Full wwPDB EM Validation Report ⓘ

Nov 29, 2022 – 10:50 AM JST

PDB ID	:	7W85
EMDB ID	:	EMD-32352
Title	:	Structural of the filamentous Escherichia coli glutamine synthetase
Authors	:	Huang, P.-C.; Chen, S.-K.; Wu, K.-P.
Deposited on	:	2021-12-07
Resolution	:	2.94 Å(reported)
Based on initial model	:	2LGS

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:

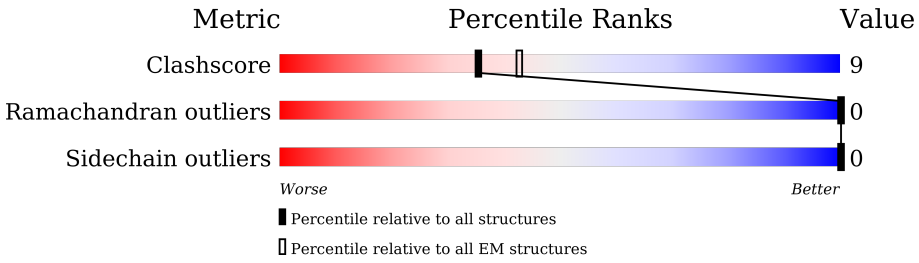
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 2.94 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	469	7% 72% 20% 7%
1	B	469	7% 73% 19% 7%
1	C	469	7% 74% 19% 7%
1	D	469	7% 74% 19% 7%
1	E	469	7% 73% 19% 7%
1	F	469	7% 74% 19% 7%
1	G	469	7% 73% 19% 7%
1	H	469	7% 72% 20% 7%

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Mol	Chain	Length	Quality of chain
1	I	469	6% 72% 21% 7%
1	J	469	6% 73% 20% 7%
1	K	469	6% 72% 21% 7%
1	L	469	6% 73% 19% 7%
1	M	469	89% 73% 20% 7%
1	N	469	89% 74% 18% 7%
1	O	469	89% 73% 20% 7%
1	P	469	89% 73% 19% 7%
1	Q	469	89% 73% 20% 7%
1	R	469	89% 72% 21% 7%
1	S	469	93% 72% 21% 7%
1	U	469	93% 73% 19% 7%
1	V	469	93% 72% 20% 7%
1	W	469	93% 73% 19% 7%
1	X	469	93% 72% 21% 7%
1	Y	469	93% 75% 18% 7%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 81522 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Glutamine synthetase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	435	Total	C	N	O	S	0	0
			3395	2146	580	648	21		
1	B	435	Total	C	N	O	S	0	0
			3395	2146	580	648	21		
1	C	435	Total	C	N	O	S	0	0
			3395	2146	580	648	21		
1	D	435	Total	C	N	O	S	0	0
			3395	2146	580	648	21		
1	E	435	Total	C	N	O	S	0	0
			3395	2146	580	648	21		
1	F	435	Total	C	N	O	S	0	0
			3395	2146	580	648	21		
1	G	435	Total	C	N	O	S	0	0
			3395	2146	580	648	21		
1	H	435	Total	C	N	O	S	0	0
			3395	2146	580	648	21		
1	I	435	Total	C	N	O	S	0	0
			3395	2146	580	648	21		
1	J	435	Total	C	N	O	S	0	0
			3395	2146	580	648	21		
1	K	435	Total	C	N	O	S	0	0
			3395	2146	580	648	21		
1	L	435	Total	C	N	O	S	0	0
			3395	2146	580	648	21		
1	M	435	Total	C	N	O	S	0	0
			3395	2146	580	648	21		
1	N	435	Total	C	N	O	S	0	0
			3395	2146	580	648	21		
1	O	435	Total	C	N	O	S	0	0
			3395	2146	580	648	21		
1	P	435	Total	C	N	O	S	0	0
			3395	2146	580	648	21		
1	Q	435	Total	C	N	O	S	0	0
			3395	2146	580	648	21		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	435	Total 3395	C 2146	N 580	O 648	S 21	0	0
1	S	435	Total 3395	C 2146	N 580	O 648	S 21	0	0
1	U	435	Total 3395	C 2146	N 580	O 648	S 21	0	0
1	V	435	Total 3395	C 2146	N 580	O 648	S 21	0	0
1	W	435	Total 3395	C 2146	N 580	O 648	S 21	0	0
1	X	435	Total 3395	C 2146	N 580	O 648	S 21	0	0
1	Y	435	Total 3395	C 2146	N 580	O 648	S 21	0	0

- Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
2	A	2	Total 2	Ni 2	0
2	B	2	Total 2	Ni 2	0
2	C	2	Total 2	Ni 2	0
2	D	2	Total 2	Ni 2	0
2	E	2	Total 2	Ni 2	0
2	F	2	Total 2	Ni 2	0
2	G	2	Total 2	Ni 2	0
2	H	2	Total 2	Ni 2	0
2	I	2	Total 2	Ni 2	0
2	J	2	Total 2	Ni 2	0
2	K	2	Total 2	Ni 2	0
2	L	2	Total 2	Ni 2	0

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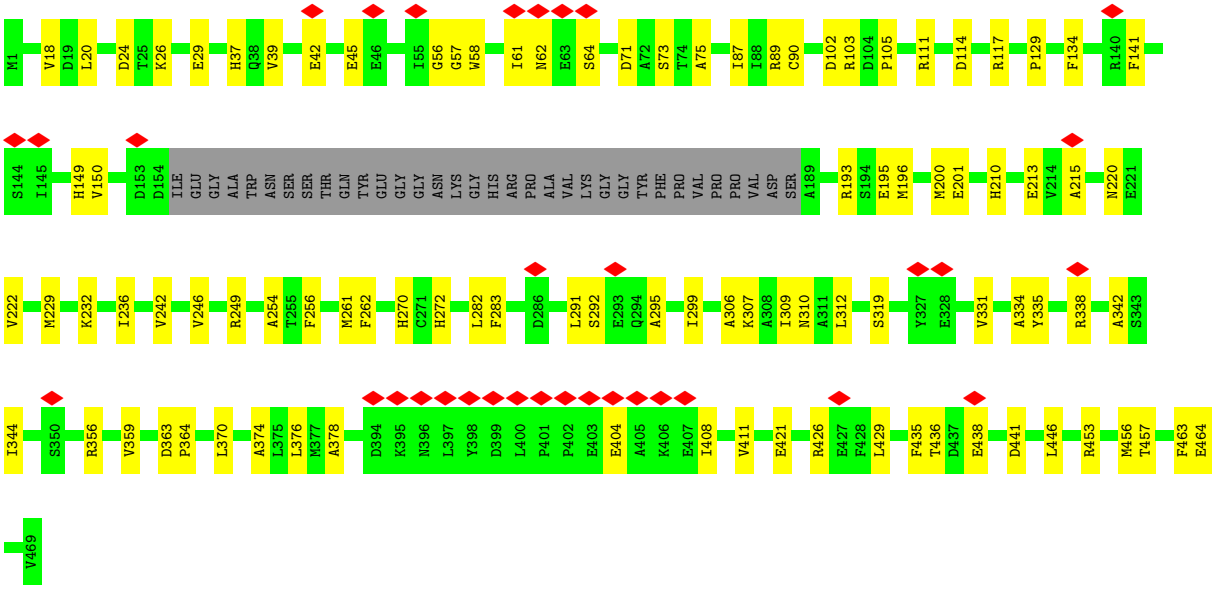
Mol	Chain	Residues	Atoms	AltConf
2	M	1	Total Ni 1 1	0
2	N	1	Total Ni 1 1	0
2	O	1	Total Ni 1 1	0
2	P	1	Total Ni 1 1	0
2	Q	1	Total Ni 1 1	0
2	R	1	Total Ni 1 1	0
2	S	2	Total Ni 2 2	0
2	U	2	Total Ni 2 2	0
2	V	2	Total Ni 2 2	0
2	W	2	Total Ni 2 2	0
2	X	2	Total Ni 2 2	0
2	Y	2	Total Ni 2 2	0

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.

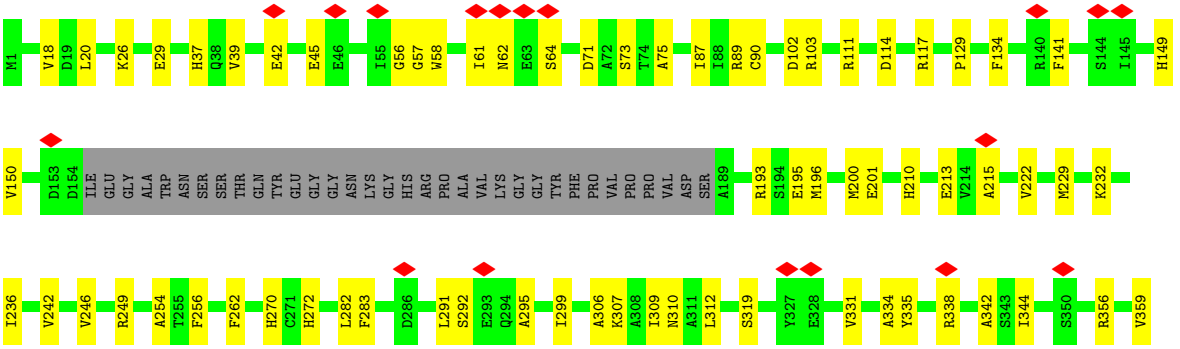
• Molecule 1: Glutamine synthetase

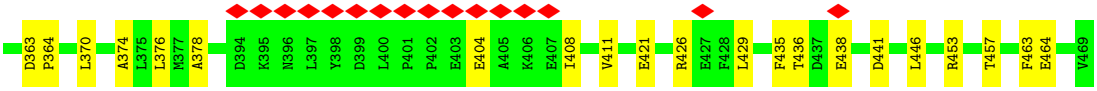
Chain A:



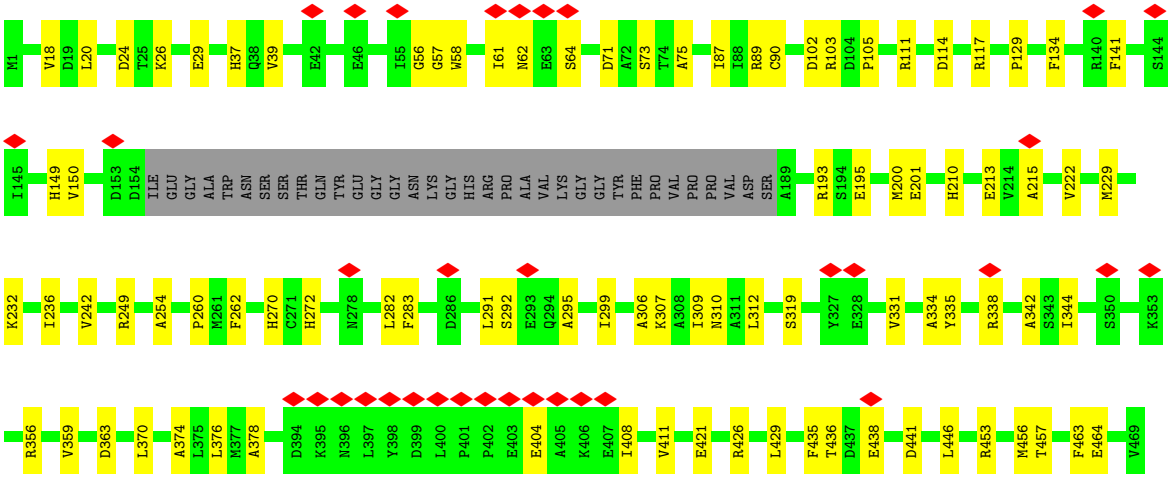
• Molecule 1: Glutamine synthetase

Chain B:

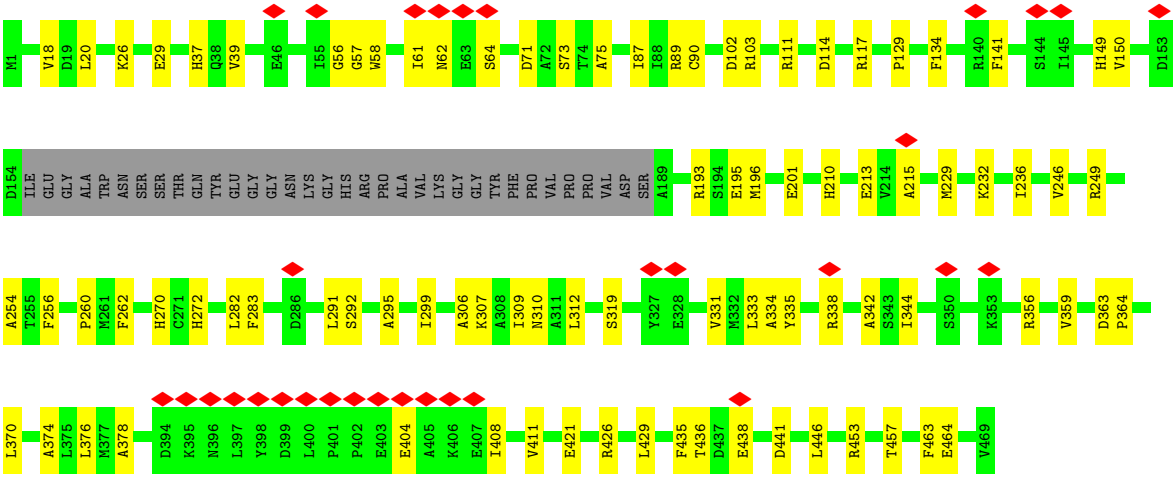




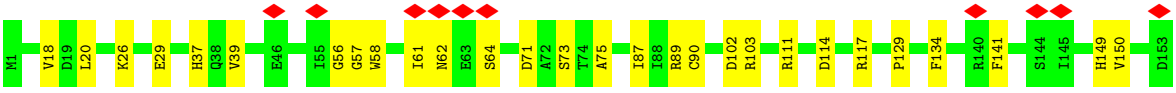
• Molecule 1: Glutamine synthetase

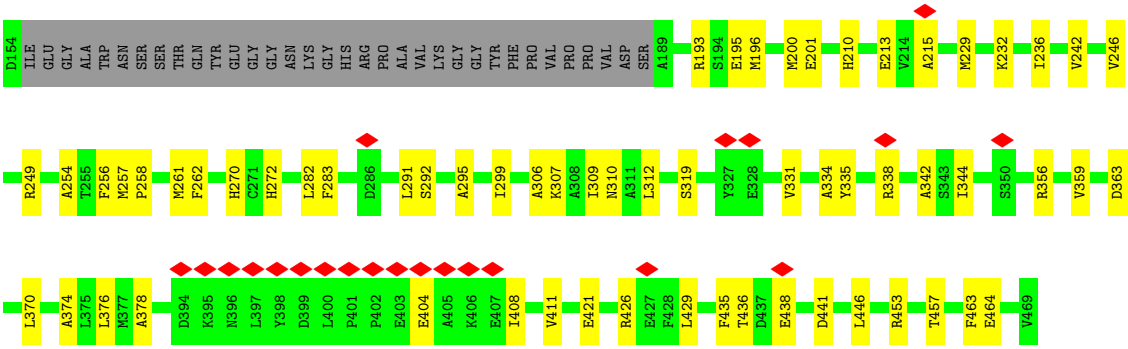


• Molecule 1: Glutamine synthetase



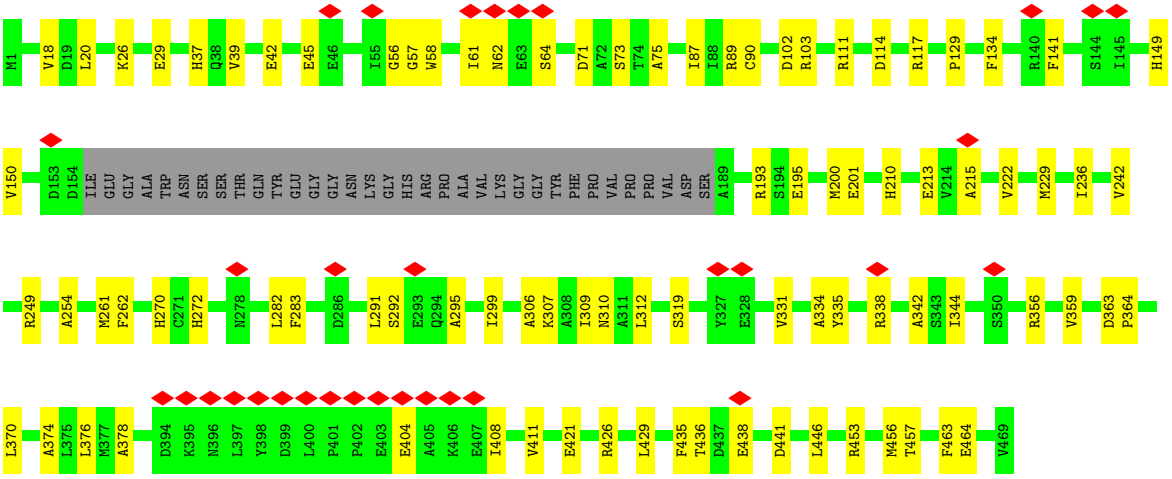
• Molecule 1: Glutamine synthetase





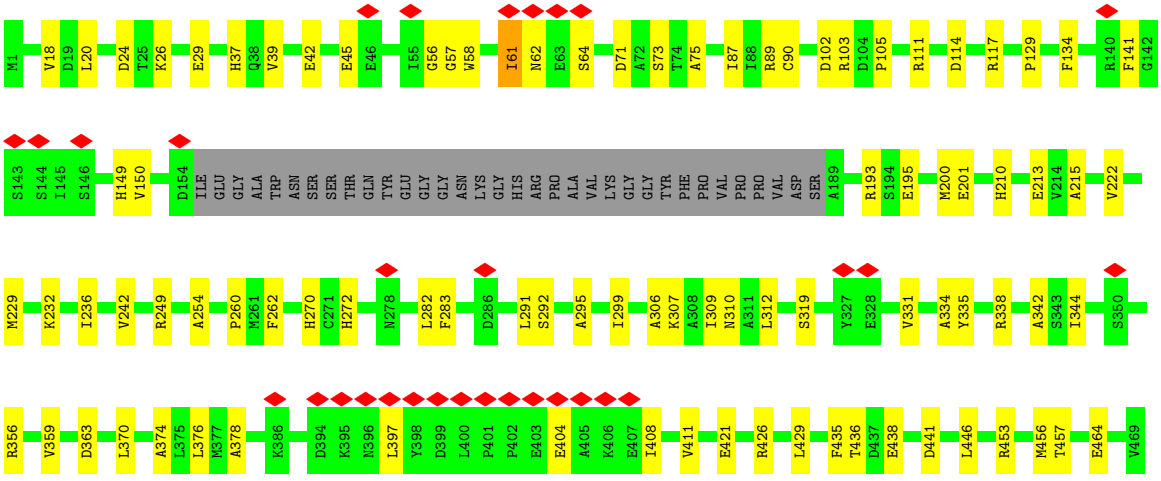
• Molecule 1: Glutamine synthetase

Chain F:



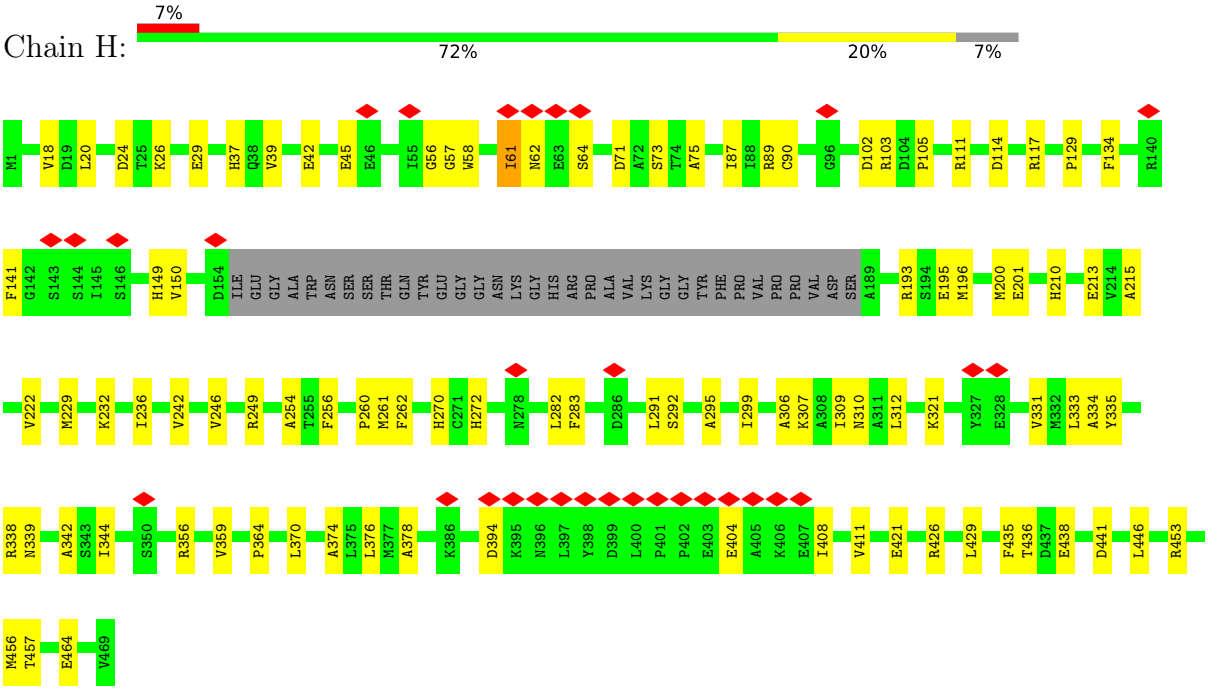
• Molecule 1: Glutamine synthetase

Chain G:



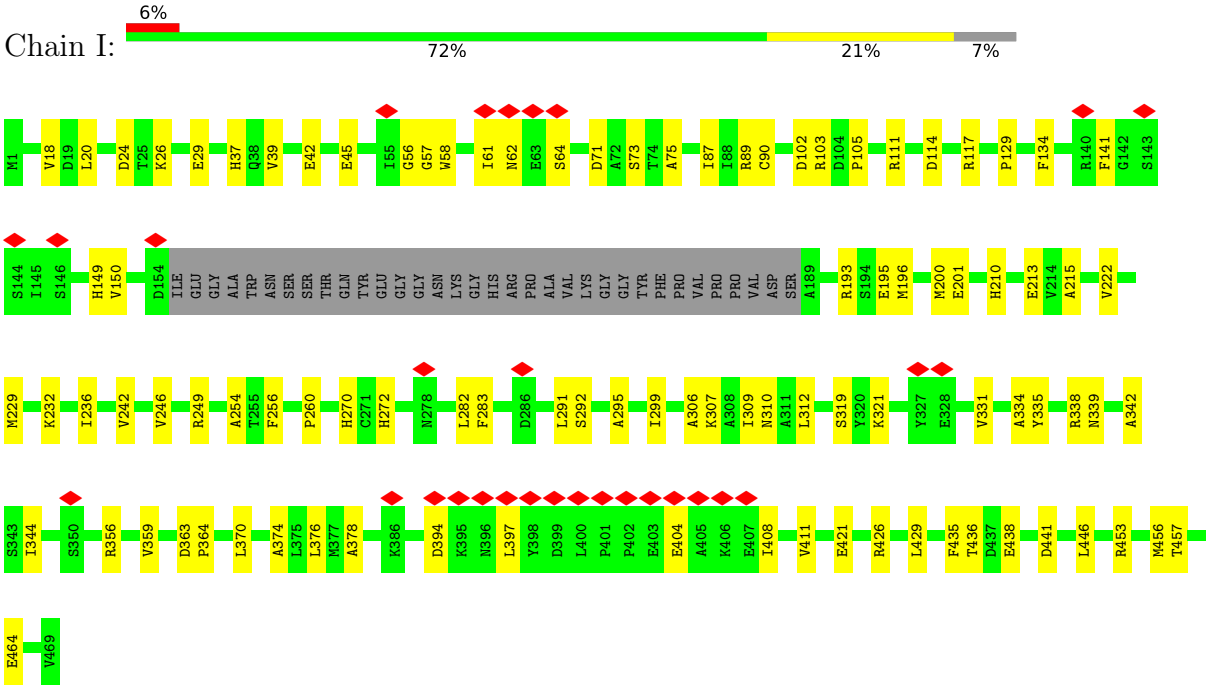
• Molecule 1: Glutamine synthetase

Chain H:



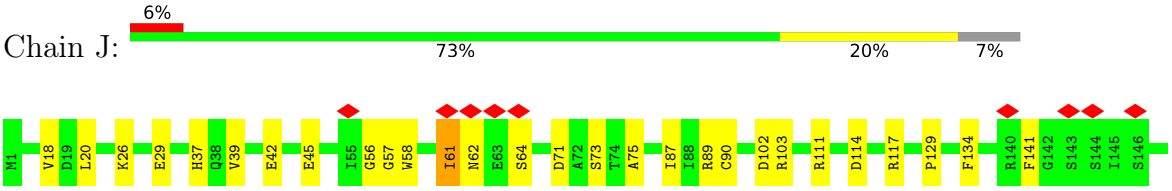
• Molecule 1: Glutamine synthetase

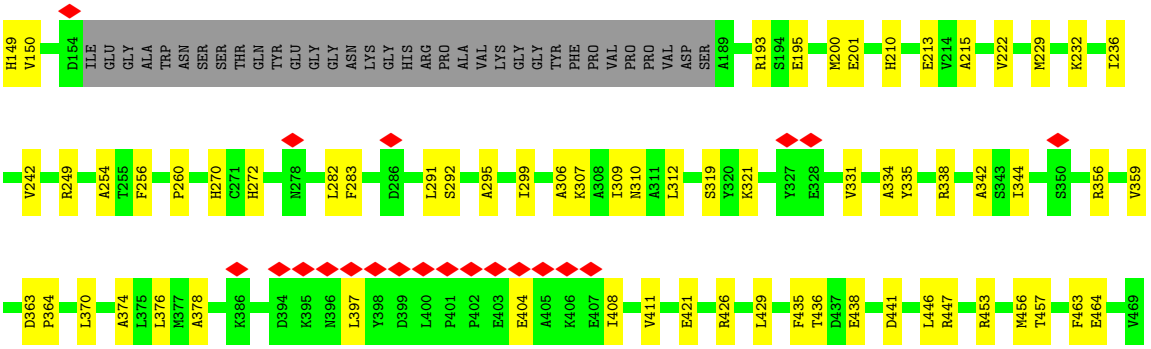
Chain I:



• Molecule 1: Glutamine synthetase

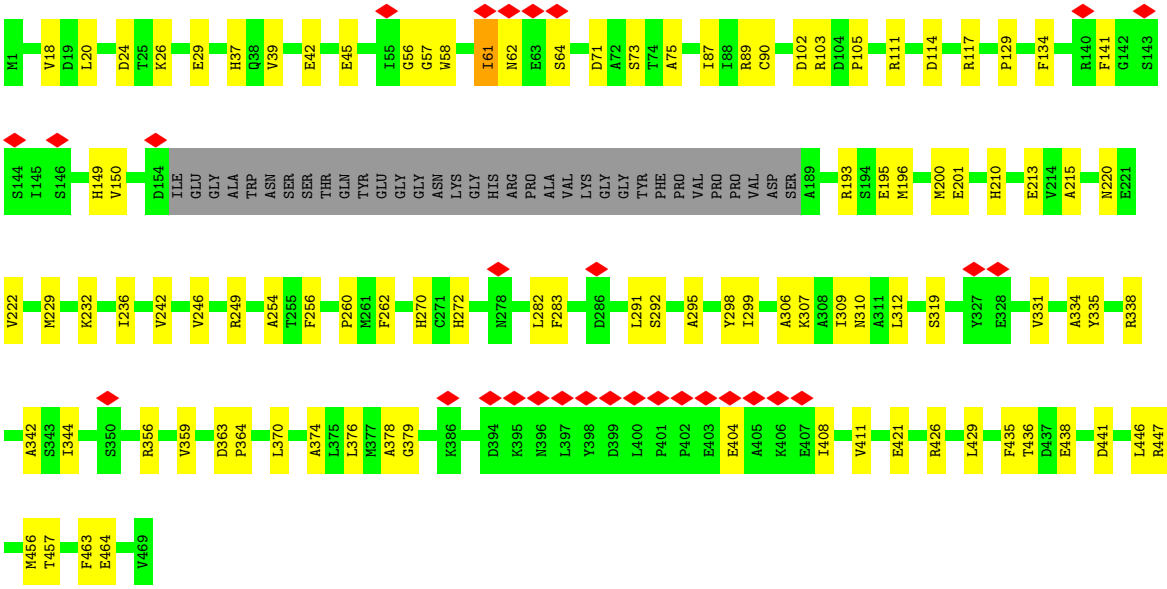
Chain J:





