Full wwPDB NMR Structure Validation Report (i)

Apr 27, 2016 – 03:16 AM BST

PDB ID	:	2M6I
Title	:	Putative pentameric open-channel structure of full-length transmembrane domains of human glycine receptor alpha1 subunit
Authors	:	Mowrey, D.; Cui, T.; Jia, Y.; Ma, D.; Makhov, A.M.; Zhang, P.; Tang, P.; Xu, Y.
Deposited on	:	2013-03-29

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

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

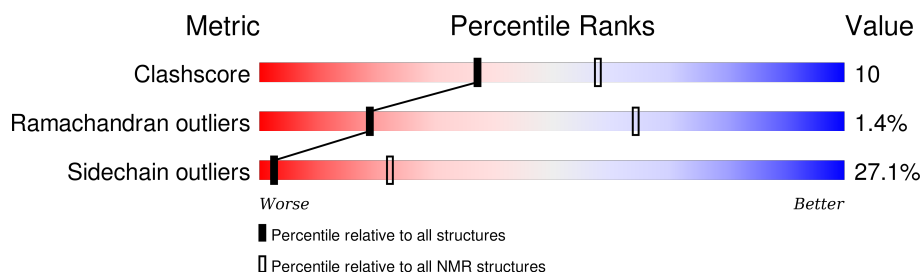|		
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027457

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 10%.

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	Percentile Ranks	Value
Clashscore		10
Ramachandran outliers		1.4%
Sidechain outliers		27.1%

Worse   *Better*

▌ Percentile relative to all structures
▯ Percentile relative to all NMR structures

Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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%

Mol	Chain	Length	Quality of chain
1	A	150	53% 38% • 8%
1	B	150	52% 39% • 8%
1	C	150	57% 35% • 7%
1	D	150	53% 39% • 7%
1	E	150	51% 41% • 7%

2 Ensemble composition and analysis ⓘ

This entry contains 15 models. Model 1 is the overall representative, medoid model (most similar to other models).

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:216-A:318,　A:389-A:423, B:216-B:318,　B:389-B:423, C:215-C:318,　C:389-C:423, D:215-D:318,　D:389-D:423, E:215-E:318,　　E:389-E:423 (693)	0.58	1

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 4 clusters and 2 single-model clusters were found.

Cluster number	Models
1	1, 6, 10, 12
2	7, 8, 11, 15
3	3, 5, 13
4	2, 4
Single-model clusters	9; 14

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 12445 atoms, of which 6300 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit.

Mol	Chain	Residues	Atoms						Trace
1	A	150	Total	C	H	N	O	S	0
			2489	819	1260	207	201	2	
1	B	150	Total	C	H	N	O	S	0
			2489	819	1260	207	201	2	
1	C	150	Total	C	H	N	O	S	0
			2489	819	1260	207	201	2	
1	D	150	Total	C	H	N	O	S	0
			2489	819	1260	207	201	2	
1	E	150	Total	C	H	N	O	S	0
			2489	819	1260	207	201	2	

4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

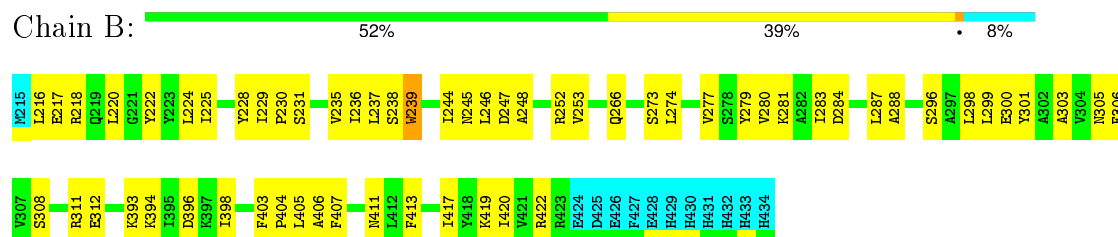- Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit
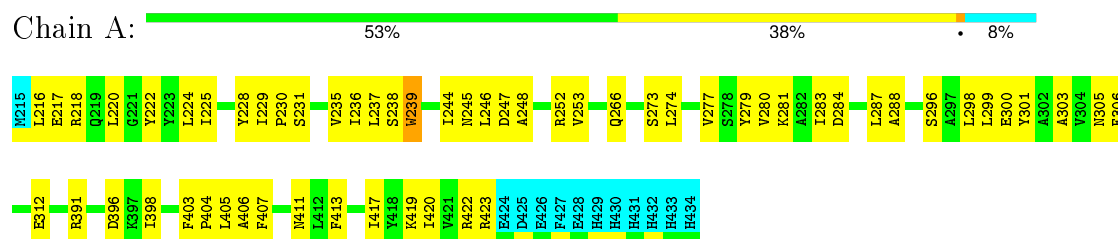
- Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

- Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

- Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain E:

4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain A:

• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain B:

• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain C:

- Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain D:

- Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain E:

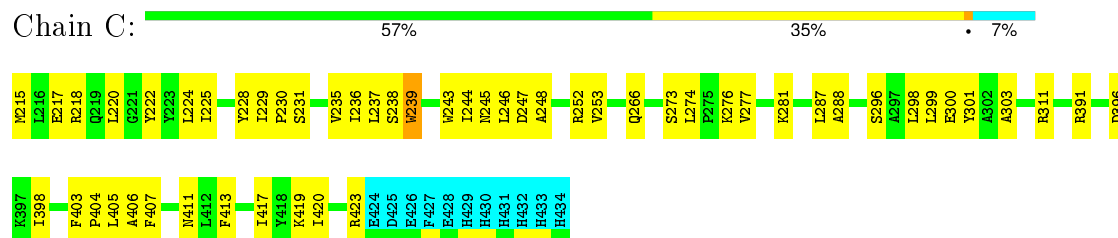### 4.2.2 Score per residue for model 2

- Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain A:

- Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain B:

• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain C:

• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain D:

• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit
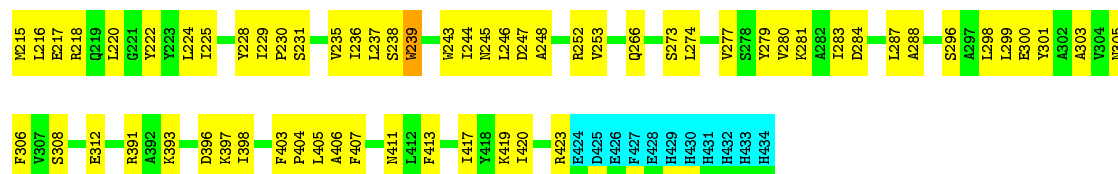
Chain E:

4.2.3 Score per residue for model 3

• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit
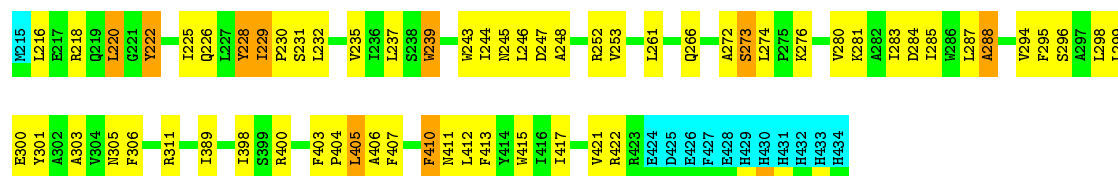
Chain A:

• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain B:

• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain C:

• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain D:

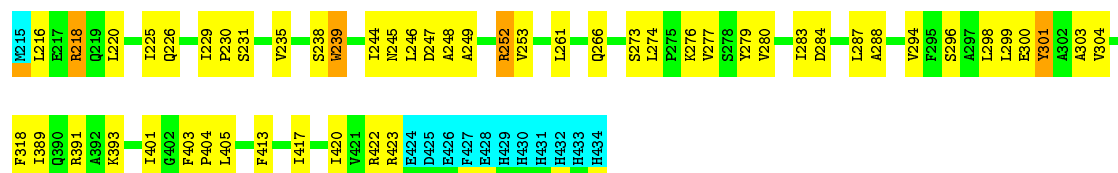• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain E:
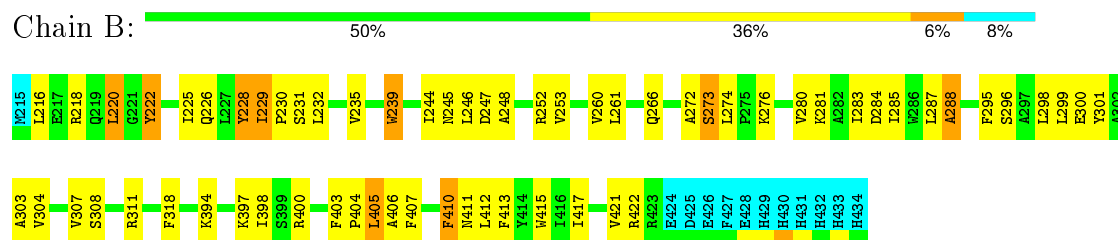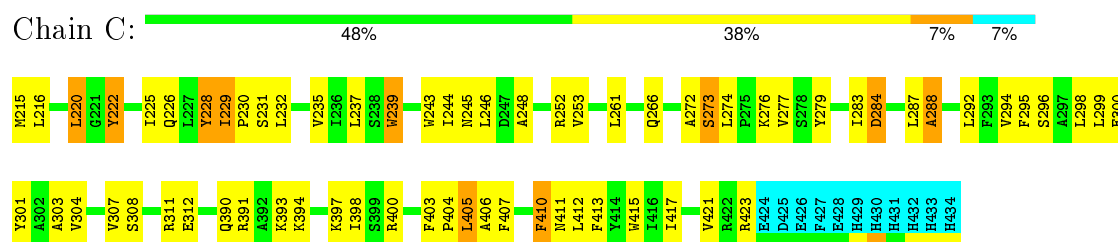
4.2.4 Score per residue for model 4

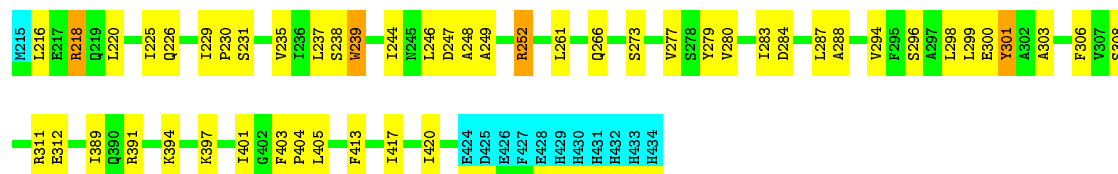• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain A:

• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain B: 55% 32% 5% 8%

• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain C: 60% 31% • 7%

• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain D: 55% 33% 5% 7%

• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain E: 55% 33% • 7%

4.2.5 Score per residue for model 5

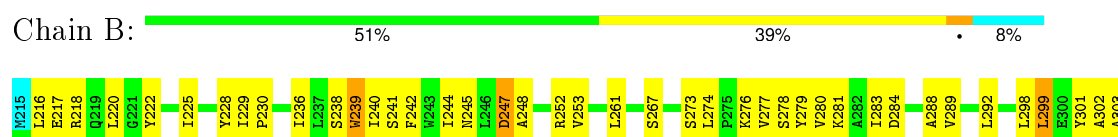• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit
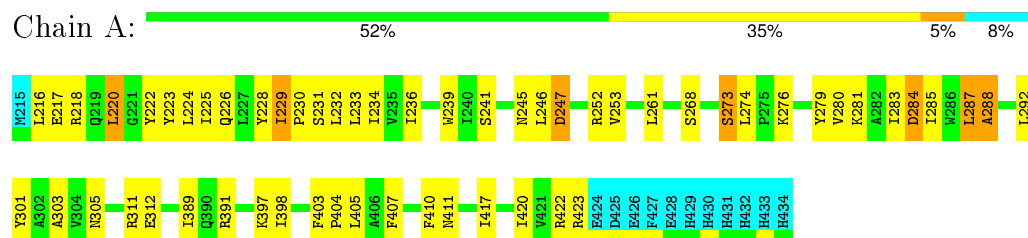
Chain A:

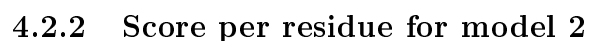

• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain B:

• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain C:
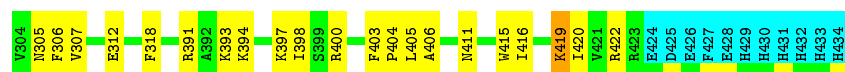

• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain D:

• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain E:

4.2.6 Score per residue for model 6

• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain A:

• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit
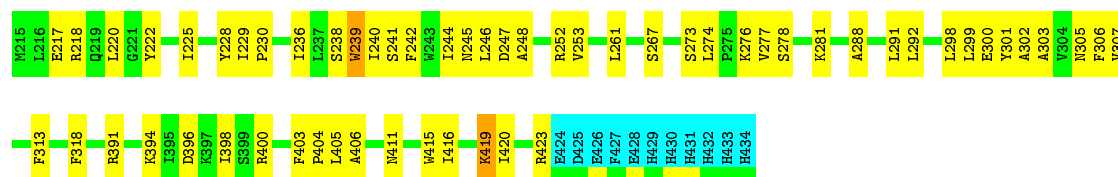
Chain B:

• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain C:

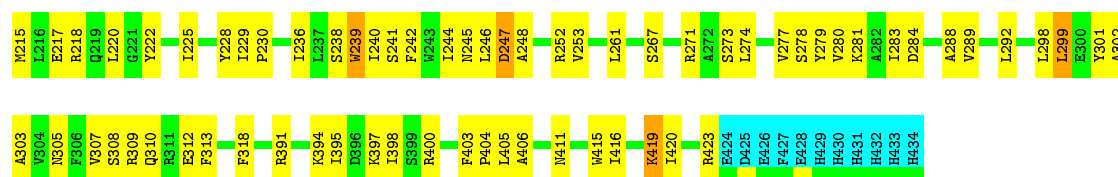• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain D:

A297 L298 L299 E300 Y301 A302 A303 V304 N305 F306 E312 R391 A392 K393 D396 S399 R400 I401 G402 F403 P404 L405 A406 F407 L408 N411 L412 F413 Y414 W415 I416 I417 Y418 K419 R423 A424 D425 E426 F427 E428 H429 H430 H431 H432 H433 H434

• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain E:　　48%　　41%　　·　　7%

M215 L216 E217 R218 Q219 L220 G221 Y222 I225 Y228 I229 P230 S231 L232 L233 I234 V235 I236 L237 S238 W239 W243 I244 N245 L246 D247 R252 V253 G254 L255 V260 Q266 R271 L274 P275 K276 V277 S278 Y279 V280 K281 A282 I283 W286 L287 A288 V289 C290 L291 S296

A297 L298 L299 E300 Y301 A302 A303 V304 N305 F306 R311 E312 K393 K394 I395 D396 S399 R400 I401 G402 F403 P404 L405 A406 F407 L408 N411 L412 F413 Y414 W415 I416 I417 Y418 K419 I420 V421 R422 R423 A424 D425 E426 E427 E428 H429 H430 H431 H432 H433 H434

4.2.7　Score per residue for model 7

• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain A:　　47%　　41%　　·　　8%

M215 L216 E217 R218 Q219 L220 G221 Y222 I225 I229 P230 S231 L232 L233 I234 V235 I236 L237 S238 W239 W243 I244 N245 L246 D247 A248 A249 R252 Q266 S267 R271 A272 S273 L274 V277 S278 Y279 V280 K281 A282 I283 D284 I285 A288 V294 F295 S296 A297 L298 L299 E300

Y301 A302 A303 V304 N305 F306 Q310 R311 E312 F313 G314 F318 I389 Q390 R391 A392 K393 D396 K397 I398 F403 P404 L405 A406 F407 L408 I409 F410 N411 L412 F413 I417 Y418 K419 I420 V421 R422 R423 A424 D425 E426 F427 E428 H429 H430 H431 H432 H433 H434

• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain B:　　50%　　39%　　·　　8%

M215 L216 E217 R218 Q219 L220 G221 Y222 I225 I229 P230 S231 L232 L233 I234 V235 I236 L237 S238 W239 I244 N245 L246 D247 A248 A249 R252 Q266 S267 S273 L274 P275 K276 V277 S278 Y279 V280 K281 A282 I283 D284 I285 A288 V294 F295 S296 A297 L298 L299 E300 Y301 A302

A303 V304 N305 S308 R311 E312 F313 G314 I389 Q390 R391 A392 K393 K394 I395 I398 F403 P404 L405 A406 F407 L408 I409 F410 N411 L412 F413 I417 Y418 K419 I420 V421 R422 R423 E424 D425 E426 F427 E428 H429 H430 H431 H432 H433 H434

• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain C:　　53%　　36%　　·　　7%

M215 L216 E217 R218 Q219 L220 G221 Y222 I225 I229 P230 S231 L232 I234 V235 I236 L237 S238 W239 I244 N245 L246 D247 A248 A249 R252 Q266 S267 S273 L274 P275 K276 V277 I285 A288 L291 V294 F295 S296 A297 L298 L299 E300 Y301 A302 A303 V304 N305

S308 R309 Q310 R311 E312 F313 G314 Q390 R391 K397 I398 F403 P404 L405 A406 F407 L408 I409 F410 N411 L412 F413 I417 Y418 K419 I420 V421 R422 R423 E424 D425 E426 F427 E428 H429 H430 H431 H432 H433 H434
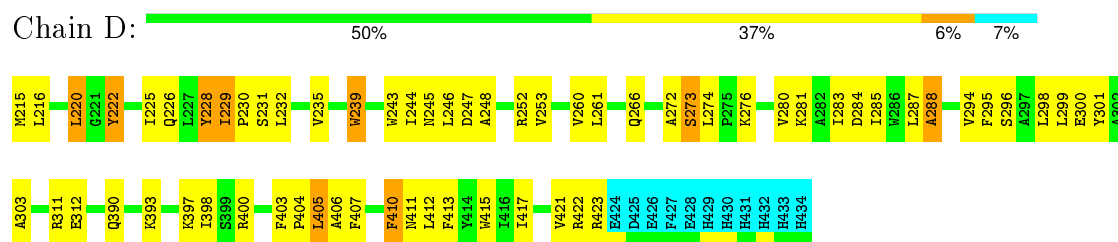
• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain D:

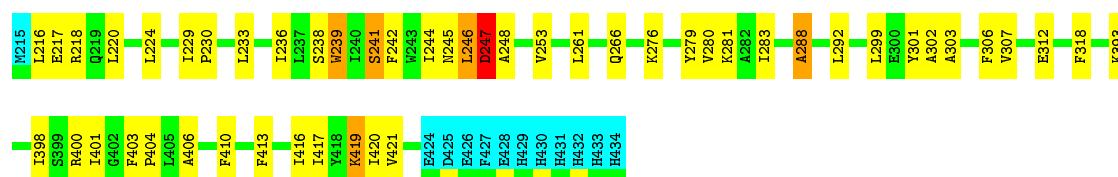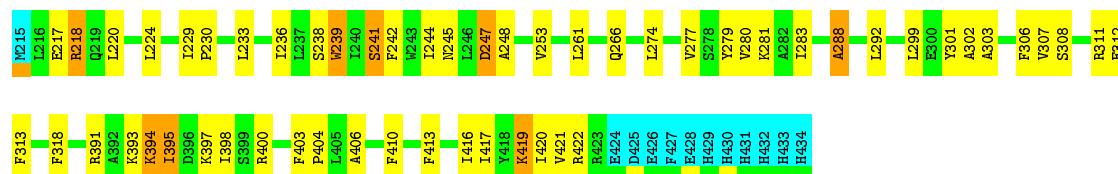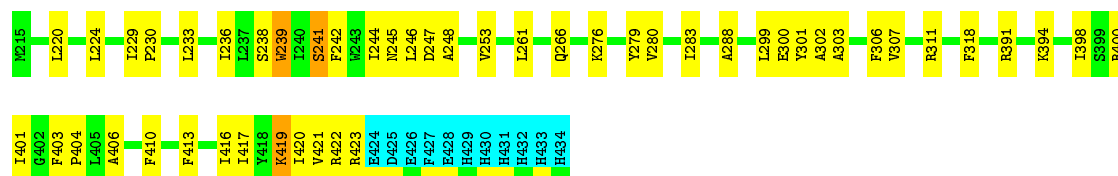• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain E:

4.2.8 Score per residue for model 8

• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain A:
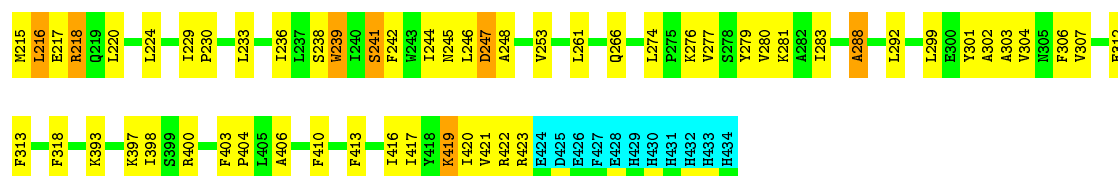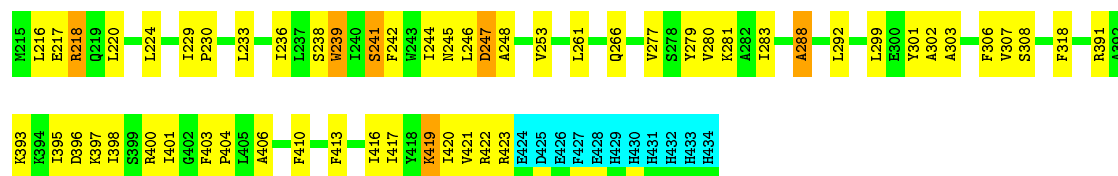

• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain B:

• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain C:

M215 L216 E217 R218 Q219 L220 L224 I225 I229 P230 S231 L232 L233 I234 V235 I236 L237 S238 W239 I240 I244 N245 L246 D247 A248 A249 R252 L255 Q266 S267 S270 S273 L274 P275 K276 V277 V280 K281 A282 I283 D284 I285 W286 L287 A288 V294 F295 S296 A297 L298

L299 E300 Y301 A302 A303 V304 N305 F306 V307 S308 R309 Q310 R311 E312 F313 R391 D396 K397 I398 F403 P404 L405 A406 F407 L408 N411 L412 Y414 W415 I416 I417 I420 V421 E424 D425 E426 F427 E428 H429 H430 H431 H432 H433 H434

• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain D: 55% 33% 5% 7%

M215 L216 E217 R218 Q219 L220 L224 I225 I229 P230 S231 L232 L233 I234 V235 I236 L237 S238 W239 I240 I244 N245 L246 D247 A248 A249 R252 L255 Q266 S267 S270 S273 L274 V277 S278 Y279 V280 K281 D284 L287 A288 V294 F295 S296 A297 L298 E299 E300

Y301 A302 A303 V304 N305 S308 R309 Q310 R311 E312 F318 K397 I398 F403 P404 L405 A406 F407 L408 N411 L412 F413 Y414 W415 I416 I417 I420 V421 R422 R423 E424 D425 E426 F427 E428 H429 H430 H431 H432 H433 H434

• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain E: 56% 31% 5% 7%

M215 L216 E217 R218 Q219 L220 L224 I225 I229 P230 S231 L232 L233 I234 V235 I236 L237 S238 W239 I240 I244 N245 L246 D247 A248 A249 R252 L255 Q266 S267 S270 S273 L274 V277 S278 Y279 V280 K281 D284 L287 A288 V294 F295 S296 A297 L298 E299 E300

Y301 A302 A303 V304 N305 F306 Q310 R311 K397 I398 F403 P404 L405 A406 F407 L408 N411 L412 F413 Y414 W415 I416 I417 I420 E424 D425 E426 F427 E428 H429 H430 H431 H432 H433 H434
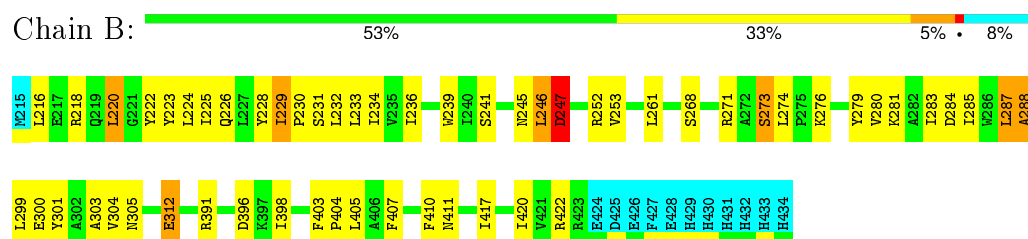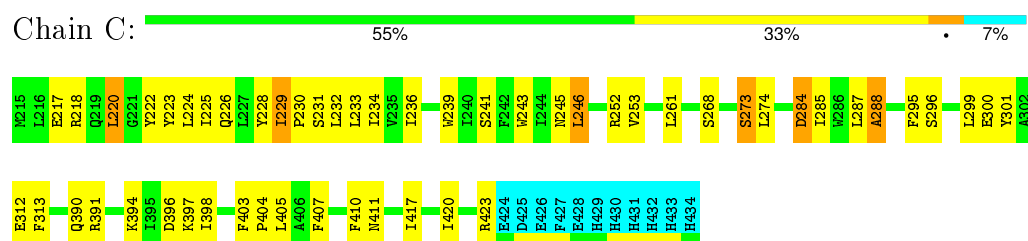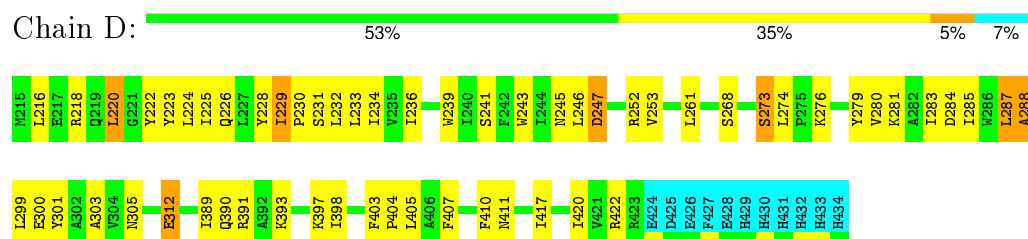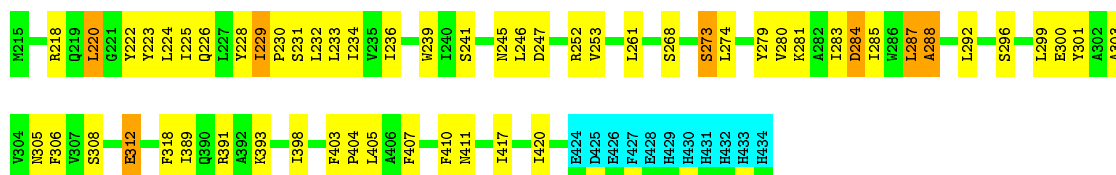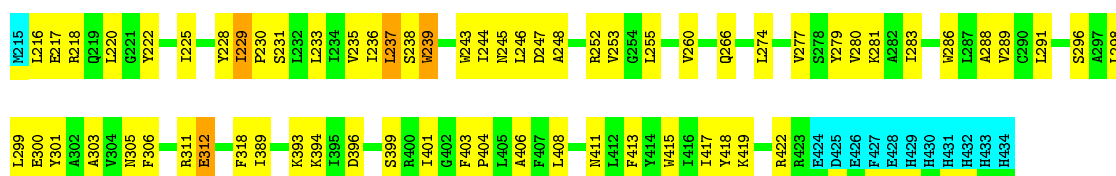
4.2.9 Score per residue for model 9

• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain A: 56% 33% • 8%

M215 L216 E217 R218 Q219 L220 L224 I229 P230 V235 I236 L237 S238 W239 W243 I244 N245 L246 D247 A248 V253 V260 T264 T265 Q266 S273 L274 V277 S278 Y279 V280 I283 L287 A288 F293 S296 L299 E300 Y301 A302 A303 V304 N305 F306 R311

E312 F318 R391 I395 D396 K397 I398 S399 F403 P404 L405 A406 N411 L412 F413 I420 V421 R422 R423 E424 D425 E426 F427 E428 H429 H430 H431 H432 H433 H434

• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain B: 57% 31% • 8%

M215 L216 E217 R218 Q219 L220 G221 Y222 Y223 L224 I225 I229 P230 V235 I236 L237 S238 W239 I244 N245 L246 D247 A248 V253 V260 T264 T265 Q266 S273 L274 V277 S278 Y279 V280 I283 W286 L287 A288 V289 F293 S296 L299 E300 Y301 A302 A303 V304

N305 F306 R309 Q310 R311 I395 D396 K397 I398 S399 F403 P404 L405 A406 N411 L412 F413 I420 E424 D425 E426 F427 E428 H429 H430 H431 H432 H433 H434

• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain C: 55% 35% • 7%

M215 L216 E217 R218 Q219 L220 G221 Y222 Y223 L224 I225 I229 P230 V235 I236 L237 S238 W239 I244 N245 L246 D247 A248 V253 V260 T264 T265 Q266 S273 L274 P275 K276 V277 S278 Y279 V280 I283 W286 L287 A288 V289 F293 S296 L299 E300 Y301 A302 A303

F306 R311 F318 I389 Q390 K394 I395 D396 K397 I398 S399 F403 P404 L405 A406 N411 L412 F413 I420 E424 D425 E426 F427 E428 H429 H430 H431 H432 H433 H434

• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain D: 57% 31% 5% 7%

M215 L216 E217 R218 Q219 L220 G221 Y222 Y223 L224 I225 I229 P230 V235 I236 L237 S238 W239 W243 I244 N245 L246 D247 A248 V253 V260 T264 T265 Q266 R271 A272 S273 L274 V277 S278 Y279 V280 I283 L287 A288 F293 S296 L299 E300 Y301 A302 A303

V304 N305 I395 D396 K397 I398 S399 F403 P404 L405 A406 N411 L412 F413 I420 V421 R422 R423 E424 D425 E426 F427 E428 H429 H430 H431 H432 H433 H434

• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain E: 58% 31% • 7%

M215 L216 E217 R218 Q219 L220 G221 Y222 Y223 L224 I225 I229 P230 V235 I236 L237 S238 W239 I244 N245 L246 D247 A248 V253 V260 T264 T265 Q266 S273 L274 V277 S278 Y279 V280 I283 L287 A288 F293 S296 L299 E300 Y301 A302 A303 V304 N305 F306

R311 E312 K394 I395 D396 K397 I398 S399 F403 P404 L405 A406 N411 L412 F413 I420 E424 D425 E426 F427 E428 H429 H430 H431 H432 H433 H434

4.2.10 Score per residue for model 10

• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain A: 57% 30% 5% 8%

M215 L216 E217 R218 Q219 L220 G221 Y222 Y223 L224 I225 Q226 L227 Y28 I229 P230 S231 L232 L233 I234 V235 I236 L237 S238 W239 I244 N245 L246 D247 A248 V253 L261 Q266 R271 A272 S273 L274 P275 K276 V277 S278 Y279 V280 I283 L287 A288 L298 L299 E300 Y301 A302 A303

V304 N305 F306 R391 K397 I398 F403 P404 L405 A406 N411 L412 F413 I417 I420 R423 E424 D425 E426 F427 E428 H429 H430 H431 H432 H433 H434
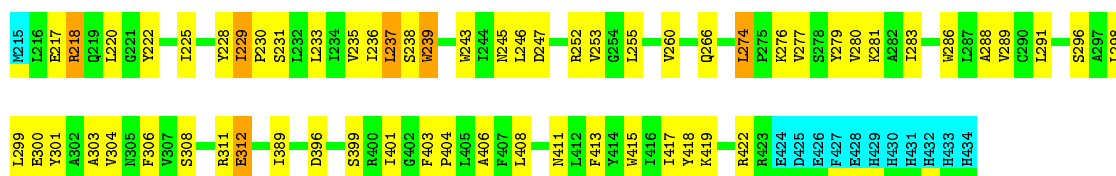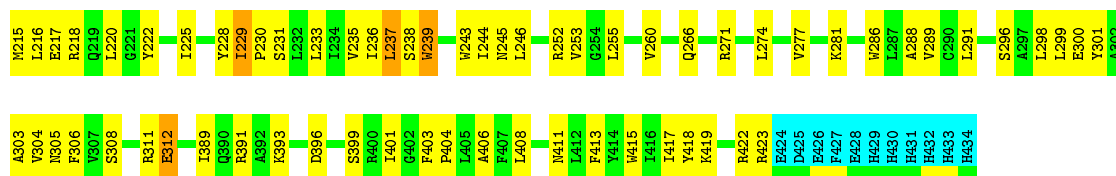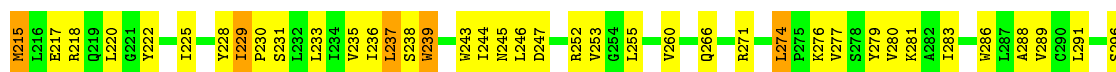
• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain B:

• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain C:

