:D:532:SER:HG	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:555:VAL:O	1:E:615:MET:HA	2.21	0.40
1:G:57:THR:HA	1:G:60:TYR:CD2	2.56	0.40
1:G:63:LEU:HD22	1:G:91:ALA:CB	2.28	0.40
1:G:140:ILE:HB	1:G:426:VAL:HG12	2.02	0.40
1:G:267:VAL:HG13	1:G:270:ARG:NH2	2.36	0.40
1:I:272:ARG:NH1	1:I:315:GLU:O	2.54	0.40
1:K:97:LEU:HD11	1:K:528:THR:CG2	2.51	0.40
1:K:150:ILE:O	1:L:467:LEU:HD22	2.21	0.40
1:M:57:THR:HA	1:M:60:TYR:CD2	2.56	0.40
1:M:60:TYR:O	1:M:64:TYR:HD2	2.04	0.40
1:C:362:ARG:HD3	1:C:362:ARG:HA	1.84	0.40
1:D:190:LYS:HD3	1:D:190:LYS:HA	1.88	0.40
1:D:473:PRO:HA	1:D:476:GLN:HB2	2.03	0.40
1:E:16:LEU:HD12	1:E:19:LEU:HD12	2.04	0.40
1:F:60:TYR:O	1:F:64:TYR:HD2	2.03	0.40
1:G:80:ARG:HA	1:G:83:VAL:HG22	2.03	0.40
1:I:60:TYR:O	1:I:64:TYR:HD2	2.04	0.40
1:J:272:ARG:HB3	1:J:316:TYR:CE2	2.57	0.40
1:J:337:ARG:NH2	1:K:251:GLU:OE1	2.55	0.40
1:J:474:ASP:HA	1:J:477:ARG:HE	1.86	0.40
1:J:555:VAL:O	1:J:615:MET:HA	2.21	0.40
1:L:19:LEU:HD22	1:L:80:ARG:NH1	2.25	0.40
1:L:57:THR:HA	1:L:60:TYR:CD2	2.56	0.40
1:M:12:LEU:HD13	1:M:80:ARG:NH2	2.37	0.40
1:M:323:TRP:O	1:M:326:VAL:HG23	2.22	0.40
1:A:69:PHE:CE1	1:A:96:VAL:HG23	2.57	0.40
1:D:16:LEU:HD12	1:D:19:LEU:HD12	2.04	0.40
1:E:24:LEU:HD11	1:E:78:GLN:HE21	1.86	0.40
1:E:99:ARG:O	1:E:99:ARG:NH1	2.55	0.40
1:E:162:GLU:HG2	1:E:353:ARG:CB	2.47	0.40
1:E:499:ARG:NH1	1:E:503:ASP:O	2.53	0.40
1:F:107:VAL:HG21	1:F:528:THR:HG1	1.85	0.40
1:F:269:TRP:O	1:F:273:ILE:HG13	2.21	0.40
1:H:161:ARG:HB3	1:H:353:ARG:HA	2.03	0.40
1:H:323:TRP:O	1:H:326:VAL:HG23	2.22	0.40
1:L:323:TRP:O	1:L:326:VAL:HG23	2.22	0.40
1:A:323:TRP:O	1:A:326:VAL:HG23	2.22	0.40
1:C:161:ARG:HB3	1:C:353:ARG:HA	2.03	0.40
1:C:555:VAL:O	1:C:615:MET:HA	2.21	0.40
1:D:323:TRP:O	1:D:326:VAL:HG23	2.22	0.40
1:F:99:ARG:NH1	1:F:99:ARG:O	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:529:GLU:HA	1:F:533:CYS:HB2	2.03	0.40
1:G:175:ILE:HG21	1:G:528:THR:HG21	2.02	0.40
1:G:530:TYR:HD2	1:G:531:CYS:HG	1.62	0.40
1:H:107:VAL:HB	1:H:528:THR:HG23	2.04	0.40
1:H:506:VAL:HG12	1:H:579:SER:HB2	2.03	0.40
1:I:160:PHE:HD1	1:I:539:MET:HE2	1.86	0.40
1:I:362:ARG:HD3	1:I:362:ARG:HA	1.84	0.40
1:I:473:PRO:HA	1:I:476:GLN:HB2	2.03	0.40
1:J:231:GLU:O	1:J:249:ARG:HD2	2.21	0.40
1:J:506:VAL:HG12	1:J:579:SER:HB2	2.04	0.40
1:K:67:LYS:HB3	1:K:71:ASP:HB3	2.03	0.40
1:L:5:LYS:CD	1:L:69:PHE:CE1	3.04	0.40
1:L:16:LEU:HD12	1:L:19:LEU:HD12	2.04	0.40
1:L:190:LYS:HA	1:L:190:LYS:HD3	1.88	0.40
1:L:531:CYS:SG	1:L:532:SER:N	2.95	0.40
1:L:555:VAL:O	1:L:615:MET:HA	2.21	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	624/626 (100%)	527 (84%)	77 (12%)	20 (3%)	4 26
1	C	622/626 (99%)	526 (85%)	84 (14%)	12 (2%)	8 38
1	D	624/626 (100%)	526 (84%)	82 (13%)	16 (3%)	5 31
1	E	624/626 (100%)	529 (85%)	81 (13%)	14 (2%)	6 35
1	F	624/626 (100%)	529 (85%)	77 (12%)	18 (3%)	4 29
1	G	624/626 (100%)	532 (85%)	76 (12%)	16 (3%)	5 31
1	H	624/626 (100%)	528 (85%)	78 (12%)	18 (3%)	4 29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	I	622/626 (99%)	529 (85%)	79 (13%)	14 (2%)	6 34
1	J	624/626 (100%)	533 (85%)	75 (12%)	16 (3%)	5 31
1	K	624/626 (100%)	532 (85%)	81 (13%)	11 (2%)	8 40
1	L	624/626 (100%)	531 (85%)	81 (13%)	12 (2%)	8 38
1	M	624/626 (100%)	526 (84%)	82 (13%)	16 (3%)	5 31
All	All	7484/7512 (100%)	6348 (85%)	953 (13%)	183 (2%)	9 33

All (183) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	LYS
1	A	351	SER
1	A	530	TYR
1	C	34	LYS
1	C	351	SER
1	D	34	LYS
1	D	45	PHE
1	D	351	SER
1	D	530	TYR
1	E	34	LYS
1	E	351	SER
1	F	34	LYS
1	F	351	SER
1	F	524	SER
1	G	34	LYS
1	G	351	SER
1	G	530	TYR
1	H	34	LYS
1	H	351	SER
1	H	530	TYR
1	I	25	PRO
1	I	285	LYS
1	I	351	SER
1	J	32	ARG
1	J	311	SER
1	J	351	SER
1	J	530	TYR
1	K	34	LYS
1	K	351	SER
1	K	530	TYR