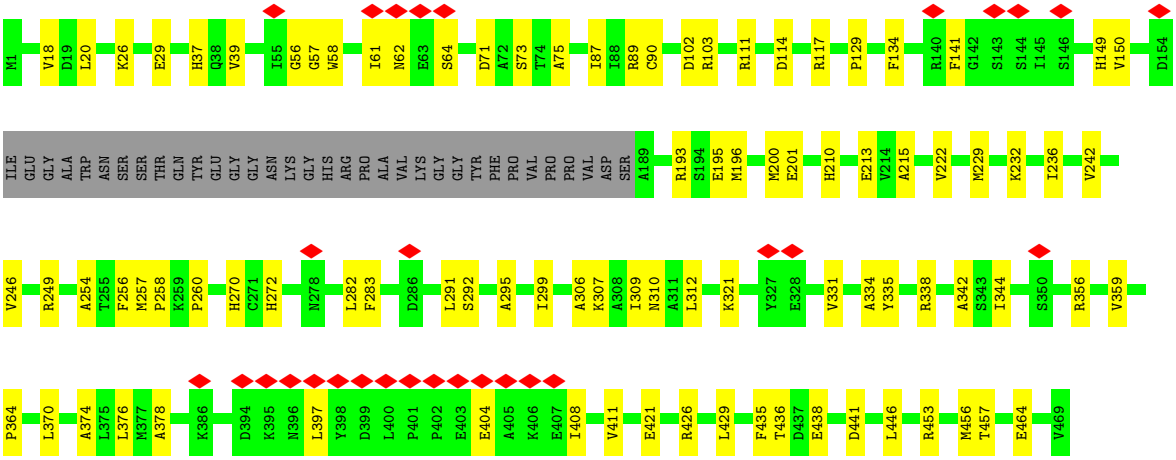
• Molecule 1: Glutamine synthetase

Chain K:



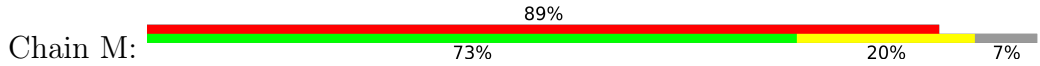
• Molecule 1: Glutamine synthetase

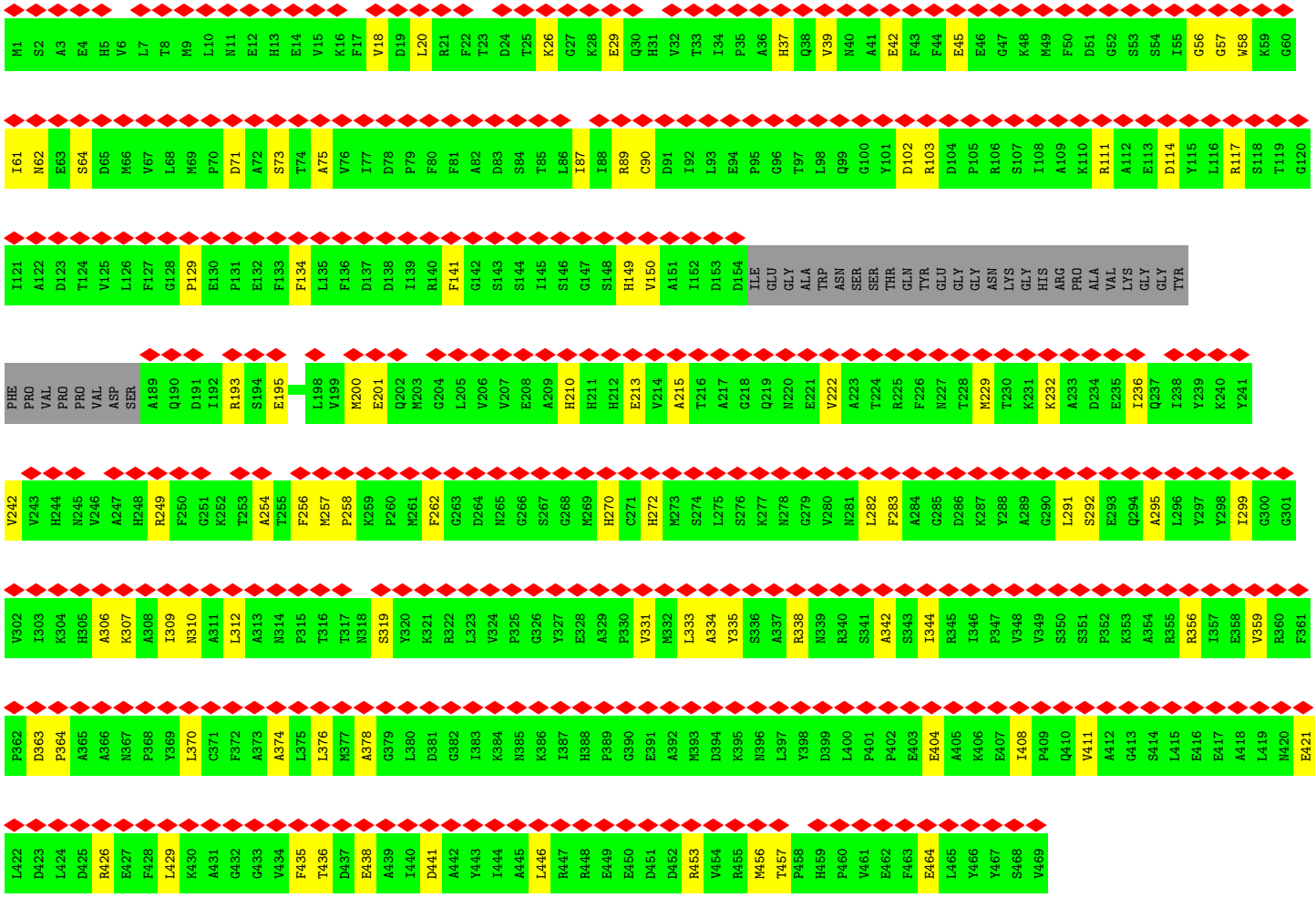
Chain L:



• Molecule 1: Glutamine synthetase

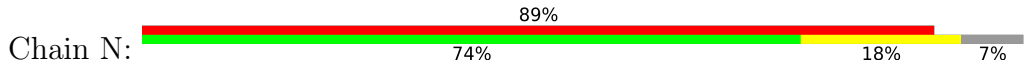
Chain M:

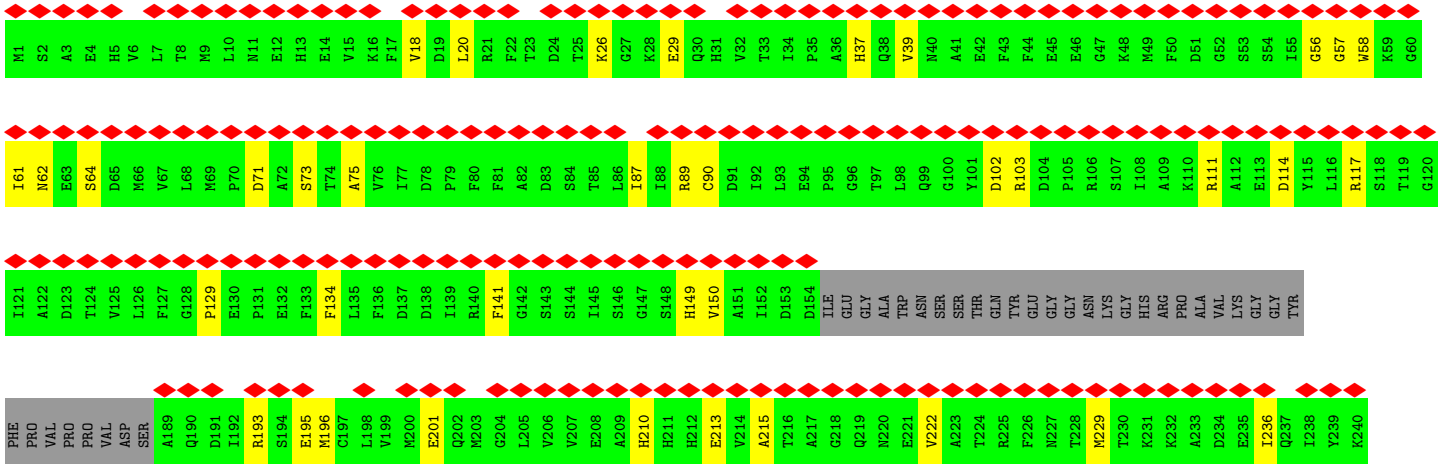


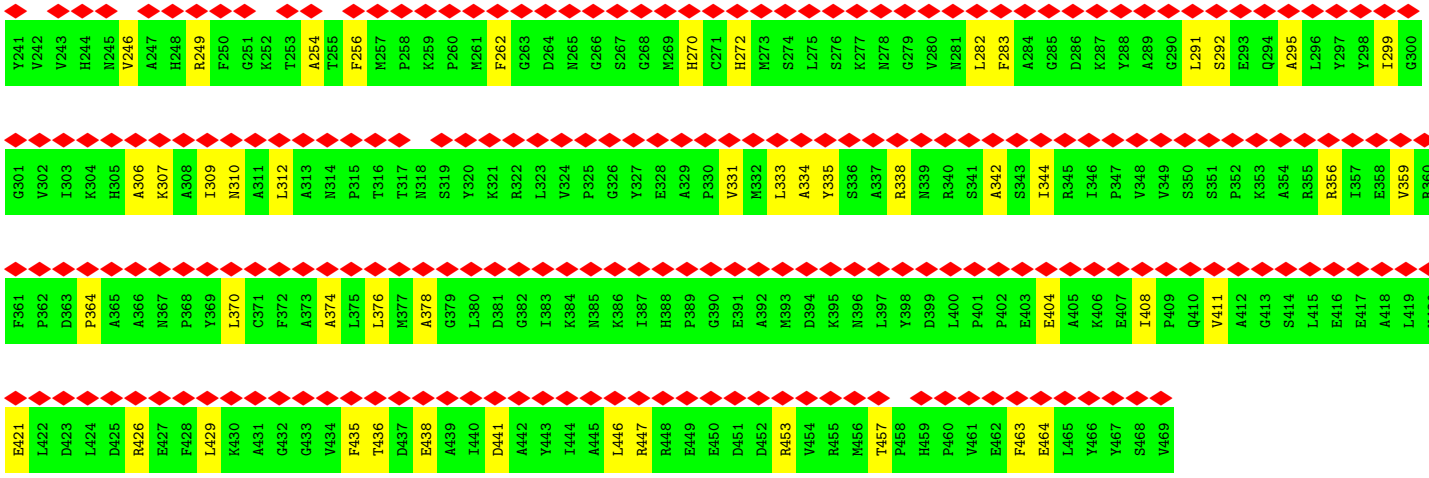


• Molecule 1: Glutamine synthetase

Chain N:

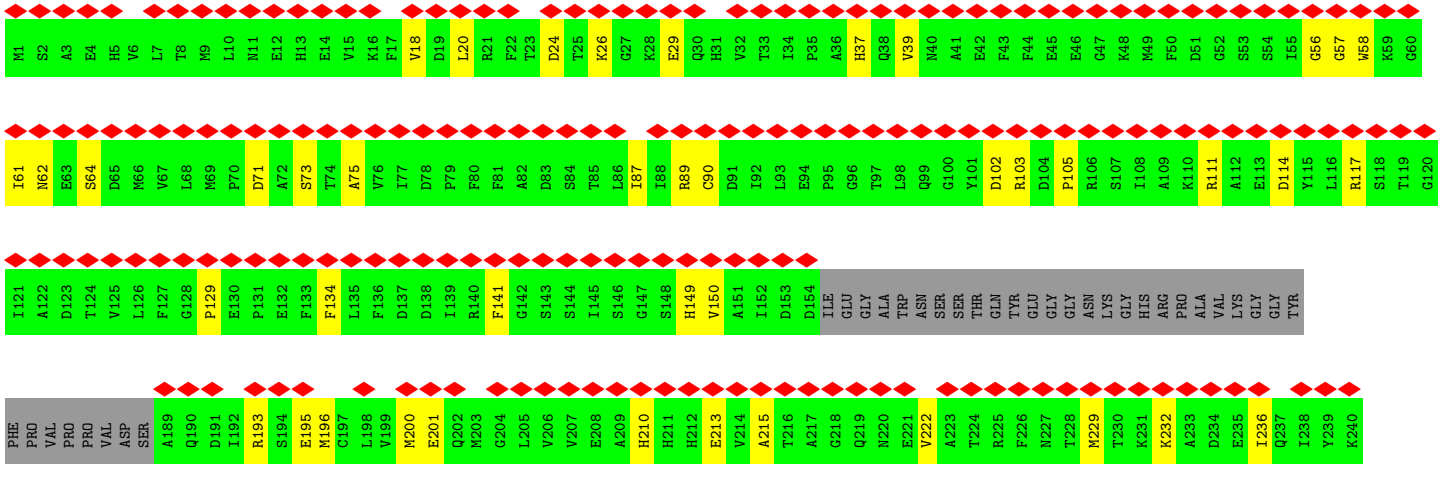






• Molecule 1: Glutamine synthetase

Chain O:



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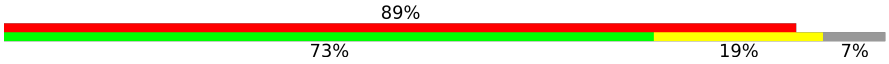
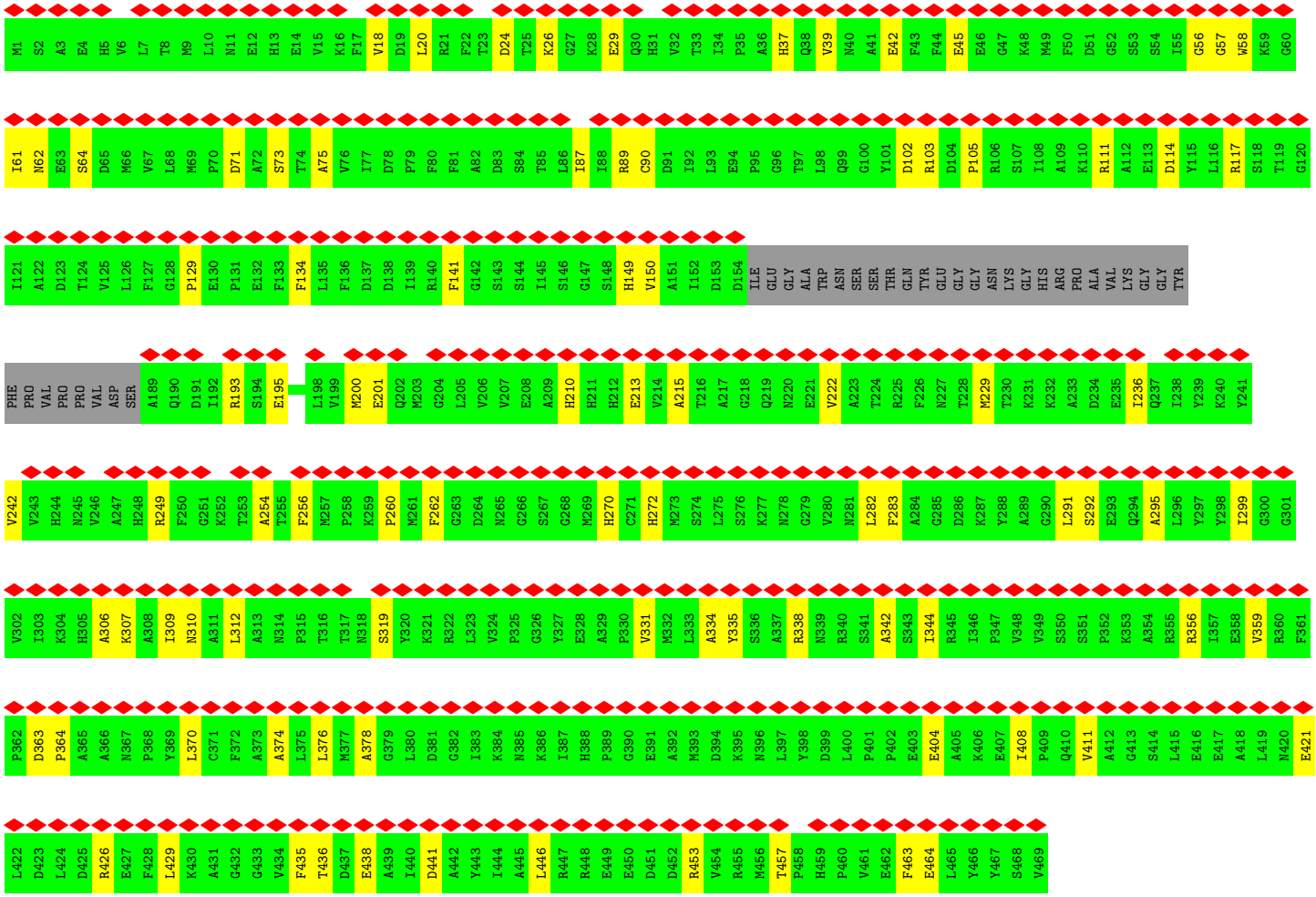
G301 V302 I303 K304 H305 A306 K307 A308 I309 N310 A311 L312 A313 N314 P315 T316 T317 N318 S319 Y320 K321 R322 L323 V324 P325 G326 Y327 E328 A329 P330 V331 M332 L333 A334 Y335 S336 A337 R338 N339 R340 S341 A342 S343 I344 R345 I346 P347 Y348 V349 S350 S351 P352 K353 A354 R355 R356 I357 E358 V359 R360
F361 P362 D363 P364 A365 A366 N367 P368 Y369 L370 C371 F372 A373 A374 L375 L376 M377 A378 G379 L380 D381 G382 I383 K384 N385 K386 I387 H388 P389 G390 E391 A392 M393 D394 K395 N396 L397 Y398 D399 L400 P401 P402 E403 E404 A405 K406 E407 I408 P409 Q410 V411 A412 G413 S414 L415 E416 E417 A418 L419 N420
E421 L422 D423 L424 D425 R426 E427 F428 L429 K430 A431 G432 G433 V434 F435 T436 D437 E438 A439 I440 D441 A442 Y443 I444 A445 L446 R447 R448 E449 E450 D451 D452 R453 V454 R455 M456 T457 P458 H459 P460 V461 E462 F463 E464 L465 Y466 Y467 S468 V469

• Molecule 1: Glutamine synthetase

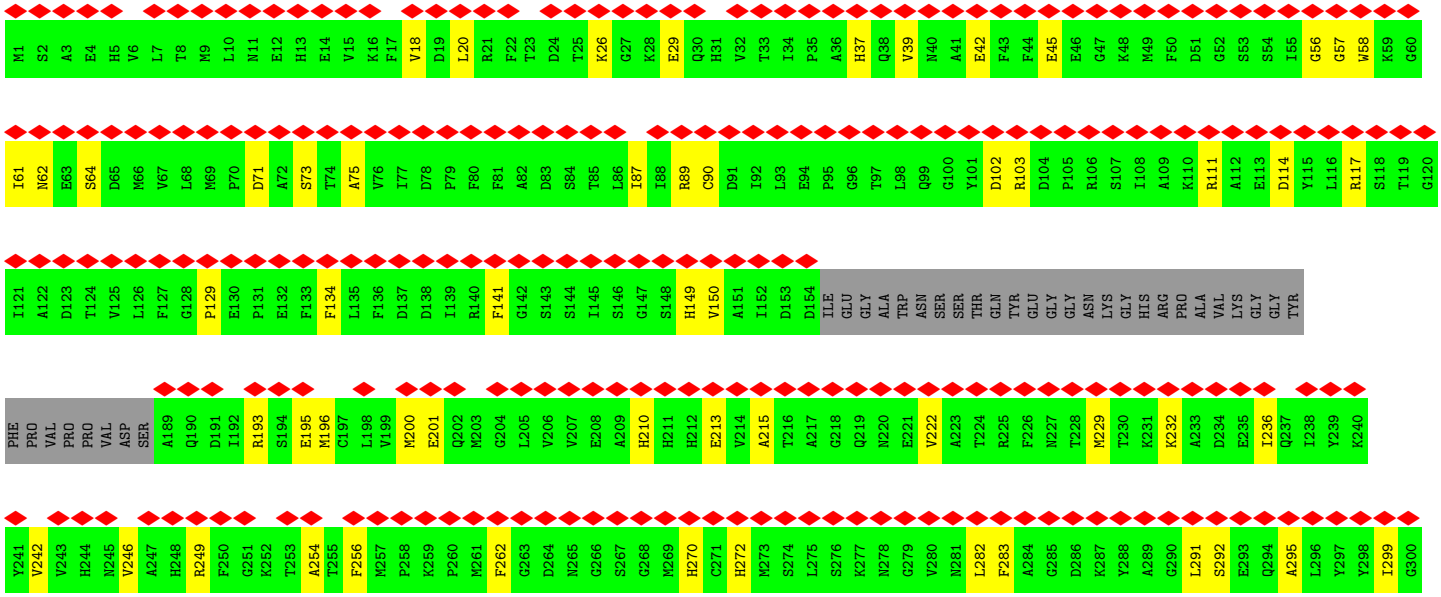
Chain P:

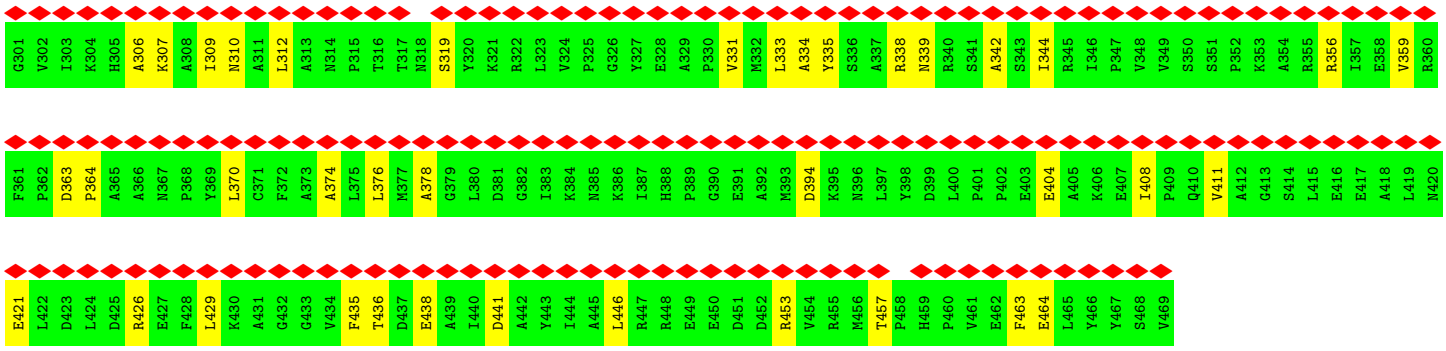




• Molecule 1: Glutamine synthetase

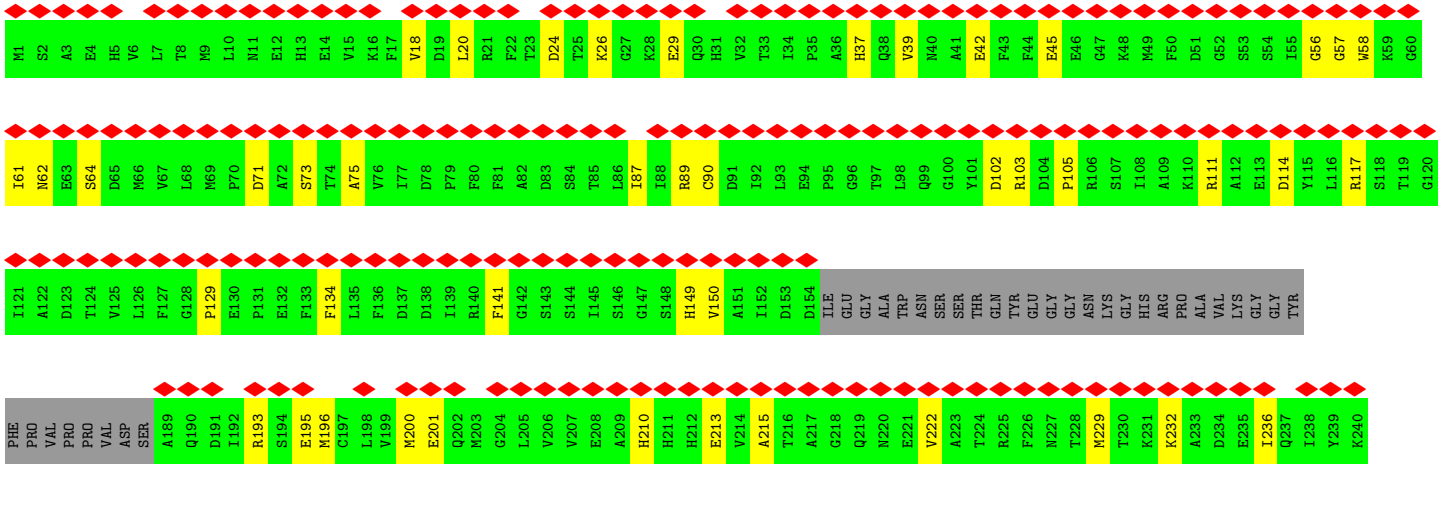
Chain Q:

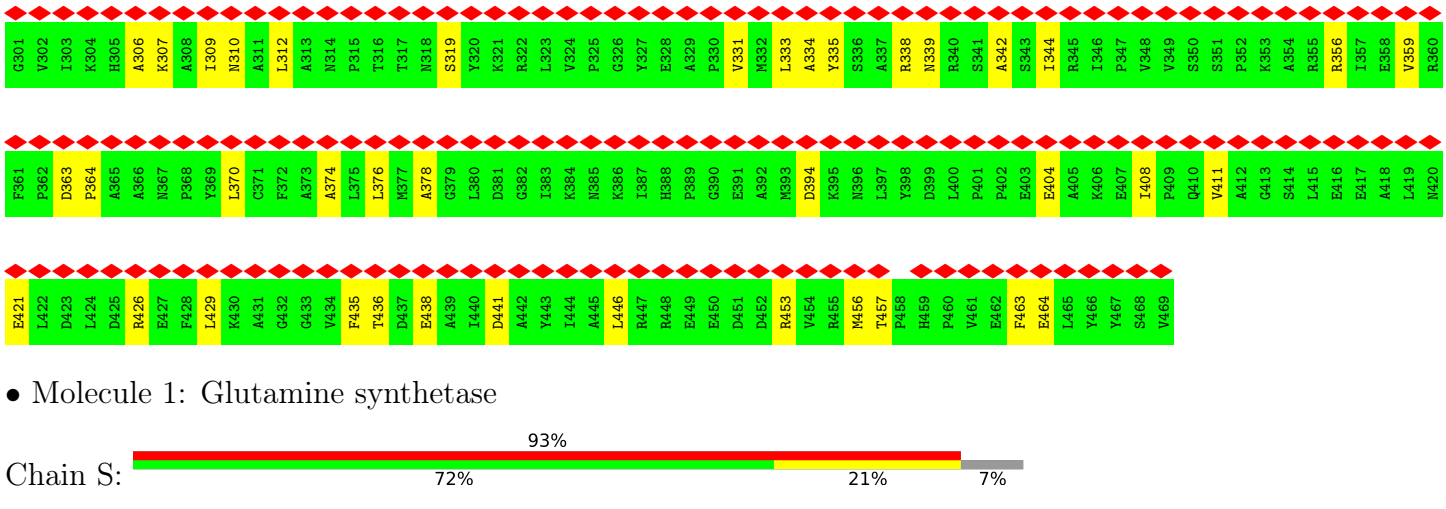




• Molecule 1: Glutamine synthetase

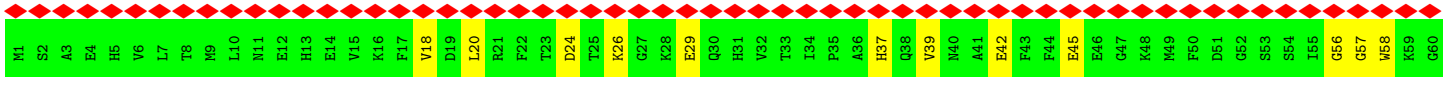
Chain R:

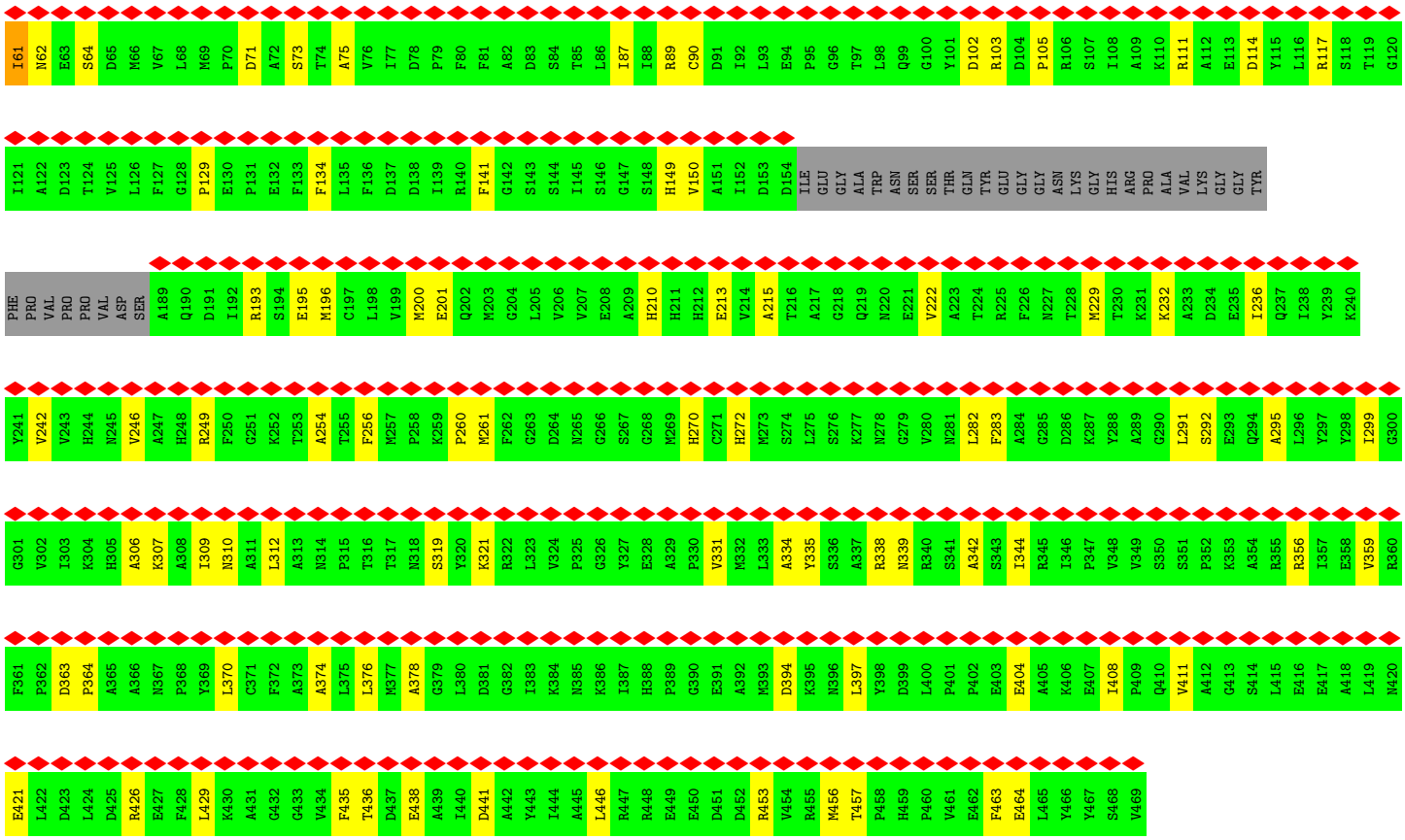




• Molecule 1: Glutamine synthetase

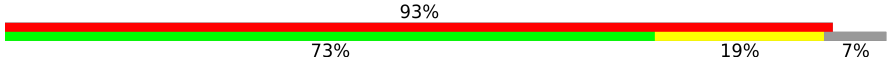
Chain S:

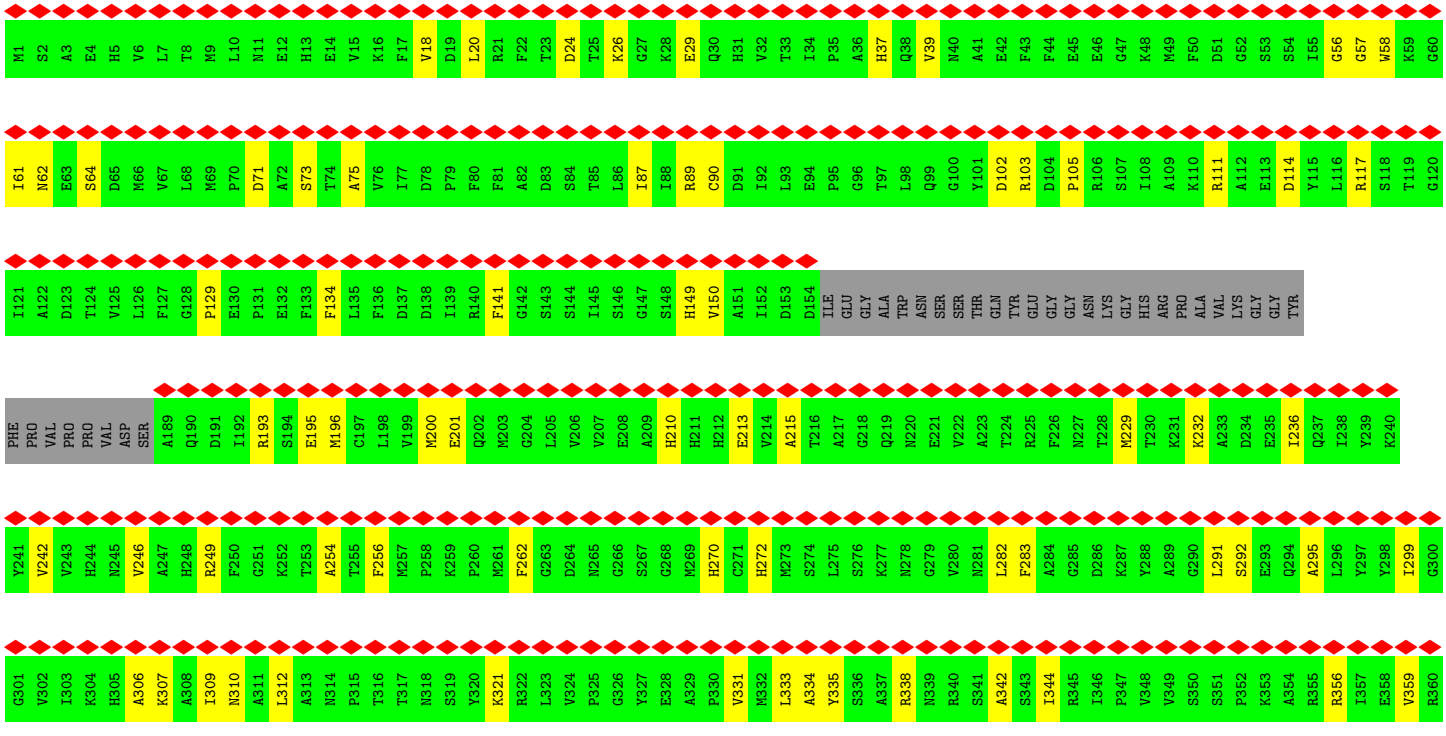




• Molecule 1: Glutamine synthetase

Chain U:





F361 P362 D363 P364 A365 A366 N367 P368 Y369 L370 C371 F372 A373 A374 L375 L376 M377 A378 G379 L380 D381 G382 I383 K384 N385 K386 I387 H388 P389 G390 E391 A392 M393 D394 K395 N396 L397 Y398 D399 L400 P401 P402 E403 E404 A405 K406 E407 I408 P409 Q410 V411 A412 G413 S414 L415 E416 E417 A418 L419 N420

E421 L422 D423 L424 D425 R426 E427 F428 L429 K430 A431 G432 G433 V434 F435 T436 D437 E438 A439 I440 D441 A442 Y443 I444 A445 L446 R447 R448 E449 E450 D451 D452 R453 V454 R455 M456 T457 P458 H459 P460 V461 E462 F463 E464 L465 Y466 Y467 S468 V469

- Molecule 1: Glutamine synthetase

Chain V: 93% 72% 20% 7%

M1 S2 A3 E4 H5 V6 L7 T8 M9 L10 N11 E12 H13 E14 V15 K16 F17 V18 D19 L20 R21 F22 T23 D24 T25 K26 G27 K28 E29 Q30 H31 V32 T33 I34 P35 A36 H37 Q38 V39 N40 A41 E42 F43 F44 E45 E46 G47 K48 M49 F50 D51 G52 S53 S54 I55 G56 G57 W58 K59 G60

I61 N62 E63 S64 D65 M66 V67 L68 M69 P70 D71 A72 S73 T74 A75 V76 I77 D78 P79 F80 F81 A82 D83 S84 T85 L86 I87 I88 R89 C90 D91 I92 L93 E94 P95 G96 T97 L98 Q99 G100 Y101 D102 R103 D104 P105 R106 S107 I108 A109 K110 R111 A112 E113 D114 Y115 L116 R117 S118 T119 G120

I121 A122 D123 T124 V125 L126 F127 G128 P129 E130 P131 E132 F133 F134 L135 F136 D137 D138 I139 R140 F141 G142 S143 S144 I145 S146 G147 S148 H149 V150 A151 I152 D153 D154 ILE GLU GLY ALA TRP ASN SER SER THR GLN TYR GLU GLY GLY ASN LYS GLY HIS ARG PRO ALA VAL LYS GLY GLY TYR

PHE PRO VAL PRO PRO VAL ASP SER A189 Q190 D191 T192 R193 S194 E195 M196 C197 L198 V199 M200 E201 Q202 M203 G204 L205 V206 V207 E208 A209 H210 H211 H212 E213 V214 A215 T216 A217 G218 Q219 N220 E221 V222 A223 T224 R225 F226 N227 T228 M229 T230 K231 K232 A233 D234 E235 I236 Q237 T238 Y239 K240

Y241 V242 V243 H244 N245 V246 A247 H248 R249 F250 G251 K252 T253 A254 T255 F256 M257 P258 K259 P260 M261 F262 G263 D264 N265 G266 S267 G268 M269 H270 C271 H272 M273 S274 L275 S276 K277 N278 G279 V280 N281 L282 F283 A284 G285 D286 K287 Y288 A289 G290 L291 S292 E293 Q294 A295 L296 Y297 Y298 I299 G300

G301 V302 I303 K304 H305 A306 K307 A308 I309 N310 A311 L312 A313 N314 P315 T316 T317 N318 S319 Y320 K321 R322 L323 V324 P325 G326 Y327 E328 A329 P330 V331 M332 L333 A334 Y335 S336 A337 R338 N339 R340 S341 A342 S343 I344 R345 I346 P347 V348 V349 S350 S351 P352 K353 A354 R355 R356 I357 E358 V359 R360

F361 P362 D363 P364 A365 A366 N367 P368 Y369 L370 C371 F372 A373 A374 L375 L376 M377 A378 G379 L380 D381 G382 I383 K384 N385 K386 I387 H388 P389 G390 E391 A392 M393 D394 K395 N396 L397 Y398 D399 L400 P401 P402 E403 E404 A405 K406 E407 I408 P409 Q410 V411 A412 G413 S414 L415 E416 E417 A418 L419 N420

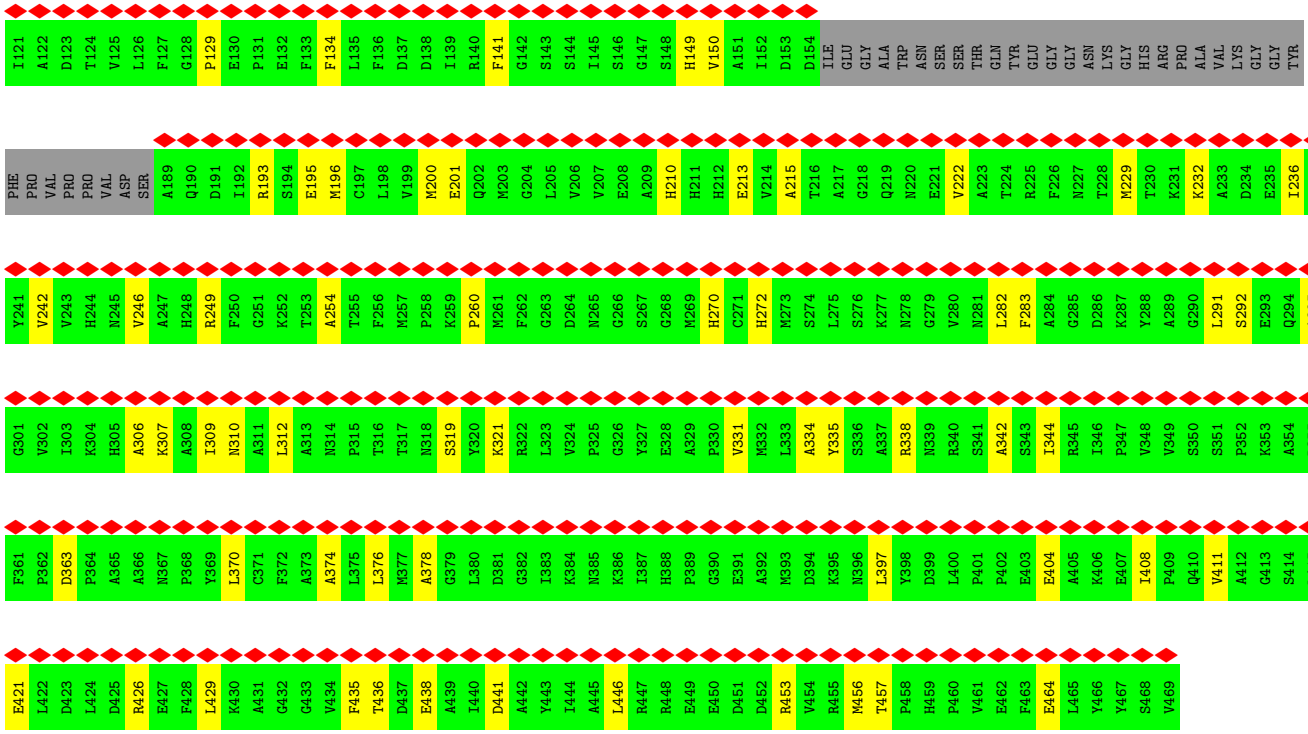
E421 L422 D423 L424 D425 R426 E427 F428 L429 K430 A431 G432 G433 V434 F435 T436 D437 E438 A439 I440 D441 A442 Y443 I444 A445 L446 R447 R448 E449 E450 D451 D452 R453 V454 R455 M456 T457 P458 H459 P460 V461 E462 F463 E464 L465 Y466 Y467 S468 V469

- Molecule 1: Glutamine synthetase

Chain W: 93% 73% 19% 7%

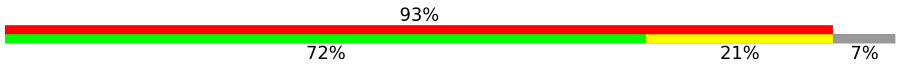
M1 S2 A3 E4 H5 V6 L7 T8 M9 L10 N11 E12 H13 E14 V15 K16 F17 V18 D19 L20 R21 F22 T23 D24 T25 K26 G27 K28 E29 Q30 H31 V32 T33 I34 P35 A36 H37 Q38 V39 N40 A41 E42 F43 F44 E45 E46 G47 K48 M49 F50 D51 G52 S53 S54 I55 G56 G57 W58 K59 G60

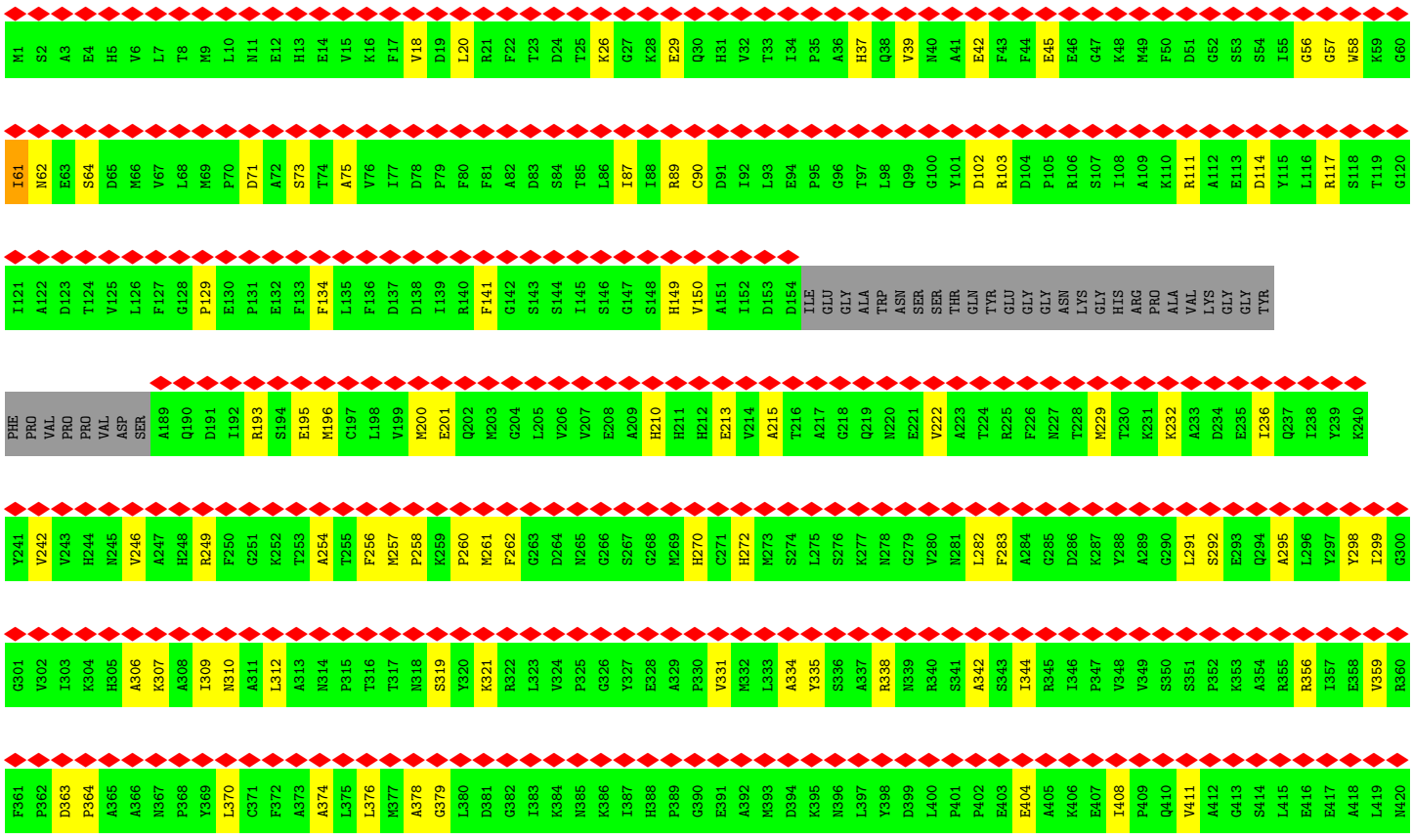
I61 N62 E63 S64 D65 M66 V67 L68 M69 P70 D71 A72 S73 T74 A75 V76 I77 D78 P79 F80 F81 A82 D83 S84 T85 L86 I87 I88 R89 C90 D91 I92 L93 E94 P95 G96 T97 L98 Q99 G100 Y101 D102 R103 D104 P105 R106 S107 I108 A109 K110 R111 A112 E113 D114 Y115 L116 R117 S118 T119 G120

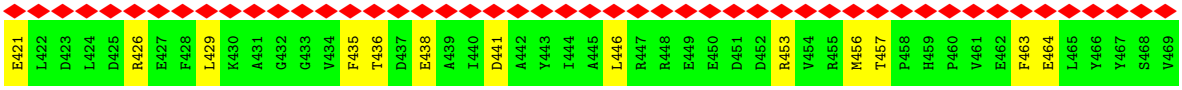


- Molecule 1: Glutamine synthetase

Chain X:

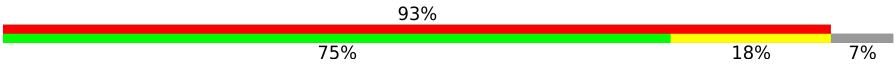


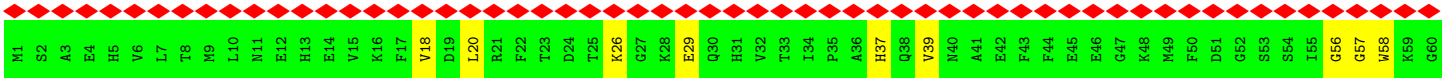


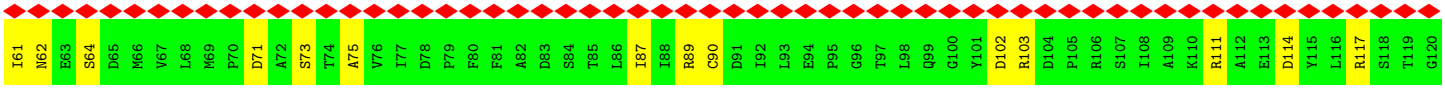


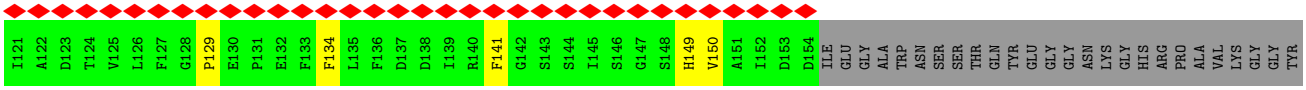
• Molecule 1: Glutamine synthetase

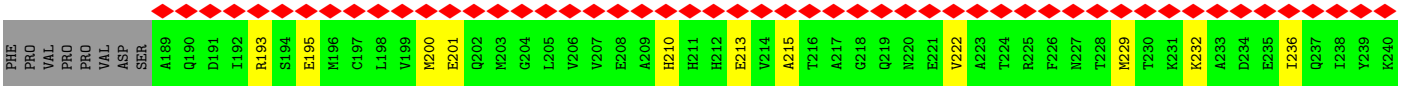
Chain Y:

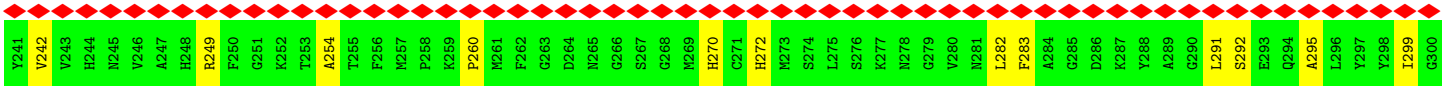


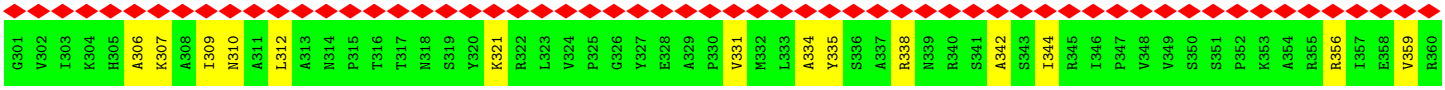


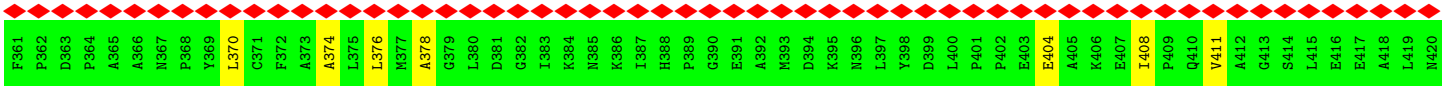


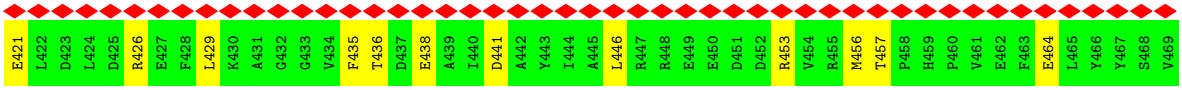












4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of particles used	117242	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	59.6	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.228	Depositor
Minimum map value	-2.136	Depositor
Average map value	0.020	Depositor
Map value standard deviation	0.096	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	353.46002, 353.46002, 353.46002	wwPDB
Map dimensions	430, 430, 430	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.822, 0.822, 0.822	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.41	0/3470	0.49	0/4694
1	B	0.41	0/3470	0.49	0/4694
1	C	0.41	0/3470	0.49	0/4694
1	D	0.41	0/3470	0.49	0/4694
1	E	0.41	0/3470	0.49	0/4694
1	F	0.41	0/3470	0.49	0/4694
1	G	0.41	0/3470	0.49	0/4694
1	H	0.41	0/3470	0.49	0/4694
1	I	0.41	0/3470	0.49	0/4694
1	J	0.41	0/3470	0.49	0/4694
1	K	0.41	0/3470	0.49	0/4694
1	L	0.41	0/3470	0.49	0/4694
1	M	0.41	0/3470	0.49	0/4694
1	N	0.41	0/3470	0.49	0/4694
1	O	0.41	0/3470	0.49	0/4694
1	P	0.41	0/3470	0.49	0/4694
1	Q	0.41	0/3470	0.49	0/4694
1	R	0.41	0/3470	0.49	0/4694
1	S	0.41	0/3470	0.49	0/4694
1	U	0.41	0/3470	0.49	0/4694
1	V	0.41	0/3470	0.49	0/4694
1	W	0.41	0/3470	0.49	0/4694
1	X	0.41	0/3470	0.49	0/4694
1	Y	0.41	0/3470	0.49	0/4694
All	All	0.41	0/83280	0.49	0/112656

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	2
1	B	0	2
1	C	0	2
1	D	0	2
1	E	0	2
1	F	0	2
1	G	0	2
1	H	0	2
1	I	0	2
1	J	0	2
1	K	0	2
1	L	0	2
1	M	0	2
1	N	0	2
1	O	0	2
1	P	0	2
1	Q	0	2
1	R	0	2
1	S	0	2
1	U	0	2
1	V	0	2
1	W	0	2
1	X	0	2
1	Y	0	2
All	All	0	48

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (48) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	61	ILE	Peptide
1	A	62	ASN	Peptide
1	B	61	ILE	Peptide
1	B	62	ASN	Peptide
1	C	61	ILE	Peptide
1	C	62	ASN	Peptide
1	D	61	ILE	Peptide
1	D	62	ASN	Peptide
1	E	61	ILE	Peptide
1	E	62	ASN	Peptide

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Mol	Chain	Res	Type	Group
1	F	61	ILE	Peptide
1	F	62	ASN	Peptide
1	G	61	ILE	Peptide
1	G	62	ASN	Peptide
1	H	61	ILE	Peptide
1	H	62	ASN	Peptide
1	I	61	ILE	Peptide
1	I	62	ASN	Peptide
1	J	61	ILE	Peptide
1	J	62	ASN	Peptide
1	K	61	ILE	Peptide
1	K	62	ASN	Peptide
1	L	61	ILE	Peptide
1	L	62	ASN	Peptide
1	M	61	ILE	Peptide
1	M	62	ASN	Peptide
1	N	61	ILE	Peptide
1	N	62	ASN	Peptide
1	O	61	ILE	Peptide
1	O	62	ASN	Peptide
1	P	61	ILE	Peptide
1	P	62	ASN	Peptide
1	Q	61	ILE	Peptide
1	Q	62	ASN	Peptide
1	R	61	ILE	Peptide
1	R	62	ASN	Peptide
1	S	61	ILE	Peptide
1	S	62	ASN	Peptide
1	U	61	ILE	Peptide
1	U	62	ASN	Peptide
1	V	61	ILE	Peptide
1	V	62	ASN	Peptide
1	W	61	ILE	Peptide
1	W	62	ASN	Peptide
1	X	61	ILE	Peptide
1	X	62	ASN	Peptide
1	Y	61	ILE	Peptide
1	Y	62	ASN	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	3395	0	3315	65	0
1	B	3395	0	3315	61	0
1	C	3395	0	3315	61	0
1	D	3395	0	3315	61	0
1	E	3395	0	3315	61	0
1	F	3395	0	3315	62	0
1	G	3395	0	3315	63	0
1	H	3395	0	3315	67	0
1	I	3395	0	3315	64	0
1	J	3395	0	3315	67	0
1	K	3395	0	3315	69	0
1	L	3395	0	3315	61	0
1	M	3395	0	3315	64	0
1	N	3395	0	3315	60	0
1	O	3395	0	3315	63	0
1	P	3395	0	3315	62	0
1	Q	3395	0	3315	64	0
1	R	3395	0	3315	66	0
1	S	3395	0	3315	69	0
1	U	3395	0	3315	62	0
1	V	3395	0	3315	66	0
1	W	3395	0	3315	62	0
1	X	3395	0	3315	68	0
1	Y	3395	0	3315	58	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
2	M	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	N	1	0	0	0	0
2	O	1	0	0	0	0
2	P	1	0	0	0	0
2	Q	1	0	0	0	0
2	R	1	0	0	0	0
2	S	2	0	0	0	0
2	U	2	0	0	0	0
2	V	2	0	0	0	0
2	W	2	0	0	0	0
2	X	2	0	0	0	0
2	Y	2	0	0	0	0
All	All	81522	0	79560	1392	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 9.