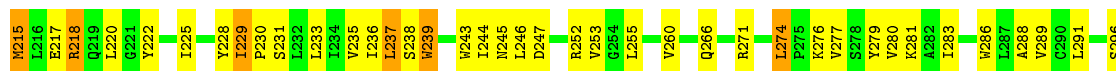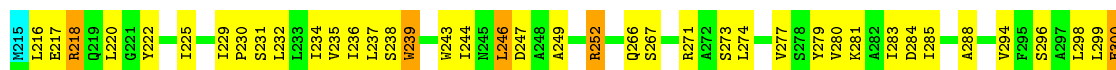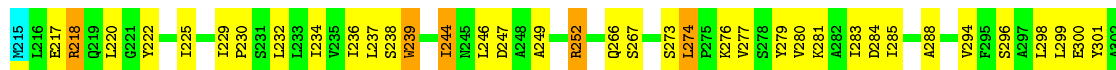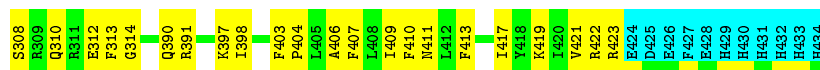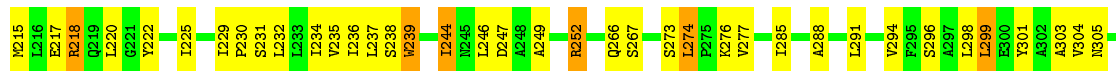• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain D:

• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit
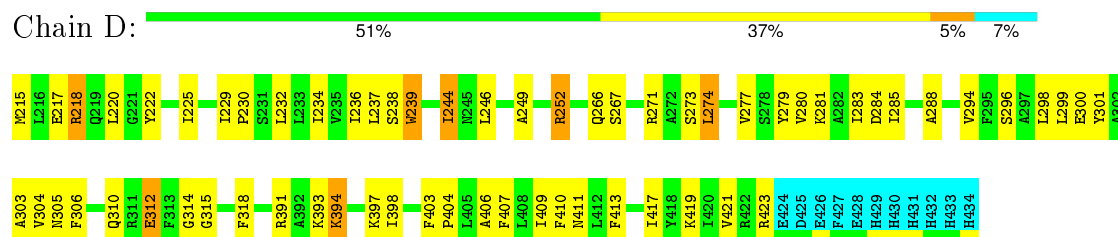
Chain E:

4.2.11 Score per residue for model 11

• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain A:

• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain B:

• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain C:

• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain D:

• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain E:

4.2.12 Score per residue for model 12

• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain A:

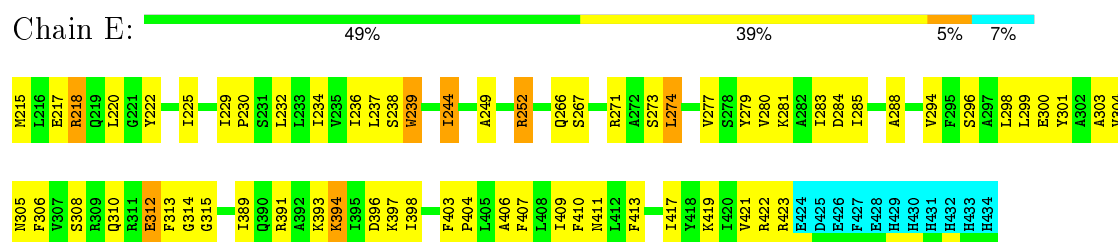• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain B:

• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain C:

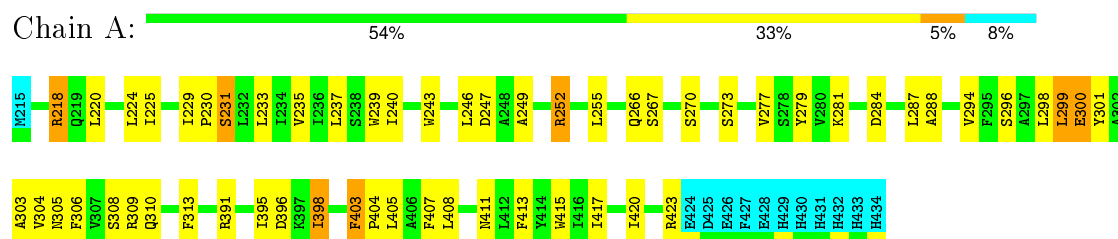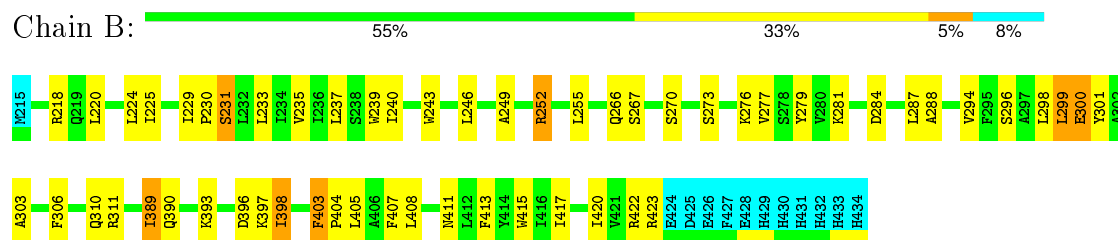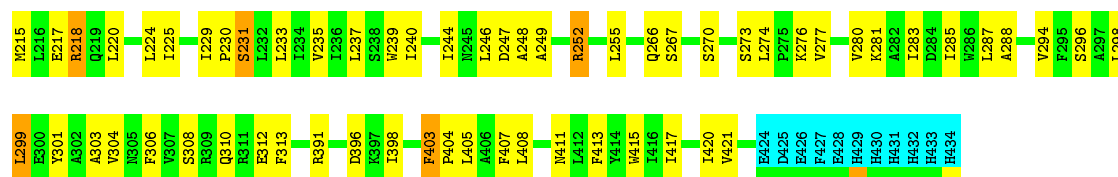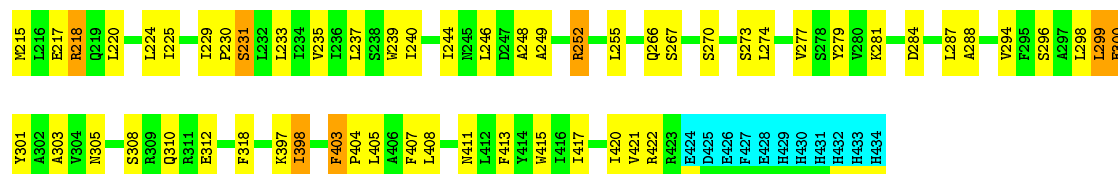• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain D:

• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit
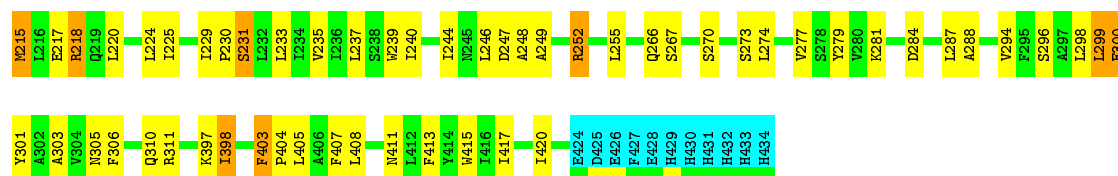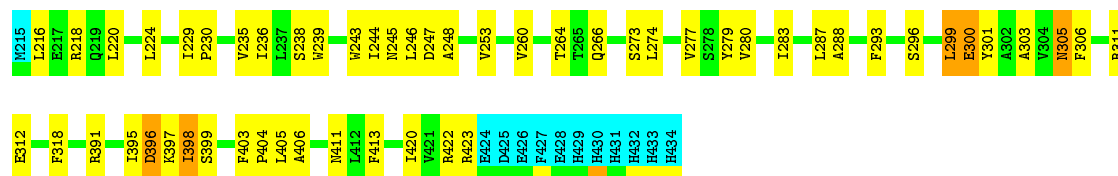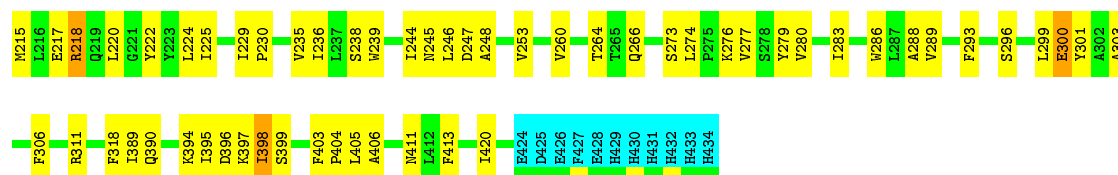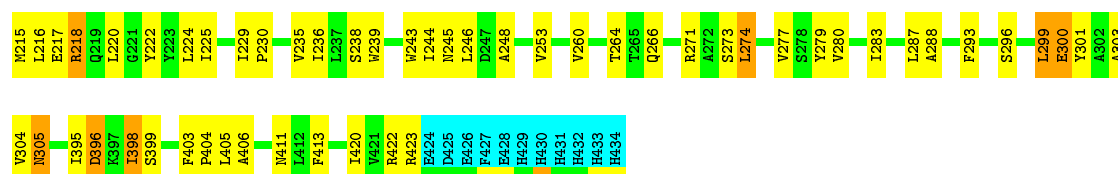
Chain E:

M215 L216 E217 R218 Q219 L220 L224 I225 I229 P230 S231 L232 L233 I234 V235 I236 L237 S238 W239 W243 I244 N245 L246 D247 A248 R252 V253 G254 L255 L261 T264 T265 Q266 S267 S268 S273 L274 Y279 V280 K281 A282 I283 D284 I285 W286 L287 A288 L291 V294 F295

S296 A297 L298 L299 E300 Y301 A302 A303 S308 E312 D396 R400 I401 G402 F403 P404 L405 A406 F407 N411 L412 F413 Y414 W415 I416 I417 I420 V421 R422 R423 E424 D425 E426 F427 E428 H429 H430 H431 H432 H433 H434

4.2.13 Score per residue for model 13

• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain A:

| 52% | 37% | • | 8% |

M215 L220 G221 Y222 Y223 L224 I225 Q226 I229 P230 S231 V235 I236 L237 S238 W239 I244 N245 L246 D247 A248 R252 V253 V260 Q266 S273 L274 V277 K281 W286 L287 A288 V289 C290 L291 L292 F295 S296 A297 L298 L299 E300 Y301 A302 A303 V304 N305 F306

R309 F318 I389 Q390 R391 D396 K397 I398 F403 P404 L405 A406 F407 L408 I409 F410 F413 Y414 W415 I416 I417 Y418 K419 I420 R423 E424 D425 E426 F427 E428 H429 H430 H431 H432 H433 H434

• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain B:

| 49% | 40% | • | 8% |

M215 L216 Q219 L220 G221 Y222 Y223 L224 I225 Q226 I229 P230 S231 I234 V235 I236 L237 S238 W239 W243 I244 N245 L246 D247 A248 R252 V253 V260 Q266 R271 A272 S273 L274 V277 K281 W286 L287 A288 V289 C290 L291 L292 F295 S296 A297 L298 L299 E300

Y301 A302 A303 V304 N305 F306 V307 S308 R309 Q310 R311 E312 F313 D396 K397 I398 F403 P404 L405 A406 F407 L408 I409 F410 F413 Y414 W415 I416 I417 Y418 K419 I420 E424 D425 E426 F427 E428 H429 H430 H431 H432 H433 H434

• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain C:

| 53% | 37% | • | 7% |

M215 L216 Q219 L220 G221 Y222 Y223 L224 I225 Q226 I229 P230 S231 I234 V235 I236 L237 S238 W239 W243 I244 N245 R252 V253 V260 Q266 R271 A272 S273 L274 P275 K276 V277 W286 L287 A288 V289 C290 L291 S296 A297 L298 L299 E300 Y301 A302 A303 F306 V307

S308 R309 Q310 R311 D396 K397 I398 F403 P404 L405 A406 F407 L408 I409 F410 F413 Y414 W415 I416 I417 Y418 K419 I420 R423 E424 D425 E426 F427 E428 H429 H430 H431 H432 H433 H434

• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain D:

| 51% | 39% | • | 7% |

M215 L220 G221 Y222 Y223 L224 I225 Q226 I229 P230 S231 V235 I236 L237 S238 W239 W243 I244 N245 L246 D247 A248 R252 V253 V260 Q266 S273 L274 P275 K276 V277 K281 W286 L287 A288 V289 C290 L291 L292 F295 S296 A297 L298 L299 E300 Y301 A302 A303 V304

N305 F306 V307 S308 R311 E312 R391 D396 K397 I398 F403 P404 L405 A406 F407 L408 I409 F410 F413 Y414 W415 I416 I417 Y418 K419 I420 R423 E424 D425 E426 F427 E428 H429 H430 H431 H432 H433 H434

• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain E: 49% 40% • 7%

M215 L216 E217 R218 Q219 L220 G221 Y222 Y223 L224 I225 Q226 I229 P230 S231 V235 I236 L237 S238 W239 W243 I244 N245 L246 D247 R252 V253 V260 Q266 R271 A272 S273 L274 P275 K276 V277 K281 W286 L287 A288 V289 C290 L291 L292 F295 S296 A297 L298 L299 E300

Y301 A302 A303 V304 N305 F306 V307 S308 R309 Q310 F318 I395 D396 K397 I398 F403 P404 L405 A406 F407 L408 I409 F410 F413 Y414 W415 I416 I417 Y418 K419 I420 E424 D425 E426 F427 E428 H429 H430 H431 H432 H433 H434

4.2.14 Score per residue for model 14

• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain A: 60% 30% • 8%

M215 L216 E217 R218 L224 I225 Q226 L227 Y228 I229 P230 S231 L232 V235 I236 L237 S238 W239 I240 S241 I244 N245 L246 D247 A248 R252 V253 G254 L255 V260 L274 P275 K276 V277 R278 Y279 V280 K281 L287 A288 S296 A297 L298 L299 E300 Y301 N305 S308 E312

R391 A392 K393 K397 I398 S399 F403 P404 L405 A406 I409 I417 I420 E424 D425 E426 F427 E428 H429 H430 H431 H432 H433 H434

• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain B: 57% 33% • 8%

M215 L216 E217 R218 L224 I225 Q226 L227 Y228 I229 P230 S231 L232 V235 I236 L237 S238 W239 I240 S241 I244 N245 L246 D247 A248 R252 V253 G254 L255 V260 L274 V277 S278 Y279 V280 K281 L287 A288 S296 A297 L298 L299 E300 Y301 A302 A303 V304 N305 F306 R311

E312 F313 R391 A392 K393 I398 S399 F403 P404 L405 A406 I409 I417 I420 V421 R422 R423 E424 D425 E426 F427 E428 H429 H430 H431 H432 H433 H434

• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain C: 59% 33% • 7%

M215 L216 E217 R218 L224 I225 Q226 L227 Y228 I229 P230 S231 L232 V235 I236 L237 S238 W239 I240 S241 I244 N245 L246 D247 A248 R252 V253 G254 L255 V260 L274 Y279 V280 K281 I285 W286 L287 A288 V289 S296 A297 L298 L299 E300 Y301 A302 A303 V304 N305 R309

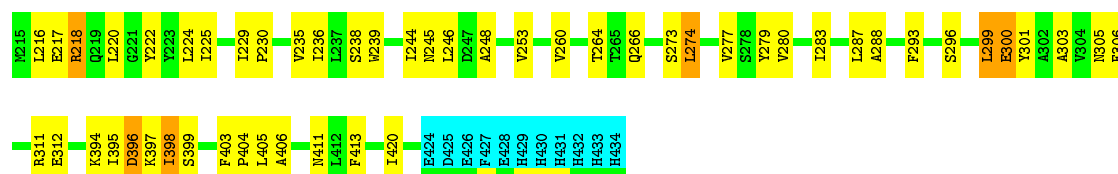Q310 R311 E312 K393 I398 S399 F403 P404 L405 A406 I409 I417 I420 R423 E424 D425 E426 F427 E428 H429 H430 H431 H432 H433 H434

• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain D:

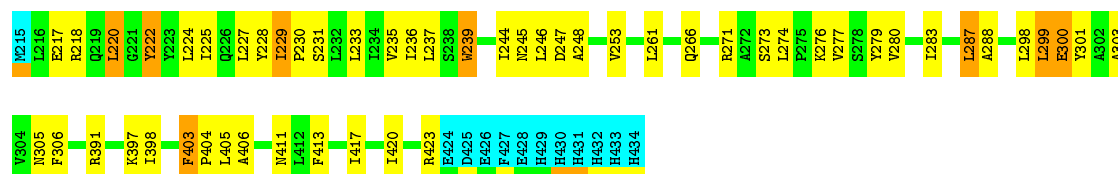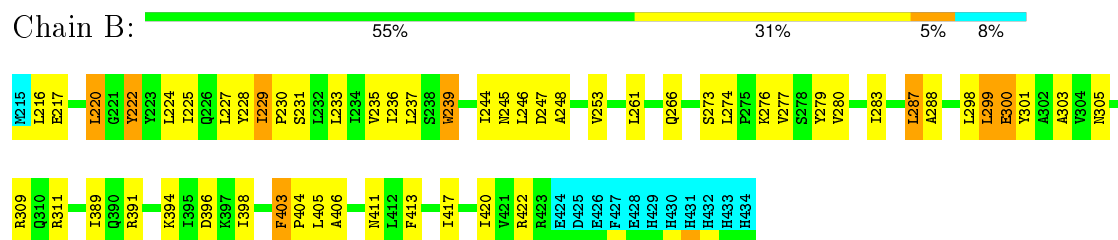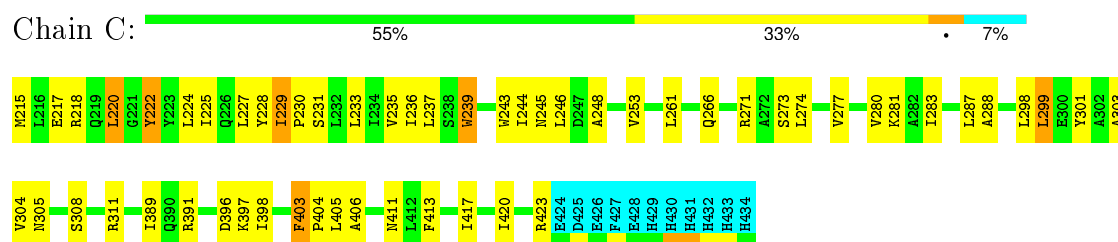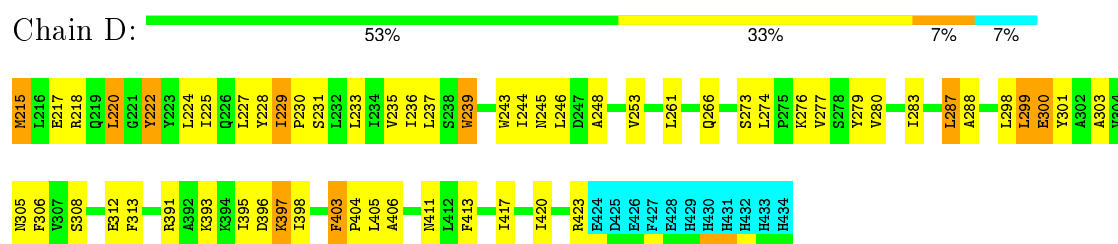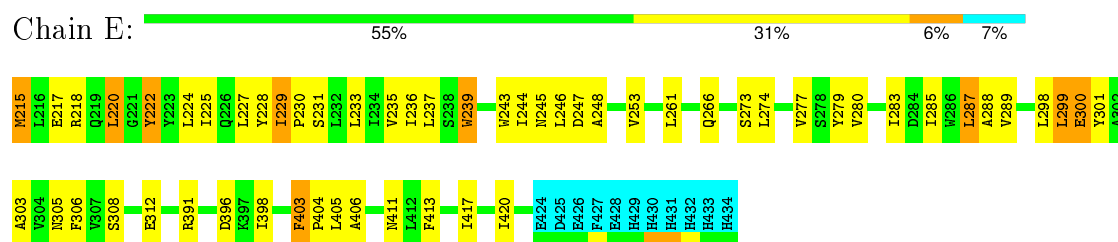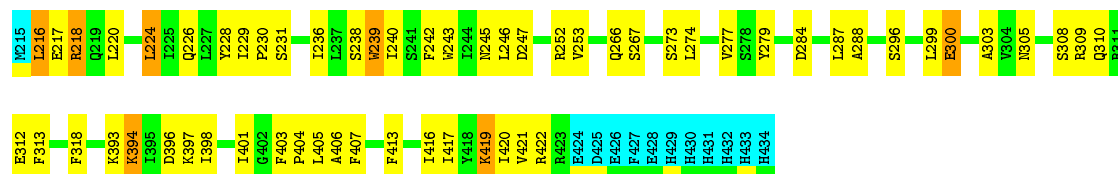• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain E:

4.2.15 Score per residue for model 15

• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain A:
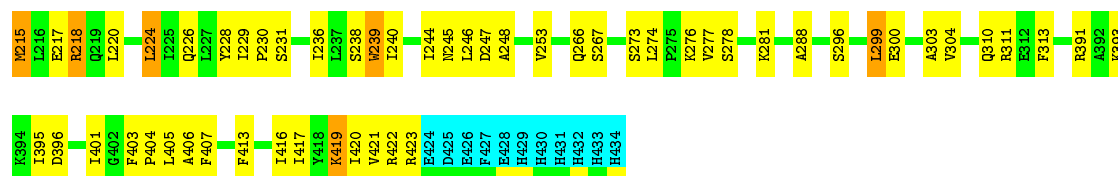

• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit
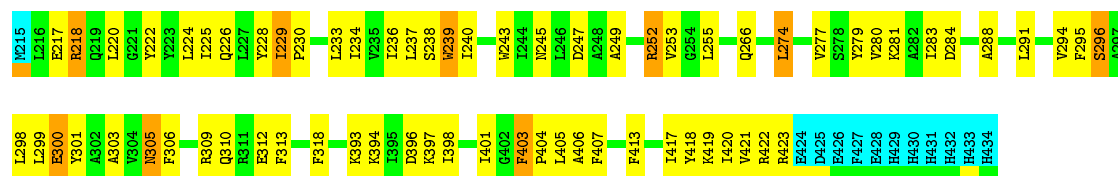
Chain B:

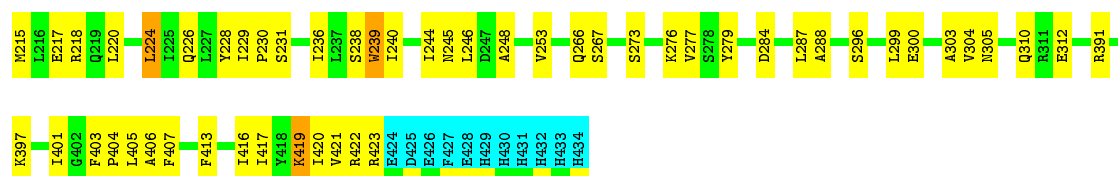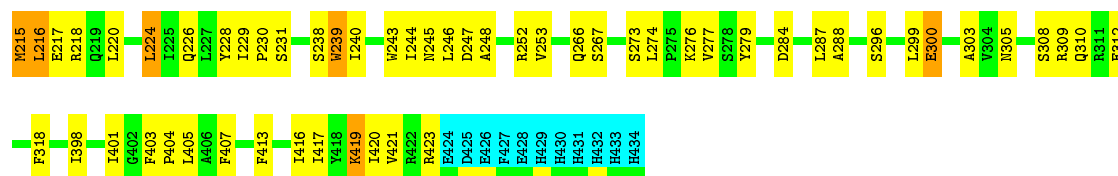• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit
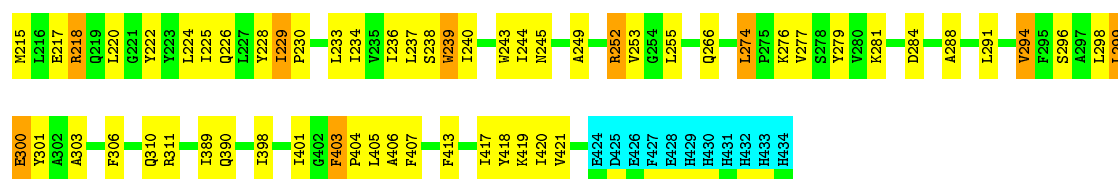
Chain C:

• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit
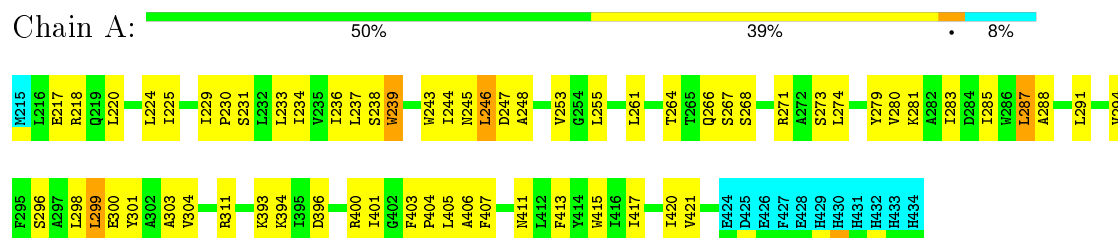
Chain D:

• Molecule 1: Full-Length Transmembrane Domains of Human Glycine Receptor alpha1 Subunit

Chain E:

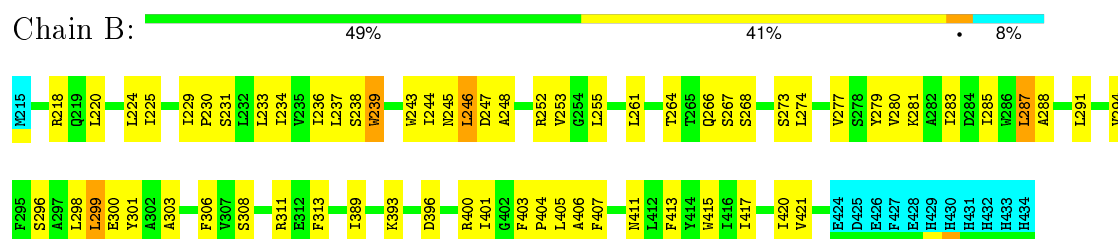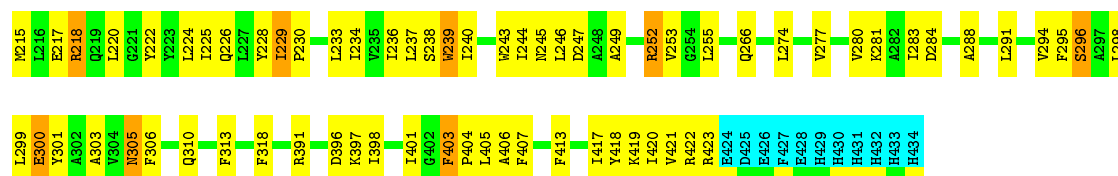# 5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *simulated annealing*.

Of the 100 calculated structures, 15 were deposited, based on the following criterion: *target function*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
CYANA	refinement	3.0

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	2m6i_cs.str
Number of chemical shift lists	1
Total number of shifts	1145
Number of shifts mapped to atoms	1145
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	10%

No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality (i)

6.1 Standard geometry (i)

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1115	1178	1178	25±6
1	B	1115	1178	1178	25±6
1	C	1123	1187	1186	25±5
1	D	1123	1187	1186	25±6
1	E	1123	1187	1186	25±6
All	All	83985	88755	88710	1705