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Mol	Chain	Res	Type
1	L	34	LYS
1	L	351	SER
1	L	574	CYS
1	M	34	LYS
1	M	351	SER
1	M	530	TYR
1	A	32	ARG
1	A	144	ALA
1	A	524	SER
1	A	573	VAL
1	C	448	SER
1	D	41	ARG
1	D	82	ILE
1	D	573	VAL
1	E	573	VAL
1	F	16	LEU
1	F	17	THR
1	F	20	THR
1	F	27	ASP
1	F	573	VAL
1	G	524	SER
1	G	573	VAL
1	H	524	SER
1	H	573	VAL
1	I	527	SER
1	I	573	VAL
1	J	573	VAL
1	K	525	GLU
1	K	573	VAL
1	M	45	PHE
1	M	81	GLN
1	M	524	SER
1	M	573	VAL
1	A	15	HIS
1	A	44	LEU
1	A	532	SER
1	C	15	HIS
1	C	44	LEU
1	D	15	HIS
1	E	15	HIS
1	E	44	LEU
1	F	15	HIS

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Mol	Chain	Res	Type
1	F	44	LEU
1	F	530	TYR
1	G	15	HIS
1	G	311	SER
1	H	15	HIS
1	H	44	LEU
1	I	44	LEU
1	I	525	GLU
1	J	15	HIS
1	J	28	GLN
1	J	31	GLU
1	L	15	HIS
1	L	44	LEU
1	M	15	HIS
1	A	31	GLU
1	A	181	TRP
1	A	344	VAL
1	A	571	ASN
1	C	181	TRP
1	C	344	VAL
1	C	415	SER
1	D	37	GLY
1	D	181	TRP
1	D	344	VAL
1	D	415	SER
1	D	524	SER
1	D	571	ASN
1	E	181	TRP
1	E	344	VAL
1	E	415	SER
1	E	571	ASN
1	F	181	TRP
1	F	344	VAL
1	F	415	SER
1	F	571	ASN
1	G	37	GLY
1	G	67	LYS
1	G	181	TRP
1	G	344	VAL
1	G	415	SER
1	G	571	ASN
1	H	22	GLU

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Mol	Chain	Res	Type
1	H	181	TRP
1	H	344	VAL
1	H	415	SER
1	H	571	ASN
1	I	37	GLY
1	I	344	VAL
1	I	415	SER
1	J	181	TRP
1	J	304	ILE
1	J	344	VAL
1	J	415	SER
1	J	571	ASN
1	K	181	TRP
1	K	344	VAL
1	K	415	SER
1	K	571	ASN
1	L	181	TRP
1	L	344	VAL
1	L	415	SER
1	L	524	SER
1	M	181	TRP
1	M	344	VAL
1	M	415	SER
1	M	571	ASN
1	A	415	SER
1	A	521	GLU
1	C	45	PHE
1	D	83	VAL
1	E	37	GLY
1	E	45	PHE
1	E	524	SER
1	F	45	PHE
1	G	82	ILE
1	H	45	PHE
1	H	81	GLN
1	I	45	PHE
1	I	181	TRP
1	I	523	VAL
1	J	37	GLY
1	L	37	GLY
1	L	45	PHE
1	M	69	PHE

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Mol	Chain	Res	Type
1	M	70	ASN
1	A	37	GLY
1	A	45	PHE
1	A	285	LYS
1	C	285	LYS
1	E	285	LYS
1	F	285	LYS
1	G	285	LYS
1	H	37	GLY
1	H	285	LYS
1	J	285	LYS
1	K	285	LYS
1	M	82	ILE
1	H	82	ILE
1	K	377	PRO
1	M	377	PRO
1	A	377	PRO
1	C	377	PRO
1	C	449	GLY
1	D	377	PRO
1	E	150	ILE
1	F	377	PRO
1	G	377	PRO
1	H	377	PRO
1	I	377	PRO
1	J	377	PRO
1	L	377	PRO

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	556/556 (100%)	496 (89%)	60 (11%)	6 23
1	C	556/556 (100%)	508 (91%)	48 (9%)	10 32
1	D	556/556 (100%)	503 (90%)	53 (10%)	8 27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	556/556 (100%)	506 (91%)	50 (9%)	9 30
1	F	556/556 (100%)	505 (91%)	51 (9%)	9 29
1	G	556/556 (100%)	508 (91%)	48 (9%)	10 32
1	H	556/556 (100%)	505 (91%)	51 (9%)	9 29
1	I	556/556 (100%)	504 (91%)	52 (9%)	8 28
1	J	556/556 (100%)	503 (90%)	53 (10%)	8 27
1	K	556/556 (100%)	505 (91%)	51 (9%)	9 29
1	L	556/556 (100%)	504 (91%)	52 (9%)	8 28
1	M	556/556 (100%)	504 (91%)	52 (9%)	8 28
All	All	6672/6672 (100%)	6051 (91%)	621 (9%)	12 28

All (621) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ASP
1	A	11	PRO
1	A	22	GLU
1	A	24	LEU
1	A	30	ASP
1	A	57	THR
1	A	78	GLN
1	A	84	ASN
1	A	85	GLU
1	A	96	VAL
1	A	97	LEU
1	A	99	ARG
1	A	100	GLU
1	A	101	ASP
1	A	105	ILE
1	A	111	GLN
1	A	122	GLU
1	A	134	HIS
1	A	142	VAL
1	A	220	MET
1	A	251	GLU
1	A	264	GLN
1	A	265	ASP
1	A	268	ARG
1	A	271	GLU

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Mol	Chain	Res	Type
1	A	305	ILE
1	A	319	SER
1	A	326	VAL
1	A	347	ASP
1	A	349	SER
1	A	353	ARG
1	A	379	THR
1	A	398	LYS
1	A	405	THR
1	A	407	ILE
1	A	414	LEU
1	A	418	ILE
1	A	425	SER
1	A	426	VAL
1	A	439	THR
1	A	442	ILE
1	A	455	THR
1	A	465	ASP
1	A	469	ASN
1	A	483	LEU
1	A	501	HIS
1	A	507	THR
1	A	512	ARG
1	A	516	GLN
1	A	528	THR
1	A	532	SER
1	A	545	SER
1	A	554	PHE
1	A	564	THR
1	A	570	GLU
1	A	578	VAL
1	A	584	ARG
1	A	591	LYS
1	A	601	LYS
1	A	620	ILE
1	C	4	ASP
1	C	11	PRO
1	C	57	THR
1	C	85	GLU
1	C	96	VAL
1	C	97	LEU
1	C	99	ARG