All (1392) 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:D:57:GLY:O	1:D:103:ARG:NH1	2.07	0.88
1:P:57:GLY:O	1:P:103:ARG:NH1	2.07	0.88
1:H:57:GLY:O	1:H:103:ARG:NH1	2.07	0.88
1:V:57:GLY:O	1:V:103:ARG:NH1	2.07	0.88
1:U:57:GLY:O	1:U:103:ARG:NH1	2.07	0.87
1:L:57:GLY:O	1:L:103:ARG:NH1	2.07	0.87
1:Q:57:GLY:O	1:Q:103:ARG:NH1	2.07	0.87
1:C:57:GLY:O	1:C:103:ARG:NH1	2.07	0.87
1:N:57:GLY:O	1:N:103:ARG:NH1	2.07	0.87
1:A:57:GLY:O	1:A:103:ARG:NH1	2.07	0.86
1:O:57:GLY:O	1:O:103:ARG:NH1	2.07	0.86
1:S:57:GLY:O	1:S:103:ARG:NH1	2.07	0.86
1:X:57:GLY:O	1:X:103:ARG:NH1	2.07	0.86
1:F:57:GLY:O	1:F:103:ARG:NH1	2.07	0.86
1:M:57:GLY:O	1:M:103:ARG:NH1	2.07	0.86
1:E:57:GLY:O	1:E:103:ARG:NH1	2.07	0.86
1:G:57:GLY:O	1:G:103:ARG:NH1	2.07	0.86
1:Y:57:GLY:O	1:Y:103:ARG:NH1	2.07	0.86
1:W:57:GLY:O	1:W:103:ARG:NH1	2.07	0.86
1:B:57:GLY:O	1:B:103:ARG:NH1	2.07	0.86
1:K:57:GLY:O	1:K:103:ARG:NH1	2.07	0.86
1:I:57:GLY:O	1:I:103:ARG:NH1	2.07	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:57:GLY:O	1:R:103:ARG:NH1	2.07	0.86
1:J:57:GLY:O	1:J:103:ARG:NH1	2.07	0.85
1:J:338:ARG:NH2	1:K:64:SER:OG	2.21	0.73
1:E:201:GLU:OE2	1:F:37:HIS:NE2	2.23	0.72
1:F:129:PRO:HG3	1:F:236:ILE:HD11	1.73	0.71
1:Q:201:GLU:OE2	1:R:37:HIS:NE2	2.23	0.71
1:W:129:PRO:HG3	1:W:236:ILE:HD11	1.73	0.70
1:A:37:HIS:NE2	1:F:201:GLU:OE2	2.24	0.70
1:Y:129:PRO:HG3	1:Y:236:ILE:HD11	1.73	0.70
1:J:129:PRO:HG3	1:J:236:ILE:HD11	1.73	0.70
1:O:129:PRO:HG3	1:O:236:ILE:HD11	1.73	0.70
1:Q:129:PRO:HG3	1:Q:236:ILE:HD11	1.73	0.70
1:U:129:PRO:HG3	1:U:236:ILE:HD11	1.73	0.70
1:C:129:PRO:HG3	1:C:236:ILE:HD11	1.73	0.70
1:G:129:PRO:HG3	1:G:236:ILE:HD11	1.73	0.70
1:N:129:PRO:HG3	1:N:236:ILE:HD11	1.73	0.70
1:B:129:PRO:HG3	1:B:236:ILE:HD11	1.73	0.70
1:H:129:PRO:HG3	1:H:236:ILE:HD11	1.73	0.70
1:L:129:PRO:HG3	1:L:236:ILE:HD11	1.73	0.70
1:M:129:PRO:HG3	1:M:236:ILE:HD11	1.73	0.70
1:D:129:PRO:HG3	1:D:236:ILE:HD11	1.73	0.70
1:K:129:PRO:HG3	1:K:236:ILE:HD11	1.73	0.69
1:S:338:ARG:NH2	1:X:64:SER:OG	2.21	0.69
1:B:201:GLU:OE2	1:C:37:HIS:NE2	2.24	0.69
1:I:129:PRO:HG3	1:I:236:ILE:HD11	1.73	0.69
1:I:338:ARG:NH2	1:J:64:SER:OG	2.20	0.69
1:S:129:PRO:HG3	1:S:236:ILE:HD11	1.73	0.69
1:M:201:GLU:OE2	1:N:37:HIS:NE2	2.24	0.69
1:R:129:PRO:HG3	1:R:236:ILE:HD11	1.73	0.69
1:R:282:LEU:O	1:R:292:SER:OG	2.11	0.69
1:X:129:PRO:HG3	1:X:236:ILE:HD11	1.73	0.69
1:A:129:PRO:HG3	1:A:236:ILE:HD11	1.73	0.69
1:E:129:PRO:HG3	1:E:236:ILE:HD11	1.73	0.69
1:E:282:LEU:O	1:E:292:SER:OG	2.11	0.69
1:P:129:PRO:HG3	1:P:236:ILE:HD11	1.73	0.69
1:V:282:LEU:O	1:V:292:SER:OG	2.11	0.69
1:S:282:LEU:O	1:S:292:SER:OG	2.11	0.69
1:V:129:PRO:HG3	1:V:236:ILE:HD11	1.73	0.68
1:A:282:LEU:O	1:A:292:SER:OG	2.11	0.68
1:N:201:GLU:OE2	1:O:37:HIS:NE2	2.24	0.68
1:P:282:LEU:O	1:P:292:SER:OG	2.11	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:102:ASP:HA	1:D:111:ARG:HH12	1.59	0.68
1:E:102:ASP:HA	1:E:111:ARG:HH12	1.59	0.68
1:J:282:LEU:O	1:J:292:SER:OG	2.11	0.68
1:U:102:ASP:HA	1:U:111:ARG:HH12	1.59	0.68
1:V:102:ASP:HA	1:V:111:ARG:HH12	1.59	0.68
1:W:102:ASP:HA	1:W:111:ARG:HH12	1.59	0.68
1:Y:102:ASP:HA	1:Y:111:ARG:HH12	1.59	0.68
1:F:282:LEU:O	1:F:292:SER:OG	2.11	0.68
1:G:282:LEU:O	1:G:292:SER:OG	2.11	0.68
1:C:102:ASP:HA	1:C:111:ARG:HH12	1.59	0.68
1:D:201:GLU:OE2	1:E:37:HIS:NE2	2.24	0.68
1:S:102:ASP:HA	1:S:111:ARG:HH12	1.59	0.68
1:X:102:ASP:HA	1:X:111:ARG:HH12	1.59	0.68
1:A:201:GLU:OE2	1:B:37:HIS:NE2	2.24	0.68
1:K:282:LEU:O	1:K:292:SER:OG	2.11	0.68
1:X:282:LEU:O	1:X:292:SER:OG	2.11	0.68
1:G:102:ASP:HA	1:G:111:ARG:HH12	1.59	0.68
1:H:282:LEU:O	1:H:292:SER:OG	2.11	0.68
1:P:201:GLU:OE2	1:Q:37:HIS:NE2	2.24	0.68
1:U:64:SER:OG	1:Y:338:ARG:NH2	2.23	0.68
1:M:102:ASP:HA	1:M:111:ARG:HH12	1.59	0.67
1:F:102:ASP:HA	1:F:111:ARG:HH12	1.59	0.67
1:C:201:GLU:OE2	1:D:37:HIS:NE2	2.26	0.67
1:M:282:LEU:O	1:M:292:SER:OG	2.11	0.67
1:N:282:LEU:O	1:N:292:SER:OG	2.11	0.67
1:R:102:ASP:HA	1:R:111:ARG:HH12	1.59	0.67
1:B:102:ASP:HA	1:B:111:ARG:HH12	1.59	0.67
1:C:282:LEU:O	1:C:292:SER:OG	2.11	0.67
1:Y:282:LEU:O	1:Y:292:SER:OG	2.11	0.67
1:A:102:ASP:HA	1:A:111:ARG:HH12	1.59	0.67
1:H:102:ASP:HA	1:H:111:ARG:HH12	1.59	0.67
1:X:338:ARG:NH2	1:Y:64:SER:OG	2.24	0.67
1:B:282:LEU:O	1:B:292:SER:OG	2.11	0.67
1:N:102:ASP:HA	1:N:111:ARG:HH12	1.59	0.67
1:L:102:ASP:HA	1:L:111:ARG:HH12	1.59	0.67
1:S:64:SER:OG	1:W:338:ARG:NH2	2.20	0.67
1:J:102:ASP:HA	1:J:111:ARG:HH12	1.59	0.67
1:M:37:HIS:NE2	1:R:201:GLU:OE2	2.24	0.67
1:P:102:ASP:HA	1:P:111:ARG:HH12	1.59	0.67
1:Q:282:LEU:O	1:Q:292:SER:OG	2.11	0.67
1:D:282:LEU:O	1:D:292:SER:OG	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:102:ASP:HA	1:K:111:ARG:HH12	1.59	0.66
1:W:282:LEU:O	1:W:292:SER:OG	2.11	0.66
1:O:201:GLU:OE2	1:P:37:HIS:NE2	2.26	0.66
1:O:102:ASP:HA	1:O:111:ARG:HH12	1.59	0.66
1:Q:102:ASP:HA	1:Q:111:ARG:HH12	1.59	0.66
1:O:282:LEU:O	1:O:292:SER:OG	2.11	0.66
1:U:282:LEU:O	1:U:292:SER:OG	2.11	0.66
1:I:102:ASP:HA	1:I:111:ARG:HH12	1.59	0.66
1:U:201:GLU:OE2	1:V:37:HIS:NE2	2.28	0.66
1:L:282:LEU:O	1:L:292:SER:OG	2.11	0.66
1:F:464:GLU:OE1	1:H:453:ARG:NH2	2.30	0.65
1:R:464:GLU:OE1	1:V:453:ARG:NH2	2.30	0.65
1:G:201:GLU:OE2	1:H:37:HIS:NE2	2.28	0.65
1:O:338:ARG:NH2	1:P:64:SER:OG	2.27	0.64
1:G:338:ARG:NH2	1:H:64:SER:OG	2.26	0.64
1:K:201:GLU:OE2	1:L:37:HIS:NE2	2.30	0.64
1:G:64:SER:OG	1:L:338:ARG:NH2	2.23	0.63
1:C:103:ARG:HH21	1:C:438:GLU:HG3	1.64	0.63
1:I:201:GLU:OE2	1:J:37:HIS:NE2	2.31	0.63
1:N:103:ARG:HH21	1:N:438:GLU:HG3	1.64	0.63
1:Y:103:ARG:HH21	1:Y:438:GLU:HG3	1.64	0.63
1:I:282:LEU:O	1:I:292:SER:OG	2.11	0.63
1:H:103:ARG:HH21	1:H:438:GLU:HG3	1.64	0.63
1:U:37:HIS:NE2	1:Y:201:GLU:OE2	2.30	0.63
1:V:201:GLU:OE2	1:W:37:HIS:NE2	2.28	0.63
1:D:103:ARG:HH21	1:D:438:GLU:HG3	1.64	0.62
1:E:464:GLU:OE1	1:I:453:ARG:NH2	2.32	0.62
1:Q:464:GLU:OE1	1:W:453:ARG:NH2	2.32	0.62
1:G:37:HIS:NE2	1:L:201:GLU:OE2	2.30	0.62
1:O:103:ARG:HH21	1:O:438:GLU:HG3	1.64	0.62
1:S:306:ALA:O	1:S:310:ASN:ND2	2.33	0.62
1:Y:306:ALA:O	1:Y:310:ASN:ND2	2.33	0.62
1:A:306:ALA:O	1:A:310:ASN:ND2	2.33	0.62
1:F:306:ALA:O	1:F:310:ASN:ND2	2.33	0.62
1:G:103:ARG:HH21	1:G:438:GLU:HG3	1.64	0.62
1:X:306:ALA:O	1:X:310:ASN:ND2	2.33	0.62
1:B:306:ALA:O	1:B:310:ASN:ND2	2.33	0.62
1:U:103:ARG:HH21	1:U:438:GLU:HG3	1.64	0.62
1:X:103:ARG:HH21	1:X:438:GLU:HG3	1.64	0.62
1:I:103:ARG:HH21	1:I:438:GLU:HG3	1.64	0.62
1:K:103:ARG:HH21	1:K:438:GLU:HG3	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:103:ARG:HH21	1:M:438:GLU:HG3	1.64	0.62
1:N:306:ALA:O	1:N:310:ASN:ND2	2.33	0.62
1:O:306:ALA:O	1:O:310:ASN:ND2	2.33	0.62
1:B:103:ARG:HH21	1:B:438:GLU:HG3	1.64	0.62
1:X:201:GLU:OE2	1:Y:37:HIS:NE2	2.30	0.62
1:C:306:ALA:O	1:C:310:ASN:ND2	2.33	0.62
1:H:201:GLU:OE2	1:I:37:HIS:NE2	2.28	0.62
1:J:103:ARG:HH21	1:J:438:GLU:HG3	1.64	0.62
1:W:306:ALA:O	1:W:310:ASN:ND2	2.33	0.62
1:M:306:ALA:O	1:M:310:ASN:ND2	2.33	0.62
1:Q:103:ARG:HH21	1:Q:438:GLU:HG3	1.64	0.62
1:R:103:ARG:HH21	1:R:438:GLU:HG3	1.64	0.62
1:S:103:ARG:HH21	1:S:438:GLU:HG3	1.64	0.62
1:W:103:ARG:HH21	1:W:438:GLU:HG3	1.64	0.62
1:F:103:ARG:HH21	1:F:438:GLU:HG3	1.64	0.62
1:G:306:ALA:O	1:G:310:ASN:ND2	2.33	0.62
1:H:306:ALA:O	1:H:310:ASN:ND2	2.33	0.62
1:L:306:ALA:O	1:L:310:ASN:ND2	2.33	0.62
1:U:306:ALA:O	1:U:310:ASN:ND2	2.33	0.62
1:A:103:ARG:HH21	1:A:438:GLU:HG3	1.64	0.61
1:B:464:GLU:OE1	1:L:453:ARG:NH2	2.33	0.61
1:E:306:ALA:O	1:E:310:ASN:ND2	2.33	0.61
1:P:306:ALA:O	1:P:310:ASN:ND2	2.33	0.61
1:R:306:ALA:O	1:R:310:ASN:ND2	2.33	0.61
1:I:306:ALA:O	1:I:310:ASN:ND2	2.33	0.61
1:K:338:ARG:NH2	1:L:64:SER:OG	2.24	0.61
1:E:103:ARG:HH21	1:E:438:GLU:HG3	1.64	0.61
1:J:319:SER:OG	1:J:363:ASP:OD2	2.19	0.61
1:S:37:HIS:NE2	1:W:201:GLU:OE2	2.31	0.61
1:K:306:ALA:O	1:K:310:ASN:ND2	2.33	0.61
1:L:103:ARG:HH21	1:L:438:GLU:HG3	1.64	0.61
1:N:464:GLU:OE1	1:Y:453:ARG:NH2	2.33	0.61
1:J:306:ALA:O	1:J:310:ASN:ND2	2.33	0.61
1:V:103:ARG:HH21	1:V:438:GLU:HG3	1.64	0.61
1:Q:306:ALA:O	1:Q:310:ASN:ND2	2.33	0.61
1:A:464:GLU:OE1	1:G:453:ARG:NH2	2.34	0.61
1:M:464:GLU:OE1	1:U:453:ARG:NH2	2.34	0.61
1:J:201:GLU:OE2	1:K:37:HIS:NE2	2.31	0.61
1:P:103:ARG:HH21	1:P:438:GLU:HG3	1.64	0.61
1:D:306:ALA:O	1:D:310:ASN:ND2	2.33	0.60
1:V:306:ALA:O	1:V:310:ASN:ND2	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:ASP:OD1	1:A:117:ARG:NH2	2.35	0.60
1:C:338:ARG:NH2	1:D:64:SER:OG	2.27	0.60
1:C:464:GLU:OE1	1:K:453:ARG:NH2	2.34	0.60
1:H:114:ASP:OD1	1:H:117:ARG:NH2	2.35	0.60
1:K:114:ASP:OD1	1:K:117:ARG:NH2	2.35	0.60
1:N:114:ASP:OD1	1:N:117:ARG:NH2	2.35	0.60
1:Q:114:ASP:OD1	1:Q:117:ARG:NH2	2.35	0.60
1:S:114:ASP:OD1	1:S:117:ARG:NH2	2.35	0.60
1:C:114:ASP:OD1	1:C:117:ARG:NH2	2.35	0.60
1:G:114:ASP:OD1	1:G:117:ARG:NH2	2.35	0.60
1:I:114:ASP:OD1	1:I:117:ARG:NH2	2.35	0.60
1:O:464:GLU:OE1	1:X:453:ARG:NH2	2.34	0.60
1:P:114:ASP:OD1	1:P:117:ARG:NH2	2.35	0.60
1:R:114:ASP:OD1	1:R:117:ARG:NH2	2.35	0.60
1:Y:114:ASP:OD1	1:Y:117:ARG:NH2	2.35	0.60
1:U:114:ASP:OD1	1:U:117:ARG:NH2	2.35	0.60
1:E:114:ASP:OD1	1:E:117:ARG:NH2	2.35	0.60
1:S:201:GLU:OE2	1:X:37:HIS:NE2	2.31	0.60
1:V:114:ASP:OD1	1:V:117:ARG:NH2	2.35	0.60
1:D:114:ASP:OD1	1:D:117:ARG:NH2	2.35	0.59
1:W:114:ASP:OD1	1:W:117:ARG:NH2	2.35	0.59
1:L:295:ALA:O	1:L:299:ILE:HG13	2.03	0.59
1:M:114:ASP:OD1	1:M:117:ARG:NH2	2.35	0.59
1:O:114:ASP:OD1	1:O:117:ARG:NH2	2.35	0.59
1:U:338:ARG:NH2	1:V:64:SER:OG	2.26	0.59
1:B:114:ASP:OD1	1:B:117:ARG:NH2	2.35	0.59
1:H:295:ALA:O	1:H:299:ILE:HG13	2.03	0.59
1:J:114:ASP:OD1	1:J:117:ARG:NH2	2.35	0.59
1:L:114:ASP:OD1	1:L:117:ARG:NH2	2.35	0.59
1:R:26:LYS:HG2	1:R:446:LEU:HD21	1.85	0.59
1:G:295:ALA:O	1:G:299:ILE:HG13	2.03	0.59
1:I:295:ALA:O	1:I:299:ILE:HG13	2.03	0.59
1:O:26:LYS:HG2	1:O:446:LEU:HD21	1.85	0.59
1:X:114:ASP:OD1	1:X:117:ARG:NH2	2.35	0.59
1:J:295:ALA:O	1:J:299:ILE:HG13	2.03	0.59
1:P:338:ARG:NH2	1:Q:64:SER:OG	2.28	0.59
1:F:295:ALA:O	1:F:299:ILE:HG13	2.03	0.59
1:I:26:LYS:HG2	1:I:446:LEU:HD21	1.85	0.59
1:L:26:LYS:HG2	1:L:446:LEU:HD21	1.85	0.59
1:N:295:ALA:O	1:N:299:ILE:HG13	2.03	0.59
1:S:26:LYS:HG2	1:S:446:LEU:HD21	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:ALA:O	1:A:299:ILE:HG13	2.03	0.59
1:Y:295:ALA:O	1:Y:299:ILE:HG13	2.03	0.59
1:A:26:LYS:HG2	1:A:446:LEU:HD21	1.85	0.59
1:U:26:LYS:HG2	1:U:446:LEU:HD21	1.85	0.59
1:X:295:ALA:O	1:X:299:ILE:HG13	2.03	0.59
1:B:26:LYS:HG2	1:B:446:LEU:HD21	1.85	0.59
1:B:295:ALA:O	1:B:299:ILE:HG13	2.03	0.59
1:D:26:LYS:HG2	1:D:446:LEU:HD21	1.85	0.59
1:E:26:LYS:HG2	1:E:446:LEU:HD21	1.85	0.59
1:F:114:ASP:OD1	1:F:117:ARG:NH2	2.35	0.59
1:M:295:ALA:O	1:M:299:ILE:HG13	2.03	0.59
1:R:295:ALA:O	1:R:299:ILE:HG13	2.03	0.59
1:V:26:LYS:HG2	1:V:446:LEU:HD21	1.85	0.59
1:S:295:ALA:O	1:S:299:ILE:HG13	2.03	0.58
1:E:295:ALA:O	1:E:299:ILE:HG13	2.02	0.58
1:K:295:ALA:O	1:K:299:ILE:HG13	2.03	0.58
1:O:295:ALA:O	1:O:299:ILE:HG13	2.03	0.58
1:X:26:LYS:HG2	1:X:446:LEU:HD21	1.85	0.58
1:D:295:ALA:O	1:D:299:ILE:HG13	2.03	0.58
1:H:26:LYS:HG2	1:H:446:LEU:HD21	1.85	0.58
1:Q:26:LYS:HG2	1:Q:446:LEU:HD21	1.85	0.58
1:Q:295:ALA:O	1:Q:299:ILE:HG13	2.02	0.58
1:U:295:ALA:O	1:U:299:ILE:HG13	2.03	0.58
1:V:295:ALA:O	1:V:299:ILE:HG13	2.03	0.58
1:P:295:ALA:O	1:P:299:ILE:HG13	2.03	0.58
1:W:295:ALA:O	1:W:299:ILE:HG13	2.03	0.58
1:G:26:LYS:HG2	1:G:446:LEU:HD21	1.85	0.58
1:P:26:LYS:HG2	1:P:446:LEU:HD21	1.85	0.58
1:B:344:ILE:HG12	1:B:359:VAL:HG12	1.86	0.58
1:C:295:ALA:O	1:C:299:ILE:HG13	2.03	0.58
1:K:26:LYS:HG2	1:K:446:LEU:HD21	1.85	0.58
1:D:344:ILE:HG12	1:D:359:VAL:HG12	1.86	0.58
1:N:26:LYS:HG2	1:N:446:LEU:HD21	1.85	0.58
1:J:344:ILE:HG12	1:J:359:VAL:HG12	1.86	0.58
1:W:344:ILE:HG12	1:W:359:VAL:HG12	1.86	0.58
1:E:344:ILE:HG12	1:E:359:VAL:HG12	1.86	0.58
1:N:344:ILE:HG12	1:N:359:VAL:HG12	1.86	0.58
1:Q:344:ILE:HG12	1:Q:359:VAL:HG12	1.86	0.58
1:V:344:ILE:HG12	1:V:359:VAL:HG12	1.86	0.58
1:C:26:LYS:HG2	1:C:446:LEU:HD21	1.85	0.58
1:J:26:LYS:HG2	1:J:446:LEU:HD21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:56:GLY:HA2	1:P:446:LEU:HD13	1.86	0.58
1:Y:344:ILE:HG12	1:Y:359:VAL:HG12	1.86	0.58
1:D:56:GLY:HA2	1:D:446:LEU:HD13	1.86	0.57
1:E:56:GLY:HA2	1:E:446:LEU:HD13	1.86	0.57
1:F:26:LYS:HG2	1:F:446:LEU:HD21	1.85	0.57
1:M:26:LYS:HG2	1:M:446:LEU:HD21	1.85	0.57
1:P:344:ILE:HG12	1:P:359:VAL:HG12	1.86	0.57
1:Q:56:GLY:HA2	1:Q:446:LEU:HD13	1.86	0.57
1:V:338:ARG:NH2	1:W:64:SER:OG	2.28	0.57
1:G:344:ILE:HG12	1:G:359:VAL:HG12	1.86	0.57
1:H:56:GLY:HA2	1:H:446:LEU:HD13	1.86	0.57
1:I:344:ILE:HG12	1:I:359:VAL:HG12	1.86	0.57
1:L:344:ILE:HG12	1:L:359:VAL:HG12	1.86	0.57
1:P:464:GLU:OE1	1:S:453:ARG:NH2	2.37	0.57
1:R:344:ILE:HG12	1:R:359:VAL:HG12	1.86	0.57
1:S:344:ILE:HG12	1:S:359:VAL:HG12	1.86	0.57
1:W:26:LYS:HG2	1:W:446:LEU:HD21	1.85	0.57
1:Y:26:LYS:HG2	1:Y:446:LEU:HD21	1.85	0.57
1:H:344:ILE:HG12	1:H:359:VAL:HG12	1.86	0.57
1:O:344:ILE:HG12	1:O:359:VAL:HG12	1.86	0.57
1:V:56:GLY:HA2	1:V:446:LEU:HD13	1.86	0.57
1:G:56:GLY:HA2	1:G:446:LEU:HD13	1.86	0.57
1:H:338:ARG:NH2	1:I:64:SER:OG	2.28	0.57
1:K:56:GLY:HA2	1:K:446:LEU:HD13	1.86	0.57
1:W:56:GLY:HA2	1:W:446:LEU:HD13	1.86	0.57
1:I:56:GLY:HA2	1:I:446:LEU:HD13	1.86	0.57
1:K:344:ILE:HG12	1:K:359:VAL:HG12	1.86	0.57
1:M:56:GLY:HA2	1:M:446:LEU:HD13	1.86	0.57
1:M:64:SER:OG	1:R:338:ARG:NH2	2.31	0.57
1:X:426:ARG:NH2	1:X:441:ASP:OD1	2.35	0.57
1:A:344:ILE:HG12	1:A:359:VAL:HG12	1.86	0.57
1:F:56:GLY:HA2	1:F:446:LEU:HD13	1.86	0.57
1:O:56:GLY:HA2	1:O:446:LEU:HD13	1.86	0.57
1:S:319:SER:OG	1:S:363:ASP:OD2	2.19	0.57
1:X:56:GLY:HA2	1:X:446:LEU:HD13	1.86	0.57
1:F:344:ILE:HG12	1:F:359:VAL:HG12	1.86	0.57
1:M:344:ILE:HG12	1:M:359:VAL:HG12	1.86	0.57
1:U:344:ILE:HG12	1:U:359:VAL:HG12	1.86	0.57
1:Y:18:VAL:HG21	1:Y:39:VAL:HG21	1.87	0.57
1:C:344:ILE:HG12	1:C:359:VAL:HG12	1.86	0.56
1:D:464:GLU:OE1	1:J:453:ARG:NH2	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:18:VAL:HG21	1:K:39:VAL:HG21	1.87	0.56
1:U:56:GLY:HA2	1:U:446:LEU:HD13	1.86	0.56
1:X:18:VAL:HG21	1:X:39:VAL:HG21	1.87	0.56
1:A:56:GLY:HA2	1:A:446:LEU:HD13	1.86	0.56
1:C:18:VAL:HG21	1:C:39:VAL:HG21	1.87	0.56
1:M:18:VAL:HG21	1:M:39:VAL:HG21	1.87	0.56
1:N:426:ARG:NH2	1:N:441:ASP:OD1	2.35	0.56
1:A:18:VAL:HG21	1:A:39:VAL:HG21	1.87	0.56
1:L:18:VAL:HG21	1:L:39:VAL:HG21	1.87	0.56
1:M:453:ARG:NH2	1:U:464:GLU:OE1	2.38	0.56
1:N:338:ARG:NH2	1:O:64:SER:OG	2.31	0.56
1:U:426:ARG:NH2	1:U:441:ASP:OD1	2.35	0.56
1:X:344:ILE:HG12	1:X:359:VAL:HG12	1.86	0.56
1:B:56:GLY:HA2	1:B:446:LEU:HD13	1.86	0.56
1:B:103:ARG:NH2	1:B:438:GLU:OE1	2.39	0.56
1:J:18:VAL:HG21	1:J:39:VAL:HG21	1.87	0.56
1:N:18:VAL:HG21	1:N:39:VAL:HG21	1.87	0.56
1:O:18:VAL:HG21	1:O:39:VAL:HG21	1.87	0.56
1:R:56:GLY:HA2	1:R:446:LEU:HD13	1.86	0.56
1:B:18:VAL:HG21	1:B:39:VAL:HG21	1.87	0.56
1:E:338:ARG:NH2	1:F:64:SER:OG	2.31	0.56
1:S:56:GLY:HA2	1:S:446:LEU:HD13	1.86	0.56
1:C:56:GLY:HA2	1:C:446:LEU:HD13	1.86	0.56
1:J:103:ARG:NH2	1:J:438:GLU:OE1	2.39	0.56
1:R:103:ARG:NH2	1:R:438:GLU:OE1	2.39	0.56
1:Y:103:ARG:NH2	1:Y:438:GLU:OE1	2.39	0.56
1:H:29:GLU:OE2	1:H:89:ARG:NH2	2.38	0.56
1:I:103:ARG:NH2	1:I:438:GLU:OE1	2.39	0.56
1:L:56:GLY:HA2	1:L:446:LEU:HD13	1.86	0.56
1:S:18:VAL:HG21	1:S:39:VAL:HG21	1.87	0.56
1:Y:56:GLY:HA2	1:Y:446:LEU:HD13	1.86	0.56
1:R:426:ARG:NH2	1:R:441:ASP:OD1	2.35	0.56
1:A:103:ARG:NH2	1:A:438:GLU:OE1	2.39	0.56
1:G:103:ARG:NH2	1:G:438:GLU:OE1	2.39	0.56
1:A:453:ARG:NH2	1:G:464:GLU:OE1	2.38	0.56
1:D:103:ARG:NH2	1:D:438:GLU:OE1	2.39	0.56
1:G:319:SER:OG	1:G:363:ASP:OD2	2.19	0.56
1:J:56:GLY:HA2	1:J:446:LEU:HD13	1.86	0.56
1:R:18:VAL:HG21	1:R:39:VAL:HG21	1.87	0.56
1:U:18:VAL:HG21	1:U:39:VAL:HG21	1.87	0.56
1:V:18:VAL:HG21	1:V:39:VAL:HG21	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:18:VAL:HG21	1:E:39:VAL:HG21	1.87	0.55
1:F:453:ARG:NH2	1:H:464:GLU:OE1	2.39	0.55
1:H:103:ARG:NH2	1:H:438:GLU:OE1	2.39	0.55
1:N:56:GLY:HA2	1:N:446:LEU:HD13	1.86	0.55
1:V:29:GLU:OE2	1:V:89:ARG:NH2	2.38	0.55
1:W:103:ARG:NH2	1:W:438:GLU:OE1	2.39	0.55
1:X:103:ARG:NH2	1:X:438:GLU:OE1	2.39	0.55
1:L:29:GLU:OE2	1:L:89:ARG:NH2	2.38	0.55
1:N:103:ARG:NH2	1:N:438:GLU:OE1	2.39	0.55
1:Q:103:ARG:NH2	1:Q:438:GLU:OE1	2.39	0.55
1:C:103:ARG:NH2	1:C:438:GLU:OE1	2.39	0.55
1:E:103:ARG:NH2	1:E:438:GLU:OE1	2.39	0.55
1:F:319:SER:OG	1:F:363:ASP:OD2	2.18	0.55
1:M:103:ARG:NH2	1:M:438:GLU:OE1	2.39	0.55
1:P:103:ARG:NH2	1:P:438:GLU:OE1	2.39	0.55
1:D:18:VAL:HG21	1:D:39:VAL:HG21	1.87	0.55
1:F:18:VAL:HG21	1:F:39:VAL:HG21	1.87	0.55
1:J:426:ARG:NH2	1:J:441:ASP:OD1	2.35	0.55
1:O:103:ARG:NH2	1:O:438:GLU:OE1	2.39	0.55
1:R:453:ARG:NH2	1:V:464:GLU:OE1	2.39	0.55
1:G:18:VAL:HG21	1:G:39:VAL:HG21	1.87	0.55
1:I:319:SER:OG	1:I:363:ASP:OD2	2.19	0.55
1:K:103:ARG:NH2	1:K:438:GLU:OE1	2.39	0.55
1:L:103:ARG:NH2	1:L:438:GLU:OE1	2.39	0.55
1:L:426:ARG:NH2	1:L:441:ASP:OD1	2.35	0.55
1:O:29:GLU:OE2	1:O:89:ARG:NH2	2.38	0.55
1:U:103:ARG:NH2	1:U:438:GLU:OE1	2.39	0.55
1:I:18:VAL:HG21	1:I:39:VAL:HG21	1.87	0.55
1:W:57:GLY:HA3	1:W:103:ARG:HD3	1.89	0.55
1:B:338:ARG:NH2	1:C:64:SER:OG	2.31	0.55
1:I:57:GLY:HA3	1:I:103:ARG:HD3	1.89	0.55
1:S:103:ARG:NH2	1:S:438:GLU:OE1	2.39	0.55
1:V:103:ARG:NH2	1:V:438:GLU:OE1	2.39	0.55
1:W:29:GLU:OE2	1:W:89:ARG:NH2	2.38	0.55
1:D:57:GLY:HA3	1:D:103:ARG:HD3	1.89	0.55
1:F:426:ARG:NH2	1:F:441:ASP:OD1	2.35	0.55
1:M:338:ARG:NH2	1:N:64:SER:OG	2.30	0.55
1:Q:57:GLY:HA3	1:Q:103:ARG:HD3	1.89	0.55
1:F:103:ARG:NH2	1:F:438:GLU:OE1	2.39	0.55
1:G:29:GLU:OE2	1:G:89:ARG:NH2	2.38	0.55
1:L:57:GLY:HA3	1:L:103:ARG:HD3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:18:VAL:HG21	1:P:39:VAL:HG21	1.87	0.55
1:Q:426:ARG:NH2	1:Q:441:ASP:OD1	2.35	0.55
1:W:18:VAL:HG21	1:W:39:VAL:HG21	1.87	0.55
1:A:57:GLY:HA3	1:A:103:ARG:HD3	1.89	0.55
1:V:57:GLY:HA3	1:V:103:ARG:HD3	1.89	0.55
1:C:57:GLY:HA3	1:C:103:ARG:HD3	1.89	0.54
1:E:57:GLY:HA3	1:E:103:ARG:HD3	1.89	0.54
1:P:57:GLY:HA3	1:P:103:ARG:HD3	1.89	0.54
1:Y:29:GLU:OE2	1:Y:89:ARG:NH2	2.38	0.54
1:N:29:GLU:OE2	1:N:89:ARG:NH2	2.38	0.54
1:N:57:GLY:HA3	1:N:103:ARG:HD3	1.89	0.54
1:D:338:ARG:NH2	1:E:64:SER:OG	2.28	0.54
1:H:18:VAL:HG21	1:H:39:VAL:HG21	1.87	0.54
1:K:57:GLY:HA3	1:K:103:ARG:HD3	1.89	0.54
1:Q:338:ARG:NH2	1:R:64:SER:OG	2.31	0.54
1:X:57:GLY:HA3	1:X:103:ARG:HD3	1.89	0.54
1:B:426:ARG:NH2	1:B:441:ASP:OD1	2.35	0.54
1:M:57:GLY:HA3	1:M:103:ARG:HD3	1.89	0.54
1:Q:29:GLU:OE2	1:Q:89:ARG:NH2	2.38	0.54
1:H:57:GLY:HA3	1:H:103:ARG:HD3	1.89	0.54
1:Y:57:GLY:HA3	1:Y:103:ARG:HD3	1.89	0.54
1:E:453:ARG:NH2	1:I:464:GLU:OE1	2.41	0.54
1:F:29:GLU:OE2	1:F:89:ARG:NH2	2.38	0.54
1:Q:453:ARG:NH2	1:W:464:GLU:OE1	2.41	0.54
1:R:57:GLY:HA3	1:R:103:ARG:HD3	1.89	0.54
1:U:57:GLY:HA3	1:U:103:ARG:HD3	1.89	0.54
1:D:453:ARG:NH2	1:J:464:GLU:OE1	2.41	0.54
1:J:57:GLY:HA3	1:J:103:ARG:HD3	1.89	0.54
1:Q:18:VAL:HG21	1:Q:39:VAL:HG21	1.87	0.54
1:O:57:GLY:HA3	1:O:103:ARG:HD3	1.89	0.54
1:P:453:ARG:NH2	1:S:464:GLU:OE1	2.41	0.54
1:R:319:SER:OG	1:R:363:ASP:OD2	2.18	0.54
1:B:29:GLU:OE2	1:B:89:ARG:NH2	2.38	0.54
1:R:29:GLU:OE2	1:R:89:ARG:NH2	2.38	0.54
1:B:57:GLY:HA3	1:B:103:ARG:HD3	1.89	0.54
1:E:426:ARG:NH2	1:E:441:ASP:OD1	2.35	0.54
1:A:64:SER:OG	1:F:338:ARG:NH2	2.31	0.53
1:M:229:MET:HE1	1:M:376:LEU:HD22	1.90	0.53
1:P:426:ARG:NH2	1:P:441:ASP:OD1	2.35	0.53
1:S:57:GLY:HA3	1:S:103:ARG:HD3	1.89	0.53
1:B:319:SER:OG	1:B:363:ASP:OD2	2.18	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:57:GLY:HA3	1:G:103:ARG:HD3	1.89	0.53
1:I:29:GLU:OE2	1:I:89:ARG:NH2	2.38	0.53
1:S:426:ARG:NH2	1:S:441:ASP:OD1	2.35	0.53
1:C:26:LYS:HE3	1:C:446:LEU:HG	1.91	0.53
1:C:29:GLU:OE2	1:C:89:ARG:NH2	2.38	0.53
1:F:57:GLY:HA3	1:F:103:ARG:HD3	1.89	0.53
1:I:26:LYS:HE3	1:I:446:LEU:HG	1.91	0.53
1:W:26:LYS:HE3	1:W:446:LEU:HG	1.91	0.53
1:Y:26:LYS:HE3	1:Y:446:LEU:HG	1.91	0.53
1:L:26:LYS:HE3	1:L:446:LEU:HG	1.91	0.53
1:O:26:LYS:HE3	1:O:446:LEU:HG	1.91	0.53
1:D:26:LYS:HE3	1:D:446:LEU:HG	1.91	0.53
1:F:26:LYS:HE3	1:F:446:LEU:HG	1.91	0.53
1:G:26:LYS:HE3	1:G:446:LEU:HG	1.91	0.53
1:J:29:GLU:OE2	1:J:89:ARG:NH2	2.38	0.53
1:R:26:LYS:HE3	1:R:446:LEU:HG	1.91	0.53
1:Y:20:LEU:HB3	1:Y:90:CYS:SG	2.49	0.53
1:B:20:LEU:HB3	1:B:90:CYS:SG	2.49	0.53
1:C:20:LEU:HB3	1:C:90:CYS:SG	2.49	0.53
1:E:229:MET:HE1	1:E:376:LEU:HD22	1.91	0.53
1:K:20:LEU:HB3	1:K:90:CYS:SG	2.49	0.53
1:N:26:LYS:HE3	1:N:446:LEU:HG	1.91	0.53
1:V:26:LYS:HE3	1:V:446:LEU:HG	1.91	0.53
1:A:26:LYS:HE3	1:A:446:LEU:HG	1.91	0.53
1:E:29:GLU:OE2	1:E:89:ARG:NH2	2.38	0.53
1:G:20:LEU:HB3	1:G:90:CYS:SG	2.49	0.53
1:H:26:LYS:HE3	1:H:446:LEU:HG	1.91	0.53
1:P:20:LEU:HB3	1:P:90:CYS:SG	2.49	0.53
1:P:26:LYS:HE3	1:P:446:LEU:HG	1.91	0.53
1:Q:20:LEU:HB3	1:Q:90:CYS:SG	2.49	0.53
1:S:26:LYS:HE3	1:S:446:LEU:HG	1.91	0.53
1:S:229:MET:HE1	1:S:376:LEU:HD22	1.91	0.53
1:U:26:LYS:HE3	1:U:446:LEU:HG	1.91	0.53
1:W:20:LEU:HB3	1:W:90:CYS:SG	2.49	0.53
1:X:29:GLU:OE2	1:X:89:ARG:NH2	2.38	0.53
1:F:20:LEU:HB3	1:F:90:CYS:SG	2.49	0.53
1:H:20:LEU:HB3	1:H:90:CYS:SG	2.49	0.53
1:M:20:LEU:HB3	1:M:90:CYS:SG	2.49	0.53
1:M:26:LYS:HE3	1:M:446:LEU:HG	1.91	0.53
1:N:20:LEU:HB3	1:N:90:CYS:SG	2.49	0.53
1:Q:26:LYS:HE3	1:Q:446:LEU:HG	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:20:LEU:HB3	1:R:90:CYS:SG	2.49	0.53
1:S:29:GLU:OE2	1:S:89:ARG:NH2	2.38	0.53
1:U:29:GLU:OE2	1:U:89:ARG:NH2	2.38	0.53
1:Y:229:MET:HE1	1:Y:376:LEU:HD22	1.90	0.53
1:A:29:GLU:OE2	1:A:89:ARG:NH2	2.38	0.53
1:B:26:LYS:HE3	1:B:446:LEU:HG	1.91	0.53
1:C:229:MET:HE1	1:C:376:LEU:HD22	1.90	0.53
1:C:453:ARG:NH2	1:K:464:GLU:OE1	2.42	0.53
1:I:20:LEU:HB3	1:I:90:CYS:SG	2.49	0.53
1:J:20:LEU:HB3	1:J:90:CYS:SG	2.49	0.53
1:J:26:LYS:HE3	1:J:446:LEU:HG	1.91	0.53
1:E:26:LYS:HE3	1:E:446:LEU:HG	1.91	0.52
1:P:229:MET:HE1	1:P:376:LEU:HD22	1.90	0.52
1:Q:229:MET:HE1	1:Q:376:LEU:HD22	1.91	0.52
1:X:20:LEU:HB3	1:X:90:CYS:SG	2.49	0.52
1:Y:426:ARG:NH2	1:Y:441:ASP:OD1	2.35	0.52
1:A:20:LEU:HB3	1:A:90:CYS:SG	2.49	0.52
1:J:229:MET:HE1	1:J:376:LEU:HD22	1.92	0.52
1:V:20:LEU:HB3	1:V:90:CYS:SG	2.49	0.52
1:X:26:LYS:HE3	1:X:446:LEU:HG	1.91	0.52
1:A:319:SER:OG	1:A:363:ASP:OD2	2.19	0.52
1:D:20:LEU:HB3	1:D:90:CYS:SG	2.49	0.52
1:F:229:MET:HE1	1:F:376:LEU:HD22	1.91	0.52
1:I:426:ARG:NH2	1:I:441:ASP:OD1	2.35	0.52
1:K:26:LYS:HE3	1:K:446:LEU:HG	1.91	0.52
1:L:20:LEU:HB3	1:L:90:CYS:SG	2.49	0.52
1:N:229:MET:HE1	1:N:376:LEU:HD22	1.91	0.52
1:O:453:ARG:NH2	1:X:464:GLU:OE1	2.42	0.52
1:V:229:MET:HE1	1:V:376:LEU:HD22	1.90	0.52
1:K:29:GLU:OE2	1:K:89:ARG:NH2	2.38	0.52
1:K:319:SER:OG	1:K:363:ASP:OD2	2.19	0.52
1:M:29:GLU:OE2	1:M:89:ARG:NH2	2.38	0.52
1:M:312:LEU:HD22	1:M:374:ALA:HB2	1.92	0.52
1:M:319:SER:OG	1:M:363:ASP:OD2	2.19	0.52
1:M:331:VAL:HG23	1:M:411:VAL:HG22	1.92	0.52
1:W:229:MET:HE1	1:W:376:LEU:HD22	1.92	0.52
1:C:331:VAL:HG23	1:C:411:VAL:HG22	1.92	0.52
1:D:229:MET:HE1	1:D:376:LEU:HD22	1.90	0.52
1:E:20:LEU:HB3	1:E:90:CYS:SG	2.49	0.52
1:H:312:LEU:HD22	1:H:374:ALA:HB2	1.92	0.52
1:J:331:VAL:HG23	1:J:411:VAL:HG22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:426:ARG:NH2	1:M:441:ASP:OD1	2.35	0.52
1:R:312:LEU:HD22	1:R:374:ALA:HB2	1.92	0.52
1:S:20:LEU:HB3	1:S:90:CYS:SG	2.49	0.52
1:S:312:LEU:HD22	1:S:374:ALA:HB2	1.92	0.52
1:U:20:LEU:HB3	1:U:90:CYS:SG	2.49	0.52
1:Y:331:VAL:HG23	1:Y:411:VAL:HG22	1.92	0.52
1:B:229:MET:HE1	1:B:376:LEU:HD22	1.92	0.52
1:E:312:LEU:HD22	1:E:374:ALA:HB2	1.92	0.52
1:F:331:VAL:HG23	1:F:411:VAL:HG22	1.92	0.52
1:H:229:MET:HE1	1:H:376:LEU:HD22	1.92	0.52
1:W:312:LEU:HD22	1:W:374:ALA:HB2	1.92	0.52
1:X:319:SER:OG	1:X:363:ASP:OD2	2.19	0.52
1:G:229:MET:HE1	1:G:376:LEU:HD22	1.90	0.52
1:G:331:VAL:HG23	1:G:411:VAL:HG22	1.92	0.52
1:I:229:MET:HE1	1:I:376:LEU:HD22	1.92	0.52
1:K:312:LEU:HD22	1:K:374:ALA:HB2	1.92	0.52
1:L:229:MET:HE1	1:L:376:LEU:HD22	1.91	0.52
1:O:20:LEU:HB3	1:O:90:CYS:SG	2.49	0.52
1:R:229:MET:HE1	1:R:376:LEU:HD22	1.92	0.52
1:X:312:LEU:HD22	1:X:374:ALA:HB2	1.92	0.52
1:D:312:LEU:HD22	1:D:374:ALA:HB2	1.92	0.52
1:F:312:LEU:HD22	1:F:374:ALA:HB2	1.92	0.52
1:I:312:LEU:HD22	1:I:374:ALA:HB2	1.92	0.52
1:P:307:LYS:HB2	1:P:421:GLU:HG2	1.92	0.52
1:Q:312:LEU:HD22	1:Q:374:ALA:HB2	1.92	0.52
1:W:307:LYS:HB2	1:W:421:GLU:HG2	1.92	0.52
1:A:312:LEU:HD22	1:A:374:ALA:HB2	1.92	0.52
1:B:312:LEU:HD22	1:B:374:ALA:HB2	1.92	0.52
1:E:307:LYS:HB2	1:E:421:GLU:HG2	1.92	0.52
1:G:312:LEU:HD22	1:G:374:ALA:HB2	1.92	0.52
1:J:312:LEU:HD22	1:J:374:ALA:HB2	1.92	0.52
1:K:331:VAL:HG23	1:K:411:VAL:HG22	1.92	0.52
1:N:331:VAL:HG23	1:N:411:VAL:HG22	1.92	0.52
1:Q:307:LYS:HB2	1:Q:421:GLU:HG2	1.92	0.52
1:V:312:LEU:HD22	1:V:374:ALA:HB2	1.92	0.52
1:W:331:VAL:HG23	1:W:411:VAL:HG22	1.92	0.52
1:A:331:VAL:HG23	1:A:411:VAL:HG22	1.92	0.52
1:B:331:VAL:HG23	1:B:411:VAL:HG22	1.92	0.52
1:D:307:LYS:HB2	1:D:421:GLU:HG2	1.92	0.52
1:G:307:LYS:HB2	1:G:421:GLU:HG2	1.92	0.52
1:I:307:LYS:HB2	1:I:421:GLU:HG2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:331:VAL:HG23	1:P:411:VAL:HG22	1.92	0.52
1:X:331:VAL:HG23	1:X:411:VAL:HG22	1.92	0.52
1:C:319:SER:OG	1:C:363:ASP:OD2	2.19	0.51
1:H:307:LYS:HB2	1:H:421:GLU:HG2	1.92	0.51
1:S:307:LYS:HB2	1:S:421:GLU:HG2	1.92	0.51
1:U:229:MET:HE1	1:U:376:LEU:HD22	1.91	0.51
1:U:307:LYS:HB2	1:U:421:GLU:HG2	1.92	0.51
1:U:312:LEU:HD22	1:U:374:ALA:HB2	1.92	0.51
1:V:307:LYS:HB2	1:V:421:GLU:HG2	1.92	0.51
1:F:307:LYS:HB2	1:F:421:GLU:HG2	1.92	0.51
1:L:331:VAL:HG23	1:L:411:VAL:HG22	1.92	0.51
1:O:312:LEU:HD22	1:O:374:ALA:HB2	1.92	0.51
1:P:29:GLU:OE2	1:P:89:ARG:NH2	2.38	0.51
1:P:312:LEU:HD22	1:P:374:ALA:HB2	1.92	0.51
1:S:331:VAL:HG23	1:S:411:VAL:HG22	1.92	0.51
1:D:426:ARG:NH2	1:D:441:ASP:OD1	2.35	0.51
1:J:307:LYS:HB2	1:J:421:GLU:HG2	1.92	0.51
1:N:453:ARG:NH2	1:Y:464:GLU:OE1	2.43	0.51
1:O:331:VAL:HG23	1:O:411:VAL:HG22	1.92	0.51
1:Q:331:VAL:HG23	1:Q:411:VAL:HG22	1.92	0.51
1:Y:312:LEU:HD22	1:Y:374:ALA:HB2	1.92	0.51
1:A:229:MET:HE1	1:A:376:LEU:HD22	1.93	0.51
1:A:307:LYS:HB2	1:A:421:GLU:HG2	1.92	0.51
1:L:312:LEU:HD22	1:L:374:ALA:HB2	1.92	0.51
1:N:312:LEU:HD22	1:N:374:ALA:HB2	1.92	0.51
1:R:307:LYS:HB2	1:R:421:GLU:HG2	1.92	0.51
1:C:312:LEU:HD22	1:C:374:ALA:HB2	1.92	0.51
1:V:331:VAL:HG23	1:V:411:VAL:HG22	1.92	0.51
1:X:229:MET:HE1	1:X:376:LEU:HD22	1.93	0.51
1:B:453:ARG:NH2	1:L:464:GLU:OE1	2.43	0.51
1:A:338:ARG:NH2	1:B:64:SER:OG	2.30	0.51
1:E:331:VAL:HG23	1:E:411:VAL:HG22	1.92	0.51
1:H:331:VAL:HG23	1:H:411:VAL:HG22	1.92	0.51
1:L:307:LYS:HB2	1:L:421:GLU:HG2	1.92	0.51
1:M:307:LYS:HB2	1:M:421:GLU:HG2	1.92	0.51
1:O:229:MET:HE1	1:O:376:LEU:HD22	1.91	0.51
1:O:307:LYS:HB2	1:O:421:GLU:HG2	1.92	0.51
1:R:262:PHE:HE1	1:V:456:MET:HG3	1.76	0.51
1:H:426:ARG:NH2	1:H:441:ASP:OD1	2.35	0.51
1:K:426:ARG:NH2	1:K:441:ASP:OD1	2.35	0.51
1:U:331:VAL:HG23	1:U:411:VAL:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:307:LYS:HB2	1:C:421:GLU:HG2	1.92	0.50
1:D:331:VAL:HG23	1:D:411:VAL:HG22	1.92	0.50
1:I:331:VAL:HG23	1:I:411:VAL:HG22	1.92	0.50
1:N:307:LYS:HB2	1:N:421:GLU:HG2	1.92	0.50
1:Y:307:LYS:HB2	1:Y:421:GLU:HG2	1.92	0.50
1:B:307:LYS:HB2	1:B:421:GLU:HG2	1.92	0.50
1:F:262:PHE:HE1	1:H:456:MET:HG3	1.76	0.50
1:R:331:VAL:HG23	1:R:411:VAL:HG22	1.92	0.50
1:W:426:ARG:NH2	1:W:441:ASP:OD1	2.35	0.50
1:K:307:LYS:HB2	1:K:421:GLU:HG2	1.92	0.50
1:X:307:LYS:HB2	1:X:421:GLU:HG2	1.92	0.50
1:G:103:ARG:HH21	1:G:438:GLU:CG	2.25	0.50
1:O:426:ARG:NH2	1:O:441:ASP:OD1	2.35	0.50
1:H:103:ARG:HH21	1:H:438:GLU:CG	2.25	0.50
1:L:103:ARG:HH21	1:L:438:GLU:CG	2.25	0.50
1:K:229:MET:HE1	1:K:376:LEU:HD22	1.94	0.50
1:P:103:ARG:HH21	1:P:438:GLU:CG	2.25	0.49
1:V:426:ARG:NH2	1:V:441:ASP:OD1	2.35	0.49
1:I:103:ARG:HH21	1:I:438:GLU:CG	2.25	0.49
1:K:103:ARG:HH21	1:K:438:GLU:CG	2.25	0.49
1:A:272:HIS:HB3	1:A:356:ARG:HD2	1.95	0.49
1:E:272:HIS:HB3	1:E:356:ARG:HD2	1.95	0.49
1:B:262:PHE:HE1	1:L:456:MET:HG3	1.78	0.49
1:C:103:ARG:HH21	1:C:438:GLU:CG	2.25	0.49
1:G:272:HIS:HB3	1:G:356:ARG:HD2	1.95	0.49
1:I:272:HIS:HB3	1:I:356:ARG:HD2	1.95	0.49
1:P:272:HIS:HB3	1:P:356:ARG:HD2	1.95	0.49
1:V:272:HIS:HB3	1:V:356:ARG:HD2	1.95	0.49
1:A:426:ARG:NH2	1:A:441:ASP:OD1	2.35	0.49
1:J:272:HIS:HB3	1:J:356:ARG:HD2	1.95	0.49
1:N:262:PHE:HE1	1:Y:456:MET:HG3	1.78	0.49
1:R:272:HIS:HB3	1:R:356:ARG:HD2	1.95	0.49
1:W:272:HIS:HB3	1:W:356:ARG:HD2	1.95	0.49
1:D:103:ARG:HH21	1:D:438:GLU:CG	2.25	0.49
1:D:272:HIS:HB3	1:D:356:ARG:HD2	1.95	0.49
1:J:103:ARG:HH21	1:J:438:GLU:CG	2.25	0.49
1:M:272:HIS:HB3	1:M:356:ARG:HD2	1.95	0.49
1:Q:272:HIS:HB3	1:Q:356:ARG:HD2	1.95	0.49
1:X:272:HIS:HB3	1:X:356:ARG:HD2	1.95	0.49
1:C:262:PHE:HE1	1:K:456:MET:HG3	1.78	0.49
1:C:426:ARG:NH2	1:C:441:ASP:OD1	2.35	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:272:HIS:HB3	1:K:356:ARG:HD2	1.95	0.49
1:S:272:HIS:HB3	1:S:356:ARG:HD2	1.95	0.49
1:U:272:HIS:HB3	1:U:356:ARG:HD2	1.95	0.49
1:B:272:HIS:HB3	1:B:356:ARG:HD2	1.95	0.49
1:H:272:HIS:HB3	1:H:356:ARG:HD2	1.95	0.49
1:B:103:ARG:HH21	1:B:438:GLU:CG	2.25	0.48
1:Y:272:HIS:HB3	1:Y:356:ARG:HD2	1.95	0.48
1:C:272:HIS:HB3	1:C:356:ARG:HD2	1.95	0.48
1:D:29:GLU:OE2	1:D:89:ARG:NH2	2.38	0.48
1:F:272:HIS:HB3	1:F:356:ARG:HD2	1.95	0.48
1:L:272:HIS:HB3	1:L:356:ARG:HD2	1.95	0.48
1:N:272:HIS:HB3	1:N:356:ARG:HD2	1.95	0.48
1:E:103:ARG:HH21	1:E:438:GLU:CG	2.25	0.48
1:M:103:ARG:HH21	1:M:438:GLU:CG	2.25	0.48
1:O:262:PHE:HE1	1:X:456:MET:HG3	1.78	0.48
1:O:272:HIS:HB3	1:O:356:ARG:HD2	1.95	0.48
1:S:103:ARG:HH21	1:S:438:GLU:CG	2.25	0.48
1:X:103:ARG:HH21	1:X:438:GLU:CG	2.25	0.48
1:R:103:ARG:HH21	1:R:438:GLU:CG	2.25	0.48
1:Y:453:ARG:O	1:Y:457:THR:HG23	2.14	0.48
1:G:453:ARG:O	1:G:457:THR:HG23	2.14	0.48
1:K:453:ARG:O	1:K:457:THR:HG23	2.14	0.48
1:A:103:ARG:HH21	1:A:438:GLU:CG	2.25	0.48
1:A:453:ARG:O	1:A:457:THR:HG23	2.14	0.48
1:E:453:ARG:O	1:E:457:THR:HG23	2.14	0.48
1:F:103:ARG:HH21	1:F:438:GLU:CG	2.25	0.48
1:L:453:ARG:O	1:L:457:THR:HG23	2.14	0.48
1:B:453:ARG:O	1:B:457:THR:HG23	2.14	0.48
1:N:453:ARG:O	1:N:457:THR:HG23	2.14	0.48
1:R:453:ARG:O	1:R:457:THR:HG23	2.14	0.48
1:G:426:ARG:NH2	1:G:441:ASP:OD1	2.35	0.48
1:O:453:ARG:O	1:O:457:THR:HG23	2.14	0.48
1:S:397:LEU:HD21	1:X:61:ILE:HD11	1.95	0.48
1:U:453:ARG:O	1:U:457:THR:HG23	2.14	0.48
1:O:103:ARG:HH21	1:O:438:GLU:CG	2.25	0.47
1:F:453:ARG:O	1:F:457:THR:HG23	2.14	0.47
1:H:453:ARG:O	1:H:457:THR:HG23	2.14	0.47
1:R:232:LYS:HD2	1:R:232:LYS:HA	1.69	0.47
1:S:453:ARG:O	1:S:457:THR:HG23	2.14	0.47
1:A:283:PHE:HA	1:A:295:ALA:HB2	1.96	0.47
1:J:283:PHE:HA	1:J:295:ALA:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:397:LEU:HD21	1:K:61:ILE:HD11	1.95	0.47
1:N:103:ARG:HH21	1:N:438:GLU:CG	2.25	0.47
1:U:103:ARG:HH21	1:U:438:GLU:CG	2.25	0.47
1:I:453:ARG:O	1:I:457:THR:HG23	2.14	0.47
1:J:453:ARG:O	1:J:457:THR:HG23	2.14	0.47
1:M:283:PHE:HA	1:M:295:ALA:HB2	1.97	0.47
1:Q:453:ARG:O	1:Q:457:THR:HG23	2.14	0.47
1:W:453:ARG:O	1:W:457:THR:HG23	2.14	0.47
1:X:232:LYS:HD2	1:X:232:LYS:HA	1.69	0.47
1:X:283:PHE:HA	1:X:295:ALA:HB2	1.96	0.47
1:C:453:ARG:O	1:C:457:THR:HG23	2.14	0.47
1:Q:262:PHE:HE1	1:W:456:MET:HG3	1.80	0.47
1:R:283:PHE:HA	1:R:295:ALA:HB2	1.96	0.47
1:S:283:PHE:HA	1:S:295:ALA:HB2	1.97	0.47
1:W:103:ARG:HH21	1:W:438:GLU:CG	2.25	0.47
1:Y:103:ARG:HH21	1:Y:438:GLU:CG	2.25	0.47
1:K:283:PHE:HA	1:K:295:ALA:HB2	1.96	0.47
1:P:453:ARG:O	1:P:457:THR:HG23	2.14	0.47
1:D:453:ARG:O	1:D:457:THR:HG23	2.14	0.47
1:F:283:PHE:HA	1:F:295:ALA:HB2	1.96	0.47
1:V:103:ARG:HH21	1:V:438:GLU:CG	2.25	0.47
1:X:453:ARG:O	1:X:457:THR:HG23	2.14	0.47
1:B:283:PHE:HA	1:B:295:ALA:HB2	1.97	0.47
1:H:232:LYS:HD2	1:H:232:LYS:HA	1.69	0.47
1:I:283:PHE:HA	1:I:295:ALA:HB2	1.96	0.47
1:L:141:PHE:HB3	1:L:150:VAL:HG23	1.97	0.47
1:S:232:LYS:HD2	1:S:232:LYS:HA	1.69	0.47
1:V:453:ARG:O	1:V:457:THR:HG23	2.14	0.47
1:Y:141:PHE:HB3	1:Y:150:VAL:HG23	1.97	0.47
1:B:232:LYS:HD2	1:B:232:LYS:HA	1.69	0.47
1:C:141:PHE:HB3	1:C:150:VAL:HG23	1.97	0.47
1:E:262:PHE:HE1	1:I:456:MET:HG3	1.80	0.47
1:A:335:TYR:HA	1:A:344:ILE:O	2.15	0.47
1:D:195:GLU:OE2	1:D:249:ARG:NH2	2.48	0.47
1:O:141:PHE:HB3	1:O:150:VAL:HG23	1.97	0.47
1:U:195:GLU:OE2	1:U:249:ARG:NH2	2.48	0.47
1:I:335:TYR:HA	1:I:344:ILE:O	2.15	0.46
1:N:283:PHE:HA	1:N:295:ALA:HB2	1.97	0.46
1:Q:103:ARG:HH21	1:Q:438:GLU:CG	2.25	0.46
1:X:335:TYR:HA	1:X:344:ILE:O	2.15	0.46
1:B:141:PHE:HB3	1:B:150:VAL:HG23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:334:ALA:O	1:D:342:ALA:HB1	2.16	0.46
1:K:213:GLU:HG2	1:K:215:ALA:O	2.16	0.46
1:L:213:GLU:HG2	1:L:215:ALA:O	2.16	0.46
1:M:195:GLU:OE2	1:M:249:ARG:NH2	2.49	0.46
1:M:213:GLU:HG2	1:M:215:ALA:O	2.16	0.46
1:N:195:GLU:OE2	1:N:249:ARG:NH2	2.49	0.46
1:R:213:GLU:HG2	1:R:215:ALA:O	2.16	0.46
1:V:334:ALA:O	1:V:342:ALA:HB1	2.16	0.46
1:W:283:PHE:HA	1:W:295:ALA:HB2	1.96	0.46
1:X:141:PHE:HB3	1:X:150:VAL:HG23	1.97	0.46
1:E:195:GLU:OE2	1:E:249:ARG:NH2	2.48	0.46
1:I:195:GLU:OE2	1:I:249:ARG:NH2	2.49	0.46
1:J:195:GLU:OE2	1:J:249:ARG:NH2	2.49	0.46
1:K:141:PHE:HB3	1:K:150:VAL:HG23	1.97	0.46
1:M:453:ARG:O	1:M:457:THR:HG23	2.14	0.46
1:N:141:PHE:HB3	1:N:150:VAL:HG23	1.97	0.46
1:S:195:GLU:OE2	1:S:249:ARG:NH2	2.49	0.46
1:V:283:PHE:HA	1:V:295:ALA:HB2	1.96	0.46
1:Y:283:PHE:HA	1:Y:295:ALA:HB2	1.97	0.46
1:B:71:ASP:OD1	1:B:73:SER:OG	2.34	0.46
1:D:335:TYR:HA	1:D:344:ILE:O	2.15	0.46
1:F:334:ALA:O	1:F:342:ALA:HB1	2.15	0.46
1:H:334:ALA:O	1:H:342:ALA:HB1	2.16	0.46
1:K:195:GLU:OE2	1:K:249:ARG:NH2	2.49	0.46
1:M:141:PHE:HB3	1:M:150:VAL:HG23	1.97	0.46
1:N:71:ASP:OD1	1:N:73:SER:OG	2.34	0.46
1:N:213:GLU:HG2	1:N:215:ALA:O	2.16	0.46
1:O:195:GLU:OE2	1:O:249:ARG:NH2	2.49	0.46
1:O:232:LYS:HD2	1:O:232:LYS:HA	1.69	0.46
1:Q:334:ALA:O	1:Q:342:ALA:HB1	2.15	0.46
1:Y:195:GLU:OE2	1:Y:249:ARG:NH2	2.49	0.46
1:A:71:ASP:OD1	1:A:73:SER:OG	2.34	0.46
1:B:213:GLU:HG2	1:B:215:ALA:O	2.16	0.46
1:B:335:TYR:HA	1:B:344:ILE:O	2.16	0.46
1:C:195:GLU:OE2	1:C:249:ARG:NH2	2.49	0.46
1:E:334:ALA:O	1:E:342:ALA:HB1	2.16	0.46
1:H:283:PHE:HA	1:H:295:ALA:HB2	1.96	0.46
1:J:213:GLU:HG2	1:J:215:ALA:O	2.16	0.46
1:L:195:GLU:OE2	1:L:249:ARG:NH2	2.48	0.46
1:M:71:ASP:OD1	1:M:73:SER:OG	2.34	0.46
1:O:213:GLU:HG2	1:O:215:ALA:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:283:PHE:HA	1:O:295:ALA:HB2	1.97	0.46
1:Q:283:PHE:HA	1:Q:295:ALA:HB2	1.96	0.46
1:Q:335:TYR:HA	1:Q:344:ILE:O	2.16	0.46
1:U:71:ASP:OD1	1:U:73:SER:OG	2.34	0.46
1:W:213:GLU:HG2	1:W:215:ALA:O	2.16	0.46
1:X:195:GLU:OE2	1:X:249:ARG:NH2	2.49	0.46
1:C:71:ASP:OD1	1:C:73:SER:OG	2.34	0.46
1:F:195:GLU:OE2	1:F:249:ARG:NH2	2.49	0.46
1:H:195:GLU:OE2	1:H:249:ARG:NH2	2.49	0.46
1:L:71:ASP:OD1	1:L:73:SER:OG	2.34	0.46
1:L:283:PHE:HA	1:L:295:ALA:HB2	1.97	0.46
1:O:71:ASP:OD1	1:O:73:SER:OG	2.34	0.46
1:P:213:GLU:HG2	1:P:215:ALA:O	2.16	0.46
1:P:283:PHE:HA	1:P:295:ALA:HB2	1.96	0.46
1:Q:195:GLU:OE2	1:Q:249:ARG:NH2	2.48	0.46
1:R:335:TYR:HA	1:R:344:ILE:O	2.15	0.46
1:U:283:PHE:HA	1:U:295:ALA:HB2	1.97	0.46
1:U:335:TYR:HA	1:U:344:ILE:O	2.16	0.46
1:A:195:GLU:OE2	1:A:249:ARG:NH2	2.49	0.46
1:C:213:GLU:HG2	1:C:215:ALA:O	2.16	0.46
1:E:283:PHE:HA	1:E:295:ALA:HB2	1.96	0.46
1:F:335:TYR:HA	1:F:344:ILE:O	2.15	0.46
1:G:71:ASP:OD1	1:G:73:SER:OG	2.34	0.46
1:G:213:GLU:HG2	1:G:215:ALA:O	2.16	0.46
1:G:334:ALA:O	1:G:342:ALA:HB1	2.16	0.46
1:J:335:TYR:HA	1:J:344:ILE:O	2.16	0.46
1:M:335:TYR:HA	1:M:344:ILE:O	2.15	0.46
1:N:335:TYR:HA	1:N:344:ILE:O	2.15	0.46
1:O:335:TYR:HA	1:O:344:ILE:O	2.16	0.46
1:P:334:ALA:O	1:P:342:ALA:HB1	2.16	0.46
1:Q:213:GLU:HG2	1:Q:215:ALA:O	2.16	0.46
1:R:195:GLU:OE2	1:R:249:ARG:NH2	2.49	0.46
1:U:141:PHE:HB3	1:U:150:VAL:HG23	1.97	0.46
1:V:195:GLU:OE2	1:V:249:ARG:NH2	2.49	0.46
1:V:213:GLU:HG2	1:V:215:ALA:O	2.16	0.46
1:Y:71:ASP:OD1	1:Y:73:SER:OG	2.34	0.46
1:A:141:PHE:HB3	1:A:150:VAL:HG23	1.97	0.46
1:C:283:PHE:HA	1:C:295:ALA:HB2	1.97	0.46
1:D:141:PHE:HB3	1:D:150:VAL:HG23	1.97	0.46
1:G:141:PHE:HB3	1:G:150:VAL:HG23	1.97	0.46
1:G:232:LYS:HD2	1:G:232:LYS:HA	1.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:141:PHE:HB3	1:H:150:VAL:HG23	1.97	0.46
1:M:262:PHE:HE1	1:U:456:MET:HG3	1.81	0.46
1:O:334:ALA:O	1:O:342:ALA:HB1	2.16	0.46
1:Q:141:PHE:HB3	1:Q:150:VAL:HG23	1.97	0.46
1:Y:335:TYR:HA	1:Y:344:ILE:O	2.16	0.46
1:B:195:GLU:OE2	1:B:249:ARG:NH2	2.49	0.46
1:C:58:TRP:CD1	1:C:58:TRP:N	2.84	0.46
1:D:71:ASP:OD1	1:D:73:SER:OG	2.34	0.46
1:F:71:ASP:OD1	1:F:73:SER:OG	2.34	0.46
1:G:195:GLU:OE2	1:G:249:ARG:NH2	2.48	0.46
1:H:335:TYR:HA	1:H:344:ILE:O	2.15	0.46
1:J:141:PHE:HB3	1:J:150:VAL:HG23	1.97	0.46
1:L:58:TRP:CD1	1:L:58:TRP:N	2.84	0.46
1:M:334:ALA:O	1:M:342:ALA:HB1	2.16	0.46
1:P:71:ASP:OD1	1:P:73:SER:OG	2.34	0.46
1:R:71:ASP:OD1	1:R:73:SER:OG	2.34	0.46
1:S:335:TYR:HA	1:S:344:ILE:O	2.16	0.46
1:U:58:TRP:CD1	1:U:58:TRP:N	2.84	0.46
1:Y:334:ALA:O	1:Y:342:ALA:HB1	2.15	0.46
1:C:312:LEU:HD23	1:C:370:LEU:HB3	1.98	0.46
1:D:283:PHE:HA	1:D:295:ALA:HB2	1.96	0.46
1:G:312:LEU:HD23	1:G:370:LEU:HB3	1.98	0.46
1:I:213:GLU:HG2	1:I:215:ALA:O	2.16	0.46
1:J:291:LEU:HD21	1:J:299:ILE:HD11	1.98	0.46
1:J:334:ALA:O	1:J:342:ALA:HB1	2.15	0.46
1:K:334:ALA:O	1:K:342:ALA:HB1	2.15	0.46
1:L:312:LEU:HD23	1:L:370:LEU:HB3	1.98	0.46
1:L:335:TYR:HA	1:L:344:ILE:O	2.16	0.46
1:N:334:ALA:O	1:N:342:ALA:HB1	2.16	0.46
1:O:312:LEU:HD23	1:O:370:LEU:HB3	1.98	0.46
1:P:195:GLU:OE2	1:P:249:ARG:NH2	2.49	0.46
1:S:213:GLU:HG2	1:S:215:ALA:O	2.16	0.46
1:X:291:LEU:HD21	1:X:299:ILE:HD11	1.99	0.46
1:X:334:ALA:O	1:X:342:ALA:HB1	2.15	0.46
1:Y:213:GLU:HG2	1:Y:215:ALA:O	2.16	0.46
1:A:262:PHE:HE1	1:G:456:MET:HG3	1.81	0.45
1:D:291:LEU:HD21	1:D:299:ILE:HD11	1.98	0.45
1:D:312:LEU:HD23	1:D:370:LEU:HB3	1.99	0.45
1:E:71:ASP:OD1	1:E:73:SER:OG	2.34	0.45
1:E:213:GLU:HG2	1:E:215:ALA:O	2.16	0.45
1:G:283:PHE:HA	1:G:295:ALA:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:213:GLU:HG2	1:H:215:ALA:O	2.16	0.45
1:I:334:ALA:O	1:I:342:ALA:HB1	2.16	0.45
1:L:232:LYS:HD2	1:L:232:LYS:HA	1.69	0.45
1:N:312:LEU:HD23	1:N:370:LEU:HB3	1.98	0.45
1:P:141:PHE:HB3	1:P:150:VAL:HG23	1.97	0.45
1:P:291:LEU:HD21	1:P:299:ILE:HD11	1.98	0.45
1:Q:71:ASP:OD1	1:Q:73:SER:OG	2.34	0.45
1:S:334:ALA:O	1:S:342:ALA:HB1	2.15	0.45
1:U:291:LEU:HD21	1:U:299:ILE:HD11	1.99	0.45
1:V:71:ASP:OD1	1:V:73:SER:OG	2.34	0.45
1:W:141:PHE:HB3	1:W:150:VAL:HG23	1.97	0.45
1:W:195:GLU:OE2	1:W:249:ARG:NH2	2.49	0.45
1:Y:312:LEU:HD23	1:Y:370:LEU:HB3	1.98	0.45
1:A:213:GLU:HG2	1:A:215:ALA:O	2.16	0.45
1:F:213:GLU:HG2	1:F:215:ALA:O	2.16	0.45
1:G:291:LEU:HD21	1:G:299:ILE:HD11	1.98	0.45
1:K:291:LEU:HD21	1:K:299:ILE:HD11	1.99	0.45
1:L:291:LEU:HD21	1:L:299:ILE:HD11	1.99	0.45
1:R:334:ALA:O	1:R:342:ALA:HB1	2.15	0.45
1:U:312:LEU:HD23	1:U:370:LEU:HB3	1.99	0.45
1:Y:291:LEU:HD21	1:Y:299:ILE:HD11	1.99	0.45
1:A:291:LEU:HD21	1:A:299:ILE:HD11	1.98	0.45
1:G:58:TRP:N	1:G:58:TRP:CD1	2.84	0.45
1:H:312:LEU:HD23	1:H:370:LEU:HB3	1.98	0.45
1:I:141:PHE:HB3	1:I:150:VAL:HG23	1.97	0.45
1:K:71:ASP:OD1	1:K:73:SER:OG	2.34	0.45
1:M:58:TRP:N	1:M:58:TRP:CD1	2.84	0.45
1:N:291:LEU:HD21	1:N:299:ILE:HD11	1.98	0.45
1:O:291:LEU:HD21	1:O:299:ILE:HD11	1.99	0.45
1:S:141:PHE:HB3	1:S:150:VAL:HG23	1.97	0.45
1:S:291:LEU:HD21	1:S:299:ILE:HD11	1.98	0.45
1:W:334:ALA:O	1:W:342:ALA:HB1	2.16	0.45
1:W:335:TYR:HA	1:W:344:ILE:O	2.15	0.45
1:X:71:ASP:OD1	1:X:73:SER:OG	2.34	0.45
1:B:334:ALA:O	1:B:342:ALA:HB1	2.16	0.45
1:E:312:LEU:HD23	1:E:370:LEU:HB3	1.98	0.45
1:F:141:PHE:HB3	1:F:150:VAL:HG23	1.97	0.45
1:H:291:LEU:HD21	1:H:299:ILE:HD11	1.98	0.45
1:M:291:LEU:HD21	1:M:299:ILE:HD11	1.98	0.45
1:P:312:LEU:HD23	1:P:370:LEU:HB3	1.99	0.45
1:R:291:LEU:HD21	1:R:299:ILE:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:232:LYS:HD2	1:W:232:LYS:HA	1.69	0.45
1:X:213:GLU:HG2	1:X:215:ALA:O	2.16	0.45
1:A:58:TRP:N	1:A:58:TRP:CD1	2.84	0.45
1:B:291:LEU:HD21	1:B:299:ILE:HD11	1.98	0.45
1:C:291:LEU:HD21	1:C:299:ILE:HD11	1.98	0.45
1:C:334:ALA:O	1:C:342:ALA:HB1	2.15	0.45
1:E:291:LEU:HD21	1:E:299:ILE:HD11	1.98	0.45
1:F:291:LEU:HD21	1:F:299:ILE:HD11	1.98	0.45
1:P:335:TYR:HA	1:P:344:ILE:O	2.16	0.45
1:R:141:PHE:HB3	1:R:150:VAL:HG23	1.97	0.45
1:V:141:PHE:HB3	1:V:150:VAL:HG23	1.97	0.45
1:V:291:LEU:HD21	1:V:299:ILE:HD11	1.98	0.45
1:V:312:LEU:HD23	1:V:370:LEU:HB3	1.98	0.45
1:G:129:PRO:CG	1:G:236:ILE:HD11	2.46	0.45
1:H:71:ASP:OD1	1:H:73:SER:OG	2.34	0.45
1:K:335:TYR:HA	1:K:344:ILE:O	2.16	0.45
1:L:334:ALA:O	1:L:342:ALA:HB1	2.15	0.45
1:U:334:ALA:O	1:U:342:ALA:HB1	2.16	0.45
1:V:335:TYR:HA	1:V:344:ILE:O	2.15	0.45
1:W:291:LEU:HD21	1:W:299:ILE:HD11	1.98	0.45
1:B:312:LEU:HD23	1:B:370:LEU:HB3	1.98	0.45
1:C:335:TYR:HA	1:C:344:ILE:O	2.16	0.45
1:D:58:TRP:CD1	1:D:58:TRP:N	2.84	0.45
1:J:58:TRP:CD1	1:J:58:TRP:N	2.84	0.45
1:K:312:LEU:HD23	1:K:370:LEU:HB3	1.98	0.45
1:Q:312:LEU:HD23	1:Q:370:LEU:HB3	1.98	0.45
1:S:71:ASP:OD1	1:S:73:SER:OG	2.34	0.45
1:W:71:ASP:OD1	1:W:73:SER:OG	2.34	0.45
1:X:312:LEU:HD23	1:X:370:LEU:HB3	1.98	0.45
1:D:213:GLU:HG2	1:D:215:ALA:O	2.16	0.45
1:J:71:ASP:OD1	1:J:73:SER:OG	2.34	0.45
1:R:149:HIS:HA	1:V:149:HIS:HA	1.99	0.45
1:W:312:LEU:HD23	1:W:370:LEU:HB3	1.98	0.45
1:A:334:ALA:O	1:A:342:ALA:HB1	2.16	0.45
1:G:335:TYR:HA	1:G:344:ILE:O	2.16	0.45
1:P:58:TRP:N	1:P:58:TRP:CD1	2.84	0.45
1:P:436:THR:HG22	1:P:438:GLU:H	1.82	0.45
1:Q:291:LEU:HD21	1:Q:299:ILE:HD11	1.98	0.45
1:U:436:THR:HG22	1:U:438:GLU:H	1.82	0.45
1:E:335:TYR:HA	1:E:344:ILE:O	2.16	0.45
1:I:71:ASP:OD1	1:I:73:SER:OG	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:312:LEU:HD23	1:M:370:LEU:HB3	1.98	0.45
1:U:213:GLU:HG2	1:U:215:ALA:O	2.16	0.45
1:V:436:THR:HG22	1:V:438:GLU:H	1.82	0.45
1:A:436:THR:HG22	1:A:438:GLU:H	1.82	0.44
1:I:291:LEU:HD21	1:I:299:ILE:HD11	1.99	0.44
1:K:58:TRP:CD1	1:K:58:TRP:N	2.84	0.44
1:M:129:PRO:CG	1:M:236:ILE:HD11	2.46	0.44
1:X:58:TRP:N	1:X:58:TRP:CD1	2.84	0.44
1:X:436:THR:HG22	1:X:438:GLU:H	1.82	0.44
1:A:312:LEU:HD23	1:A:370:LEU:HB3	1.98	0.44
1:C:232:LYS:HA	1:C:232:LYS:HD2	1.69	0.44
1:E:141:PHE:HB3	1:E:150:VAL:HG23	1.97	0.44
1:S:58:TRP:CD1	1:S:58:TRP:N	2.84	0.44
1:V:58:TRP:CD1	1:V:58:TRP:N	2.84	0.44
1:J:129:PRO:CG	1:J:236:ILE:HD11	2.46	0.44
1:J:312:LEU:HD23	1:J:370:LEU:HB3	1.98	0.44
1:J:436:THR:HG22	1:J:438:GLU:H	1.82	0.44
1:Q:436:THR:HG22	1:Q:438:GLU:H	1.82	0.44
1:R:58:TRP:N	1:R:58:TRP:CD1	2.84	0.44
1:R:312:LEU:HD23	1:R:370:LEU:HB3	1.98	0.44
1:Y:436:THR:HG22	1:Y:438:GLU:H	1.82	0.44
1:I:312:LEU:HD23	1:I:370:LEU:HB3	1.98	0.44
1:I:436:THR:HG22	1:I:438:GLU:H	1.82	0.44
1:S:436:THR:HG22	1:S:438:GLU:H	1.82	0.44
1:U:309:ILE:HD11	1:U:378:ALA:CB	2.48	0.44
1:D:232:LYS:HD2	1:D:232:LYS:HA	1.69	0.44
1:E:309:ILE:HD11	1:E:378:ALA:CB	2.48	0.44
1:F:58:TRP:CD1	1:F:58:TRP:N	2.84	0.44
1:F:312:LEU:HD23	1:F:370:LEU:HB3	1.98	0.44
1:G:397:LEU:HD21	1:H:61:ILE:HD11	1.99	0.44
1:M:149:HIS:HA	1:U:149:HIS:HA	2.00	0.44
1:R:436:THR:HG22	1:R:438:GLU:H	1.82	0.44
1:B:436:THR:HG22	1:B:438:GLU:H	1.82	0.44
1:C:309:ILE:HD11	1:C:378:ALA:CB	2.48	0.44
1:E:58:TRP:CD1	1:E:58:TRP:N	2.84	0.44
1:F:149:HIS:HA	1:H:149:HIS:HA	1.99	0.44
1:F:436:THR:HG22	1:F:438:GLU:H	1.82	0.44
1:H:58:TRP:N	1:H:58:TRP:CD1	2.84	0.44
1:O:436:THR:HG22	1:O:438:GLU:H	1.82	0.44
1:P:309:ILE:HD11	1:P:378:ALA:CB	2.48	0.44
1:S:312:LEU:HD23	1:S:370:LEU:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:309:ILE:HD11	1:W:378:ALA:CB	2.48	0.44
1:C:129:PRO:CG	1:C:236:ILE:HD11	2.46	0.44
1:Q:58:TRP:N	1:Q:58:TRP:CD1	2.84	0.44
1:W:58:TRP:N	1:W:58:TRP:CD1	2.84	0.44
1:F:129:PRO:CG	1:F:236:ILE:HD11	2.46	0.44
1:G:309:ILE:HD11	1:G:378:ALA:CB	2.48	0.44
1:H:309:ILE:HD11	1:H:378:ALA:CB	2.48	0.44
1:L:436:THR:HG22	1:L:438:GLU:H	1.82	0.44
1:U:397:LEU:HD21	1:V:61:ILE:HD11	1.99	0.44
1:U:429:LEU:O	1:U:435:PHE:HB2	2.18	0.44
1:W:129:PRO:CG	1:W:236:ILE:HD11	2.46	0.44
1:C:429:LEU:O	1:C:435:PHE:HB2	2.18	0.43
1:I:58:TRP:N	1:I:58:TRP:CD1	2.84	0.43
1:W:436:THR:HG22	1:W:438:GLU:H	1.82	0.43
1:Y:129:PRO:CG	1:Y:236:ILE:HD11	2.46	0.43
1:A:309:ILE:HD11	1:A:378:ALA:CB	2.48	0.43
1:G:436:THR:HG22	1:G:438:GLU:H	1.82	0.43
1:P:429:LEU:O	1:P:435:PHE:HB2	2.18	0.43
1:U:232:LYS:HD2	1:U:232:LYS:HA	1.68	0.43
1:Y:429:LEU:O	1:Y:435:PHE:HB2	2.18	0.43
1:B:429:LEU:O	1:B:435:PHE:HB2	2.18	0.43
1:I:232:LYS:HD2	1:I:232:LYS:HA	1.69	0.43
1:O:429:LEU:O	1:O:435:PHE:HB2	2.18	0.43
1:A:149:HIS:HA	1:G:149:HIS:HA	2.00	0.43
1:G:429:LEU:O	1:G:435:PHE:HB2	2.18	0.43
1:H:429:LEU:O	1:H:435:PHE:HB2	2.18	0.43
1:O:309:ILE:HD11	1:O:378:ALA:CB	2.48	0.43
1:C:436:THR:HG22	1:C:438:GLU:H	1.82	0.43
1:D:463:PHE:HZ	1:J:260:PRO:O	2.02	0.43
1:Y:58:TRP:N	1:Y:58:TRP:CD1	2.84	0.43
1:B:309:ILE:HD11	1:B:378:ALA:CB	2.48	0.43
1:K:436:THR:HG22	1:K:438:GLU:H	1.82	0.43
1:M:436:THR:HG22	1:M:438:GLU:H	1.82	0.43
1:Q:309:ILE:HD11	1:Q:378:ALA:CB	2.48	0.43
1:R:309:ILE:HD11	1:R:378:ALA:CB	2.48	0.43
1:R:429:LEU:O	1:R:435:PHE:HB2	2.18	0.43
1:V:319:SER:OG	1:V:363:ASP:OD2	2.19	0.43
1:D:309:ILE:HD11	1:D:378:ALA:CB	2.48	0.43
1:E:436:THR:HG22	1:E:438:GLU:H	1.82	0.43
1:F:309:ILE:HD11	1:F:378:ALA:CB	2.48	0.43
1:I:429:LEU:O	1:I:435:PHE:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:75:ALA:HA	1:J:87:ILE:O	2.19	0.43
1:K:429:LEU:O	1:K:435:PHE:HB2	2.18	0.43
1:L:309:ILE:HD11	1:L:378:ALA:CB	2.48	0.43
1:L:429:LEU:O	1:L:435:PHE:HB2	2.18	0.43
1:N:436:THR:HG22	1:N:438:GLU:H	1.82	0.43
1:P:262:PHE:HE1	1:S:456:MET:HG3	1.84	0.43
1:P:319:SER:OG	1:P:363:ASP:OD2	2.18	0.43
1:Q:232:LYS:HD2	1:Q:232:LYS:HA	1.69	0.43
1:Q:333:LEU:HD23	1:Q:333:LEU:HA	1.90	0.43
1:R:75:ALA:HA	1:R:87:ILE:O	2.19	0.43
1:A:429:LEU:O	1:A:435:PHE:HB2	2.18	0.43
1:B:134:PHE:O	1:B:254:ALA:HA	2.19	0.43
1:B:463:PHE:HZ	1:L:260:PRO:O	2.02	0.43
1:H:333:LEU:HD23	1:H:333:LEU:HA	1.90	0.43
1:I:134:PHE:O	1:I:254:ALA:HA	2.19	0.43
1:M:309:ILE:HD11	1:M:378:ALA:CB	2.48	0.43
1:S:75:ALA:HA	1:S:87:ILE:O	2.19	0.43
1:S:429:LEU:O	1:S:435:PHE:HB2	2.19	0.43
1:V:134:PHE:O	1:V:254:ALA:HA	2.19	0.43
1:V:429:LEU:O	1:V:435:PHE:HB2	2.18	0.43
1:D:134:PHE:O	1:D:254:ALA:HA	2.19	0.43
1:D:436:THR:HG22	1:D:438:GLU:H	1.82	0.43
1:F:75:ALA:HA	1:F:87:ILE:O	2.19	0.43
1:K:309:ILE:HD11	1:K:378:ALA:CB	2.48	0.43
1:S:134:PHE:O	1:S:254:ALA:HA	2.19	0.43
1:W:404:GLU:O	1:W:408:ILE:HG12	2.19	0.43
1:C:134:PHE:O	1:C:254:ALA:HA	2.19	0.43
1:D:262:PHE:HE1	1:J:456:MET:HG3	1.84	0.43
1:D:429:LEU:O	1:D:435:PHE:HB2	2.18	0.43
1:E:457:THR:O	1:I:321:LYS:HE3	2.19	0.43
1:G:75:ALA:HA	1:G:87:ILE:O	2.19	0.43
1:H:75:ALA:HA	1:H:87:ILE:O	2.19	0.43
1:I:309:ILE:HD11	1:I:378:ALA:CB	2.48	0.43
1:Q:429:LEU:O	1:Q:435:PHE:HB2	2.18	0.43
1:R:134:PHE:O	1:R:254:ALA:HA	2.19	0.43
1:S:309:ILE:HD11	1:S:378:ALA:CB	2.48	0.43
1:V:309:ILE:HD11	1:V:378:ALA:CB	2.48	0.43
1:X:309:ILE:HD11	1:X:378:ALA:CB	2.48	0.43
1:Y:309:ILE:HD11	1:Y:378:ALA:CB	2.48	0.43
1:B:75:ALA:HA	1:B:87:ILE:O	2.19	0.42
1:E:149:HIS:HA	1:I:149:HIS:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:436:THR:HG22	1:H:438:GLU:H	1.82	0.42
1:J:309:ILE:HD11	1:J:378:ALA:CB	2.48	0.42
1:L:75:ALA:HA	1:L:87:ILE:O	2.19	0.42
1:Q:134:PHE:O	1:Q:254:ALA:HA	2.19	0.42
1:Q:149:HIS:HA	1:W:149:HIS:HA	2.01	0.42
1:U:134:PHE:O	1:U:254:ALA:HA	2.19	0.42
1:V:404:GLU:O	1:V:408:ILE:HG12	2.19	0.42
1:Y:134:PHE:O	1:Y:254:ALA:HA	2.19	0.42
1:C:75:ALA:HA	1:C:87:ILE:O	2.19	0.42
1:D:75:ALA:HA	1:D:87:ILE:O	2.19	0.42
1:D:149:HIS:HA	1:J:149:HIS:HA	2.02	0.42
1:E:134:PHE:O	1:E:254:ALA:HA	2.19	0.42
1:H:129:PRO:CG	1:H:236:ILE:HD11	2.46	0.42
1:H:404:GLU:O	1:H:408:ILE:HG12	2.19	0.42
1:J:134:PHE:O	1:J:254:ALA:HA	2.19	0.42
1:J:232:LYS:HD2	1:J:232:LYS:HA	1.69	0.42
1:M:134:PHE:O	1:M:254:ALA:HA	2.19	0.42
1:P:463:PHE:HZ	1:S:260:PRO:O	2.02	0.42
1:Q:129:PRO:CG	1:Q:236:ILE:HD11	2.46	0.42
1:X:134:PHE:O	1:X:254:ALA:HA	2.19	0.42
1:A:134:PHE:O	1:A:254:ALA:HA	2.19	0.42
1:E:319:SER:OG	1:E:363:ASP:OD2	2.19	0.42
1:E:429:LEU:O	1:E:435:PHE:HB2	2.18	0.42
1:I:75:ALA:HA	1:I:87:ILE:O	2.19	0.42
1:N:75:ALA:HA	1:N:87:ILE:O	2.19	0.42
1:N:309:ILE:HD11	1:N:378:ALA:CB	2.48	0.42
1:P:134:PHE:O	1:P:254:ALA:HA	2.19	0.42
1:U:75:ALA:HA	1:U:87:ILE:O	2.19	0.42
1:V:75:ALA:HA	1:V:87:ILE:O	2.19	0.42
1:W:75:ALA:HA	1:W:87:ILE:O	2.19	0.42
1:A:75:ALA:HA	1:A:87:ILE:O	2.19	0.42
1:D:299:ILE:HG23	1:D:344:ILE:HG21	2.02	0.42
1:E:75:ALA:HA	1:E:87:ILE:O	2.19	0.42
1:G:404:GLU:O	1:G:408:ILE:HG12	2.19	0.42
1:H:134:PHE:O	1:H:254:ALA:HA	2.19	0.42
1:J:429:LEU:O	1:J:435:PHE:HB2	2.18	0.42
1:K:134:PHE:O	1:K:254:ALA:HA	2.19	0.42
1:M:75:ALA:HA	1:M:87:ILE:O	2.19	0.42
1:N:463:PHE:HZ	1:Y:260:PRO:O	2.02	0.42
1:X:404:GLU:O	1:X:408:ILE:HG12	2.19	0.42
1:X:429:LEU:O	1:X:435:PHE:HB2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:404:GLU:O	1:B:408:ILE:HG12	2.19	0.42
1:D:193:ARG:HB3	1:D:210:HIS:CD2	2.55	0.42
1:D:404:GLU:O	1:D:408:ILE:HG12	2.19	0.42
1:I:193:ARG:HB3	1:I:210:HIS:CD2	2.55	0.42
1:M:429:LEU:O	1:M:435:PHE:HB2	2.18	0.42
1:N:429:LEU:O	1:N:435:PHE:HB2	2.18	0.42
1:O:75:ALA:HA	1:O:87:ILE:O	2.19	0.42
1:P:299:ILE:HG23	1:P:344:ILE:HG21	2.02	0.42
1:Q:75:ALA:HA	1:Q:87:ILE:O	2.19	0.42
1:Q:404:GLU:O	1:Q:408:ILE:HG12	2.19	0.42
1:R:404:GLU:O	1:R:408:ILE:HG12	2.19	0.42
1:S:404:GLU:O	1:S:408:ILE:HG12	2.19	0.42
1:Y:75:ALA:HA	1:Y:87:ILE:O	2.19	0.42
1:Y:404:GLU:O	1:Y:408:ILE:HG12	2.19	0.42
1:D:319:SER:OG	1:D:363:ASP:OD2	2.18	0.42
1:E:404:GLU:O	1:E:408:ILE:HG12	2.19	0.42
1:G:299:ILE:HG23	1:G:344:ILE:HG21	2.02	0.42
1:H:193:ARG:HB3	1:H:210:HIS:CD2	2.55	0.42
1:N:129:PRO:CG	1:N:236:ILE:HD11	2.46	0.42
1:N:193:ARG:HB3	1:N:210:HIS:CD2	2.55	0.42
1:O:193:ARG:HB3	1:O:210:HIS:CD2	2.55	0.42
1:O:299:ILE:HG23	1:O:344:ILE:HG21	2.02	0.42
1:P:75:ALA:HA	1:P:87:ILE:O	2.19	0.42
1:U:193:ARG:HB3	1:U:210:HIS:CD2	2.55	0.42
1:U:299:ILE:HG23	1:U:344:ILE:HG21	2.02	0.42
1:V:299:ILE:HG23	1:V:344:ILE:HG21	2.02	0.42
1:Y:232:LYS:HA	1:Y:232:LYS:HD2	1.69	0.42
1:A:404:GLU:O	1:A:408:ILE:HG12	2.19	0.42
1:B:58:TRP:N	1:B:58:TRP:CD1	2.84	0.42
1:E:193:ARG:HB3	1:E:210:HIS:CD2	2.55	0.42
1:E:299:ILE:HG23	1:E:344:ILE:HG21	2.02	0.42
1:H:299:ILE:HG23	1:H:344:ILE:HG21	2.02	0.42
1:I:397:LEU:HD21	1:J:61:ILE:HD11	2.00	0.42
1:K:193:ARG:HB3	1:K:210:HIS:CD2	2.55	0.42
1:L:193:ARG:HB3	1:L:210:HIS:CD2	2.55	0.42
1:Q:193:ARG:HB3	1:Q:210:HIS:CD2	2.55	0.42
1:Q:457:THR:O	1:W:321:LYS:HE3	2.19	0.42
1:R:193:ARG:HB3	1:R:210:HIS:CD2	2.55	0.42
1:S:193:ARG:HB3	1:S:210:HIS:CD2	2.55	0.42
1:W:134:PHE:O	1:W:254:ALA:HA	2.19	0.42
1:A:193:ARG:HB3	1:A:210:HIS:CD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:299:ILE:HG23	1:C:344:ILE:HG21	2.02	0.42
1:D:333:LEU:HD23	1:D:333:LEU:HA	1.90	0.42
1:F:429:LEU:O	1:F:435:PHE:HB2	2.18	0.42
1:G:193:ARG:HB3	1:G:210:HIS:CD2	2.55	0.42
1:K:75:ALA:HA	1:K:87:ILE:O	2.19	0.42
1:L:299:ILE:HG23	1:L:344:ILE:HG21	2.02	0.42
1:N:58:TRP:N	1:N:58:TRP:CD1	2.84	0.42
1:N:404:GLU:O	1:N:408:ILE:HG12	2.19	0.42
1:O:58:TRP:CD1	1:O:58:TRP:N	2.84	0.42
1:O:134:PHE:O	1:O:254:ALA:HA	2.19	0.42
1:Q:299:ILE:HG23	1:Q:344:ILE:HG21	2.02	0.42
1:S:61:ILE:HD11	1:W:397:LEU:HD21	2.00	0.42
1:W:299:ILE:HG23	1:W:344:ILE:HG21	2.02	0.42
1:C:463:PHE:HZ	1:K:260:PRO:O	2.03	0.42
1:D:129:PRO:CG	1:D:236:ILE:HD11	2.46	0.42
1:I:299:ILE:HG23	1:I:344:ILE:HG21	2.02	0.42
1:N:134:PHE:O	1:N:254:ALA:HA	2.19	0.42
1:O:404:GLU:O	1:O:408:ILE:HG12	2.19	0.42
1:P:193:ARG:HB3	1:P:210:HIS:CD2	2.55	0.42
1:U:404:GLU:O	1:U:408:ILE:HG12	2.19	0.42
1:V:193:ARG:HB3	1:V:210:HIS:CD2	2.55	0.42
1:W:429:LEU:O	1:W:435:PHE:HB2	2.18	0.42
1:Y:193:ARG:HB3	1:Y:210:HIS:CD2	2.55	0.42
1:C:193:ARG:HB3	1:C:210:HIS:CD2	2.55	0.42
1:F:299:ILE:HG23	1:F:344:ILE:HG21	2.02	0.42
1:K:232:LYS:HD2	1:K:232:LYS:HA	1.69	0.42
1:X:193:ARG:HB3	1:X:210:HIS:CD2	2.55	0.42
1:B:193:ARG:HB3	1:B:210:HIS:CD2	2.55	0.41
1:I:404:GLU:O	1:I:408:ILE:HG12	2.19	0.41
1:J:404:GLU:O	1:J:408:ILE:HG12	2.19	0.41
1:K:129:PRO:CG	1:K:236:ILE:HD11	2.46	0.41
1:L:404:GLU:O	1:L:408:ILE:HG12	2.19	0.41
1:P:149:HIS:HA	1:S:149:HIS:HA	2.02	0.41
1:Y:299:ILE:HG23	1:Y:344:ILE:HG21	2.02	0.41
1:B:457:THR:O	1:L:321:LYS:HE3	2.20	0.41
1:C:149:HIS:HA	1:K:149:HIS:HA	2.02	0.41
1:E:129:PRO:HA	1:E:270:HIS:O	2.21	0.41
1:F:129:PRO:HA	1:F:270:HIS:O	2.21	0.41
1:L:134:PHE:O	1:L:254:ALA:HA	2.19	0.41
1:P:260:PRO:O	1:S:463:PHE:HZ	2.03	0.41
1:Q:129:PRO:HA	1:Q:270:HIS:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:319:SER:OG	1:Q:363:ASP:OD2	2.19	0.41
1:R:129:PRO:HA	1:R:270:HIS:O	2.21	0.41
1:R:200:MET:HG3	1:R:242:VAL:HG11	2.02	0.41
1:R:299:ILE:HG23	1:R:344:ILE:HG21	2.02	0.41
1:U:129:PRO:CG	1:U:236:ILE:HD11	2.46	0.41
1:A:129:PRO:HA	1:A:270:HIS:O	2.21	0.41
1:A:256:PHE:HB3	1:A:364:PRO:HB2	2.03	0.41
1:F:134:PHE:O	1:F:254:ALA:HA	2.19	0.41
1:F:200:MET:HG3	1:F:242:VAL:HG11	2.02	0.41
1:I:256:PHE:HB3	1:I:364:PRO:HB2	2.03	0.41
1:K:404:GLU:O	1:K:408:ILE:HG12	2.19	0.41
1:P:129:PRO:HA	1:P:270:HIS:O	2.21	0.41
1:R:42:GLU:HA	1:R:45:GLU:OE1	2.21	0.41
1:R:256:PHE:HB3	1:R:364:PRO:HB2	2.03	0.41
1:W:193:ARG:HB3	1:W:210:HIS:CD2	2.55	0.41
1:X:75:ALA:HA	1:X:87:ILE:O	2.19	0.41
1:A:232:LYS:HD2	1:A:232:LYS:HA	1.69	0.41
1:G:134:PHE:O	1:G:254:ALA:HA	2.19	0.41
1:M:129:PRO:HA	1:M:270:HIS:O	2.21	0.41
1:S:42:GLU:HA	1:S:45:GLU:OE1	2.21	0.41
1:S:256:PHE:HB3	1:S:364:PRO:HB2	2.03	0.41
1:S:299:ILE:HG23	1:S:344:ILE:HG21	2.02	0.41
1:U:333:LEU:HD23	1:U:333:LEU:HA	1.90	0.41
1:V:129:PRO:CG	1:V:236:ILE:HD11	2.46	0.41
1:A:42:GLU:HA	1:A:45:GLU:OE1	2.21	0.41
1:D:129:PRO:HA	1:D:270:HIS:O	2.21	0.41
1:E:256:PHE:HB3	1:E:364:PRO:HB2	2.03	0.41
1:E:463:PHE:HZ	1:I:260:PRO:O	2.04	0.41
1:F:457:THR:O	1:H:321:LYS:HE3	2.20	0.41
1:G:129:PRO:HA	1:G:270:HIS:O	2.21	0.41
1:I:200:MET:HG3	1:I:242:VAL:HG11	2.02	0.41
1:M:232:LYS:HD2	1:M:232:LYS:HA	1.69	0.41
1:M:333:LEU:HD23	1:M:333:LEU:HA	1.90	0.41
1:M:404:GLU:O	1:M:408:ILE:HG12	2.19	0.41
1:O:149:HIS:HA	1:X:149:HIS:HA	2.02	0.41
1:O:456:MET:HG3	1:X:262:PHE:HE1	1.86	0.41
1:R:333:LEU:HD23	1:R:333:LEU:HA	1.90	0.41
1:S:210:HIS:CD2	1:S:222:VAL:HG22	2.56	0.41
1:V:129:PRO:HA	1:V:270:HIS:O	2.21	0.41
1:X:42:GLU:HA	1:X:45:GLU:OE1	2.21	0.41
1:X:257:MET:HA	1:X:258:PRO:HD3	1.97	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:HIS:CD2	1:A:222:VAL:HG22	2.56	0.41
1:C:404:GLU:O	1:C:408:ILE:HG12	2.19	0.41
1:C:456:MET:HG3	1:K:262:PHE:HE1	1.86	0.41
1:F:193:ARG:HB3	1:F:210:HIS:CD2	2.55	0.41
1:J:42:GLU:HA	1:J:45:GLU:OE1	2.21	0.41
1:J:299:ILE:HG23	1:J:344:ILE:HG21	2.02	0.41
1:J:447:ARG:HD3	1:J:447:ARG:HA	1.90	0.41
1:K:256:PHE:HB3	1:K:364:PRO:HB2	2.03	0.41
1:L:210:HIS:CD2	1:L:222:VAL:HG22	2.56	0.41
1:N:149:HIS:HA	1:Y:149:HIS:HA	2.02	0.41
1:N:299:ILE:HG23	1:N:344:ILE:HG21	2.02	0.41
1:N:457:THR:O	1:Y:321:LYS:HE3	2.20	0.41
1:O:200:MET:HG3	1:O:242:VAL:HG11	2.02	0.41
1:O:260:PRO:O	1:X:463:PHE:HZ	2.04	0.41
1:O:463:PHE:HZ	1:X:260:PRO:O	2.03	0.41
1:P:404:GLU:O	1:P:408:ILE:HG12	2.19	0.41
1:S:200:MET:HG3	1:S:242:VAL:HG11	2.02	0.41
1:U:129:PRO:HA	1:U:270:HIS:O	2.21	0.41
1:W:200:MET:HG3	1:W:242:VAL:HG11	2.02	0.41
1:X:256:PHE:HB3	1:X:364:PRO:HB2	2.03	0.41
1:A:200:MET:HG3	1:A:242:VAL:HG11	2.02	0.41
1:A:299:ILE:HG23	1:A:344:ILE:HG21	2.02	0.41
1:B:210:HIS:CD2	1:B:222:VAL:HG22	2.56	0.41
1:D:260:PRO:O	1:J:463:PHE:HZ	2.03	0.41
1:F:42:GLU:HA	1:F:45:GLU:OE1	2.21	0.41
1:F:404:GLU:O	1:F:408:ILE:HG12	2.19	0.41
1:G:200:MET:HG3	1:G:242:VAL:HG11	2.02	0.41
1:I:129:PRO:HA	1:I:270:HIS:O	2.21	0.41
1:J:200:MET:HG3	1:J:242:VAL:HG11	2.02	0.41
1:L:200:MET:HG3	1:L:242:VAL:HG11	2.02	0.41
1:Q:42:GLU:HA	1:Q:45:GLU:OE1	2.21	0.41
1:S:129:PRO:HA	1:S:270:HIS:O	2.21	0.41
1:W:42:GLU:HA	1:W:45:GLU:OE1	2.21	0.41
1:W:129:PRO:HA	1:W:270:HIS:O	2.21	0.41
1:Y:129:PRO:HA	1:Y:270:HIS:O	2.20	0.41
1:B:42:GLU:HA	1:B:45:GLU:OE1	2.21	0.41
1:B:196:MET:HG3	1:B:246:VAL:HG11	2.03	0.41
1:B:256:PHE:HB3	1:B:364:PRO:HB2	2.03	0.41
1:C:200:MET:HG3	1:C:242:VAL:HG11	2.02	0.41
1:F:210:HIS:CD2	1:F:222:VAL:HG22	2.56	0.41
1:H:129:PRO:HA	1:H:270:HIS:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:196:MET:HG3	1:H:246:VAL:HG11	2.03	0.41
1:K:42:GLU:HA	1:K:45:GLU:OE1	2.21	0.41
1:K:299:ILE:HG23	1:K:344:ILE:HG21	2.02	0.41
1:L:129:PRO:HA	1:L:270:HIS:O	2.20	0.41
1:L:196:MET:HG3	1:L:246:VAL:HG11	2.03	0.41
1:Q:200:MET:HG3	1:Q:242:VAL:HG11	2.02	0.41
1:V:256:PHE:HB3	1:V:364:PRO:HB2	2.03	0.41
1:W:210:HIS:CD2	1:W:222:VAL:HG22	2.56	0.41
1:B:129:PRO:HA	1:B:270:HIS:O	2.21	0.41
1:B:299:ILE:HG23	1:B:344:ILE:HG21	2.02	0.41
1:C:129:PRO:HA	1:C:270:HIS:O	2.20	0.41
1:C:210:HIS:CD2	1:C:222:VAL:HG22	2.56	0.41
1:C:260:PRO:O	1:K:463:PHE:HZ	2.03	0.41
1:D:196:MET:HG3	1:D:246:VAL:HG11	2.03	0.41
1:F:463:PHE:HZ	1:H:260:PRO:O	2.04	0.41
1:G:210:HIS:CD2	1:G:222:VAL:HG22	2.56	0.41
1:I:42:GLU:HA	1:I:45:GLU:OE1	2.21	0.41
1:I:196:MET:HG3	1:I:246:VAL:HG11	2.03	0.41
1:I:210:HIS:CD2	1:I:222:VAL:HG22	2.56	0.41
1:J:129:PRO:HA	1:J:270:HIS:O	2.21	0.41
1:J:193:ARG:HB3	1:J:210:HIS:CD2	2.55	0.41
1:K:210:HIS:CD2	1:K:222:VAL:HG22	2.56	0.41
1:L:256:PHE:HB3	1:L:364:PRO:HB2	2.03	0.41
1:M:200:MET:HG3	1:M:242:VAL:HG11	2.02	0.41
1:M:299:ILE:HG23	1:M:344:ILE:HG21	2.02	0.41
1:M:457:THR:O	1:U:321:LYS:HE3	2.21	0.41
1:N:129:PRO:HA	1:N:270:HIS:O	2.21	0.41
1:N:256:PHE:HB3	1:N:364:PRO:HB2	2.03	0.41
1:N:447:ARG:HD3	1:N:447:ARG:HA	1.90	0.41
1:O:129:PRO:HA	1:O:270:HIS:O	2.21	0.41
1:O:196:MET:HG3	1:O:246:VAL:HG11	2.03	0.41
1:O:210:HIS:CD2	1:O:222:VAL:HG22	2.56	0.41
1:P:200:MET:HG3	1:P:242:VAL:HG11	2.02	0.41
1:Q:196:MET:HG3	1:Q:246:VAL:HG11	2.03	0.41
1:Q:463:PHE:HZ	1:W:260:PRO:O	2.04	0.41
1:R:196:MET:HG3	1:R:246:VAL:HG11	2.03	0.41
1:R:210:HIS:CD2	1:R:222:VAL:HG22	2.56	0.41
1:R:457:THR:O	1:V:321:LYS:HE3	2.20	0.41
1:S:196:MET:HG3	1:S:246:VAL:HG11	2.03	0.41
1:S:363:ASP:HB2	1:S:364:PRO:HD2	2.03	0.41
1:X:200:MET:HG3	1:X:242:VAL:HG11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:210:HIS:CD2	1:X:222:VAL:HG22	2.56	0.41
1:A:129:PRO:CG	1:A:236:ILE:HD11	2.46	0.41
1:A:196:MET:HG3	1:A:246:VAL:HG11	2.03	0.41
1:A:456:MET:HG3	1:G:262:PHE:HE1	1.86	0.41
1:B:149:HIS:HA	1:L:149:HIS:HA	2.02	0.41
1:H:42:GLU:HA	1:H:45:GLU:OE1	2.21	0.41
1:H:200:MET:HG3	1:H:242:VAL:HG11	2.02	0.41
1:K:196:MET:HG3	1:K:246:VAL:HG11	2.03	0.41
1:M:193:ARG:HB3	1:M:210:HIS:CD2	2.55	0.41
1:N:196:MET:HG3	1:N:246:VAL:HG11	2.03	0.41
1:N:210:HIS:CD2	1:N:222:VAL:HG22	2.56	0.41
1:N:333:LEU:HD23	1:N:333:LEU:HA	1.90	0.41
1:P:210:HIS:CD2	1:P:222:VAL:HG22	2.56	0.41
1:Q:210:HIS:CD2	1:Q:222:VAL:HG22	2.56	0.41
1:R:463:PHE:HZ	1:V:260:PRO:O	2.04	0.41
1:U:196:MET:HG3	1:U:246:VAL:HG11	2.03	0.41
1:V:42:GLU:HA	1:V:45:GLU:OE1	2.21	0.41
1:X:196:MET:HG3	1:X:246:VAL:HG11	2.03	0.41
1:X:299:ILE:HG23	1:X:344:ILE:HG21	2.02	0.41
1:B:200:MET:HG3	1:B:242:VAL:HG11	2.02	0.40
1:E:134:PHE:HE2	1:E:261:MET:HE1	1.86	0.40
1:G:61:ILE:HD11	1:L:397:LEU:HD21	2.02	0.40
1:H:256:PHE:HB3	1:H:364:PRO:HB2	2.03	0.40
1:J:363:ASP:HB2	1:J:364:PRO:HD2	2.03	0.40
1:K:363:ASP:HB2	1:K:364:PRO:HD2	2.04	0.40
1:M:257:MET:HA	1:M:258:PRO:HD3	1.97	0.40
1:O:24:ASP:O	1:O:105:PRO:HG2	2.22	0.40
1:O:256:PHE:HB3	1:O:364:PRO:HB2	2.03	0.40
1:O:257:MET:HA	1:O:258:PRO:HD3	1.97	0.40
1:R:339:ASN:HB2	1:R:394:ASP:O	2.21	0.40
1:S:24:ASP:O	1:S:105:PRO:HG2	2.22	0.40
1:U:24:ASP:O	1:U:105:PRO:HG2	2.22	0.40
1:Y:200:MET:HG3	1:Y:242:VAL:HG11	2.02	0.40
1:A:24:ASP:O	1:A:105:PRO:HG2	2.22	0.40
1:D:256:PHE:HB3	1:D:364:PRO:HB2	2.03	0.40
1:E:200:MET:HG3	1:E:242:VAL:HG11	2.02	0.40
1:F:456:MET:HG3	1:H:262:PHE:HE1	1.86	0.40
1:H:210:HIS:CD2	1:H:222:VAL:HG22	2.56	0.40
1:J:256:PHE:HB3	1:J:364:PRO:HB2	2.03	0.40
1:K:200:MET:HG3	1:K:242:VAL:HG11	2.02	0.40
1:M:42:GLU:HA	1:M:45:GLU:OE1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:457:THR:O	1:S:321:LYS:HE3	2.22	0.40
1:Q:256:PHE:HB3	1:Q:364:PRO:HB2	2.03	0.40
1:R:24:ASP:O	1:R:105:PRO:HG2	2.22	0.40
1:R:363:ASP:HB2	1:R:364:PRO:HD2	2.04	0.40
1:S:129:PRO:CG	1:S:236:ILE:HD11	2.46	0.40
1:U:256:PHE:HB3	1:U:364:PRO:HB2	2.03	0.40
1:X:129:PRO:HA	1:X:270:HIS:O	2.20	0.40
1:Y:210:HIS:CD2	1:Y:222:VAL:HG22	2.56	0.40
1:A:463:PHE:HZ	1:G:260:PRO:O	2.05	0.40
1:C:24:ASP:O	1:C:105:PRO:HG2	2.22	0.40
1:D:457:THR:O	1:J:321:LYS:HE3	2.22	0.40
1:E:196:MET:HG3	1:E:246:VAL:HG11	2.03	0.40
1:F:363:ASP:HB2	1:F:364:PRO:HD2	2.04	0.40
1:H:24:ASP:O	1:H:105:PRO:HG2	2.22	0.40
1:I:24:ASP:O	1:I:105:PRO:HG2	2.22	0.40
1:I:339:ASN:HB2	1:I:394:ASP:O	2.22	0.40
1:J:210:HIS:CD2	1:J:222:VAL:HG22	2.56	0.40
1:L:257:MET:HA	1:L:258:PRO:HD3	1.97	0.40
1:M:210:HIS:CD2	1:M:222:VAL:HG22	2.56	0.40
1:M:256:PHE:HB3	1:M:364:PRO:HB2	2.03	0.40
1:P:24:ASP:O	1:P:105:PRO:HG2	2.22	0.40
1:P:256:PHE:HB3	1:P:364:PRO:HB2	2.03	0.40
1:V:134:PHE:HE2	1:V:261:MET:HE1	1.87	0.40
1:V:196:MET:HG3	1:V:246:VAL:HG11	2.03	0.40
1:X:134:PHE:HE2	1:X:261:MET:HE1	1.87	0.40
1:A:210:HIS:HE1	1:A:220:ASN:HB3	1.87	0.40
1:E:232:LYS:HD2	1:E:232:LYS:HA	1.69	0.40
1:G:24:ASP:O	1:G:105:PRO:HG2	2.22	0.40
1:H:134:PHE:HE2	1:H:261:MET:HE1	1.87	0.40
1:H:339:ASN:HB2	1:H:394:ASP:O	2.22	0.40
1:K:210:HIS:HE1	1:K:220:ASN:HB3	1.87	0.40
1:K:447:ARG:HD3	1:K:447:ARG:HA	1.90	0.40
1:M:363:ASP:HB2	1:M:364:PRO:HD2	2.04	0.40
1:M:456:MET:HG3	1:U:262:PHE:HE1	1.86	0.40
1:P:129:PRO:CG	1:P:236:ILE:HD11	2.46	0.40
1:Q:339:ASN:HB2	1:Q:394:ASP:O	2.22	0.40
1:S:134:PHE:HE2	1:S:261:MET:HE1	1.87	0.40
1:V:24:ASP:O	1:V:105:PRO:HG2	2.22	0.40
1:V:200:MET:HG3	1:V:242:VAL:HG11	2.02	0.40
1:V:210:HIS:CD2	1:V:222:VAL:HG22	2.56	0.40
1:W:196:MET:HG3	1:W:246:VAL:HG11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:319:SER:OG	1:W:363:ASP:OD2	2.19	0.40
1:X:298:TYR:CE2	1:X:379:GLY:HA3	2.57	0.40
1:X:363:ASP:HB2	1:X:364:PRO:HD2	2.04	0.40
1:A:134:PHE:HE2	1:A:261:MET:HE1	1.87	0.40
1:E:257:MET:HA	1:E:258:PRO:HD3	1.97	0.40
1:F:134:PHE:HE2	1:F:261:MET:HE1	1.87	0.40
1:G:42:GLU:HA	1:G:45:GLU:OE1	2.21	0.40
1:J:193:ARG:HD2	1:J:210:HIS:CE1	2.57	0.40
1:K:24:ASP:O	1:K:105:PRO:HG2	2.22	0.40
1:K:129:PRO:HA	1:K:270:HIS:O	2.21	0.40
1:K:298:TYR:CE2	1:K:379:GLY:HA3	2.57	0.40
1:O:457:THR:O	1:X:321:LYS:HE3	2.22	0.40
1:P:42:GLU:HA	1:P:45:GLU:OE1	2.21	0.40
1:R:456:MET:HG3	1:V:262:PHE:HE1	1.86	0.40
1:S:339:ASN:HB2	1:S:394:ASP:O	2.22	0.40
1:U:200:MET:HG3	1:U:242:VAL:HG11	2.02	0.40
1:V:298:TYR:CE2	1:V:379:GLY:HA3	2.57	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	431/469 (92%)	407 (94%)	24 (6%)	0	100	100
1	B	431/469 (92%)	407 (94%)	24 (6%)	0	100	100
1	C	431/469 (92%)	407 (94%)	24 (6%)	0	100	100
1	D	431/469 (92%)	407 (94%)	24 (6%)	0	100	100
1	E	431/469 (92%)	407 (94%)	24 (6%)	0	100	100
1	F	431/469 (92%)	407 (94%)	24 (6%)	0	100	100
1	G	431/469 (92%)	407 (94%)	24 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	431/469 (92%)	407 (94%)	24 (6%)	0	100	100
1	I	431/469 (92%)	407 (94%)	24 (6%)	0	100	100
1	J	431/469 (92%)	407 (94%)	24 (6%)	0	100	100
1	K	431/469 (92%)	407 (94%)	24 (6%)	0	100	100
1	L	431/469 (92%)	407 (94%)	24 (6%)	0	100	100
1	M	431/469 (92%)	408 (95%)	23 (5%)	0	100	100
1	N	431/469 (92%)	407 (94%)	24 (6%)	0	100	100
1	O	431/469 (92%)	407 (94%)	24 (6%)	0	100	100
1	P	431/469 (92%)	407 (94%)	24 (6%)	0	100	100
1	Q	431/469 (92%)	407 (94%)	24 (6%)	0	100	100
1	R	431/469 (92%)	407 (94%)	24 (6%)	0	100	100
1	S	431/469 (92%)	407 (94%)	24 (6%)	0	100	100
1	U	431/469 (92%)	407 (94%)	24 (6%)	0	100	100
1	V	431/469 (92%)	407 (94%)	24 (6%)	0	100	100
1	W	431/469 (92%)	407 (94%)	24 (6%)	0	100	100
1	X	431/469 (92%)	407 (94%)	24 (6%)	0	100	100
1	Y	431/469 (92%)	407 (94%)	24 (6%)	0	100	100
All	All	10344/11256 (92%)	9769 (94%)	575 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	362/388 (93%)	362 (100%)	0	100	100
1	B	362/388 (93%)	362 (100%)	0	100	100
1	C	362/388 (93%)	362 (100%)	0	100	100
1	D	362/388 (93%)	362 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	362/388 (93%)	362 (100%)	0	100	100
1	F	362/388 (93%)	362 (100%)	0	100	100
1	G	362/388 (93%)	362 (100%)	0	100	100
1	H	362/388 (93%)	362 (100%)	0	100	100
1	I	362/388 (93%)	362 (100%)	0	100	100
1	J	362/388 (93%)	362 (100%)	0	100	100
1	K	362/388 (93%)	362 (100%)	0	100	100
1	L	362/388 (93%)	362 (100%)	0	100	100
1	M	362/388 (93%)	362 (100%)	0	100	100
1	N	362/388 (93%)	362 (100%)	0	100	100
1	O	362/388 (93%)	362 (100%)	0	100	100
1	P	362/388 (93%)	362 (100%)	0	100	100
1	Q	362/388 (93%)	362 (100%)	0	100	100
1	R	362/388 (93%)	362 (100%)	0	100	100
1	S	362/388 (93%)	362 (100%)	0	100	100
1	U	362/388 (93%)	362 (100%)	0	100	100
1	V	362/388 (93%)	362 (100%)	0	100	100
1	W	362/388 (93%)	362 (100%)	0	100	100
1	X	362/388 (93%)	362 (100%)	0	100	100
1	Y	362/388 (93%)	362 (100%)	0	100	100
All	All	8688/9312 (93%)	8688 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	210	HIS
1	B	210	HIS
1	C	210	HIS
1	D	210	HIS
1	E	210	HIS
1	F	210	HIS
1	G	210	HIS
1	H	210	HIS

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Mol	Chain	Res	Type
1	I	210	HIS
1	J	210	HIS
1	K	210	HIS
1	L	210	HIS
1	M	210	HIS
1	N	210	HIS
1	O	210	HIS
1	P	210	HIS
1	Q	210	HIS
1	R	210	HIS
1	S	210	HIS
1	U	210	HIS
1	V	210	HIS
1	W	210	HIS
1	X	210	HIS
1	Y	210	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

Of 42 ligands modelled in this entry, 42 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

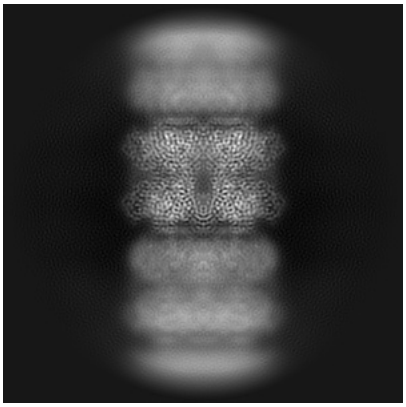
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-32352. These allow visual inspection of the internal detail of the map and identification of artifacts.

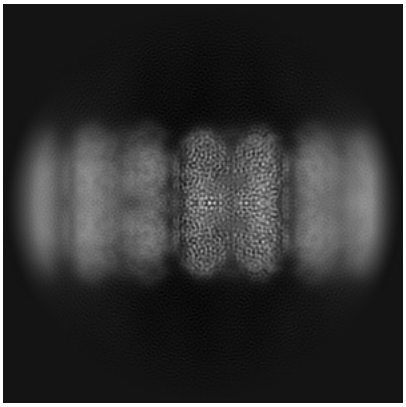
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

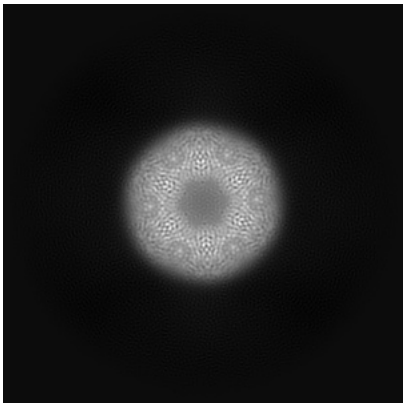
6.1.1 Primary map



X



Y

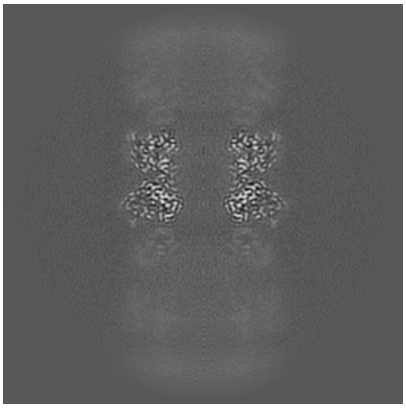


Z

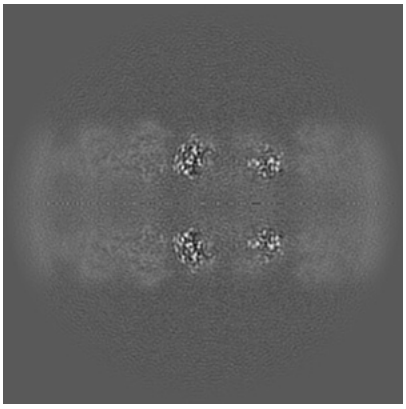
The images above show the map projected in three orthogonal directions.

6.2 Central slices

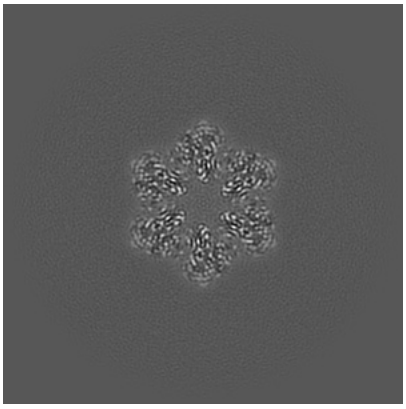
6.2.1 Primary map



X Index: 215



Y Index: 215

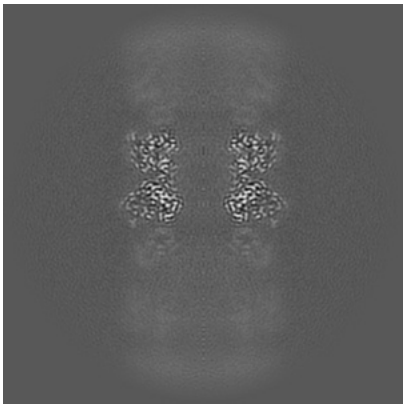


Z Index: 215

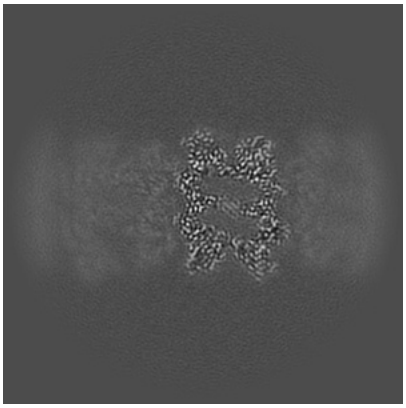
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

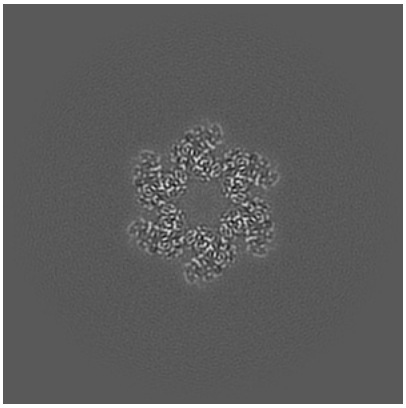
6.3.1 Primary map



X Index: 215



Y Index: 248

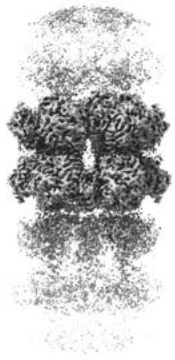


Z Index: 210

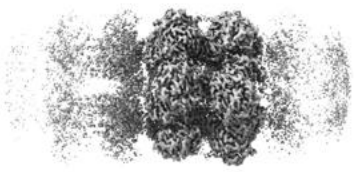
The images above show the largest variance slices of the map in three orthogonal directions.

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 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

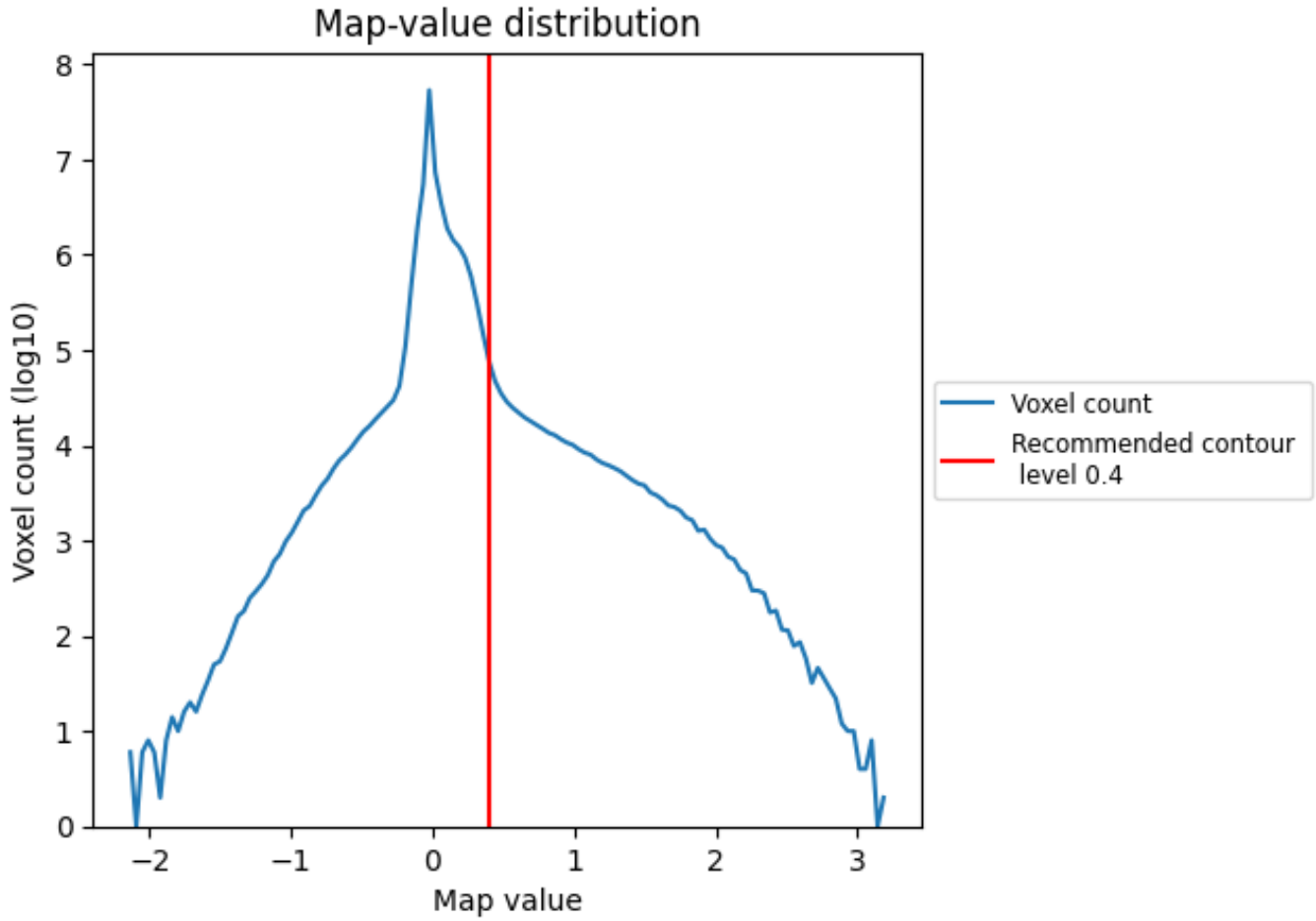
6.5 Mask visualisation (i)

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

7 Map analysis

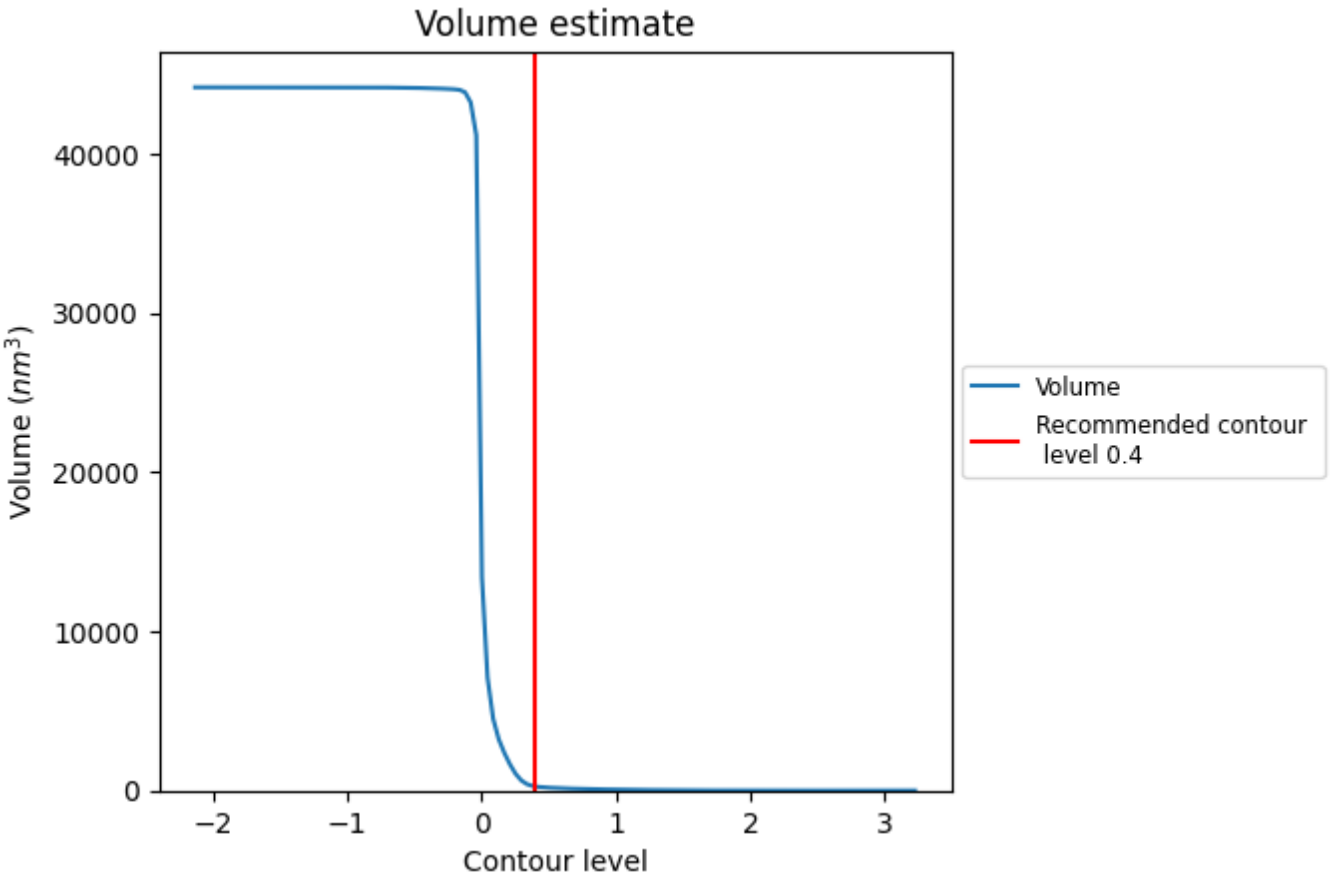
This section contains the results of statistical analysis of the map.

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.

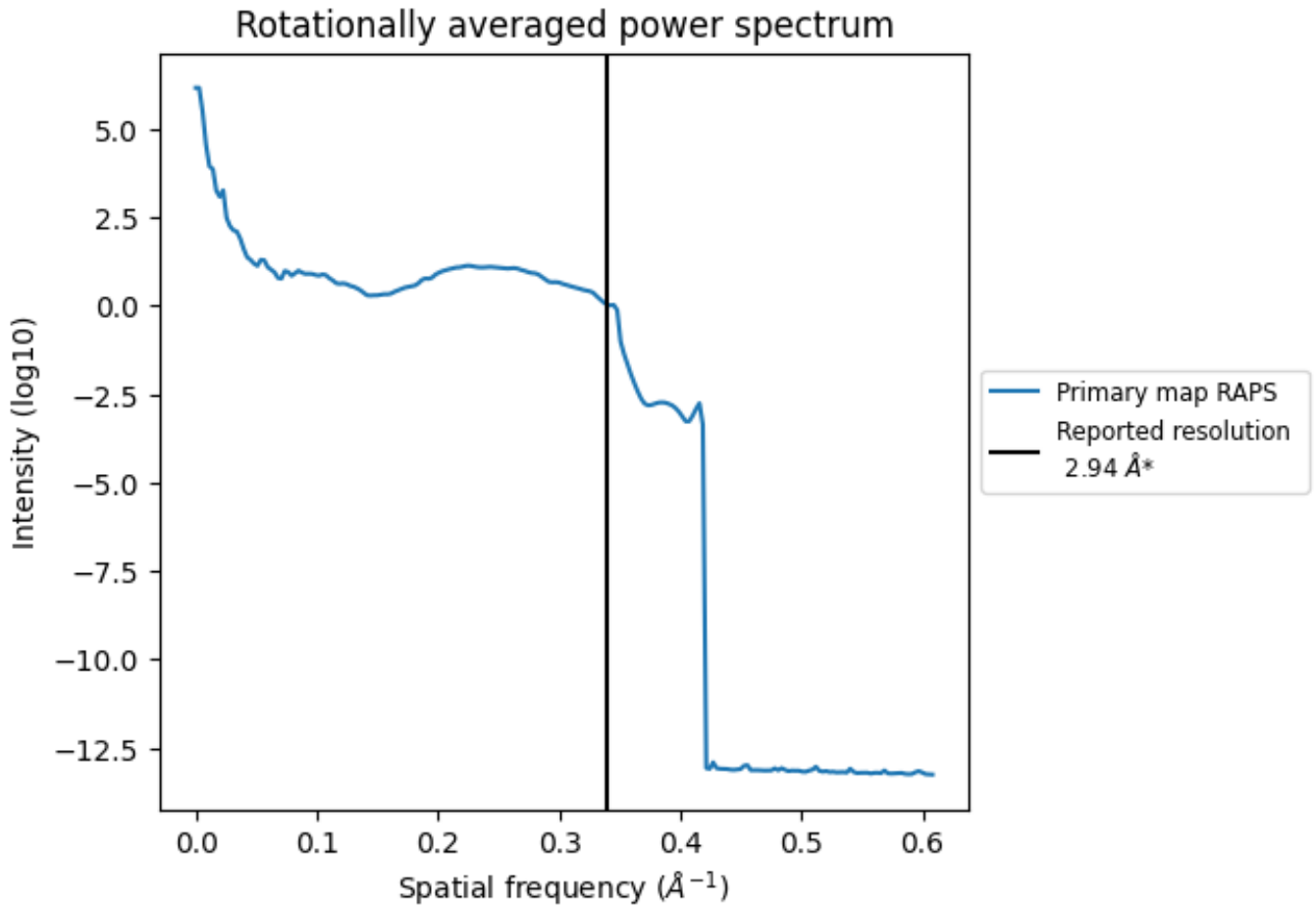
7.2 Volume estimate



The volume at the recommended contour level is 259 nm^3; this corresponds to an approximate mass of 234 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 0.340 $Å^{-1}$

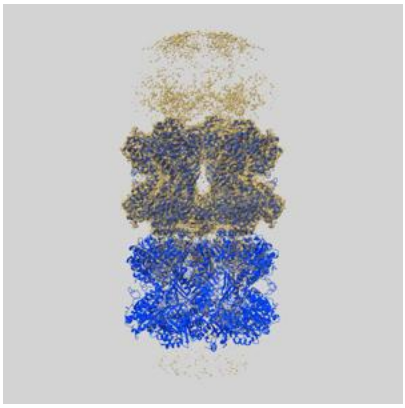
8 Fourier-Shell correlation (i)

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

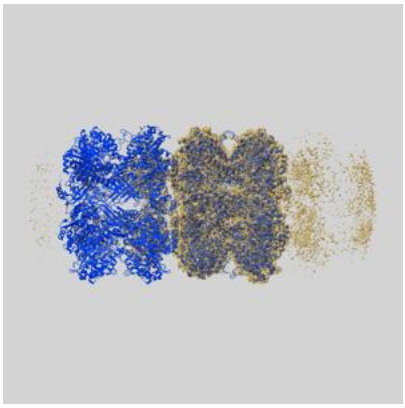
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-32352 and PDB model 7W85. Per-residue inclusion information can be found in section 3 on page 7.

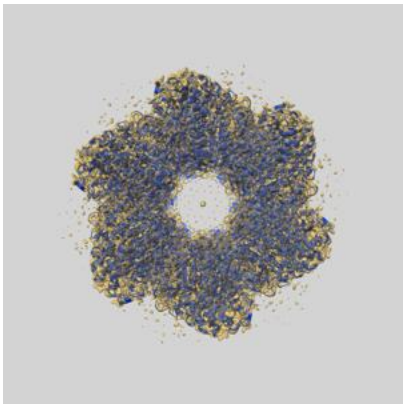
9.1 Map-model overlay



X



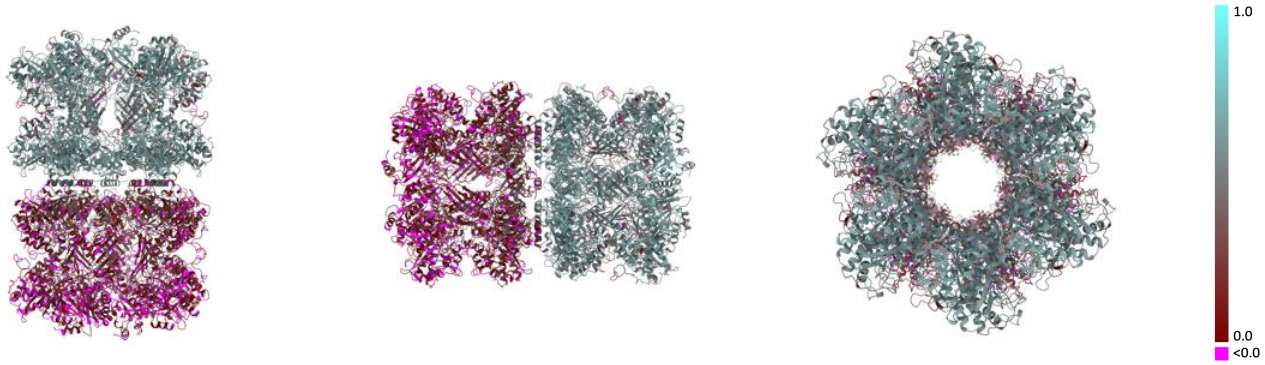
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.4 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.

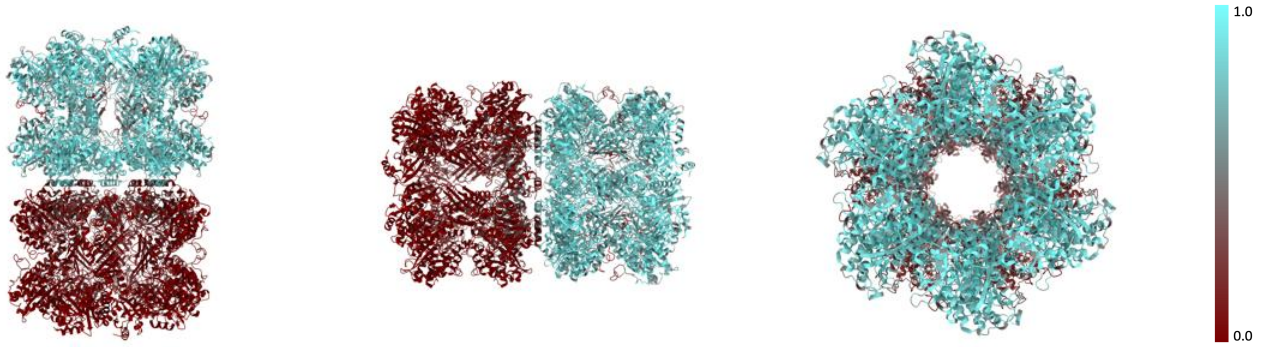
9.2 Q-score mapped to coordinate model (i)



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.

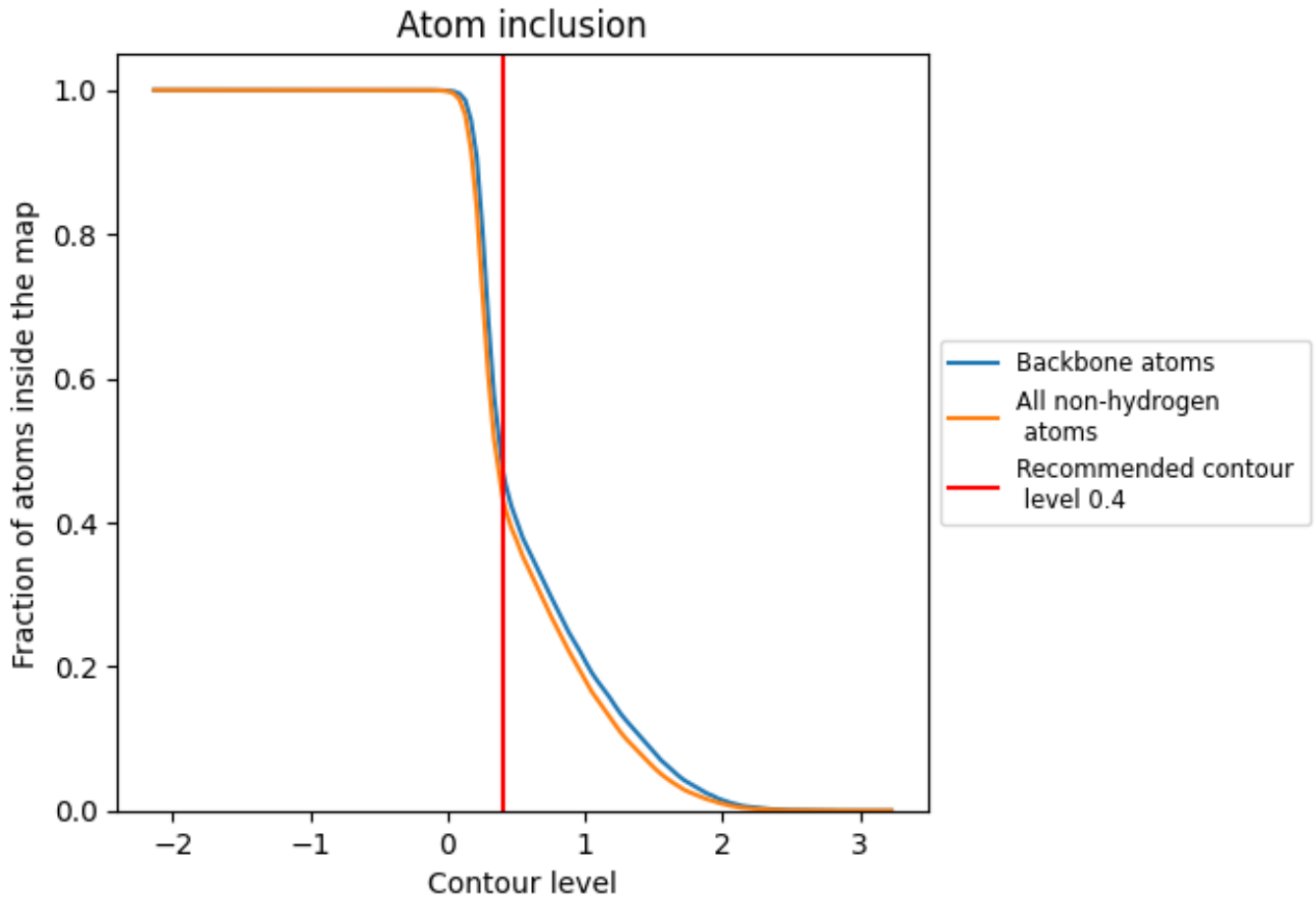
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.4).

9.4 Atom inclusion (i)



At the recommended contour level, 47% of all backbone atoms, 43% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4338	0.3450
A	0.8082	0.5480
B	0.8085	0.5480
C	0.8064	0.5470
D	0.8094	0.5480
E	0.8091	0.5460
F	0.8082	0.5470
G	0.8265	0.5620
H	0.8253	0.5610
I	0.8250	0.5610
J	0.8262	0.5600
K	0.8244	0.5600
L	0.8265	0.5610
M	0.0902	0.1840
N	0.0887	0.1830
O	0.0878	0.1820
P	0.0899	0.1820
Q	0.0884	0.1850
R	0.0881	0.1850
S	0.0126	0.0850
U	0.0132	0.0880
V	0.0126	0.0860
W	0.0114	0.0850
X	0.0129	0.0870
Y	0.0114	0.0880