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 10.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:D:246:LEU:HD21	1:D:304:VAL:HG21	0.93	1.39	6	2
1:E:246:LEU:HD21	1:E:304:VAL:HG21	0.89	1.42	6	1
1:B:246:LEU:HD21	1:B:304:VAL:HG21	0.89	1.45	6	2
1:C:246:LEU:HD21	1:C:304:VAL:HG21	0.84	1.46	3	4
1:A:225:ILE:HG23	1:A:417:ILE:HD13	0.68	1.65	8	5
1:A:246:LEU:HD21	1:A:304:VAL:CG2	0.67	2.19	8	2
1:E:225:ILE:HG23	1:E:417:ILE:HD13	0.67	1.66	8	5
1:C:225:ILE:HG23	1:C:417:ILE:HD13	0.67	1.65	8	5
1:A:298:LEU:HD13	1:E:237:LEU:HB3	0.66	1.68	15	5
1:D:218:ARG:HD2	1:D:277:VAL:HG11	0.66	1.68	8	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Models Total
1:B:225:ILE:HG23	1:B:417:ILE:HD13	0.66	1.67	14	5
1:B:237:LEU:HB3	1:C:298:LEU:HD13	0.65	1.68	7	5
1:D:225:ILE:HG23	1:D:417:ILE:HD13	0.65	1.68	1	5
1:C:237:LEU:HB3	1:D:298:LEU:HD13	0.65	1.69	15	5
1:D:218:ARG:CD	1:D:277:VAL:HG11	0.65	2.22	8	6
1:E:218:ARG:CD	1:E:277:VAL:HG11	0.65	2.22	9	6
1:E:218:ARG:HD2	1:E:277:VAL:HG11	0.65	1.69	8	5
1:C:218:ARG:HD2	1:C:277:VAL:HG11	0.64	1.69	8	5
1:B:300:GLU:OE2	1:B:398:ILE:HD12	0.64	1.93	15	1
1:C:246:LEU:HD21	1:C:304:VAL:CG2	0.64	2.22	11	2
1:C:218:ARG:CD	1:C:277:VAL:HG11	0.63	2.24	15	8
1:E:218:ARG:HD3	1:E:277:VAL:HG11	0.63	1.69	9	1
1:B:218:ARG:CD	1:B:277:VAL:HG11	0.63	2.24	15	9
1:A:218:ARG:HD3	1:A:277:VAL:HG11	0.63	1.71	9	3
1:B:218:ARG:HD3	1:B:277:VAL:HG11	0.62	1.71	2	4
1:C:225:ILE:CG1	1:C:417:ILE:HG21	0.62	2.23	3	3
1:B:389:ILE:HG23	1:B:390:GLN:HG2	0.62	1.72	8	2
1:E:300:GLU:OE2	1:E:398:ILE:HD12	0.62	1.93	15	1
1:A:300:GLU:OE2	1:A:398:ILE:HD12	0.62	1.94	15	1
1:A:218:ARG:CD	1:A:277:VAL:HG11	0.62	2.25	15	7
1:C:300:GLU:OE2	1:C:398:ILE:HD12	0.62	1.94	15	1
1:B:242:PHE:CD1	1:B:253:VAL:HG22	0.62	2.29	11	1
1:B:218:ARG:HD2	1:B:277:VAL:HG11	0.62	1.72	1	4
1:D:246:LEU:HD21	1:D:304:VAL:CG2	0.62	2.25	11	4
1:C:218:ARG:HD3	1:C:277:VAL:HG11	0.61	1.70	2	3
1:D:300:GLU:OE2	1:D:398:ILE:HD12	0.61	1.94	15	1
1:A:298:LEU:HD12	1:E:252:ARG:NH1	0.61	2.11	13	2
1:D:237:LEU:HB3	1:E:298:LEU:HD13	0.61	1.72	7	5
1:C:225:ILE:HG12	1:C:417:ILE:HG21	0.61	1.73	15	5
1:A:218:ARG:HD2	1:A:277:VAL:HG11	0.61	1.70	8	4
1:C:246:LEU:HD13	1:C:300:GLU:OE1	0.61	1.95	2	2
1:D:225:ILE:CG1	1:D:417:ILE:HG21	0.61	2.26	3	3
1:D:215:MET:N	1:D:274:LEU:HD13	0.61	2.11	8	4
1:A:225:ILE:HG12	1:A:417:ILE:HG21	0.61	1.73	15	5
1:A:280:VAL:HA	1:A:283:ILE:HD12	0.61	1.73	2	11
1:E:215:MET:N	1:E:274:LEU:HD13	0.61	2.11	12	5
1:B:281:LYS:HE3	1:B:285:ILE:HD11	0.60	1.74	3	1
1:B:239:TRP:CH2	1:B:398:ILE:HD11	0.60	2.32	3	5
1:D:280:VAL:HA	1:D:283:ILE:HD12	0.60	1.73	1	11
1:C:215:MET:N	1:C:274:LEU:HD13	0.60	2.12	12	5
1:D:218:ARG:HD3	1:D:277:VAL:HG11	0.60	1.72	12	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:281:LYS:HE3	1:A:285:ILE:HD11	0.60	1.74	3	1
1:B:280:VAL:HA	1:B:283:ILE:HD12	0.60	1.73	2	11
1:E:239:TRP:CH2	1:E:401:ILE:HD11	0.60	2.31	6	5
1:A:239:TRP:CH2	1:A:401:ILE:HD11	0.60	2.32	6	5
1:D:225:ILE:HG12	1:D:417:ILE:HG21	0.60	1.74	15	5
1:E:280:VAL:HA	1:E:283:ILE:HD12	0.60	1.73	2	11
1:A:225:ILE:CG1	1:A:417:ILE:HG21	0.59	2.27	3	4
1:E:239:TRP:CH2	1:E:398:ILE:HD11	0.59	2.32	3	5
1:C:239:TRP:CH2	1:C:401:ILE:HD11	0.59	2.32	6	5
1:E:225:ILE:HG12	1:E:417:ILE:HG21	0.59	1.74	15	5
1:A:237:LEU:HB3	1:B:298:LEU:HD13	0.59	1.75	15	5
1:D:215:MET:O	1:D:274:LEU:HD13	0.59	1.97	2	3
1:A:300:GLU:OE2	1:A:398:ILE:HD13	0.59	1.98	10	3
1:B:225:ILE:HG12	1:B:417:ILE:HG21	0.59	1.75	15	5
1:E:279:TYR:CZ	1:E:283:ILE:HD11	0.59	2.33	5	1
1:B:239:TRP:CH2	1:B:401:ILE:HD11	0.59	2.33	6	5
1:E:215:MET:O	1:E:274:LEU:HD13	0.59	1.97	6	1
1:A:236:ILE:HG12	1:A:406:ALA:HB1	0.58	1.73	10	3
1:A:299:LEU:HD23	1:A:300:GLU:OE1	0.58	1.98	10	1
1:A:252:ARG:NH1	1:B:298:LEU:HD12	0.58	2.13	13	1
1:A:244:ILE:HD13	1:B:305:ASN:OD1	0.58	1.97	7	1
1:E:281:LYS:HE3	1:E:285:ILE:HD11	0.58	1.75	3	1
1:B:225:ILE:CG1	1:B:417:ILE:HG21	0.58	2.28	3	3
1:D:244:ILE:HD13	1:E:305:ASN:CG	0.58	2.19	13	1
1:E:225:ILE:CG1	1:E:417:ILE:HG21	0.58	2.29	5	3
1:D:239:TRP:CH2	1:D:401:ILE:HD11	0.58	2.32	6	4
1:D:279:TYR:CZ	1:D:283:ILE:HD11	0.58	2.33	5	1
1:B:279:TYR:CZ	1:B:283:ILE:HD11	0.58	2.33	5	1
1:D:281:LYS:HE3	1:D:285:ILE:HD11	0.58	1.74	3	1
1:D:300:GLU:OE2	1:D:398:ILE:HD13	0.58	1.99	10	2
1:E:307:VAL:HG12	1:E:318:PHE:CZ	0.58	2.33	13	1
1:B:296:SER:HA	1:B:299:LEU:HD12	0.57	1.75	15	1
1:C:234:ILE:HA	1:C:237:LEU:HD12	0.57	1.75	15	3
1:E:215:MET:HA	1:E:274:LEU:HD13	0.57	1.77	10	1
1:D:296:SER:HA	1:D:299:LEU:HD12	0.57	1.76	15	1
1:A:305:ASN:OD1	1:E:244:ILE:HD12	0.57	2.00	9	2
1:E:220:LEU:HD13	1:E:273:SER:CB	0.57	2.29	11	6
1:A:296:SER:HA	1:A:299:LEU:HD12	0.57	1.76	15	1
1:D:220:LEU:HD13	1:D:273:SER:CB	0.57	2.30	7	7
1:D:299:LEU:HD23	1:D:300:GLU:OE1	0.57	2.00	10	1
1:E:299:LEU:HD23	1:E:300:GLU:OE1	0.57	2.00	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:B:279:TYR:CD2	1:B:283:ILE:HD11	0.57	2.35	12	1
1:E:234:ILE:HA	1:E:237:LEU:HD12	0.57	1.75	15	2
1:C:236:ILE:HG12	1:C:406:ALA:HB1	0.57	1.75	10	3
1:D:252:ARG:NH1	1:E:298:LEU:HD12	0.57	2.15	13	1
1:E:279:TYR:CD2	1:E:283:ILE:HD11	0.57	2.35	12	1
1:E:300:GLU:OE2	1:E:398:ILE:HD13	0.57	2.00	10	3
1:D:244:ILE:HD13	1:E:305:ASN:OD1	0.57	1.99	13	1
1:A:220:LEU:HD11	1:A:272:ALA:HB3	0.56	1.76	3	1
1:A:279:TYR:CD2	1:A:283:ILE:HD11	0.56	2.35	12	1
1:D:279:TYR:CD2	1:D:283:ILE:HD11	0.56	2.35	12	1
1:B:220:LEU:HD11	1:B:272:ALA:HB3	0.56	1.76	3	1
1:B:234:ILE:HA	1:B:237:LEU:HD12	0.56	1.75	15	3
1:E:236:ILE:HG12	1:E:406:ALA:HB1	0.56	1.76	10	3
1:E:296:SER:HA	1:E:299:LEU:HD12	0.56	1.76	15	1
1:B:220:LEU:HD13	1:B:273:SER:CB	0.56	2.31	7	7
1:C:215:MET:O	1:C:274:LEU:HD13	0.56	2.00	14	1
1:A:239:TRP:CH2	1:A:398:ILE:HD11	0.56	2.35	3	5
1:D:220:LEU:HD11	1:D:272:ALA:HB3	0.56	1.76	3	1
1:B:236:ILE:HG12	1:B:406:ALA:HB1	0.56	1.76	10	3
1:E:232:LEU:HD11	1:E:409:ILE:CG2	0.56	2.31	14	2
1:D:239:TRP:CH2	1:D:398:ILE:HD11	0.55	2.36	3	5
1:A:246:LEU:HD11	1:A:304:VAL:CG2	0.55	2.32	12	1
1:D:243:TRP:O	1:D:246:LEU:HD22	0.55	2.00	5	1
1:C:232:LEU:HD11	1:C:409:ILE:CG2	0.55	2.31	14	2
1:D:220:LEU:HD22	1:D:273:SER:HB2	0.55	1.77	3	2
1:A:232:LEU:HD11	1:A:409:ILE:CG2	0.55	2.31	14	2
1:C:294:VAL:O	1:C:298:LEU:HD12	0.55	2.02	15	5
1:C:220:LEU:HD13	1:C:273:SER:CB	0.55	2.32	7	6
1:D:236:ILE:HG12	1:D:406:ALA:HB1	0.55	1.77	10	3
1:A:246:LEU:HD23	1:A:247:ASP:HB3	0.55	1.79	4	1
1:E:220:LEU:HD22	1:E:273:SER:HB2	0.55	1.79	3	2
1:A:236:ILE:HD13	1:A:406:ALA:HB1	0.55	1.79	4	7
1:B:307:VAL:HG11	1:B:318:PHE:CE1	0.55	2.36	4	2
1:D:246:LEU:O	1:D:246:LEU:HD23	0.55	2.02	8	1
1:C:239:TRP:CH2	1:C:398:ILE:HD11	0.55	2.36	3	5
1:E:288:ALA:O	1:E:292:LEU:HD12	0.55	2.02	4	2
1:C:215:MET:HA	1:C:274:LEU:HD13	0.55	1.78	11	1
1:C:249:ALA:HB1	1:D:301:TYR:OH	0.54	2.01	15	4
1:D:288:ALA:O	1:D:292:LEU:HD12	0.54	2.02	4	2
1:A:302:ALA:HB2	1:E:241:SER:HB3	0.54	1.79	2	1
1:A:220:LEU:HD13	1:A:273:SER:CB	0.54	2.32	7	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:E:307:VAL:HG11	1:E:318:PHE:CD1	0.54	2.38	4	1
1:A:288:ALA:O	1:A:292:LEU:HD12	0.54	2.03	4	2
1:E:220:LEU:HD11	1:E:272:ALA:HB3	0.54	1.80	3	1
1:D:217:GLU:OE1	1:D:274:LEU:HD22	0.54	2.02	12	2
1:A:307:VAL:HG11	1:A:318:PHE:CD1	0.54	2.38	4	1
1:C:244:ILE:HD13	1:D:305:ASN:ND2	0.54	2.17	15	1
1:B:231:SER:O	1:B:235:VAL:HG23	0.54	2.03	13	6
1:E:233:LEU:HA	1:E:236:ILE:HD12	0.54	1.80	5	2
1:D:233:LEU:HA	1:D:236:ILE:HD12	0.54	1.80	5	2
1:B:232:LEU:HD11	1:B:409:ILE:CG2	0.54	2.33	14	2
1:E:417:ILE:O	1:E:421:VAL:HG23	0.54	2.02	3	6
1:B:220:LEU:HD22	1:B:273:SER:HB2	0.54	1.80	3	2
1:A:318:PHE:CD2	1:A:389:ILE:HG23	0.54	2.37	6	3
1:B:252:ARG:NH1	1:C:298:LEU:HD12	0.54	2.17	13	1
1:C:231:SER:O	1:C:235:VAL:HG23	0.54	2.03	13	7
1:D:307:VAL:HG11	1:D:318:PHE:CE1	0.54	2.38	2	2
1:D:231:SER:O	1:D:235:VAL:HG23	0.54	2.03	13	6
1:B:299:LEU:HD23	1:B:300:GLU:OE1	0.54	2.03	10	1
1:D:307:VAL:HG11	1:D:318:PHE:CD1	0.54	2.38	4	2
1:C:252:ARG:NH1	1:D:298:LEU:HD12	0.54	2.17	13	1
1:E:231:SER:O	1:E:235:VAL:HG23	0.54	2.03	13	6
1:E:217:GLU:OE1	1:E:274:LEU:HD22	0.54	2.03	12	2
1:C:280:VAL:HA	1:C:283:ILE:HD12	0.54	1.79	10	5
1:A:233:LEU:HA	1:A:236:ILE:HD12	0.54	1.80	5	2
1:E:307:VAL:HG11	1:E:318:PHE:CE1	0.54	2.38	4	1
1:E:246:LEU:HD23	1:E:246:LEU:O	0.54	2.02	8	1
1:E:252:ARG:HA	1:E:255:LEU:HD12	0.54	1.80	15	1
1:C:228:TYR:O	1:C:232:LEU:HD12	0.54	2.03	3	2
1:E:228:TYR:O	1:E:232:LEU:HD12	0.54	2.03	3	2
1:B:300:GLU:OE2	1:B:398:ILE:HD13	0.54	2.02	10	3
1:C:307:VAL:HG11	1:C:318:PHE:CE1	0.54	2.37	2	2
1:D:294:VAL:O	1:D:298:LEU:HD12	0.53	2.03	15	6
1:D:232:LEU:HD11	1:D:409:ILE:CG2	0.53	2.33	14	2
1:C:220:LEU:HD11	1:C:272:ALA:HB3	0.53	1.81	3	1