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Mol	Chain	Res	Type
1	C	101	ASP
1	C	105	ILE
1	C	111	GLN
1	C	122	GLU
1	C	220	MET
1	C	251	GLU
1	C	265	ASP
1	C	268	ARG
1	C	271	GLU
1	C	305	ILE
1	C	319	SER
1	C	326	VAL
1	C	347	ASP
1	C	349	SER
1	C	353	ARG
1	C	379	THR
1	C	398	LYS
1	C	405	THR
1	C	407	ILE
1	C	418	ILE
1	C	425	SER
1	C	426	VAL
1	C	439	THR
1	C	442	ILE
1	C	455	THR
1	C	465	ASP
1	C	467	LEU
1	C	469	ASN
1	C	483	LEU
1	C	501	HIS
1	C	507	THR
1	C	516	GLN
1	C	545	SER
1	C	554	PHE
1	C	564	THR
1	C	578	VAL
1	C	584	ARG
1	C	591	LYS
1	C	601	LYS
1	C	603	GLU
1	C	620	ILE
1	D	4	ASP

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Mol	Chain	Res	Type
1	D	11	PRO
1	D	41	ARG
1	D	57	THR
1	D	84	ASN
1	D	85	GLU
1	D	96	VAL
1	D	97	LEU
1	D	99	ARG
1	D	101	ASP
1	D	105	ILE
1	D	111	GLN
1	D	122	GLU
1	D	220	MET
1	D	262	ASP
1	D	265	ASP
1	D	271	GLU
1	D	305	ILE
1	D	309	ASP
1	D	319	SER
1	D	326	VAL
1	D	347	ASP
1	D	349	SER
1	D	353	ARG
1	D	379	THR
1	D	398	LYS
1	D	405	THR
1	D	407	ILE
1	D	418	ILE
1	D	425	SER
1	D	426	VAL
1	D	439	THR
1	D	442	ILE
1	D	455	THR
1	D	465	ASP
1	D	469	ASN
1	D	483	LEU
1	D	501	HIS
1	D	507	THR
1	D	512	ARG
1	D	516	GLN
1	D	528	THR
1	D	532	SER

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Mol	Chain	Res	Type
1	D	545	SER
1	D	554	PHE
1	D	564	THR
1	D	570	GLU
1	D	578	VAL
1	D	584	ARG
1	D	591	LYS
1	D	601	LYS
1	D	603	GLU
1	D	620	ILE
1	E	4	ASP
1	E	11	PRO
1	E	38	ILE
1	E	57	THR
1	E	85	GLU
1	E	96	VAL
1	E	97	LEU
1	E	99	ARG
1	E	101	ASP
1	E	105	ILE
1	E	111	GLN
1	E	122	GLU
1	E	220	MET
1	E	264	GLN
1	E	265	ASP
1	E	271	GLU
1	E	305	ILE
1	E	319	SER
1	E	326	VAL
1	E	347	ASP
1	E	349	SER
1	E	353	ARG
1	E	379	THR
1	E	398	LYS
1	E	405	THR
1	E	407	ILE
1	E	418	ILE
1	E	425	SER
1	E	426	VAL
1	E	439	THR
1	E	442	ILE
1	E	455	THR

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Mol	Chain	Res	Type
1	E	465	ASP
1	E	469	ASN
1	E	483	LEU
1	E	501	HIS
1	E	507	THR
1	E	512	ARG
1	E	516	GLN
1	E	532	SER
1	E	545	SER
1	E	554	PHE
1	E	564	THR
1	E	570	GLU
1	E	578	VAL
1	E	584	ARG
1	E	591	LYS
1	E	601	LYS
1	E	603	GLU
1	E	620	ILE
1	F	4	ASP
1	F	11	PRO
1	F	17	THR
1	F	20	THR
1	F	24	LEU
1	F	38	ILE
1	F	57	THR
1	F	85	GLU
1	F	96	VAL
1	F	97	LEU
1	F	99	ARG
1	F	101	ASP
1	F	105	ILE
1	F	111	GLN
1	F	122	GLU
1	F	220	MET
1	F	265	ASP
1	F	271	GLU
1	F	305	ILE
1	F	319	SER
1	F	326	VAL
1	F	347	ASP
1	F	349	SER
1	F	353	ARG

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Mol	Chain	Res	Type
1	F	379	THR
1	F	398	LYS
1	F	405	THR
1	F	407	ILE
1	F	418	ILE
1	F	425	SER
1	F	426	VAL
1	F	439	THR
1	F	442	ILE
1	F	455	THR
1	F	465	ASP
1	F	469	ASN
1	F	483	LEU
1	F	501	HIS
1	F	507	THR
1	F	528	THR
1	F	529	GLU
1	F	545	SER
1	F	554	PHE
1	F	564	THR
1	F	570	GLU
1	F	578	VAL
1	F	584	ARG
1	F	591	LYS
1	F	601	LYS
1	F	603	GLU
1	F	620	ILE
1	G	4	ASP
1	G	11	PRO
1	G	57	THR
1	G	85	GLU
1	G	96	VAL
1	G	97	LEU
1	G	99	ARG
1	G	101	ASP
1	G	105	ILE
1	G	111	GLN
1	G	122	GLU
1	G	220	MET
1	G	265	ASP
1	G	271	GLU
1	G	305	ILE

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Mol	Chain	Res	Type
1	G	319	SER
1	G	326	VAL
1	G	347	ASP
1	G	349	SER
1	G	353	ARG
1	G	379	THR
1	G	398	LYS
1	G	405	THR
1	G	407	ILE
1	G	418	ILE
1	G	425	SER
1	G	426	VAL
1	G	439	THR
1	G	442	ILE
1	G	455	THR
1	G	465	ASP
1	G	469	ASN
1	G	483	LEU
1	G	501	HIS
1	G	507	THR
1	G	512	ARG
1	G	528	THR
1	G	532	SER
1	G	545	SER
1	G	554	PHE
1	G	564	THR
1	G	570	GLU
1	G	578	VAL
1	G	584	ARG
1	G	591	LYS
1	G	601	LYS
1	G	603	GLU
1	G	620	ILE
1	H	4	ASP
1	H	5	LYS
1	H	11	PRO
1	H	22	GLU
1	H	57	THR
1	H	85	GLU
1	H	96	VAL
1	H	97	LEU
1	H	99	ARG

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Mol	Chain	Res	Type
1	H	101	ASP
1	H	105	ILE
1	H	111	GLN
1	H	122	GLU
1	H	220	MET
1	H	265	ASP
1	H	268	ARG
1	H	305	ILE
1	H	319	SER
1	H	326	VAL
1	H	347	ASP
1	H	349	SER
1	H	353	ARG
1	H	379	THR
1	H	398	LYS
1	H	405	THR
1	H	407	ILE
1	H	418	ILE
1	H	425	SER
1	H	426	VAL
1	H	439	THR
1	H	442	ILE
1	H	455	THR
1	H	465	ASP
1	H	469	ASN
1	H	483	LEU
1	H	501	HIS
1	H	507	THR
1	H	512	ARG
1	H	516	GLN
1	H	528	THR
1	H	532	SER
1	H	545	SER
1	H	554	PHE
1	H	564	THR
1	H	570	GLU
1	H	578	VAL
1	H	584	ARG
1	H	591	LYS
1	H	601	LYS
1	H	603	GLU
1	H	620	ILE