1:D:235:VAL:HG22	1:D:260:VAL:HG21	0.53	1.80	13	6
1:B:228:TYR:O	1:B:232:LEU:HD12	0.53	2.03	3	2
1:B:307:VAL:HG11	1:B:318:PHE:CD1	0.53	2.38	4	3
1:B:236:ILE:HD13	1:B:406:ALA:HB1	0.53	1.80	2	7
1:A:301:TYR:OH	1:E:249:ALA:HB1	0.53	2.02	7	4
1:C:233:LEU:HA	1:C:236:ILE:HD12	0.53	1.80	5	2
1:B:235:VAL:HG22	1:B:260:VAL:HG21	0.53	1.80	13	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:234:ILE:HA	1:A:237:LEU:HD12	0.53	1.81	15	2
1:B:233:LEU:HD22	1:C:291:LEU:HD11	0.53	1.80	12	1
1:A:220:LEU:HD22	1:A:273:SER:HB2	0.53	1.80	3	2
1:B:245:ASN:CB	1:B:253:VAL:HG23	0.53	2.34	11	11
1:E:235:VAL:HG22	1:E:260:VAL:HG21	0.53	1.79	13	5
1:A:231:SER:O	1:A:235:VAL:HG23	0.53	2.03	13	7
1:C:235:VAL:HG22	1:C:260:VAL:HG21	0.53	1.80	13	4
1:A:232:LEU:HD11	1:A:409:ILE:HG21	0.53	1.80	7	1
1:A:228:TYR:O	1:A:232:LEU:HD12	0.53	2.03	3	2
1:A:294:VAL:O	1:A:298:LEU:HD12	0.53	2.03	15	6
1:A:417:ILE:O	1:A:421:VAL:HG23	0.53	2.04	3	6
1:D:228:TYR:O	1:D:232:LEU:HD12	0.53	2.03	3	2
1:E:294:VAL:O	1:E:298:LEU:HD12	0.52	2.04	8	6
1:C:233:LEU:HD22	1:D:291:LEU:HD11	0.52	1.80	12	1
1:E:236:ILE:HD13	1:E:406:ALA:HB1	0.52	1.80	4	7
1:A:279:TYR:CZ	1:A:283:ILE:HD11	0.52	2.39	5	1
1:C:220:LEU:HD22	1:C:273:SER:HB2	0.52	1.80	3	2
1:C:232:LEU:HD11	1:C:409:ILE:HG21	0.52	1.81	7	1
1:A:233:LEU:HD22	1:B:291:LEU:HD11	0.52	1.79	12	1
1:B:220:LEU:HD13	1:B:273:SER:HB3	0.52	1.80	9	5
1:D:416:ILE:HD13	1:D:419:LYS:HE2	0.52	1.82	4	2
1:A:246:LEU:HD23	1:A:246:LEU:O	0.52	2.04	11	5
1:D:233:LEU:HD22	1:E:291:LEU:HD11	0.52	1.80	12	1
1:C:307:VAL:HG11	1:C:318:PHE:CD1	0.52	2.38	4	2
1:B:237:LEU:CB	1:C:298:LEU:HD13	0.52	2.33	7	4
1:D:236:ILE:HD13	1:D:406:ALA:HB1	0.52	1.82	2	6
1:B:233:LEU:HD13	1:C:291:LEU:CD2	0.52	2.35	15	2
1:A:235:VAL:HG22	1:A:260:VAL:HG21	0.52	1.80	13	4
1:D:249:ALA:HB1	1:E:301:TYR:OH	0.52	2.05	7	4
1:C:233:LEU:HD13	1:D:291:LEU:CD2	0.52	2.35	15	2
1:A:307:VAL:HG11	1:A:318:PHE:CE1	0.52	2.39	4	1
1:A:302:ALA:HB2	1:E:241:SER:CB	0.52	2.34	4	1
1:B:252:ARG:HA	1:B:255:LEU:HD12	0.52	1.80	15	1
1:D:241:SER:HB3	1:E:302:ALA:HB2	0.52	1.81	2	1
1:C:236:ILE:HD13	1:C:406:ALA:HB1	0.52	1.80	4	6
1:E:235:VAL:HG22	1:E:260:VAL:CG2	0.52	2.35	13	2
1:D:417:ILE:O	1:D:421:VAL:HG23	0.52	2.04	3	7
1:B:294:VAL:O	1:B:298:LEU:HD12	0.52	2.03	15	5
1:B:233:LEU:HA	1:B:236:ILE:HD12	0.52	1.80	5	2
1:B:288:ALA:O	1:B:292:LEU:HD12	0.52	2.04	4	2
1:A:300:GLU:HG3	1:A:398:ILE:HD12	0.52	1.82	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:C:252:ARG:HA	1:C:255:LEU:HD12	0.52	1.80	15	1
1:A:305:ASN:ND2	1:E:244:ILE:HD13	0.52	2.20	15	1
1:E:284:ASP:O	1:E:288:ALA:HB3	0.51	2.05	3	2
1:D:217:GLU:HG3	1:D:277:VAL:HG21	0.51	1.81	6	8
1:C:220:LEU:HD23	1:C:278:SER:CB	0.51	2.35	2	1
1:C:417:ILE:O	1:C:421:VAL:HG23	0.51	2.04	3	7
1:A:416:ILE:HD13	1:A:419:LYS:HE2	0.51	1.82	4	2
1:B:417:ILE:O	1:B:421:VAL:HG23	0.51	2.04	3	6
1:D:235:VAL:HG22	1:D:260:VAL:CG2	0.51	2.35	13	2
1:A:298:LEU:HD21	1:E:252:ARG:NH1	0.51	2.20	8	3
1:A:241:SER:CB	1:B:302:ALA:HB2	0.51	2.35	4	1
1:A:241:SER:HB3	1:B:302:ALA:HB2	0.51	1.81	2	1
1:B:241:SER:HB3	1:C:302:ALA:HB2	0.51	1.82	2	1
1:C:237:LEU:CB	1:D:298:LEU:HD13	0.51	2.35	12	5
1:A:298:LEU:HD13	1:E:237:LEU:CB	0.51	2.34	15	4
1:C:241:SER:CB	1:D:302:ALA:HB2	0.51	2.35	4	1
1:B:235:VAL:HG22	1:B:260:VAL:CG2	0.51	2.35	13	1
1:C:241:SER:HB3	1:D:302:ALA:HB2	0.51	1.83	2	1
1:D:245:ASN:CB	1:D:253:VAL:HG23	0.51	2.36	10	13
1:A:245:ASN:CB	1:A:253:VAL:HG23	0.51	2.36	10	12
1:B:217:GLU:HG3	1:B:277:VAL:HG21	0.51	1.82	6	8
1:B:246:LEU:O	1:B:246:LEU:HD23	0.51	2.06	1	3
1:A:235:VAL:HG22	1:A:260:VAL:CG2	0.51	2.35	13	1
1:B:246:LEU:HD23	1:B:247:ASP:HB3	0.51	1.82	5	1
1:D:234:ILE:HA	1:D:237:LEU:HD12	0.51	1.81	15	1
1:C:222:TYR:HA	1:C:225:ILE:HD12	0.51	1.83	10	9
1:C:405:LEU:HD23	1:C:406:ALA:N	0.51	2.21	3	1
1:E:217:GLU:HG3	1:E:277:VAL:HG21	0.51	1.83	11	7
1:B:416:ILE:HD13	1:B:419:LYS:HE2	0.51	1.82	4	2
1:D:252:ARG:HA	1:D:255:LEU:HD12	0.51	1.83	15	1
1:D:220:LEU:HD13	1:D:273:SER:HB3	0.51	1.83	9	6
1:D:405:LEU:HD23	1:D:406:ALA:N	0.51	2.21	3	1
1:A:217:GLU:HG3	1:A:277:VAL:HG21	0.51	1.83	11	7
1:E:220:LEU:HD13	1:E:273:SER:HB3	0.51	1.83	9	4
1:B:232:LEU:HD21	1:B:409:ILE:HG22	0.51	1.83	7	1
1:A:405:LEU:HD23	1:A:406:ALA:N	0.50	2.21	3	1
1:A:403:PHE:N	1:A:404:PRO:HD2	0.50	2.21	2	15
1:B:224:LEU:HD23	1:B:228:TYR:CE1	0.50	2.42	11	1
1:E:245:ASN:CB	1:E:253:VAL:HG23	0.50	2.36	10	11
1:C:403:PHE:N	1:C:404:PRO:HD2	0.50	2.21	2	15
1:E:239:TRP:CZ3	1:E:401:ILE:HD11	0.50	2.41	6	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Models Total
1:B:244:ILE:HG13	1:B:248:ALA:HB3	0.50	1.83	4	4
1:E:416:ILE:HD13	1:E:419:LYS:HE2	0.50	1.82	2	2
1:C:224:LEU:HD23	1:C:228:TYR:CE1	0.50	2.42	11	1
1:C:232:LEU:HD21	1:C:409:ILE:HG22	0.50	1.83	7	1
1:A:222:TYR:HA	1:A:225:ILE:HD12	0.50	1.83	6	8
1:D:220:LEU:HD22	1:D:273:SER:CB	0.50	2.36	3	2
1:C:279:TYR:CZ	1:C:283:ILE:HD11	0.50	2.42	3	1
1:A:246:LEU:HD21	1:A:304:VAL:HG21	0.50	1.82	8	3
1:D:239:TRP:CZ3	1:D:401:ILE:HD11	0.50	2.42	6	3
1:A:244:ILE:HG13	1:A:248:ALA:HB3	0.50	1.82	2	4
1:B:249:ALA:HB1	1:C:301:TYR:OH	0.50	2.05	7	4
1:A:232:LEU:HD21	1:A:409:ILE:HG22	0.50	1.83	7	1
1:B:222:TYR:HA	1:B:225:ILE:HD12	0.50	1.84	15	9
1:D:233:LEU:HD13	1:E:291:LEU:CD2	0.50	2.36	15	2
1:E:244:ILE:HG13	1:E:248:ALA:HB3	0.50	1.82	2	2
1:C:300:GLU:HG2	1:C:398:ILE:HD12	0.50	1.82	13	1
1:E:246:LEU:O	1:E:246:LEU:HD23	0.50	2.07	5	1
1:A:224:LEU:HD23	1:A:228:TYR:CE1	0.50	2.42	11	1
1:C:245:ASN:CB	1:C:253:VAL:HG23	0.50	2.36	10	10
1:C:244:ILE:HG13	1:C:248:ALA:HB3	0.50	1.82	2	3
1:B:232:LEU:HD11	1:B:409:ILE:HG21	0.50	1.82	7	1
1:A:284:ASP:O	1:A:288:ALA:HB3	0.50	2.07	3	2
1:E:405:LEU:HD23	1:E:406:ALA:N	0.50	2.21	3	1
1:C:220:LEU:HD13	1:C:273:SER:HB3	0.50	1.81	9	6
1:B:220:LEU:HD23	1:B:278:SER:CB	0.50	2.37	2	1
1:E:222:TYR:HA	1:E:225:ILE:HD12	0.50	1.83	6	9
1:C:416:ILE:HD13	1:C:419:LYS:HE2	0.50	1.82	4	2
1:B:284:ASP:O	1:B:288:ALA:HB3	0.50	2.06	3	1
1:D:403:PHE:N	1:D:404:PRO:HD2	0.50	2.21	2	15
1:D:222:TYR:HA	1:D:225:ILE:HD12	0.50	1.83	6	9
1:D:284:ASP:O	1:D:288:ALA:HB3	0.50	2.06	3	1
1:C:284:ASP:O	1:C:288:ALA:HB3	0.50	2.06	3	2
1:B:244:ILE:HG12	1:B:248:ALA:HB3	0.50	1.84	3	5
1:B:403:PHE:N	1:B:404:PRO:HD2	0.50	2.21	2	15
1:A:239:TRP:CZ3	1:A:401:ILE:HD11	0.50	2.41	1	3
1:C:235:VAL:HG22	1:C:260:VAL:CG2	0.50	2.35	13	2
1:A:249:ALA:HB1	1:B:301:TYR:OH	0.50	2.07	7	4
1:C:246:LEU:HD11	1:C:300:GLU:HG3	0.50	1.82	5	1
1:D:224:LEU:HD23	1:D:228:TYR:CE1	0.49	2.42	11	1
1:E:244:ILE:HG12	1:E:248:ALA:HB3	0.49	1.84	3	6
1:C:217:GLU:HG3	1:C:277:VAL:HG21	0.49	1.83	9	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Models Total
1:B:300:GLU:HG3	1:B:398:ILE:HD12	0.49	1.85	13	1
1:A:220:LEU:HD13	1:A:273:SER:HB3	0.49	1.84	9	5
1:A:233:LEU:HD13	1:B:291:LEU:CD2	0.49	2.37	15	2
1:D:220:LEU:HD13	1:D:273:SER:CA	0.49	2.37	5	1
1:D:232:LEU:HD11	1:D:409:ILE:HG21	0.49	1.83	7	1
1:D:220:LEU:HD13	1:D:273:SER:N	0.49	2.22	3	1
1:E:403:PHE:N	1:E:404:PRO:HD2	0.49	2.21	2	15
1:C:220:LEU:HD22	1:C:273:SER:CB	0.49	2.38	3	2
1:E:395:ILE:HD13	1:E:397:LYS:NZ	0.49	2.22	1	1
1:D:244:ILE:HG13	1:D:248:ALA:HB3	0.49	1.83	4	4
1:D:244:ILE:HG12	1:D:248:ALA:HB3	0.49	1.85	3	7
1:B:239:TRP:CZ3	1:B:401:ILE:HD11	0.49	2.42	6	3
1:A:252:ARG:NH1	1:B:298:LEU:HD21	0.49	2.23	8	4
1:D:241:SER:CB	1:E:302:ALA:HB2	0.49	2.37	4	1
1:B:405:LEU:HD23	1:B:406:ALA:N	0.49	2.21	3	1
1:B:252:ARG:NH1	1:C:298:LEU:HD21	0.49	2.22	8	3
1:E:245:ASN:HB2	1:E:253:VAL:HG23	0.49	1.85	2	5
1:A:302:ALA:HB1	1:E:240:ILE:HG22	0.49	1.85	2	1
1:E:224:LEU:HD23	1:E:228:TYR:CE1	0.49	2.42	11	1
1:A:232:LEU:HD22	1:A:410:PHE:HB2	0.49	1.84	3	1
1:E:229:ILE:N	1:E:230:PRO:HD2	0.49	2.23	5	15
1:C:279:TYR:CD2	1:C:283:ILE:HD11	0.49	2.42	4	1
1:E:246:LEU:O	1:E:246:LEU:HD13	0.49	2.07	13	1
1:D:232:LEU:HD21	1:D:409:ILE:HG22	0.49	1.84	7	1
1:C:239:TRP:CZ3	1:C:401:ILE:HD11	0.49	2.42	6	2
1:A:220:LEU:HD23	1:A:278:SER:CB	0.49	2.38	2	1
1:B:416:ILE:HD13	1:B:419:LYS:HE3	0.49	1.85	11	1
1:A:237:LEU:CB	1:B:298:LEU:HD13	0.48	2.37	12	4
1:D:237:LEU:CB	1:E:298:LEU:HD13	0.48	2.38	7	3
1:A:416:ILE:HD13	1:A:419:LYS:HE3	0.48	1.85	11	1
1:B:220:LEU:HD22	1:B:273:SER:CB	0.48	2.38	3	2
1:A:229:ILE:N	1:A:230:PRO:HD2	0.48	2.23	5	15
1:C:299:LEU:O	1:C:303:ALA:HB2	0.48	2.08	10	15
1:A:237:LEU:HD23	1:B:298:LEU:HD13	0.48	1.86	6	1
1:B:232:LEU:HD22	1:B:410:PHE:HB2	0.48	1.85	3	1
1:C:229:ILE:N	1:C:230:PRO:HD2	0.48	2.24	9	15
1:B:229:ILE:N	1:B:230:PRO:HD2	0.48	2.24	13	15
1:D:300:GLU:HG3	1:D:398:ILE:HD12	0.48	1.85	13	1
1:A:252:ARG:HA	1:A:255:LEU:HD12	0.48	1.83	15	1
1:A:220:LEU:HD22	1:A:273:SER:CB	0.48	2.38	3	2
1:D:229:ILE:N	1:D:230:PRO:HD2	0.48	2.23	5	15

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:230:PRO:O	1:A:234:ILE:HD12	0.48	2.09	7	1
1:A:252:ARG:CZ	1:B:298:LEU:HD21	0.48	2.39	2	1
1:C:230:PRO:O	1:C:234:ILE:HD12	0.48	2.08	7	1
1:A:299:LEU:O	1:A:303:ALA:HB2	0.48	2.08	2	14
1:B:299:LEU:O	1:B:303:ALA:HB2	0.48	2.09	2	15
1:B:237:LEU:HD23	1:C:298:LEU:HD13	0.48	1.85	6	1
1:D:252:ARG:NH1	1:E:298:LEU:HD21	0.48	2.24	8	4
1:D:279:TYR:CE1	1:D:283:ILE:HD11	0.48	2.44	5	1
1:D:220:LEU:HD23	1:D:278:SER:CB	0.48	2.38	2	1
1:A:298:LEU:HD11	1:E:237:LEU:O	0.48	2.08	6	2
1:C:252:ARG:NH1	1:D:298:LEU:HD21	0.48	2.24	8	3
1:B:241:SER:CB	1:C:302:ALA:HB2	0.48	2.39	4	1
1:D:230:PRO:O	1:D:234:ILE:HD12	0.48	2.08	7	1
1:E:299:LEU:O	1:E:303:ALA:HB2	0.48	2.09	12	15
1:E:295:PHE:CZ	1:E:299:LEU:HD11	0.48	2.44	15	1
1:E:416:ILE:HD13	1:E:419:LYS:HE3	0.48	1.85	11	1
1:E:232:LEU:HD21	1:E:409:ILE:HG22	0.48	1.85	7	1
1:D:237:LEU:HD23	1:E:298:LEU:HD13	0.48	1.85	6	1
1:C:287:LEU:HD21	1:C:291:LEU:HD13	0.48	1.85	13	1
1:D:245:ASN:HB2	1:D:253:VAL:HG23	0.48	1.85	2	5
1:B:220:LEU:HD13	1:B:273:SER:CA	0.48	2.39	5	1
1:E:232:LEU:HD11	1:E:409:ILE:HG21	0.48	1.85	7	1
1:D:220:LEU:HD12	1:D:273:SER:CB	0.47	2.39	10	1
1:E:220:LEU:HD13	1:E:273:SER:N	0.47	2.24	3	1
1:A:291:LEU:HD11	1:E:233:LEU:HD22	0.47	1.86	12	1
1:A:236:ILE:CD1	1:A:406:ALA:HB1	0.47	2.39	2	6
1:B:300:GLU:CD	1:B:398:ILE:HD13	0.47	2.30	9	1
1:E:300:GLU:HG3	1:E:398:ILE:HD12	0.47	1.87	13	1
1:B:230:PRO:O	1:B:234:ILE:HD12	0.47	2.10	7	1
1:E:232:LEU:HD22	1:E:410:PHE:HB2	0.47	1.86	3	1
1:C:244:ILE:HG12	1:C:248:ALA:HB3	0.47	1.86	11	6
1:C:217:GLU:OE1	1:C:274:LEU:HD22	0.47	2.09	7	2
1:E:279:TYR:CE1	1:E:283:ILE:HD11	0.47	2.44	5	1
1:C:416:ILE:HD13	1:C:419:LYS:HE3	0.47	1.85	11	1
1:A:245:ASN:HB2	1:A:253:VAL:HG23	0.47	1.85	2	8
1:B:237:LEU:O	1:C:298:LEU:HD11	0.47	2.10	6	2
1:C:304:VAL:HG23	1:C:391:ARG:CZ	0.47	2.39	8	1
1:E:300:GLU:CD	1:E:398:ILE:HD13	0.47	2.30	9	1
1:D:295:PHE:CZ	1:D:299:LEU:HD11	0.47	2.44	15	1
1:D:246:LEU:O	1:D:246:LEU:HD13	0.47	2.09	2	1
1:A:237:LEU:O	1:B:298:LEU:HD11	0.47	2.09	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Models Total
1:C:287:LEU:CD2	1:C:291:LEU:HD13	0.47	2.40	13	1
1:C:240:ILE:HG22	1:D:302:ALA:HB1	0.47	1.87	2	1
1:B:246:LEU:HD21	1:B:304:VAL:CG2	0.47	2.39	7	1
1:B:220:LEU:HD13	1:B:273:SER:N	0.47	2.25	3	1
1:D:299:LEU:O	1:D:303:ALA:HB2	0.47	2.10	10	15
1:A:291:LEU:CD2	1:E:233:LEU:HD13	0.47	2.40	15	2
1:B:394:LYS:C	1:B:395:ILE:HD12	0.47	2.30	4	1
1:A:300:GLU:CD	1:A:398:ILE:HD13	0.47	2.30	9	1
1:D:246:LEU:HD23	1:D:247:ASP:N	0.47	2.24	5	1
1:C:220:LEU:HD13	1:C:273:SER:CA	0.47	2.40	5	1
1:B:234:ILE:HD11	1:C:291:LEU:CD2	0.47	2.39	7	1
1:E:220:LEU:HD22	1:E:273:SER:CB	0.47	2.40	3	2
1:A:244:ILE:HG12	1:A:248:ALA:HB3	0.47	1.85	3	7
1:B:245:ASN:HB2	1:B:253:VAL:HG23	0.47	1.86	4	6
1:E:220:LEU:HD12	1:E:273:SER:CB	0.47	2.39	10	1
1:B:295:PHE:CZ	1:B:299:LEU:HD11	0.47	2.44	15	1
1:A:295:PHE:CZ	1:A:299:LEU:HD11	0.47	2.45	15	1
1:A:298:LEU:HD21	1:E:252:ARG:CZ	0.47	2.40	2	1
1:E:220:LEU:HD23	1:E:278:SER:CB	0.47	2.40	2	1
1:D:252:ARG:CZ	1:E:298:LEU:HD21	0.47	2.38	2	1
1:B:217:GLU:OE1	1:B:274:LEU:HD22	0.47	2.09	7	1
1:C:245:ASN:HB2	1:C:253:VAL:HG23	0.47	1.86	4	6
1:E:220:LEU:HD13	1:E:273:SER:CA	0.47	2.39	5	1
1:A:220:LEU:HD13	1:A:273:SER:N	0.46	2.25	3	1
1:D:237:LEU:O	1:E:298:LEU:HD11	0.46	2.11	6	2
1:B:279:TYR:CE1	1:B:283:ILE:HD11	0.46	2.44	5	1
1:C:215:MET:C	1:C:216:LEU:HD22	0.46	2.30	14	1
1:B:237:LEU:HB3	1:C:298:LEU:HD22	0.46	1.86	10	1
1:B:242:PHE:CE1	1:B:253:VAL:HG22	0.46	2.45	11	1
1:C:232:LEU:HD22	1:C:410:PHE:HB2	0.46	1.86	3	1
1:D:215:MET:C	1:D:216:LEU:HD22	0.46	2.31	4	1
1:D:416:ILE:HD13	1:D:419:LYS:HE3	0.46	1.85	11	1
1:D:232:LEU:HD22	1:D:410:PHE:HB2	0.46	1.86	3	1
1:D:300:GLU:CD	1:D:398:ILE:HD13	0.46	2.31	9	1
1:C:220:LEU:HD13	1:C:273:SER:N	0.46	2.26	3	1
1:A:302:ALA:HB2	1:E:241:SER:OG	0.46	2.10	4	1
1:E:236:ILE:CD1	1:E:406:ALA:HB1	0.46	2.41	4	4
1:C:287:LEU:HD13	1:C:291:LEU:HD22	0.46	1.87	13	1
1:B:236:ILE:CD1	1:B:406:ALA:HB1	0.46	2.40	2	6
1:A:220:LEU:HD13	1:A:273:SER:CA	0.46	2.40	5	1
1:B:240:ILE:HG22	1:C:302:ALA:HB1	0.46	1.88	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:237:LEU:O	1:D:298:LEU:HD11	0.46	2.11	10	2
1:A:233:LEU:HD21	1:A:410:PHE:CZ	0.45	2.46	4	1
1:C:246:LEU:HD23	1:C:246:LEU:O	0.45	2.11	14	1
1:B:403:PHE:CB	1:B:404:PRO:CD	0.45	2.94	4	14
1:A:298:LEU:HD13	1:E:237:LEU:HD23	0.45	1.89	6	1
1:D:236:ILE:CD1	1:D:406:ALA:HB1	0.45	2.41	4	5
1:D:244:ILE:HD12	1:E:305:ASN:HB2	0.45	1.87	6	2
1:C:236:ILE:CD1	1:C:406:ALA:HB1	0.45	2.40	4	7
1:C:220:LEU:HD12	1:C:273:SER:CB	0.45	2.41	10	1
1:A:220:LEU:HD12	1:A:273:SER:CB	0.45	2.42	10	1
1:C:233:LEU:HD21	1:C:410:PHE:CZ	0.45	2.47	4	1
1:B:252:ARG:CZ	1:C:298:LEU:HD21	0.45	2.41	2	1
1:C:403:PHE:CB	1:C:404:PRO:CD	0.45	2.95	6	14
1:C:252:ARG:CZ	1:D:298:LEU:HD21	0.45	2.42	2	1
1:D:403:PHE:CB	1:D:404:PRO:CD	0.45	2.95	7	14
1:A:403:PHE:CB	1:A:404:PRO:CD	0.45	2.95	7	14
1:E:403:PHE:CB	1:E:404:PRO:CD	0.45	2.95	6	14
1:C:237:LEU:HB3	1:D:298:LEU:HD22	0.44	1.89	10	1
1:A:237:LEU:HB3	1:B:298:LEU:HD22	0.44	1.89	10	1
1:E:233:LEU:HD21	1:E:410:PHE:CZ	0.44	2.47	4	1
1:C:285:ILE:O	1:C:289:VAL:HG12	0.44	2.12	14	1
1:C:237:LEU:HD23	1:D:298:LEU:HD13	0.44	1.87	6	1
1:B:233:LEU:HD21	1:B:410:PHE:CZ	0.44	2.48	4	1
1:C:300:GLU:CD	1:C:398:ILE:HD13	0.44	2.32	9	1
1:E:220:LEU:HD13	1:E:273:SER:HB2	0.44	1.88	11	1
1:D:412:LEU:O	1:D:412:LEU:HD12	0.44	2.13	3	1
1:E:217:GLU:CG	1:E:274:LEU:HD22	0.44	2.43	9	1
1:E:412:LEU:HD12	1:E:412:LEU:O	0.44	2.13	3	1
1:B:286:TRP:HA	1:B:289:VAL:HG12	0.44	1.90	6	2
1:D:395:ILE:HD12	1:D:397:LYS:CG	0.44	2.43	10	1
1:B:220:LEU:HD12	1:B:273:SER:CB	0.44	2.42	10	1
1:C:244:ILE:HD12	1:D:305:ASN:OD1	0.44	2.12	9	1
1:C:244:ILE:HD13	1:D:304:VAL:HB	0.44	1.89	7	1
1:A:412:LEU:HD12	1:A:412:LEU:O	0.44	2.12	3	1
1:B:220:LEU:HD13	1:B:273:SER:HB2	0.44	1.90	11	1
1:B:412:LEU:HD12	1:B:412:LEU:O	0.44	2.13	3	1
1:E:286:TRP:HA	1:E:289:VAL:HG12	0.44	1.90	6	1
1:B:300:GLU:CD	1:B:398:ILE:HD12	0.44	2.33	15	1
1:E:216:LEU:HD11	1:E:273:SER:OG	0.44	2.13	11	1
1:C:412:LEU:HD12	1:C:412:LEU:O	0.44	2.13	3	1
1:A:246:LEU:O	1:A:246:LEU:HD12	0.44	2.13	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:C:286:TRP:HA	1:C:289:VAL:HG12	0.43	1.89	6	2
1:C:299:LEU:O	1:C:299:LEU:HD23	0.43	2.13	5	1
1:C:236:ILE:HG23	1:C:406:ALA:CB	0.43	2.43	6	1
1:E:300:GLU:CD	1:E:398:ILE:HD12	0.43	2.33	15	1
1:C:225:ILE:HG12	1:C:417:ILE:HD12	0.43	1.90	7	1
1:A:287:LEU:HD23	1:A:287:LEU:O	0.43	2.14	10	1
1:B:236:ILE:HG23	1:B:406:ALA:CB	0.43	2.44	6	1
1:A:286:TRP:HA	1:A:289:VAL:HG12	0.43	1.90	6	1
1:D:217:GLU:CG	1:D:274:LEU:HD22	0.43	2.44	9	1
1:D:229:ILE:HG22	1:D:230:PRO:N	0.43	2.29	15	11
1:E:244:ILE:O	1:E:246:LEU:HD23	0.43	2.13	15	1
1:D:300:GLU:CD	1:D:398:ILE:HD12	0.43	2.34	15	1
1:D:246:LEU:HD12	1:D:246:LEU:O	0.43	2.14	11	1
1:D:244:ILE:HD13	1:E:304:VAL:HB	0.43	1.91	7	1
1:C:229:ILE:HG22	1:C:230:PRO:N	0.43	2.29	15	8
1:D:237:LEU:HB3	1:E:298:LEU:HD22	0.43	1.91	10	1
1:C:241:SER:OG	1:D:302:ALA:HB2	0.43	2.13	4	1
1:D:233:LEU:HD21	1:D:410:PHE:CZ	0.43	2.49	4	1
1:A:287:LEU:O	1:A:287:LEU:HD23	0.43	2.14	12	1
1:B:287:LEU:O	1:B:287:LEU:HD23	0.43	2.14	10	2
1:D:236:ILE:HG23	1:D:406:ALA:CB	0.43	2.44	6	1
1:A:300:GLU:CD	1:A:398:ILE:HD12	0.43	2.34	15	1
1:E:236:ILE:HG23	1:E:406:ALA:CB	0.43	2.43	6	1
1:B:287:LEU:HD12	1:B:287:LEU:O	0.43	2.14	5	1
1:D:220:LEU:CD1	1:D:272:ALA:HB3	0.42	2.44	3	1
1:E:229:ILE:HG22	1:E:230:PRO:N	0.42	2.30	5	13
1:B:229:ILE:HG22	1:B:230:PRO:N	0.42	2.29	5	14
1:C:220:LEU:HD22	1:C:273:SER:OG	0.42	2.14	5	1
1:A:229:ILE:HG22	1:A:230:PRO:N	0.42	2.29	3	14
1:E:287:LEU:O	1:E:287:LEU:HD23	0.42	2.14	10	1
1:D:220:LEU:HD22	1:D:273:SER:OG	0.42	2.14	5	1
1:A:287:LEU:O	1:A:287:LEU:HD12	0.42	2.13	5	1
1:E:215:MET:N	1:E:274:LEU:HD22	0.42	2.29	14	1
1:A:236:ILE:HG23	1:A:406:ALA:CB	0.42	2.45	6	1
1:A:227:LEU:HD23	1:A:227:LEU:O	0.42	2.14	10	1
1:D:287:LEU:HD12	1:D:287:LEU:O	0.42	2.14	5	1
1:A:246:LEU:HD11	1:A:304:VAL:HG21	0.42	1.91	12	1
1:E:287:LEU:HD23	1:E:287:LEU:O	0.42	2.14	12	2
1:D:287:LEU:O	1:D:287:LEU:HD23	0.42	2.14	10	2
1:C:244:ILE:HD12	1:D:305:ASN:HB2	0.42	1.90	6	1
1:C:246:LEU:HD11	1:C:300:GLU:CG	0.42	2.43	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:E:220:LEU:HD22	1:E:273:SER:OG	0.42	2.15	5	1
1:E:287:LEU:O	1:E:287:LEU:HD12	0.42	2.14	5	1
1:D:286:TRP:HA	1:D:289:VAL:HG12	0.42	1.90	6	1
1:C:227:LEU:HD23	1:C:227:LEU:O	0.42	2.14	10	1
1:E:227:LEU:HD23	1:E:227:LEU:O	0.42	2.14	10	1
1:B:244:ILE:HD13	1:C:304:VAL:HB	0.42	1.91	7	1
1:D:227:LEU:O	1:D:227:LEU:HD23	0.42	2.14	10	1
1:A:236:ILE:CG1	1:A:406:ALA:HB1	0.42	2.44	11	2
1:E:285:ILE:O	1:E:289:VAL:HG13	0.42	2.15	10	1
1:A:241:SER:OG	1:B:302:ALA:HB2	0.42	2.15	4	1
1:E:398:ILE:HD12	1:E:401:ILE:HD11	0.42	1.92	4	1
1:B:246:LEU:O	1:B:246:LEU:HD13	0.41	2.15	12	1
1:A:398:ILE:HD12	1:A:401:ILE:HD11	0.41	1.92	4	1
1:B:394:LYS:O	1:B:395:ILE:HD12	0.41	2.15	4	1
1:A:279:TYR:CE1	1:A:283:ILE:HD11	0.41	2.49	5	1
1:C:239:TRP:HH2	1:C:401:ILE:HD11	0.41	1.74	15	1
1:C:246:LEU:HD12	1:C:246:LEU:O	0.41	2.14	11	2
1:B:216:LEU:HD11	1:B:273:SER:OG	0.41	2.15	11	1
1:E:304:VAL:O	1:E:307:VAL:HG23	0.41	2.16	3	2
1:E:246:LEU:HD21	1:E:304:VAL:CG2	0.41	2.46	2	1
1:B:227:LEU:O	1:B:227:LEU:HD23	0.41	2.14	10	1
1:C:398:ILE:HD12	1:C:401:ILE:HD11	0.41	1.92	4	1
1:B:220:LEU:HD22	1:B:273:SER:OG	0.41	2.15	5	1
1:E:310:GLN:NE2	1:E:315:GLY:H	0.41	2.14	7	1
1:E:225:ILE:HG12	1:E:417:ILE:HD12	0.41	1.92	7	1
1:C:304:VAL:O	1:C:307:VAL:HG23	0.41	2.16	3	1
1:E:229:ILE:CB	1:E:230:PRO:CD	0.41	2.99	15	10
1:A:237:LEU:CD2	1:B:298:LEU:HD22	0.41	2.46	6	1
1:D:229:ILE:CB	1:D:230:PRO:CD	0.41	2.99	2	8
1:B:218:ARG:NE	1:B:277:VAL:HG11	0.41	2.30	8	1
1:C:288:ALA:O	1:C:292:LEU:HD12	0.41	2.15	3	1
1:D:220:LEU:HD12	1:D:273:SER:HB3	0.41	1.91	10	1
1:E:220:LEU:HD12	1:E:273:SER:HB3	0.41	1.91	10	1
1:D:241:SER:OG	1:E:302:ALA:HB2	0.41	2.16	4	1
1:C:300:GLU:CD	1:C:398:ILE:HD12	0.41	2.37	15	1
1:D:240:ILE:HG22	1:E:302:ALA:HB1	0.41	1.92	2	1
1:C:403:PHE:N	1:C:404:PRO:CD	0.41	2.84	2	1
1:E:403:PHE:N	1:E:404:PRO:CD	0.41	2.84	2	1
1:A:225:ILE:HG12	1:A:417:ILE:HD12	0.41	1.92	7	1
1:A:220:LEU:CD1	1:A:272:ALA:HB3	0.41	2.44	3	1
1:B:220:LEU:CD1	1:B:272:ALA:HB3	0.41	2.44	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:C:229:ILE:CB	1:C:230:PRO:CD	0.41	2.99	6	7
1:A:220:LEU:HD22	1:A:273:SER:OG	0.41	2.16	5	1
1:D:240:ILE:HD13	1:D:243:TRP:CZ2	0.40	2.51	12	1
1:E:395:ILE:HD13	1:E:397:LYS:CE	0.40	2.46	1	1
1:D:217:GLU:CG	1:D:277:VAL:HG21	0.40	2.46	8	1
1:E:239:TRP:HH2	1:E:401:ILE:HD11	0.40	1.75	15	2
1:B:236:ILE:CG1	1:B:406:ALA:HB1	0.40	2.46	11	2
1:C:236:ILE:CG1	1:C:406:ALA:HB1	0.40	2.46	11	1
1:A:304:VAL:HB	1:E:244:ILE:HD13	0.40	1.92	7	1
1:B:304:VAL:O	1:B:307:VAL:HG23	0.40	2.16	3	1
1:C:217:GLU:CG	1:C:277:VAL:HG21	0.40	2.46	6	1
1:B:237:LEU:CD2	1:C:298:LEU:HD22	0.40	2.46	6	1
1:B:229:ILE:CB	1:B:230:PRO:CD	0.40	2.99	1	3
1:C:220:LEU:HD12	1:C:273:SER:HB3	0.40	1.94	10	1
1:A:229:ILE:CB	1:A:230:PRO:CD	0.40	2.99	1	3
1:A:240:ILE:HG22	1:B:302:ALA:HB1	0.40	1.94	2	1
1:A:246:LEU:HD11	1:A:300:GLU:CD	0.40	2.37	7	1
1:A:305:ASN:HB2	1:E:244:ILE:HD12	0.40	1.93	6	1
1:A:298:LEU:HD22	1:E:237:LEU:HB3	0.40	1.92	10	1
1:D:304:VAL:O	1:D:307:VAL:HG23	0.40	2.16	1	1
1:B:241:SER:OG	1:C:302:ALA:HB2	0.40	2.16	4	1
1:C:304:VAL:HG23	1:C:391:ARG:NH1	0.40	2.30	8	1
1:A:244:ILE:HD12	1:B:305:ASN:HB2	0.40	1.94	15	1
1:C:246:LEU:O	1:C:246:LEU:HD12	0.40	2.16	2	1
1:A:403:PHE:N	1:A:404:PRO:CD	0.40	2.84	2	1
1:B:403:PHE:N	1:B:404:PRO:CD	0.40	2.84	2	1
1:B:216:LEU:HD13	1:B:219:GLN:HE21	0.40	1.76	13	1
1:D:236:ILE:CG1	1:D:406:ALA:HB1	0.40	2.47	11	1
1:A:318:PHE:HD2	1:A:389:ILE:HG23	0.40	1.77	13	1
1:D:310:GLN:NE2	1:D:315:GLY:H	0.40	2.13	7	1