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Mol	Chain	Res	Type
1	I	4	ASP
1	I	11	PRO
1	I	15	HIS
1	I	25	PRO
1	I	57	THR
1	I	85	GLU
1	I	96	VAL
1	I	97	LEU
1	I	99	ARG
1	I	101	ASP
1	I	105	ILE
1	I	111	GLN
1	I	122	GLU
1	I	186	MET
1	I	220	MET
1	I	264	GLN
1	I	265	ASP
1	I	271	GLU
1	I	305	ILE
1	I	319	SER
1	I	326	VAL
1	I	347	ASP
1	I	349	SER
1	I	353	ARG
1	I	379	THR
1	I	398	LYS
1	I	405	THR
1	I	407	ILE
1	I	418	ILE
1	I	425	SER
1	I	426	VAL
1	I	439	THR
1	I	442	ILE
1	I	455	THR
1	I	465	ASP
1	I	469	ASN
1	I	483	LEU
1	I	501	HIS
1	I	507	THR
1	I	516	GLN
1	I	524	SER
1	I	530	TYR

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Mol	Chain	Res	Type
1	I	545	SER
1	I	554	PHE
1	I	564	THR
1	I	570	GLU
1	I	578	VAL
1	I	584	ARG
1	I	591	LYS
1	I	601	LYS
1	I	603	GLU
1	I	620	ILE
1	J	4	ASP
1	J	11	PRO
1	J	34	LYS
1	J	38	ILE
1	J	57	THR
1	J	85	GLU
1	J	96	VAL
1	J	97	LEU
1	J	99	ARG
1	J	101	ASP
1	J	103	LYS
1	J	105	ILE
1	J	111	GLN
1	J	122	GLU
1	J	220	MET
1	J	251	GLU
1	J	265	ASP
1	J	304	ILE
1	J	305	ILE
1	J	309	ASP
1	J	319	SER
1	J	326	VAL
1	J	347	ASP
1	J	349	SER
1	J	353	ARG
1	J	379	THR
1	J	398	LYS
1	J	405	THR
1	J	407	ILE
1	J	418	ILE
1	J	425	SER
1	J	426	VAL

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Mol	Chain	Res	Type
1	J	439	THR
1	J	442	ILE
1	J	455	THR
1	J	465	ASP
1	J	469	ASN
1	J	483	LEU
1	J	501	HIS
1	J	507	THR
1	J	512	ARG
1	J	532	SER
1	J	533	CYS
1	J	545	SER
1	J	554	PHE
1	J	564	THR
1	J	570	GLU
1	J	578	VAL
1	J	584	ARG
1	J	591	LYS
1	J	601	LYS
1	J	603	GLU
1	J	620	ILE
1	K	4	ASP
1	K	5	LYS
1	K	11	PRO
1	K	57	THR
1	K	63	LEU
1	K	84	ASN
1	K	85	GLU
1	K	96	VAL
1	K	97	LEU
1	K	99	ARG
1	K	101	ASP
1	K	105	ILE
1	K	111	GLN
1	K	122	GLU
1	K	220	MET
1	K	265	ASP
1	K	268	ARG
1	K	305	ILE
1	K	319	SER
1	K	326	VAL
1	K	347	ASP

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Mol	Chain	Res	Type
1	K	349	SER
1	K	353	ARG
1	K	379	THR
1	K	398	LYS
1	K	405	THR
1	K	407	ILE
1	K	418	ILE
1	K	425	SER
1	K	426	VAL
1	K	439	THR
1	K	442	ILE
1	K	455	THR
1	K	465	ASP
1	K	469	ASN
1	K	483	LEU
1	K	501	HIS
1	K	507	THR
1	K	512	ARG
1	K	516	GLN
1	K	532	SER
1	K	545	SER
1	K	554	PHE
1	K	564	THR
1	K	570	GLU
1	K	578	VAL
1	K	584	ARG
1	K	591	LYS
1	K	601	LYS
1	K	603	GLU
1	K	620	ILE
1	L	4	ASP
1	L	5	LYS
1	L	11	PRO
1	L	57	THR
1	L	85	GLU
1	L	96	VAL
1	L	97	LEU
1	L	99	ARG
1	L	101	ASP
1	L	105	ILE
1	L	111	GLN
1	L	122	GLU

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Mol	Chain	Res	Type
1	L	220	MET
1	L	265	ASP
1	L	268	ARG
1	L	271	GLU
1	L	275	ASP
1	L	305	ILE
1	L	319	SER
1	L	326	VAL
1	L	347	ASP
1	L	349	SER
1	L	353	ARG
1	L	379	THR
1	L	398	LYS
1	L	405	THR
1	L	407	ILE
1	L	418	ILE
1	L	425	SER
1	L	426	VAL
1	L	439	THR
1	L	442	ILE
1	L	455	THR
1	L	465	ASP
1	L	467	LEU
1	L	469	ASN
1	L	483	LEU
1	L	501	HIS
1	L	507	THR
1	L	516	GLN
1	L	527	SER
1	L	528	THR
1	L	530	TYR
1	L	545	SER
1	L	554	PHE
1	L	571	ASN
1	L	578	VAL
1	L	584	ARG
1	L	591	LYS
1	L	601	LYS
1	L	603	GLU
1	L	620	ILE
1	M	4	ASP
1	M	11	PRO

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Mol	Chain	Res	Type
1	M	57	THR
1	M	68	ASP
1	M	85	GLU
1	M	96	VAL
1	M	97	LEU
1	M	99	ARG
1	M	101	ASP
1	M	105	ILE
1	M	111	GLN
1	M	122	GLU
1	M	220	MET
1	M	251	GLU
1	M	264	GLN
1	M	265	ASP
1	M	271	GLU
1	M	305	ILE
1	M	319	SER
1	M	326	VAL
1	M	347	ASP
1	M	349	SER
1	M	353	ARG
1	M	379	THR
1	M	398	LYS
1	M	405	THR
1	M	407	ILE
1	M	418	ILE
1	M	425	SER
1	M	426	VAL
1	M	439	THR
1	M	442	ILE
1	M	455	THR
1	M	465	ASP
1	M	469	ASN
1	M	483	LEU
1	M	501	HIS
1	M	507	THR
1	M	512	ARG
1	M	516	GLN
1	M	528	THR
1	M	532	SER
1	M	545	SER
1	M	554	PHE

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Mol	Chain	Res	Type
1	M	564	THR
1	M	570	GLU
1	M	578	VAL
1	M	584	ARG
1	M	591	LYS
1	M	601	LYS
1	M	603	GLU
1	M	620	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	GLN
1	A	84	ASN
1	A	133	ASN
1	A	169	HIS
1	A	431	HIS
1	C	81	GLN
1	C	278	ASN
1	C	431	HIS
1	D	81	GLN
1	D	125	ASN
1	D	169	HIS
1	D	278	ASN
1	D	431	HIS
1	E	81	GLN
1	E	125	ASN
1	E	169	HIS
1	E	278	ASN
1	E	431	HIS
1	F	81	GLN
1	F	169	HIS
1	F	278	ASN
1	F	431	HIS
1	G	78	GLN
1	G	81	GLN
1	G	133	ASN
1	G	169	HIS
1	G	278	ASN
1	G	431	HIS
1	H	169	HIS
1	H	224	HIS

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Mol	Chain	Res	Type
1	H	278	ASN
1	H	431	HIS
1	I	81	GLN
1	I	125	ASN
1	I	278	ASN
1	I	288	ASN
1	I	431	HIS
1	J	81	GLN
1	J	125	ASN
1	J	169	HIS
1	J	278	ASN
1	J	419	ASN
1	J	431	HIS
1	K	81	GLN
1	K	125	ASN
1	K	169	HIS
1	K	278	ASN
1	K	419	ASN
1	K	431	HIS
1	L	81	GLN
1	L	133	ASN
1	L	169	HIS
1	L	172	HIS
1	L	278	ASN
1	L	431	HIS
1	M	81	GLN
1	M	169	HIS
1	M	278	ASN
1	M	431	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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	I	2
1	C	2
1	A	1
1	E	1
1	F	1
1	H	1
1	L	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	34:LYS	C	35:GLY	N	4.15
1	C	519:ALA	C	520:GLY	N	2.61
1	A	44:LEU	C	45:PHE	N	1.71
1	C	44:LEU	C	45:PHE	N	1.71
1	E	44:LEU	C	45:PHE	N	1.71
1	F	44:LEU	C	45:PHE	N	1.71
1	H	44:LEU	C	45:PHE	N	1.71
1	I	44:LEU	C	45:PHE	N	1.71
1	L	44:LEU	C	45:PHE	N	1.71

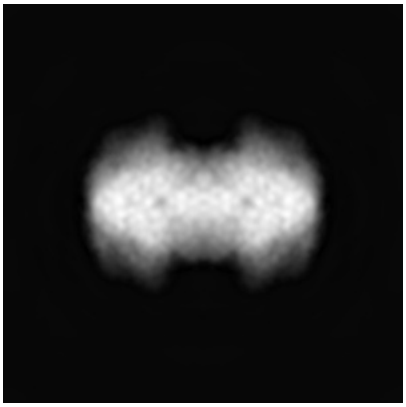
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-5101. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

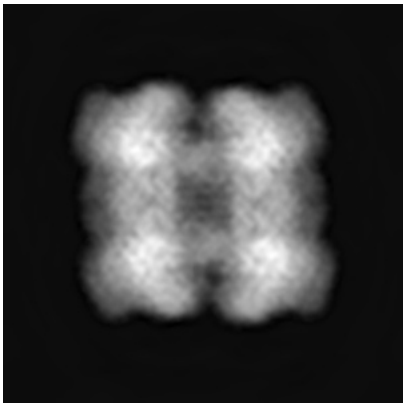
6.1 Orthogonal projections

6.1.1 Primary map



X

Y

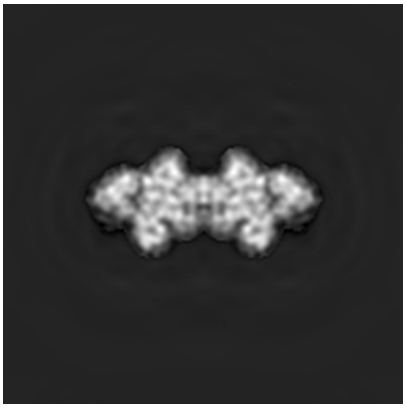


Z

The images above show the map projected in three orthogonal directions.

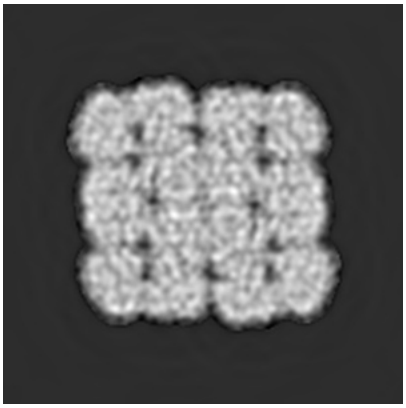
6.2 Central slices

6.2.1 Primary map



X Index: 104

Y Index: 104

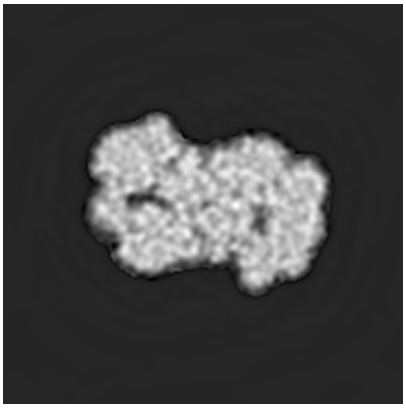


Z Index: 104

The images above show central slices of the map in three orthogonal directions.

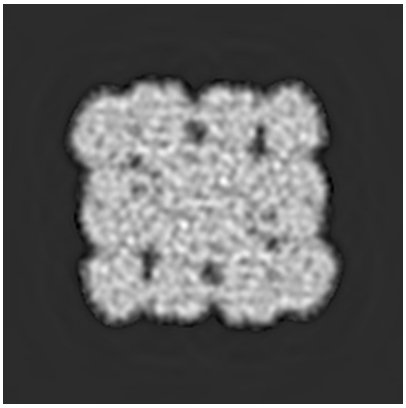
6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 75

Y Index: 133

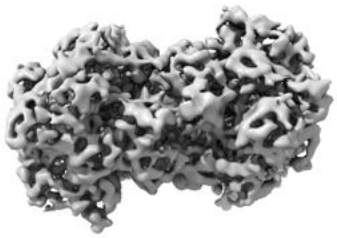


Z Index: 107

The images above show the largest variance slices of the map in three orthogonal directions.

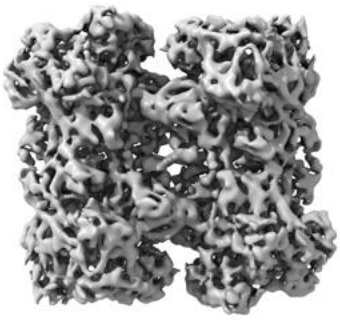
6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.16. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

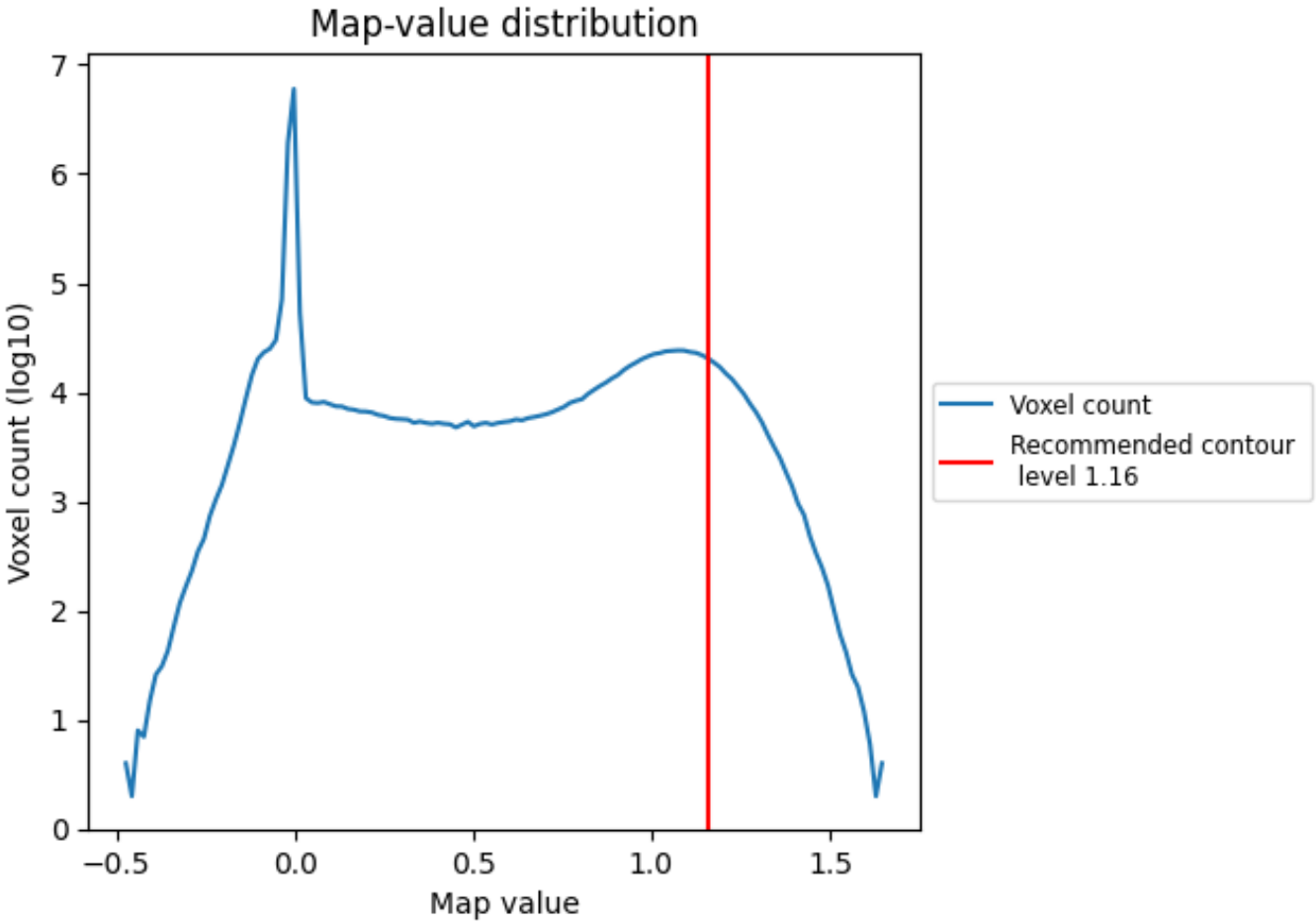
6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

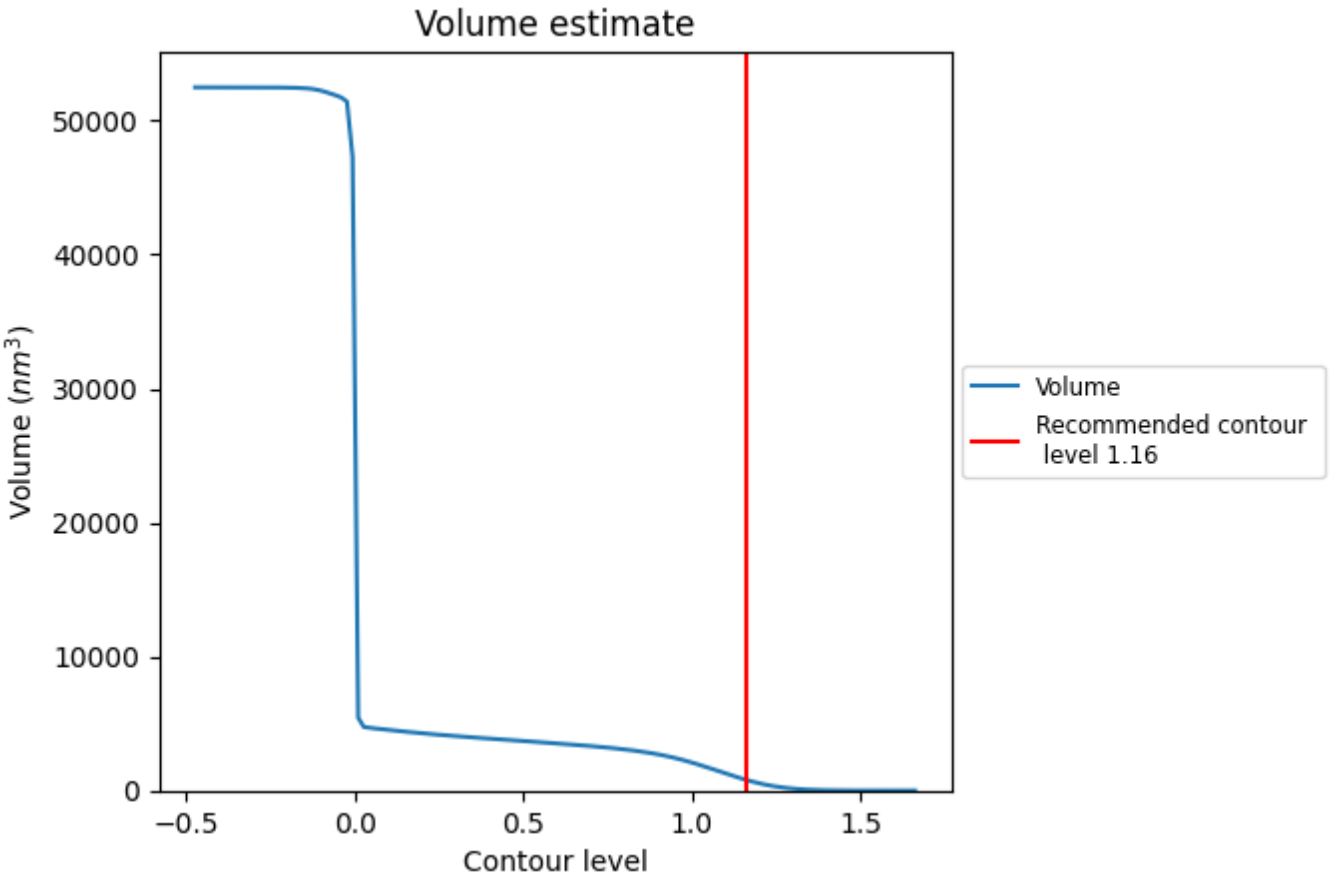
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

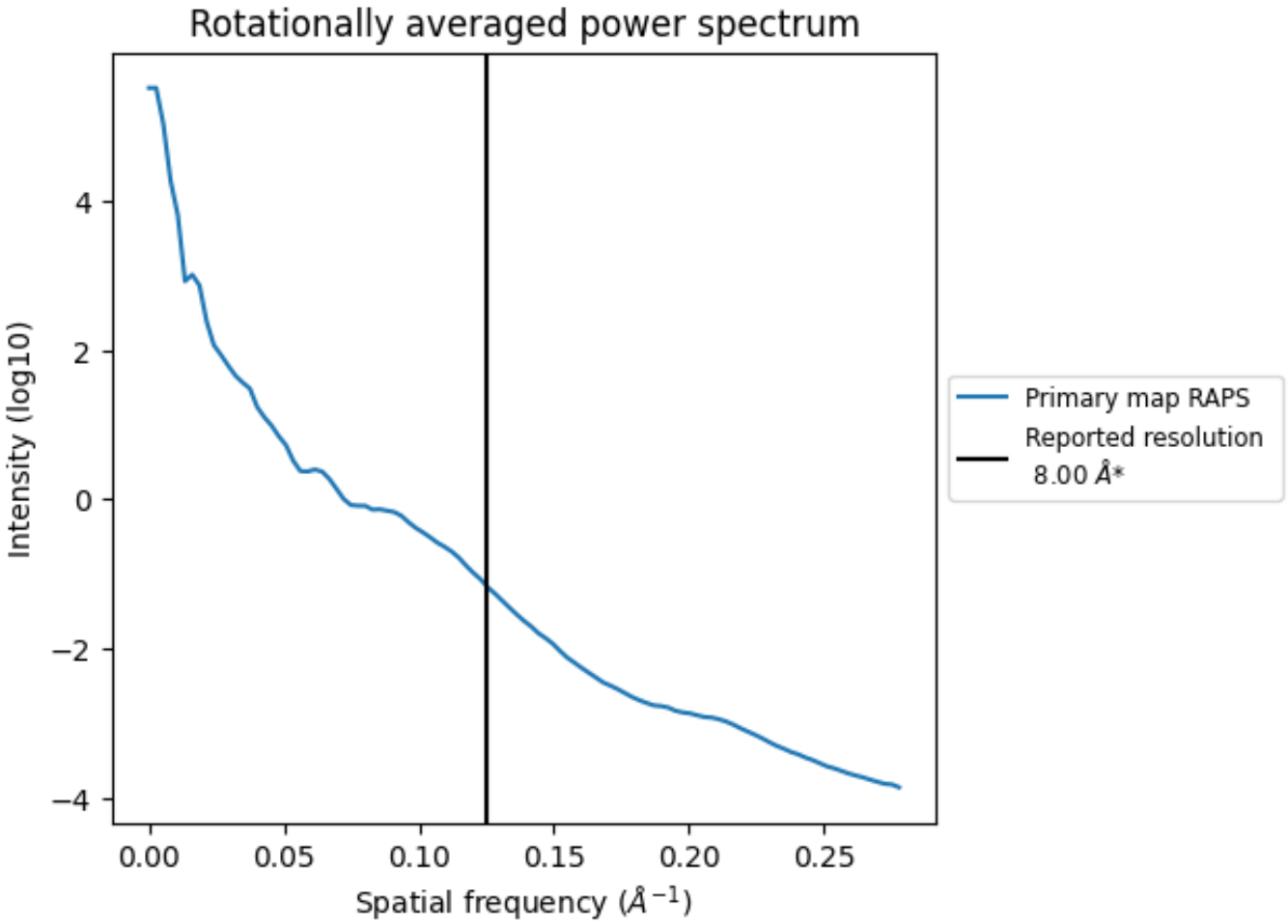
7.2 Volume estimate



The volume at the recommended contour level is 811 nm^3; this corresponds to an approximate mass of 733 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.125 Å^{-1}

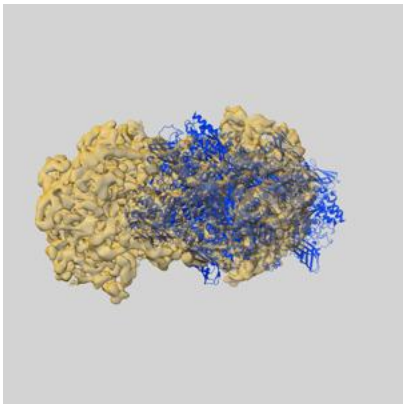
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

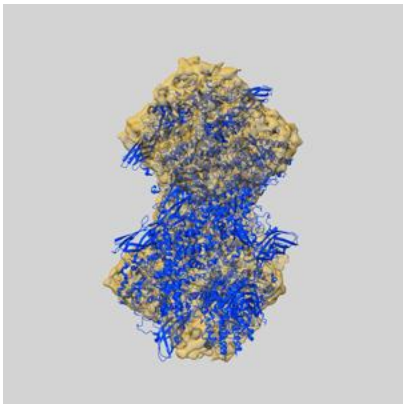
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-5101 and PDB model 3IXW. Per-residue inclusion information can be found in section 3 on page 5.

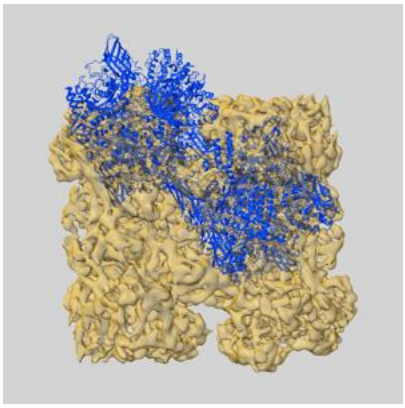
9.1 Map-model overlay



X



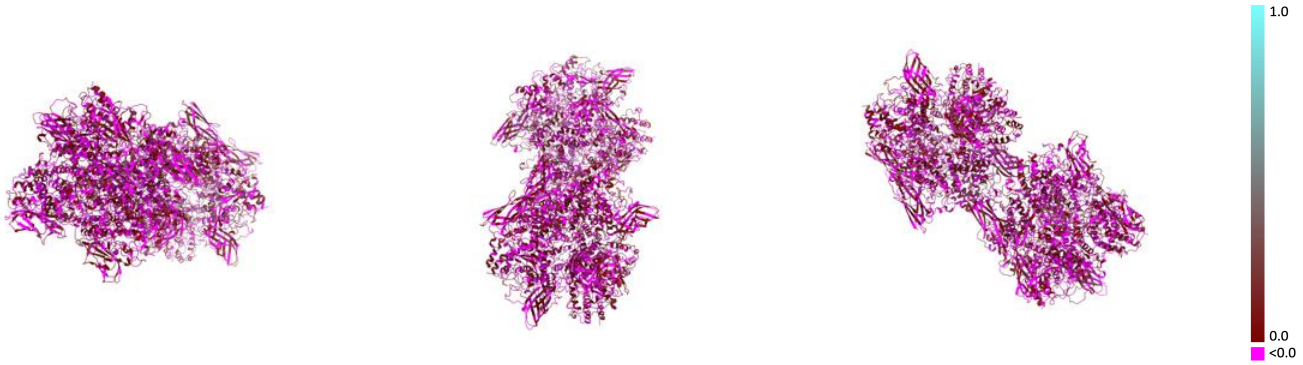
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.16 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

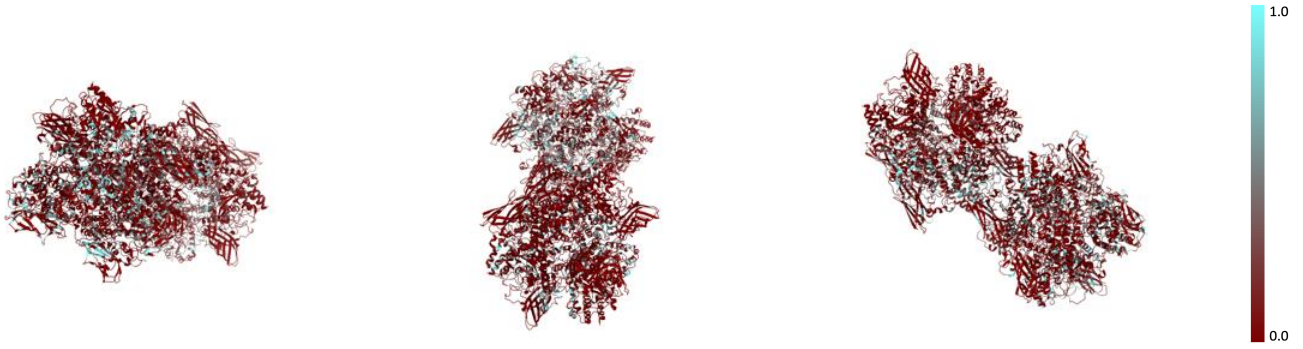
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

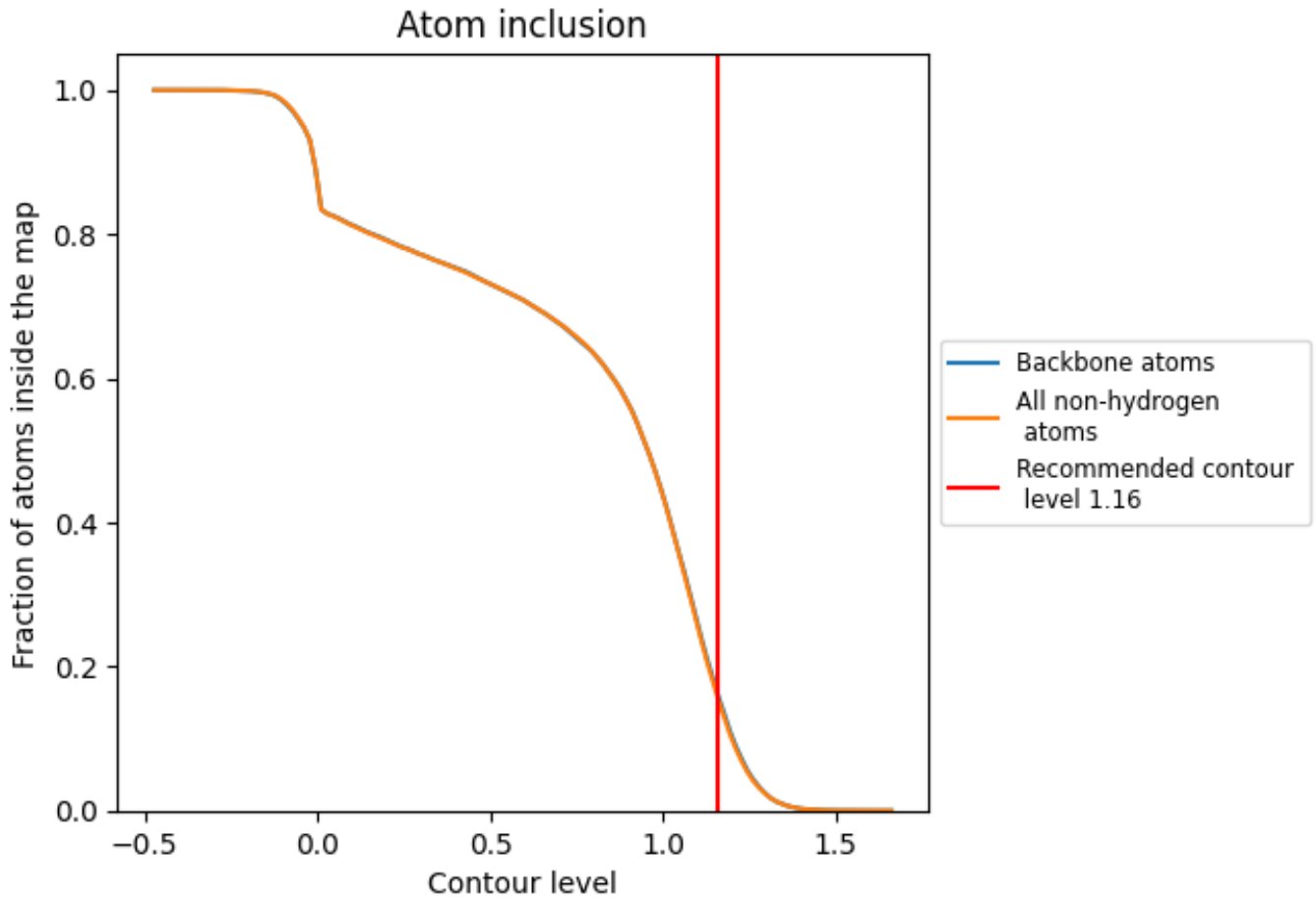
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.16).

9.4 Atom inclusion (i)



At the recommended contour level, 16% of all backbone atoms, 16% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (1.16) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.1556	0.0080
A	0.2052	-0.0000
C	0.1646	0.0050
D	0.2167	0.0110
E	0.2153	0.0120
F	0.1752	0.0040
G	0.0886	0.0030
H	0.1672	0.0100
I	0.2075	0.0090
J	0.1960	0.0100
K	0.0610	0.0080
L	0.0959	0.0110
M	0.0576	0.0090