6.3 Torsion angles (i)

6.3.1 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 NMR 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	138/150 (92%)	129±1 (93±1%)	7±1 (5±1%)	2±1 (1±1%)	19	64
1	B	138/150 (92%)	129±1 (93±1%)	7±2 (5±1%)	2±1 (1±1%)	18	63
1	C	138/150 (92%)	129±1 (93±1%)	7±2 (5±1%)	2±1 (1±1%)	20	66
1	D	138/150 (92%)	129±1 (93±1%)	7±1 (5±1%)	2±1 (1±1%)	19	64
1	E	138/150 (92%)	129±1 (93±1%)	7±2 (5±1%)	2±1 (1±1%)	19	64
All	All	10350/11250 (92%)	9653 (93%)	553 (5%)	144 (1%)	19	64

All 44 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	C	288	ALA	15
1	D	288	ALA	15
1	A	288	ALA	15
1	B	288	ALA	15
1	E	288	ALA	15
1	A	312	GLU	4
1	A	247	ASP	4
1	C	312	GLU	4
1	D	312	GLU	4
1	E	247	ASP	4
1	D	247	ASP	4
1	E	312	GLU	4
1	B	312	GLU	4
1	B	247	ASP	4
1	C	247	ASP	3
1	B	394	LYS	2
1	C	398	ILE	1
1	D	394	LYS	1
1	D	314	GLY	1
1	B	289	VAL	1
1	C	289	VAL	1
1	E	314	GLY	1
1	B	396	ASP	1
1	D	396	ASP	1
1	E	396	ASP	1
1	E	290	CYS	1
1	B	398	ILE	1
1	A	289	VAL	1
1	B	314	GLY	1
1	E	394	LYS	1

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Mol	Chain	Res	Type	Models (Total)
1	A	396	ASP	1
1	B	290	CYS	1
1	C	290	CYS	1
1	C	314	GLY	1
1	A	314	GLY	1
1	A	290	CYS	1
1	D	289	VAL	1
1	D	290	CYS	1
1	E	289	VAL	1
1	B	395	ILE	1
1	E	398	ILE	1
1	D	398	ILE	1
1	A	398	ILE	1
1	C	396	ASP	1

6.3.2 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 NMR 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	118/130 (91%)	87±5 (74±4%)	31±5 (26±4%)	3	23
1	B	118/130 (91%)	86±4 (72±4%)	32±4 (28±4%)	2	21
1	C	119/130 (92%)	88±5 (74±4%)	31±5 (26±4%)	3	24
1	D	119/130 (92%)	87±4 (73±4%)	32±4 (27±4%)	2	22
1	E	119/130 (92%)	85±3 (72±3%)	34±3 (28±3%)	2	20
All	All	8895/9750 (91%)	6487 (73%)	2408 (27%)	2	22

All 435 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	239	TRP	15
1	C	239	TRP	15
1	D	239	TRP	15
1	B	239	TRP	15
1	E	239	TRP	15
1	A	247	ASP	14

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Mol	Chain	Res	Type	Models (Total)
1	B	247	ASP	14
1	E	218	ARG	14
1	D	300	GLU	13
1	E	300	GLU	13
1	B	300	GLU	13
1	E	420	ILE	13
1	D	312	GLU	13
1	A	300	GLU	13
1	A	413	PHE	12
1	A	218	ARG	12
1	B	413	PHE	12
1	E	405	LEU	12
1	E	296	SER	12
1	D	413	PHE	12
1	D	405	LEU	12
1	C	296	SER	12
1	E	413	PHE	12
1	A	405	LEU	12
1	C	405	LEU	12
1	D	420	ILE	12
1	B	296	SER	12
1	C	266	GLN	12
1	E	266	GLN	12
1	B	266	GLN	12
1	C	423	ARG	12
1	D	266	GLN	12
1	A	420	ILE	12
1	D	296	SER	12
1	A	296	SER	12
1	C	311	ARG	12
1	A	266	GLN	12
1	D	218	ARG	12
1	B	420	ILE	12
1	C	413	PHE	12
1	B	405	LEU	12
1	C	420	ILE	12
1	B	279	TYR	11
1	D	238	SER	11
1	A	301	TYR	11
1	E	301	TYR	11
1	C	238	SER	11
1	A	279	TYR	11

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Mol	Chain	Res	Type	Models (Total)
1	D	301	TYR	11
1	B	238	SER	11
1	B	422	ARG	11
1	D	397	LYS	11
1	B	311	ARG	11
1	E	238	SER	11
1	E	252	ARG	11
1	D	423	ARG	11
1	C	301	TYR	11
1	B	252	ARG	11
1	B	301	TYR	11
1	A	238	SER	11
1	D	252	ARG	10
1	E	308	SER	10
1	E	247	ASP	10
1	E	287	LEU	10
1	D	279	TYR	10
1	E	224	LEU	10
1	E	279	TYR	10
1	A	287	LEU	10
1	E	397	LYS	10
1	B	218	ARG	10
1	E	423	ARG	10
1	E	281	LYS	10
1	B	306	PHE	10
1	A	224	LEU	10
1	C	218	ARG	10
1	E	306	PHE	10
1	A	281	LYS	10
1	B	287	LEU	10
1	D	224	LEU	10
1	C	224	LEU	10
1	C	276	LYS	10
1	D	287	LEU	10
1	D	281	LYS	10
1	B	281	LYS	10
1	A	252	ARG	10
1	B	224	LEU	10
1	C	411	ASN	9
1	E	391	ARG	9
1	D	276	LYS	9
1	E	396	ASP	9

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Mol	Chain	Res	Type	Models (Total)
1	D	393	LYS	9
1	C	391	ARG	9
1	A	305	ASN	9
1	B	274	LEU	9
1	A	306	PHE	9
1	A	411	ASN	9
1	E	215	MET	9
1	C	252	ARG	9
1	D	391	ARG	9
1	D	411	ASN	9
1	D	305	ASN	9
1	E	246	LEU	9
1	E	305	ASN	9
1	A	422	ARG	9
1	A	391	ARG	9
1	C	396	ASP	9
1	B	396	ASP	9
1	E	411	ASN	9
1	B	411	ASN	9
1	E	393	LYS	8
1	E	312	GLU	8
1	E	243	TRP	8
1	E	216	LEU	8
1	D	308	SER	8
1	A	396	ASP	8
1	C	243	TRP	8
1	A	407	PHE	8
1	A	216	LEU	8
1	C	281	LYS	8
1	B	407	PHE	8
1	C	407	PHE	8
1	B	305	ASN	8
1	D	274	LEU	8
1	D	215	MET	8
1	A	274	LEU	8
1	A	423	ARG	8
1	C	274	LEU	8
1	D	407	PHE	8
1	B	308	SER	8
1	B	393	LYS	8
1	E	407	PHE	8
1	C	287	LEU	7

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Mol	Chain	Res	Type	Models (Total)
1	E	284	ASP	7
1	B	312	GLU	7
1	C	306	PHE	7
1	D	284	ASP	7
1	A	284	ASP	7
1	B	284	ASP	7
1	D	247	ASP	7
1	C	220	LEU	7
1	A	243	TRP	7
1	A	393	LYS	7
1	C	397	LYS	7
1	B	391	ARG	7
1	D	220	LEU	7
1	C	300	GLU	7
1	D	306	PHE	7
1	B	261	LEU	7
1	A	419	LYS	7
1	A	220	LEU	7
1	B	220	LEU	7
1	C	215	MET	7
1	C	308	SER	7
1	D	396	ASP	7
1	A	261	LEU	7
1	C	419	LYS	7
1	E	274	LEU	7
1	C	261	LEU	7
1	B	419	LYS	7
1	C	305	ASN	7
1	E	261	LEU	7
1	E	419	LYS	7
1	B	216	LEU	7
1	D	419	LYS	7
1	B	397	LYS	7
1	D	261	LEU	7
1	E	220	LEU	7
1	B	276	LYS	7
1	A	226	GLN	6
1	B	246	LEU	6
1	C	313	PHE	6
1	D	415	TRP	6
1	B	313	PHE	6
1	D	226	GLN	6

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Mol	Chain	Res	Type	Models (Total)
1	D	422	ARG	6
1	B	243	TRP	6
1	C	415	TRP	6
1	A	276	LYS	6
1	A	311	ARG	6
1	E	226	GLN	6
1	B	415	TRP	6
1	C	226	GLN	6
1	B	394	LYS	6
1	B	226	GLN	6
1	E	422	ARG	6
1	E	311	ARG	6
1	E	415	TRP	6
1	A	415	TRP	6
1	C	393	LYS	6
1	A	312	GLU	5
1	C	390	GLN	5
1	C	299	LEU	5
1	D	228	TYR	5
1	C	228	TYR	5
1	C	389	ILE	5
1	A	228	TYR	5
1	C	247	ASP	5
1	B	389	ILE	5
1	A	246	LEU	5
1	E	267	SER	5
1	C	267	SER	5
1	D	216	LEU	5
1	A	229	ILE	5
1	E	310	GLN	5
1	E	228	TYR	5
1	B	299	LEU	5
1	E	276	LYS	5
1	B	229	ILE	5
1	D	229	ILE	5
1	A	267	SER	5
1	D	299	LEU	5
1	A	299	LEU	5
1	B	228	TYR	5
1	B	309	ARG	5
1	D	267	SER	5
1	E	299	LEU	5

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Mol	Chain	Res	Type	Models (Total)
1	B	267	SER	5
1	C	422	ARG	5
1	D	243	TRP	5
1	C	394	LYS	5
1	E	229	ILE	5
1	C	229	ILE	5
1	A	403	PHE	4
1	A	310	GLN	4
1	D	271	ARG	4
1	A	400	ARG	4
1	C	279	TYR	4
1	D	410	PHE	4
1	C	403	PHE	4
1	D	246	LEU	4
1	E	400	ARG	4
1	E	231	SER	4
1	C	255	LEU	4
1	B	231	SER	4
1	C	231	SER	4
1	E	410	PHE	4
1	C	216	LEU	4
1	B	400	ARG	4
1	D	400	ARG	4
1	D	255	LEU	4
1	B	410	PHE	4
1	C	285	ILE	4
1	A	231	SER	4
1	A	410	PHE	4
1	E	255	LEU	4
1	C	284	ASP	4
1	A	397	LYS	4
1	D	313	PHE	4
1	B	255	LEU	4
1	D	311	ARG	4
1	B	403	PHE	4
1	C	410	PHE	4
1	C	310	GLN	4
1	D	310	GLN	4
1	E	394	LYS	4
1	D	403	PHE	4
1	A	255	LEU	4
1	C	246	LEU	4

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Mol	Chain	Res	Type	Models (Total)
1	D	231	SER	4
1	C	400	ARG	4
1	E	403	PHE	4
1	D	389	ILE	3
1	A	241	SER	3
1	A	271	ARG	3
1	B	398	ILE	3
1	D	399	SER	3
1	C	312	GLU	3
1	E	395	ILE	3
1	C	309	ARG	3
1	A	399	SER	3
1	E	217	GLU	3
1	A	408	LEU	3
1	E	285	ILE	3
1	C	271	ARG	3
1	C	399	SER	3
1	B	285	ILE	3
1	D	408	LEU	3
1	A	390	GLN	3
1	E	318	PHE	3
1	B	399	SER	3
1	D	318	PHE	3
1	A	318	PHE	3
1	E	309	ARG	3
1	D	273	SER	3
1	A	285	ILE	3
1	B	273	SER	3
1	B	240	ILE	3
1	D	390	GLN	3
1	A	240	ILE	3
1	E	399	SER	3
1	B	408	LEU	3
1	C	408	LEU	3
1	E	241	SER	3
1	B	310	GLN	3
1	D	398	ILE	3
1	A	217	GLU	3
1	A	309	ARG	3
1	D	241	SER	3
1	E	240	ILE	3
1	A	398	ILE	3

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Mol	Chain	Res	Type	Models (Total)
1	D	285	ILE	3
1	E	271	ARG	3
1	A	308	SER	3
1	C	241	SER	3
1	A	273	SER	3
1	D	240	ILE	3
1	B	423	ARG	3
1	C	398	ILE	3
1	E	398	ILE	3
1	B	241	SER	3
1	C	240	ILE	3
1	E	408	LEU	3
1	E	273	SER	3
1	C	273	SER	3
1	C	217	GLU	3
1	D	395	ILE	2
1	D	394	LYS	2
1	A	418	TYR	2
1	B	295	PHE	2
1	E	268	SER	2
1	A	394	LYS	2
1	B	271	ARG	2
1	C	395	ILE	2
1	B	318	PHE	2
1	D	242	PHE	2
1	A	295	PHE	2
1	C	418	TYR	2
1	E	292	LEU	2
1	E	389	ILE	2
1	E	242	PHE	2
1	A	264	THR	2
1	D	264	THR	2
1	B	418	TYR	2
1	B	292	LEU	2
1	E	418	TYR	2
1	E	295	PHE	2
1	B	395	ILE	2
1	C	277	VAL	2
1	A	222	TYR	2
1	C	268	SER	2
1	C	264	THR	2
1	E	222	TYR	2

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Mol	Chain	Res	Type	Models (Total)
1	C	291	LEU	2
1	C	222	TYR	2
1	B	268	SER	2
1	D	222	TYR	2
1	B	242	PHE	2
1	D	418	TYR	2
1	E	234	ILE	2
1	A	242	PHE	2
1	A	292	LEU	2
1	E	313	PHE	2
1	A	395	ILE	2
1	C	295	PHE	2
1	D	295	PHE	2
1	B	264	THR	2
1	E	264	THR	2
1	A	389	ILE	2
1	A	268	SER	2
1	B	222	TYR	2
1	D	268	SER	2
1	D	292	LEU	2
1	C	242	PHE	2
1	D	223	TYR	1
1	A	298	LEU	1
1	C	223	TYR	1
1	B	270	SER	1
1	D	234	ILE	1
1	E	289	VAL	1
1	C	244	ILE	1
1	A	223	TYR	1
1	D	277	VAL	1
1	E	293	PHE	1
1	E	237	LEU	1
1	D	309	ARG	1
1	E	223	TYR	1
1	D	289	VAL	1
1	C	318	PHE	1
1	E	233	LEU	1
1	B	293	PHE	1
1	B	237	LEU	1
1	C	233	LEU	1
1	C	237	LEU	1
1	C	234	ILE	1

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Mol	Chain	Res	Type	Models (Total)
1	E	286	TRP	1
1	B	277	VAL	1
1	D	298	LEU	1
1	B	286	TRP	1
1	C	270	SER	1
1	C	286	TRP	1
1	B	223	TYR	1
1	D	217	GLU	1
1	E	227	LEU	1
1	B	414	TYR	1
1	E	219	GLN	1
1	C	414	TYR	1
1	C	292	LEU	1
1	D	414	TYR	1
1	A	286	TRP	1
1	A	289	VAL	1
1	A	227	LEU	1
1	A	414	TYR	1
1	D	270	SER	1
1	C	298	LEU	1
1	E	270	SER	1
1	D	286	TRP	1
1	B	244	ILE	1
1	E	390	GLN	1
1	E	244	ILE	1
1	C	278	SER	1
1	A	293	PHE	1
1	A	313	PHE	1
1	B	298	LEU	1
1	D	227	LEU	1
1	A	237	LEU	1
1	C	293	PHE	1
1	C	227	LEU	1
1	D	237	LEU	1
1	B	233	LEU	1
1	A	234	ILE	1
1	A	270	SER	1
1	A	233	LEU	1
1	D	244	ILE	1
1	E	414	TYR	1
1	C	294	VAL	1
1	B	217	GLU	1

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Mol	Chain	Res	Type	Models (Total)
1	E	298	LEU	1
1	A	277	VAL	1
1	D	293	PHE	1
1	C	219	GLN	1
1	B	289	VAL	1
1	B	227	LEU	1
1	B	234	ILE	1
1	D	233	LEU	1
1	E	277	VAL	1

6.3.3   RNA (i)

There are no RNA molecules in this entry.

6.4   Non-standard residues in protein, DNA, RNA chains (i)

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

6.5   Carbohydrates (i)

There are no carbohydrates in this entry.

6.6   Ligand geometry (i)

There are no ligands in this entry.

6.7   Other polymers (i)

There are no such molecules in this entry.

6.8   Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation ⓘ

The completeness of assignment taking into account all chemical shift lists is 10% for the well-defined parts and 10% for the entire structure.

7.1 Chemical shift list 1

File name: 2m6i_cs.str

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping ⓘ

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1145
Number of shifts mapped to atoms	1145
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	133	-0.30 ± 0.20	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	112	0.28 ± 0.07	None needed (< 0.5 ppm)
$^{13}C'$	18	-0.15 ± 0.46	None needed (< 0.5 ppm)
^{15}N	146	0.96 ± 0.18	Should be applied

7.1.3 Completeness of resonance assignments ⓘ

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 10%, i.e. 932 atoms were assigned a chemical shift out of a possible 8989. 0 out of 150 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	516/3425 (15%)	244/1366 (18%)	138/1386 (10%)	134/673 (20%)
Sidechain	399/4594 (9%)	269/2680 (10%)	121/1709 (7%)	9/205 (4%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	17/970 (2%)	17/510 (3%)	0/440 (0%)	0/20 (0%)
Overall	932/8989 (10%)	530/4556 (12%)	259/3535 (7%)	143/898 (16%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 10%, i.e. 991 atoms were assigned a chemical shift out of a possible 9775. 0 out of 150 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	558/3710 (15%)	261/1480 (18%)	151/1500 (10%)	146/730 (20%)
Sidechain	416/4840 (9%)	275/2830 (10%)	132/1805 (7%)	9/205 (4%)
Aromatic	17/1225 (1%)	17/655 (3%)	0/520 (0%)	0/50 (0%)
Overall	991/9775 (10%)	553/4965 (11%)	283/3825 (7%)	155/985 (16%)

7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots (i)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A: