Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	2KZT
Title	:	Structure of the Tandem MA-3 Region of Pdcd4
Authors	:	Waters, L.C.; Strong, S.L.; Oka, O.; Muskett, F.W.; Veverka, V.; Banerjee, S.; Schmedt, T.; Henry, A.J.; Klempnauer, K.H.; Carr, M.D.
Deposited on	:	2010-06-24

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
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

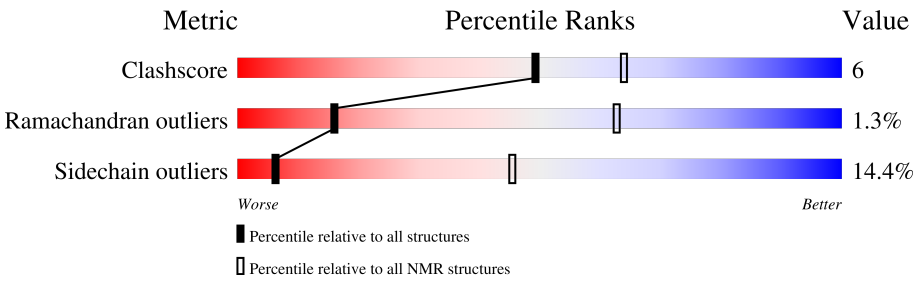
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment was not calculated.

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)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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	163	76% 16% 8%
2	B	131	76% 15% 8%

2 Ensemble composition and analysis (i)

This entry contains 73 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest haddock score*.

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:156-A:305, B:330-B:449 (270)	0.81	3

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, 2, 3, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 16, 17, 18, 22, 24, 26, 27, 29, 32, 33, 34, 37, 38, 39, 40, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 57, 60, 61, 62, 63, 64, 65, 67, 68, 70, 71, 73
2	15, 20, 21, 23, 25, 28, 30, 31, 41, 42, 58, 66, 69, 72
3	4, 35
4	56, 59
Single-model clusters	19; 36

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2792 atoms, of which 501 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Programmed cell death protein 4.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	163	1511	772	278	208	245	8	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	156	GLY	-	expression tag	UNP Q53EL6

- Molecule 2 is a protein called Programmed cell death protein 4.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	131	1281	676	223	172	203	7	0

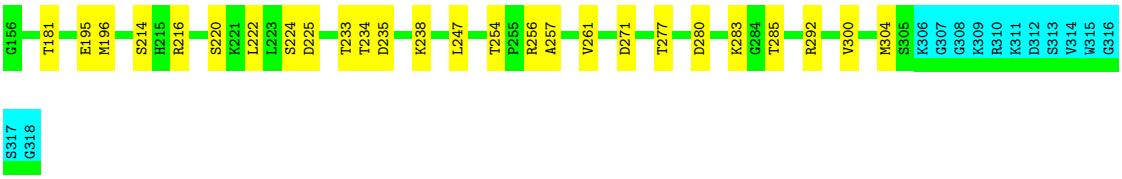
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide 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: Programmed cell death protein 4

Chain A: 76% 16% 8%



• Molecule 2: Programmed cell death protein 4

Chain B: 76% 15% 8%

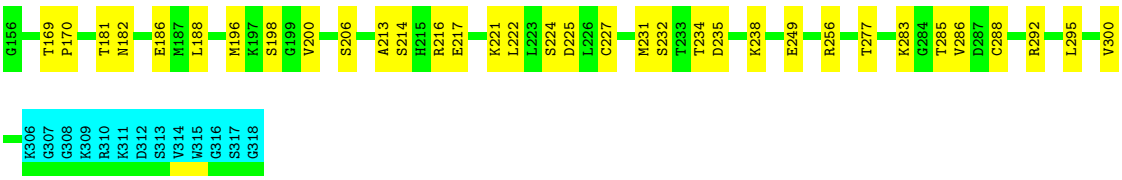
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Programmed cell death protein 4

Chain A: 71% 21% 8%



• Molecule 2: Programmed cell death protein 4

Chain B: 76% 15% 8%

G319 G320 Q321 Q322 P323 V324 N325 H326 L327 V328 K329 Y338 L339 L340 V356 E377 S378 K381 L384 D385 K388 K392 S393 T397 I398 D399 Y405 I408 I412 P413 Y423 S440 R444 S449

4.2.2 Score per residue for model 2

- Molecule 1: Programmed cell death protein 4

Chain A: 72% 19% • 8%

G156 D160 E165 I172 Y175 N182 E183 E186 D190 E195 M196 V200 P201 V202 L203 S214 S220 K221 L222 D225 M231 S232 D235 D241 D253 R256 Q263 D271 T285 R292 A298 T299 V300 L301 M304 S305 K306

G307 G308 K309 R310 K311 D312 S313 V314 W315 G316 S317 G318

- Molecule 2: Programmed cell death protein 4

Chain B: 70% 21% • 8%

G319 G320 Q321 Q322 P323 V324 N325 H326 L327 V328 K329 M333 L334 L335 K336 E337 L340 S341 S345 E346 L351 V356 F359 V364 Y365 V369 S378 S389 K392 S393 T397 M401 Y405 E406 R407 E411 N416 P420 H421 S422 Y423 S424

S449

4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: Programmed cell death protein 4

Chain A: 70% 21% • 8%

G156 I172 Y175 H178 G179 D180 T181 N182 E183 D190 L193 G194 E195 M196 S214 K221 L222 D235 K238 D246 L247 P248 E249 T254 P255 R256 A257 P258 Q259 L260 V261 G262 Q263 T277 D280 K283 G284 T285 C288 V289 Q290 A291 R292 V300

L301 L302 S303 K306 G307 G308 K309 R310 K311 D312 S313 V314 W315 G316 S317 G318

- Molecule 2: Programmed cell death protein 4

Chain B: 74% 18% 8%

G319 G320 Q321 Q322 P323 V324 N325 H326 L327 V328 K329 E337 Y338 L339 L340 E346 H361 T375 S378 L386 S389 K392 T397 R403 G404 Y405 E406 R407 I408 Y409 M410 E411 I412 P413 S424 S440 S449

4.2.4 Score per residue for model 4

• Molecule 1: Programmed cell death protein 4

Chain A: 62% 28% • 8%

G156 T169 I172 Y175 G179 E186 H187 L188 R189 D190 L191 M196 K197 S198 P201 A204 V205 S206 L207 A208 L209 S214 E217 M218 T219 S220 K221 L222 D225 L226 D235 K238 S239 F240 L244 L247 P248 E249 L250 T254 A257 P258

V261 G262 Q263 F264 D271 G272 I273 T277 D280 K283 G284 T285 V286 D287 C288 R292 D296 V300 L301 M304 S305 K306 G307 G308 K309 R310 K311 D312 S313 V314 W315 G316 S317 G318

• Molecule 2: Programmed cell death protein 4

Chain B: 57% 29% 5% 8%

G319 G320 Q321 Q322 P323 V324 N325 H326 L327 V328 K329 D332 M333 L334 E337 Y338 L339 L340 S345 E346 A347 E348 H349 C350 L351 L354 E355 V356 P357 H358 F359 V364 Y365 E366 A367 I368 V369 M370 V371 T375 S378 M382 I383 L384 D385 L386 L387 K388 S389 L390 W391 K392

S393 S394 T395 M401 K402 Y405 I412 N416 S422 I439 Q442 L443 C447 P448 S449

4.2.5 Score per residue for model 5

• Molecule 1: Programmed cell death protein 4

Chain A: 72% 20% 8%

G156 L168 H178 T181 D190 E195 M196 P201 T219 L222 L223 S224 D225 L226 C227 M231 S232 T233 T234 D235 V236 E237 K238 D246 A251 L252 D253 P258 V261 G262 Q263 V269 I273 L274 T277 T285 R292 T299 M304 S305

K306 G307 G308 K309 R310 K311 D312 S313 V314 W315 G316 S317 G318

• Molecule 2: Programmed cell death protein 4

Chain B: 73% 16% • 8%

G319 G320 Q321 Q322 P323 V324 N325 H326 L327 V328 K329 D332 M333 E337 Y338 S345 E346 A347 L351 L354 A367 V371 E377 S378 S394 D399 R403 R407 E411 I412 P413 D414 H421 S422 Y423 S424 S440 S449

4.2.6 Score per residue for model 6

• Molecule 1: Programmed cell death protein 4

Chain A: 68% 23% • 8%

G156 D160 N182 E186 D190 E195 M196 K197 S198 G199 V200 P201 V205 R216 S220 S224 D225 M231 S232 T233 T234 D235 V236 E237 L247 P248 R256 Q263 F264 I265 A266 D271 G272 I273 T277 D280 K283 G284 T285 V286 D287 C288

R292 D296 V300 L301 M304 S305 K306 G307 G308 K309 R310 K311 D312 S313 V314 W315 G316 S317 G318

• Molecule 2: Programmed cell death protein 4

Chain B: 61% 26% 5% 8%

G319 G320 Q321 Q322 P323 V324 N325 H326 L327 V328 K329 D332 M333 L334 E337 L340 D343 E346 A347 E348 V356 F359 H360 H361 E366 M370 T375 G376 E377 S378 A379 F380 I383 L386 L387 L390 S394 T395 I396 T397 Q400 G404 Y405 E406

R407 I408 E411 I412 D418 H421 S424 R428 F429 I438 I439 S440 S449

4.2.7 Score per residue for model 7

• Molecule 1: Programmed cell death protein 4

Chain A: 67% 23% • 8%

G156 D160 L168 E174 T181 V184 L188 E195 M196 K197 S198 A213 S214 H215 R216 E217 S220 K221 L222 D225 M231 S232 T233 T234 D235 K238 L244 L247 D253 T254 A257 V261 I265 A266 R267 D271 C275 N276 T277 Y278

I279 K283 G284 T285 R292 L295 T299 V300 K306 G307 G308 K309 R310 K311 D312 S313 V314 W315 G316 S317 G318

• Molecule 2: Programmed cell death protein 4

Chain B: 59% 32% • 8%

G319 G320 Q321 Q322 P323 V324 N325 H326 L327 V328 K329 E330 I331 D332 M333 L340 S345 E346 L354 V364 A367 V371 E377 S378 L384 D385 L386 L387 K388 S389 K392 T395 T396 T397 T398 D399 Q400 M401 Y405 E406 R407 I408 Y409 M410 E411 I412 P413 H421

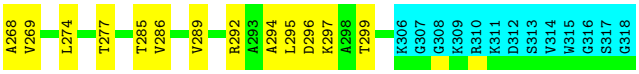
S422 Y423 S424 V425 L426 E427 R428 F429 V430 E431 E432 C433 F434 S440 K441 R444 C447 P448 S449

4.2.8 Score per residue for model 8

• Molecule 1: Programmed cell death protein 4

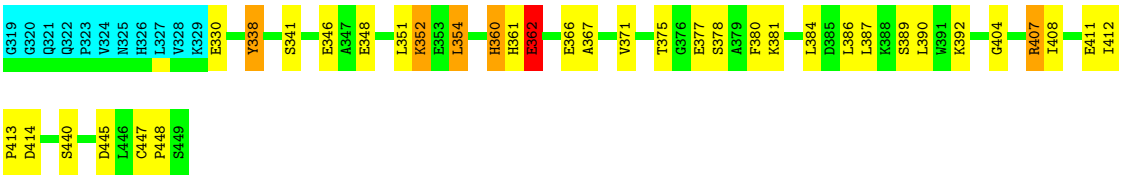
Chain A: 61% 29% • 8%

G156 I172 F176 T181 M187 D190 L191 N192 L193 G194 E195 M196 V202 L203 A204 V205 A208 L209 S214 M218 T219 S220 S224 T233 T234 D235 K238 S239 F240 D241 K245 D246 L247 P248 E249 L252 D253 T254 P255 R256 V261 I265 A266 R267



• Molecule 2: Programmed cell death protein 4

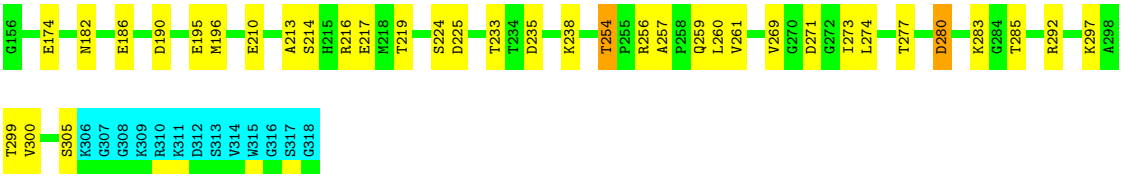
Chain B:



4.2.9 Score per residue for model 9

• Molecule 1: Programmed cell death protein 4

Chain A:



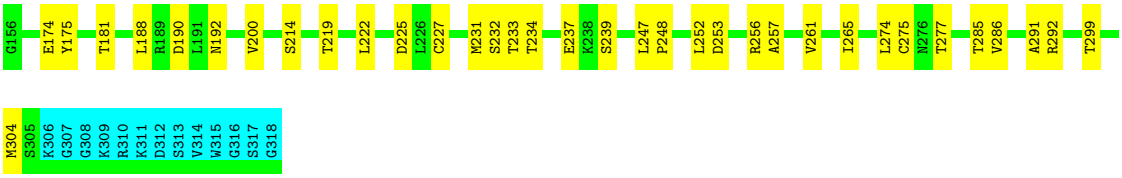
• Molecule 2: Programmed cell death protein 4

Chain B:

4.2.10 Score per residue for model 10

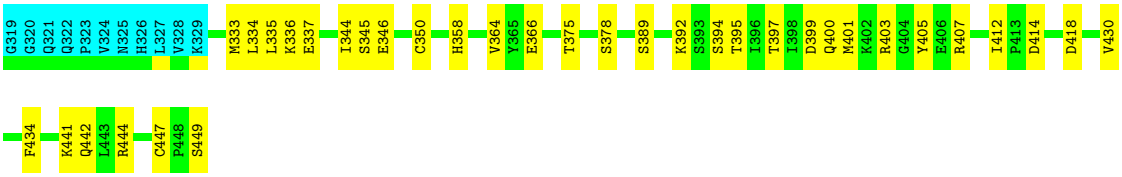
• Molecule 1: Programmed cell death protein 4

Chain A:



• Molecule 2: Programmed cell death protein 4

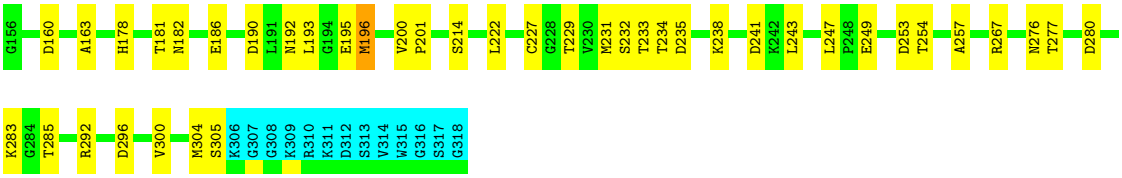
Chain B:



4.2.11 Score per residue for model 11

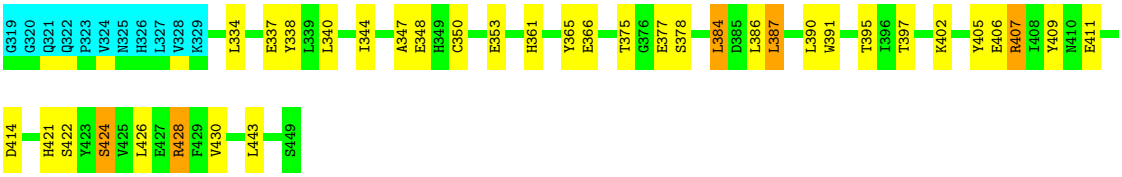
- Molecule 1: Programmed cell death protein 4

Chain A: 67% 25% • 8%



- Molecule 2: Programmed cell death protein 4

Chain B: 64% 24% • 8%



4.2.12 Score per residue for model 12

- Molecule 1: Programmed cell death protein 4

Chain A: 75% 17% 8%

- Molecule 2: Programmed cell death protein 4

Chain B: 73% 18% • 8%

4.2.13 Score per residue for model 13

- Molecule 1: Programmed cell death protein 4

Chain A: 60% 29% • 8%

G156 D160 E174 E177 T181 D190 L191 N192 E195 M196 K197 S198 V205 L209 S214 H215 M218 T219 S220 K221 L222 L223 S224 D225 L226 C227 S232 T233 T234 D235 V236 E237 K238 S239 F240 D241 K242 L243 L244 K245 D246 L247 P248 E249 L252 P255 R256

A257 P258 Q259 L260 V261 A268 I273 L274 C275 N276 T277 D280 T285 A291 R292 D296 T299 V300 K306 G307 G308 K309 R310 K311 D312 S313 V314 W315 G316 S317 G318

- Molecule 2: Programmed cell death protein 4

Chain B: 66% 25% • 8%

G319 G320 Q321 Q322 P323 V324 N325 H326 L327 V328 K329 K336 E337 Y338 L339 L340 S341 G342 D343 T344 S345 E346 A347 E348 L351 K352 E353 H361 E373 S374 T375 S378 M382 S389 L390 W391 K392 S393 S394 T395 T396 T397 T398 D399 Y405 E406 R407 I408 E411 I412

H421 S422 Y423 S424 E427 R428 F429 S440 R444 S449

4.2.14 Score per residue for model 14

- Molecule 1: Programmed cell death protein 4

Chain A: 72% 19% • 8%

G156 D160 E161 E165 Y175 L188 R189 D190 E195 V200 S214 H215 S220 K221 L222 D225 T234 D235 K238 P248 E249 T254 P255 R256 A257 D271 T277 D280 K283 G284 T285 Q290 A291 R292 D296 V300 S303 K306

G307 G308 K309 R310 K311 D312 S313 V314 W315 G316 S317 G318

- Molecule 2: Programmed cell death protein 4

Chain B: 71% 19% • 8%

G319 G320 Q321 Q322 P323 V324 N325 H326 L327 V328 K329 E330 I331 D332 M333 E337 L340 E346 H349 F359 H360 H361 E362 Y365 S378 L387 K388 S389 L390 W391 K392 I396 Q400 Y405 E406 R407 I408 I412 P413 N416 L426 V430 S440

S449

4.2.15 Score per residue for model 15

- Molecule 1: Programmed cell death protein 4

Chain A: 64% 26% • 8%

G156 D160 I172 Y175 T181 E195 M196 S206 L209 E210 S214 H215 R216 T219 S220 K221 S224 D225 L226 C227 M231 S232 T233 L244 K245 D246 L247 R256 A257 P258 Q259 L260 V261 G262 Q263 F264 I273 T277 D280 K283 G284 T285 V286

D287 C288 V289 Q290 A291 R292 K297 A298 T299 V300 L301 M304 S305 K306 G307 G308 K309 R310 K311 D312 S313 V314 W315 G316 S317 G318

• Molecule 2: Programmed cell death protein 4

Chain B: 74% 18% 8%

G319 G320 Q321 Q322 P323 V324 N325 H326 L327 V328 K329 E337 Y338 L339 L340 I344 E348 L354 E355 V356 P357 H358 S378 L386 L387 T397 Y405 E406 R407 E411 H421 S422 Y423 S424 R428 E431 S440 L443 L446 S449

4.2.16 Score per residue for model 16

• Molecule 1: Programmed cell death protein 4

Chain A: 69% 21% • 8%

G156 G179 D180 T181 D190 E195 M196 V200 P201 S214 H215 S220 K221 L222 L223 S224 T234 D235 K238 D241 K245 D246 L247 P248 T254 A257 P258 Q259 L260 V261 D271 T277 D280 K283 G284 T285 R292 K297 A298 L301 L302

S303 M304 S305 K306 G307 G308 K309 R310 K311 D312 S313 V314 W315 G316 S317 G318

• Molecule 2: Programmed cell death protein 4

Chain B: 67% 23% • 8%

G319 G320 Q321 Q322 P323 V324 N325 H326 L327 V328 K329 E330 M333 I334 L335 K336 I344 S345 E346 E353 L354 E355 V356 P357 Y365 V369 L384 L387 T395 I396 T397 Y405 E406 R407 I408 E411 I412 P413 N416 L417 D418 V419 P420 Y423 S424 V425 L426

V430 S440 K441 Q442 L443 R444 S449

4.2.17 Score per residue for model 17

• Molecule 1: Programmed cell death protein 4

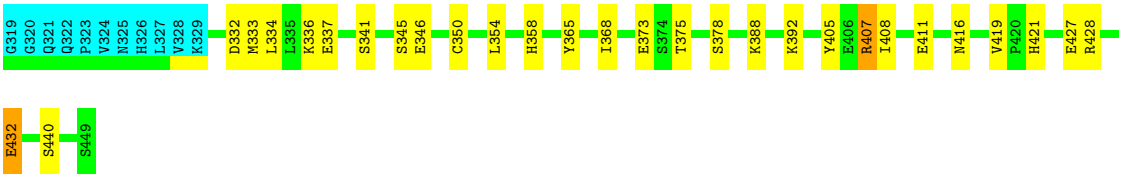
Chain A: 68% 23% • 8%

G156 T167 L168 T169 P170 I171 F176 T181 V184 L188 L193 A208 K212 A213 S214 D225 T233 T234 D235 V236 E237 K238 L244 L247 P248 E249 L250 V261 R267 D271 G272 I273 T277 Y282 T285 V286 D287 C288 R292 D296

K297 V300 L301 L302 S303 M304 S305 K306 G307 G308 K309 R310 K311 D312 S313 V314 W315 G316 S317 G318

• Molecule 2: Programmed cell death protein 4

Chain B:



4.2.18 Score per residue for model 18

• Molecule 1: Programmed cell death protein 4

Chain A:

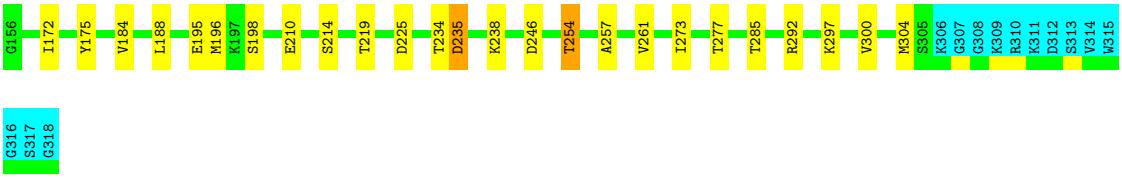
• Molecule 2: Programmed cell death protein 4

Chain B:

4.2.19 Score per residue for model 19

• Molecule 1: Programmed cell death protein 4

Chain A:



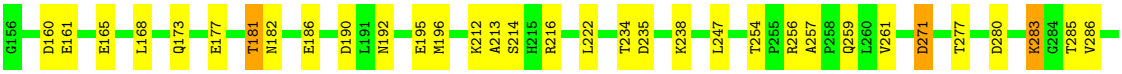
• Molecule 2: Programmed cell death protein 4

Chain B:

4.2.20 Score per residue for model 20

• Molecule 1: Programmed cell death protein 4

Chain A:



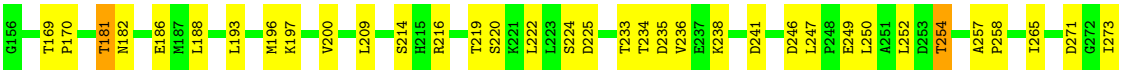
• Molecule 2: Programmed cell death protein 4

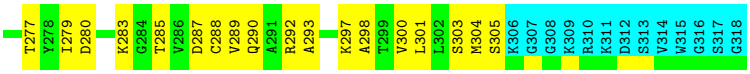
Chain B:

4.2.21 Score per residue for model 21

• Molecule 1: Programmed cell death protein 4

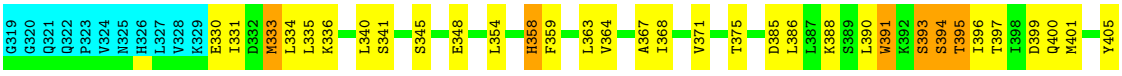
Chain A:





• Molecule 2: Programmed cell death protein 4

Chain B:



4.2.22 Score per residue for model 22

- Molecule 1: Programmed cell death protein 4

Chain A: 64% 26% • 8%

G156 L168 T169 P170 I171 I172 F176 E177 H178 G179 D180 T181 N182 E186 N192 E195 V202 L203 A204 E210 S214 T219 S224 C227 G228 T229 S232 T233 V236 E237 K238 L243 D246 L247 P248 D253 R256 Q259 Q263 I273

T285 V286 D287 C288 A291 K297 V300 L301 L302 S303 M304 S305 K306 G307 G308 K309 R310 K311 D312 S313 V314 W315 G316 S317 G318

- Molecule 2: Programmed cell death protein 4

Chain B: 61% 27% • 8%

G319 G320 Q321 Q322 P323 V324 N325 H326 L327 V328 K329 M333 K336 E337 Y338 L339 L340 S341 G342 D343 I344 S345 E346 A347 E348 H349 K352 V356 Y365 I368 V371 L372 E373 S374 T375 L387 L390 W391 S394 T395 D399 Q400 M401 K402 R403 G404 Y405 E406 R407

I408 Y409 N410 E411 H421 S422 F434 S440 K441 R444 S449

4.2.23 Score per residue for model 23

- Molecule 1: Programmed cell death protein 4

Chain A: 76% 16% 8%

G156 D190 E195 M196 V200 P201 A213 S214 H215 R216 S220 K221 S224 D225 T234 E237 T254 P258 V261 F264 D271 G272 T277 T285 R292 K297 V300 L301 K306 G307 G308 K309 R310 K311 D312 S313 V314 W315 G316 S317 G318

- Molecule 2: Programmed cell death protein 4

Chain B: 71% 20% • 8%

G319 G320 Q321 Q322 P323 V324 N325 H326 L327 V328 K329 E330 I331 D332 L340 I344 E348 K352 E353 H361 E362 L363 T375 S378 A379 I383 L384 D385 L386 L387 K388 S389 L390 Q400 Y405 E406 R407 N410 E411 I412 P413 H421 S422 Y423 S424 S440

S449

4.2.24 Score per residue for model 24

- Molecule 1: Programmed cell death protein 4

Chain A: 66% 25% • 8%

G156 D160 A163 F164 E165 P170 E174 T181 E195 M196 K197 S198 G199 V200 P201 V202 L203 S206 L209 S214 H215 R216 S220 K221 L222 D225 L226 T229 V230 M231 S232 T233 T234 D235 K238 D246 L247 P248 A251 R256 A257 P258 T277

T285 V286 V289 Q290 A291 K297 A298 T299 V300 L301 L302 K306 G307 G308 K309 R310 K311 D312 S313 V314 W315 G316 S317 G318

• Molecule 2: Programmed cell death protein 4

Chain B: 58% 32% • 8%

G319 G320 Q321 Q322 P323 V324 N325 H326 L327 V328 K329 E330 E337 Y338 S341 G342 D343 E346 A347 C350 L354 E355 V356 A367 V371 T375 S378 K381 M382 I383 L384 D385 L386 L387 K388 S389 L390 W391 K392 S393 S394 D399 K402 R403 G404 Y405 E406 R407

I408 Y409 N410 E411 D414 D418 Y423 R428 E431 F434 Q435 A436 S440 K441 S449

4.2.25 Score per residue for model 25

• Molecule 1: Programmed cell death protein 4

Chain A: 61% 29% • 8%

G156 L157 P158 L159 D160 A163 L168 T169 P170 I171 I172 G179 V184 M187 L188 R189 D190 L191 N192 L193 G194 E195 M196 V200 P201 V205 S206 L207 A213 S214 H215 R216 S224 D225 L226 C227 M231 S232 T233 T234 D235 K238 D246 L247 P248 E249 D253

T254 A257 V261 G262 Q263 D271 T277 D280 K283 G284 T285 R292 D296 V300 L301 M304 S305 K306 G307 G308 K309 R310 K311 D312 S313 V314 W315 G316 S317 G318

• Molecule 2: Programmed cell death protein 4

Chain B: 67% 24% • 8%

G319 G320 Q321 Q322 P323 V324 N325 H326 L327 V328 K329 M333 Y338 L339 L340 S341 G342 D343 T344 S345 E346 E353 L354 P357 V364 Y365 V369 S378 D385 L386 L387 W391 T395 N401 Y405 E406 R407 I408 Y409 N410 E411 I412 P413 N416 S422 Y423

S424 F429 V430 E431 S449

4.2.26 Score per residue for model 26

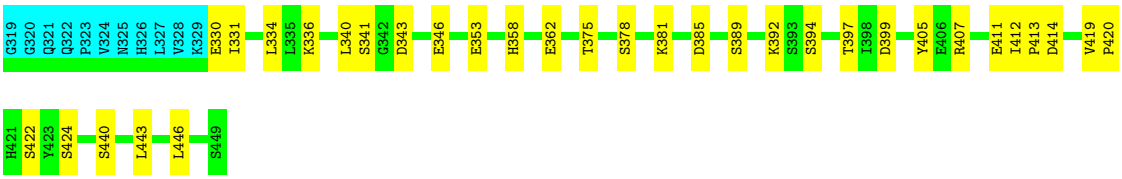
• Molecule 1: Programmed cell death protein 4

Chain A: 74% 17% • 8%

G156 L188 E195 M196 V200 S214 H215 S220 K221 S224 D225 S232 T233 T234 D235 V236 E237 K238 D241 K245 D246 L247 P248 E249 R256 V261 D271 T277 Y282 T285 D296 V300 M304 S305 K306 G307 G308 K309 R310 K311 D312 S313

• Molecule 2: Programmed cell death protein 4

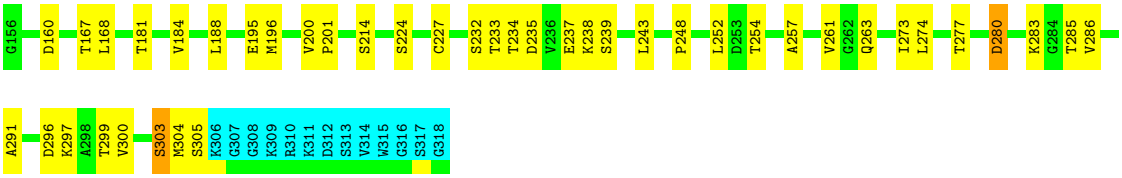
Chain B:



4.2.27 Score per residue for model 27

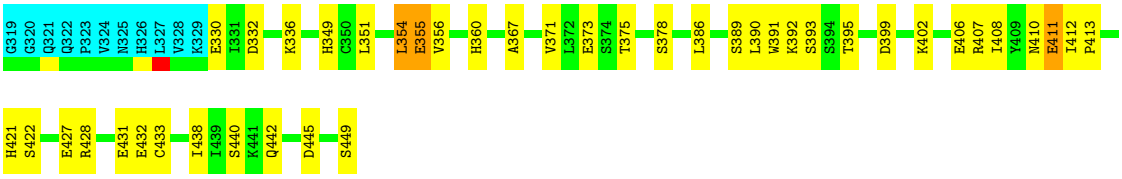
• Molecule 1: Programmed cell death protein 4

Chain A:



• Molecule 2: Programmed cell death protein 4

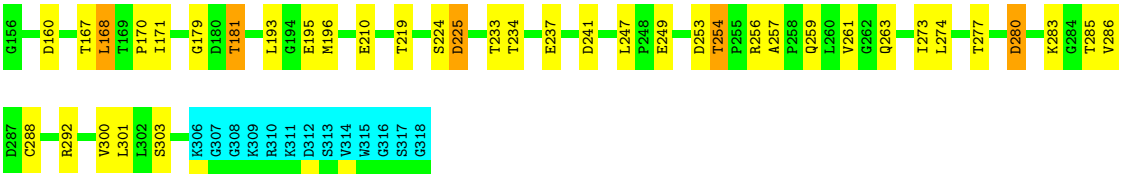
Chain B:



4.2.28 Score per residue for model 28

• Molecule 1: Programmed cell death protein 4

Chain A:



• Molecule 2: Programmed cell death protein 4

Chain B: 68% 21% • 8%

G319 G320 Q321 Q322 P323 V324 N325 H326 L327 V328 K329 E337 Y338 L339 L340 I344 S345 E346 A347 E348 K352 E353 L354 I383 L386 L387 K388 S389 K392 S393 T397 K402 Y405 E406 R407 I408 Y409 N410 E411 I412 P413 H421 S424 V425 L426 V430 E431

L443 R444 S449

4.2.29 Score per residue for model 29

- Molecule 1: Programmed cell death protein 4

Chain A: 65% 25% • 8%

G156 E174 T181 N182 N192 E195 M196 V205 L209 E210 R216 S220 K221 L222 L223 S224 D225 L226 T229 T233 T234 D235 K238 D241 K245 D246 L247 P248 E249 P255 R256 A257 P258 Q259 L260 V261 F264 A268 D271 G272 I273 L274 C275

N276 T277 Y278 I279 D280 T285 A291 R292 L295 V300 M304 S305 K306 G307 G308 K309 R310 K311 D312 S313 V314 W315 G316 S317 G318

- Molecule 2: Programmed cell death protein 4

Chain B: 67% 21% • 8%

G319 G320 Q321 Q322 P323 V324 N325 H326 L327 V328 K329 E330 I331 D332 M333 L334 L335 K336 E337 L340 D343 I344 S345 E346 A347 E348 K352 H361 V371 S378 A379 F380 K381 D385 L386 L387 K388 S389 L390 W391 T395 I396 T397 Y405 E406 R407 E411 S422 Y423

S424 E427 S440 R444 S449

4.2.30 Score per residue for model 30

- Molecule 1: Programmed cell death protein 4

Chain A: 65% 25% • 8%

G156 I172 Q173 E174 T181 E186 E195 M196 A204 V205 L209 A213 S214 H215 R216 K221 S224 D225 M231 S232 T233 T234 D235 V236 E237 L247 P248 E249 L250 T254 P255 R256 A257 P258 Q259 L260 V261 R267 A268 V269 G270 D271 T277 D280

K283 G284 T285 V286 D287 C288 R292 D296 T299 V300 L301 L302 K306 G307 G308 K309 R310 K311 D312 S313 V314 W315 G316 S317 G318

- Molecule 2: Programmed cell death protein 4

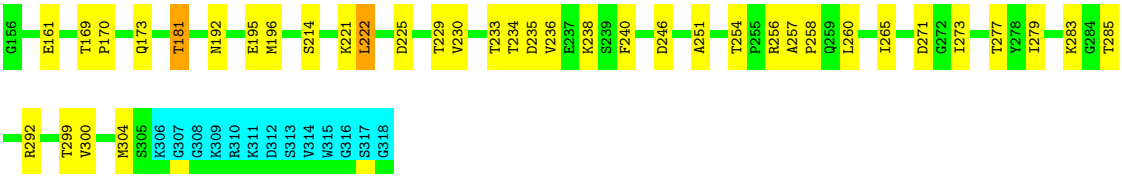
Chain B: 62% 27% • 8%

G319 G320 Q321 Q322 P323 V324 N325 H326 L327 V328 K329 E330 M333 L334 E337 Y338 L339 L340 I344 A347 E353 H358 H361 V364 Y365 I368 V371 E377 S378 M382 I383 L384 D385 L386 L387 K392 T395 Q400 M401 K402 R407 I408 Y409

4.2.31 Score per residue for model 31

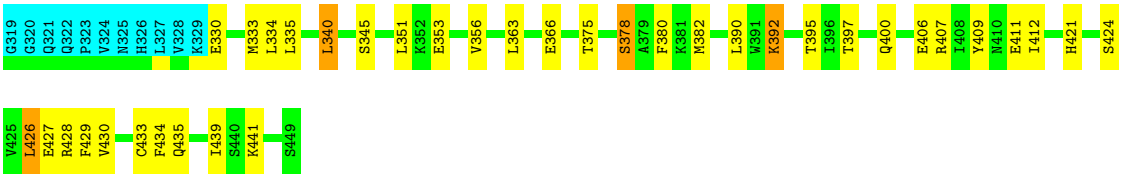
• Molecule 1: Programmed cell death protein 4

Chain A:



• Molecule 2: Programmed cell death protein 4

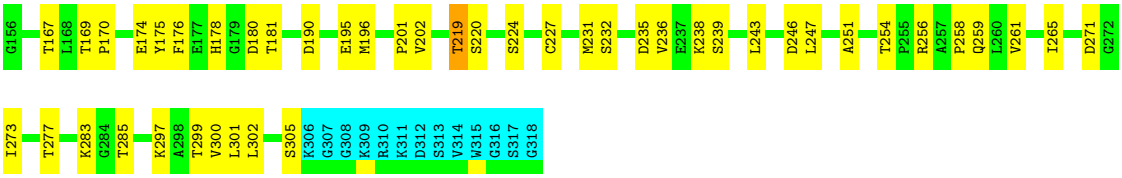
Chain B:



4.2.32 Score per residue for model 32

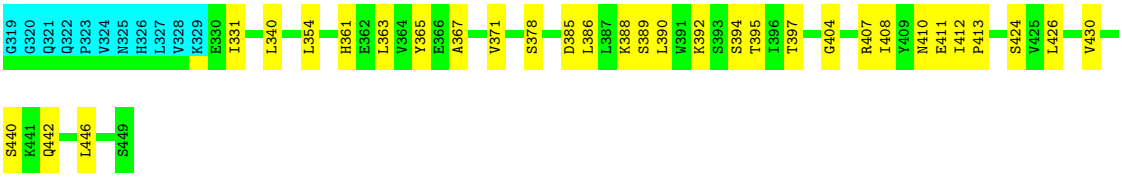
• Molecule 1: Programmed cell death protein 4

Chain A:



• Molecule 2: Programmed cell death protein 4

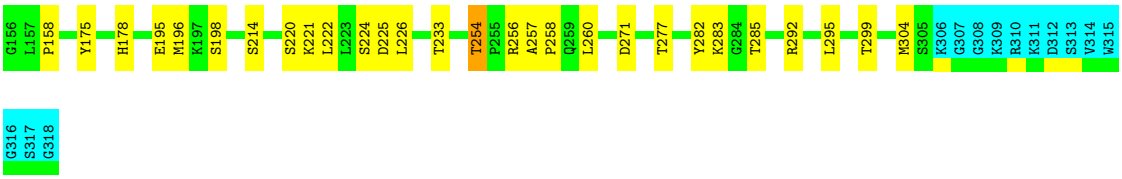
Chain B:



4.2.33 Score per residue for model 33

- Molecule 1: Programmed cell death protein 4

Chain A: 75% 17% • 8%



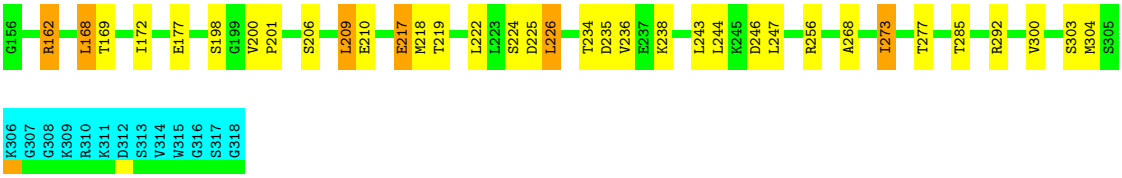
- Molecule 2: Programmed cell death protein 4

Chain B: 63% 27% • 8%

4.2.34 Score per residue for model 34

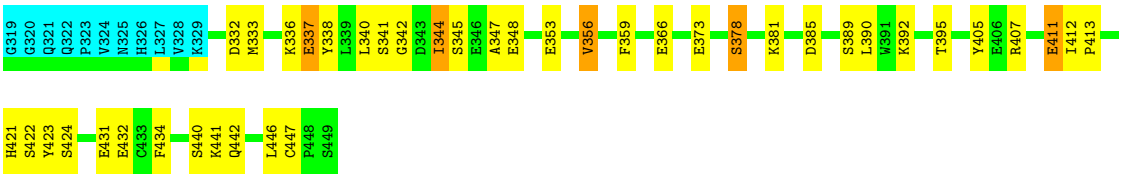
- Molecule 1: Programmed cell death protein 4

Chain A: 71% 18% • 8%



- Molecule 2: Programmed cell death protein 4

Chain B: 60% 27% • 8%



4.2.35 Score per residue for model 35

- Molecule 1: Programmed cell death protein 4

Chain A: 67% 23% • 8%

G156 D160 T169 P170 I171 T181 M187 N192 L193 G194 E195 M196 L207 A208 L209 R216 E217 S220 K221 D225 S232 T233 E237 F240 D246 L247 T254 P255 R256 A257 P258 Q259 L260 V261 F264 R267 G272 I273 Y278 T285

R292 K297 V300 S303 M304 S305 K306 G307 G308 K309 R310 K311 D312 S313 V314 W315 G316 S317 G318

• Molecule 2: Programmed cell death protein 4

Chain B: 62% 24% 5% 8%

G319 G320 Q321 Q322 P323 V324 N325 H326 L327 V328 K329 D332 K336 E337 Y338 L339 L340 H349 C350 L351 K352 E353 L354 E355 V356 H361 E366 V369 M370 V371 L372 F380 K381 D385 L386 L387 K388 S389 L390 W391 K392 S393 K402 Y405 Y409 D414 I415 N416

L417 D418 V419 P420 H421 S422 E427 E432 Q435 S440 K441 Q442 L443 L446 S449

4.2.36 Score per residue for model 36

• Molecule 1: Programmed cell death protein 4

Chain A: 67% 25% 8%

G156 L157 P158 L159 D160 E161 R162 T181 V184 L188 E195 M196 V205 L209 S214 L222 L223 S224 D225 L226 T234 D235 V236 E237 K238 S239 K242 K245 D246 L247 P248 E249 R256 V261 G262 Q263 R267 I273 T277 K283 G284 T285 V286

Q290 A291 T299 V300 L301 M304 S305 K306 G307 G308 K309 R310 K311 D312 S313 V314 W315 G316 S317 G318

• Molecule 2: Programmed cell death protein 4

Chain B: 56% 28% 7% 8%

G319 G320 Q321 Q322 P323 V324 N325 H326 L327 V328 K329 E330 L334 L335 K336 E337 Y338 L339 L340 D343 I344 S345 E346 A347 E348 H349 E353 L354 H361 A367 T375 S378 A379 F380 I383 L384 D385 L386 L390 S394 Q400 G404 Y405 E406 R407 I408 E411

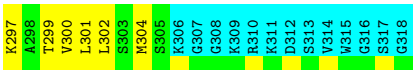
I412 N416 S422 Y423 S424 V425 L426 E427 R428 F429 V430 E431 F434 Q435 A436 G437 S440 K441 C447 P448 S449

4.2.37 Score per residue for model 37

• Molecule 1: Programmed cell death protein 4

Chain A: 69% 23% • 8%

G156 D160 L168 N182 E186 E195 M196 V200 P201 S206 S214 S220 K221 D225 T233 T234 D235 K238 L244 L247 T254 A257 P258 V261 G262 A268 L274 T277 D280 K283 G284 T285 V286 D287 C288 R292



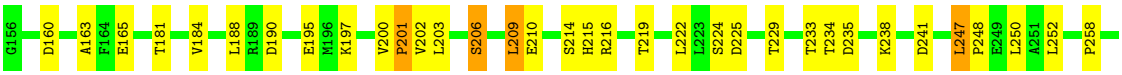
• Molecule 2: Programmed cell death protein 4

Chain B: 71% 17% • 8%

4.2.38 Score per residue for model 38

• Molecule 1: Programmed cell death protein 4

Chain A: 65% 25% • 8%



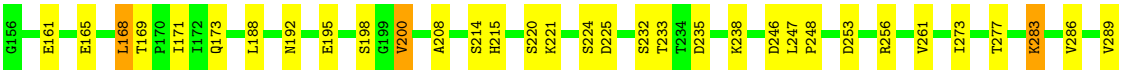
• Molecule 2: Programmed cell death protein 4

Chain B: 66% 22% • 8%

4.2.39 Score per residue for model 39

• Molecule 1: Programmed cell death protein 4

Chain A: 68% 21% • 8%



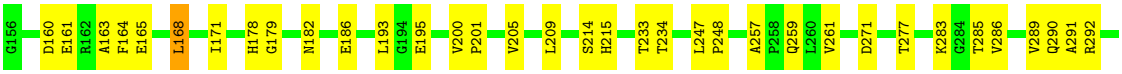
• Molecule 2: Programmed cell death protein 4

Chain B: 71% 21% 8%

4.2.40 Score per residue for model 40

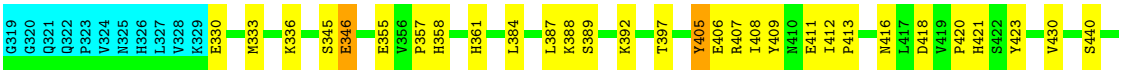
- Molecule 1: Programmed cell death protein 4

Chain A:



- Molecule 2: Programmed cell death protein 4

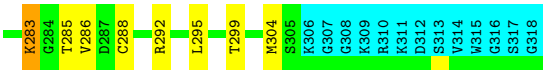
Chain B:



4.2.41 Score per residue for model 41

- Molecule 1: Programmed cell death protein 4

Chain A:



- Molecule 2: Programmed cell death protein 4

Chain B:

4.2.42 Score per residue for model 42

- Molecule 1: Programmed cell death protein 4

Chain A: 70% 21% •• 8%

G156 T169 P170 E177 E195 G199 V200 P201 V202 L203 A204 V205 S206 L207 S214 H215 R216 T219 S220 D225 S232 T233 T234 D235 K238 E249 L250 A251 L252 D253 R256 L260 I273 T277 T285 V286 D287 C288 R292 T299 V300 K306

G307 G308 K309 R310 K311 D312 S313 V314 W315 G316 S317 G318

- Molecule 2: Programmed cell death protein 4

Chain B: 59% 30% • 8%

G319 G320 Q321 Q322 P323 V324 N325 H326 L327 V328 K329 E330 I331 L334 L340 S345 E346 A347 E348 H349 C350 L354 H360 L363 V364 A367 V371 T375 S378 L386 L390 W391 K392 S393 S394 T395 I396 T397 I398 D399 Q400 M401 Y405 E406 R407 I408

I412 N416 P420 H421 S422 Y423 S424 V425 R428 E432 C433 F434 I438 I439 S440 K441 Q442 L443 S449

4.2.43 Score per residue for model 43

- Molecule 1: Programmed cell death protein 4

Chain A: 72% 20% • 8%

G156 N182 E186 D190 M196 V205 A213 S214 H215 R216 S220 L223 S224 D225 T233 T234 D235 K238 L243 D246 L247 P248 E249 R256 A257 P258 V261 G262 Q263 D271 G272 I273 T277 T285 R292 V300 L301 M304 S305 K306

G307 G308 K309 R310 K311 D312 S313 V314 W315 G316 S317 G318

- Molecule 2: Programmed cell death protein 4

Chain B: 66% 26% 8%

G319 G320 Q321 Q322 P323 V324 N325 H326 L327 V328 K329 E330 I331 D332 M333 L334 E337 L340 E346 K352 E353 L354 E355 V356 V364 A367 V371 T375 S378 K381 D385 T395 I396 T397 M401 K402 Y405 E406 R407 I408 Y409 N410 E411 I412 P413

S422 Y423 S424 E427 S440 L443 R444 S449

4.2.44 Score per residue for model 44

- Molecule 1: Programmed cell death protein 4

Chain A: 71% 20% •• 8%

G156 D160 T181 N182 E183 V184 E195 M196 V202 S214 L222 T233 T234 D235 V236 E237 K238 S239 F240 K245 D246 L247 P248 A251 R256 A257 P258 Q259 L260 V261 D271 T277 D280 K283 G284 T285 D296 K297 A298 T299 V300 L301 M304 S305

K306 G307 G308 K309 R310 K311 D312 S313 V314 W315 G316 S317 G318

• Molecule 2: Programmed cell death protein 4

Chain B: 63% 27% • 8%

G319 G320 Q321 Q322 P323 V324 N325 H326 L327 V328 K329 E330 I331 D332 M333 L334 L335 K336 E337 S341 E346 C350 L354 H361 E362 L363 V364 Y365 E366 A367 M370 V371 S378 A379 F380 K381 D385 L386 L387 K388 S389 K392 S393 Q400 G404 R407 I408

E411 I412 P413 Y423 S424 R428 E431 Q435 S440 R444 S449

4.2.45 Score per residue for model 45

• Molecule 1: Programmed cell death protein 4

Chain A: 67% 23% • 8%

G156 D160 A163 F164 L168 T169 P170 E174 E177 H178 G179 N192 L193 G194 E195 M196 S206 L209 E210 S214 M218 T219 S220 K221 L222 L223 S224 D225 T229 T233 L244 K245 D246 L247 P248 E249 R256 A266 T277 D280 T285 V286

D287 C288 V289 Q290 A298 T299 V300 M304 S305 K306 G307 G308 K309 R310 K311 D312 S313 V314 W315 G316 S317 G318

• Molecule 2: Programmed cell death protein 4

Chain B: 60% 29% • 8%

G319 G320 Q321 Q322 P323 V324 N325 H326 L327 V328 K329 E330 I331 D332 M333 L334 L335 K336 E337 Y338 L339 L340 S341 G342 D343 I344 S345 C350 V356 F359 E373 S374 T375 S378 K381 M382 L386 S389 K392 S393 T397 Q400 M401 K402 R403 E406 R407

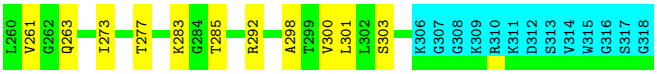
E411 I412 P413 D414 D418 H421 S422 Y423 S424 E427 S440 L443 P448 S449

4.2.46 Score per residue for model 46

• Molecule 1: Programmed cell death protein 4

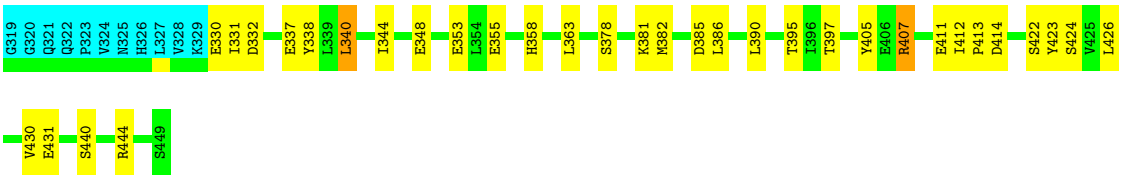
Chain A: 64% 23% • 8%

G156 D160 A163 F164 E165 I172 Q173 E174 Y175 F176 T181 N182 E186 L193 G194 E195 M196 V200 P201 V202 L203 S206 E210 A213 R216 T219 L222 D225 S232 T233 T234 D235 K238 L247 P248 E249 T254 P255 R256 A257 P258 Q259



• Molecule 2: Programmed cell death protein 4

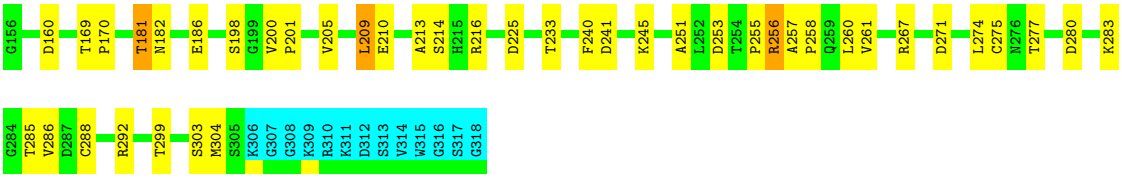
Chain B:



4.2.47 Score per residue for model 47

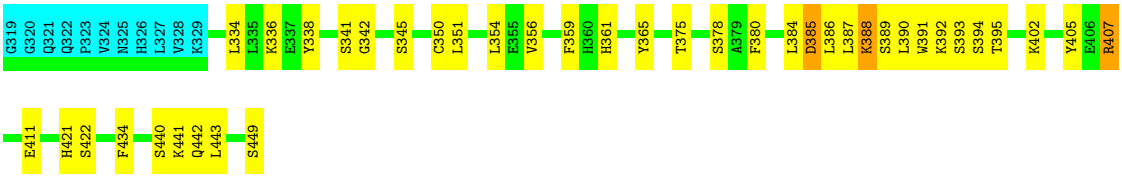
• Molecule 1: Programmed cell death protein 4

Chain A:



• Molecule 2: Programmed cell death protein 4

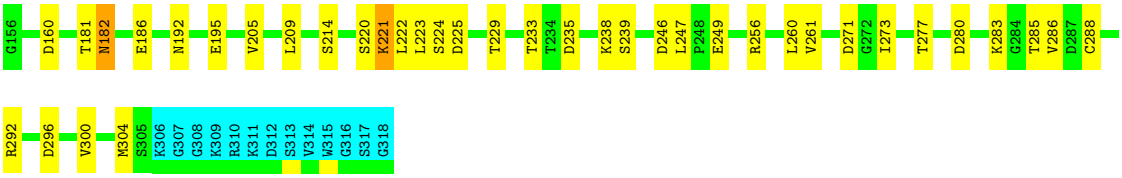
Chain B:



4.2.48 Score per residue for model 48

• Molecule 1: Programmed cell death protein 4

Chain A:



• Molecule 2: Programmed cell death protein 4

Chain B: 72% 18% • 8%

G319 G320 Q321 Q322 P323 V324 N325 H326 L327 V328 K329 E330 I331 D332 M333 L334 E337 L340 S345 E346 A347 E353 V356 I368 V371 S378 A379 F380 D385 L386 L387 K388 S389 K392 T397 R407 I408 E411 S422 F429 I438 S449

4.2.49 Score per residue for model 49

• Molecule 1: Programmed cell death protein 4

Chain A: 70% 19% • 8%

G156 E161 T181 E195 M196 V202 V205 L209 E217 M218 T219 S220 K221 L222 L226 T229 D235 D241 K242 L243 L247 P248 L252 D253 R256 A257 P258 R267 A268 G272 I273 T277 D280 K283 G284 T285 R292 T299 V300

L301 S305 K306 G307 G308 K309 R310 K311 D312 S313 V314 W315 G316 S317 G318

• Molecule 2: Programmed cell death protein 4

Chain B: 71% 18% • 8%

G319 G320 Q321 Q322 P323 V324 N325 H326 L327 V328 K329 E330 Y338 S341 G342 D343 E346 L354 E355 H358 T375 S378 M382 T395 I396 T397 I398 D399 Y405 E406 Y409 N410 E411 D414 H421 S424 E427 F434 S440 K441 R444

S449

4.2.50 Score per residue for model 50

• Molecule 1: Programmed cell death protein 4

Chain A: 74% 17% • 8%

G156 M196 A213 R216 S220 K221 T233 T234 D235 K238 D246 L247 P248 E249 R256 Q259 L260 V261 R267 T277 Y278 I279 T285 V286 D287 C288 R292 K297 A298 T299 V300 L301 L302 S303 M304 S305 K306 G307 G308 K309 R310 K311 D312 S313 V314 W315

G316 S317 G318

• Molecule 2: Programmed cell death protein 4

Chain B: 63% 26% • • 8%

G319 G320 Q321 Q322 P323 V324 N325 H326 L327 V328 K329 M333 L334 L335 K336 L340 E346 A347 C350 V356 P357 H358 F359 V364 Y365 V369 M370 V371 L372 E373 S378 I383 L387 K388 S389 K392 S393 Y405 E406 R407 I408 Y409 N410 E411 I412 P413 N416

H421 S424 V425 L426 F429 V430 I438 I439 S440 R444 S449

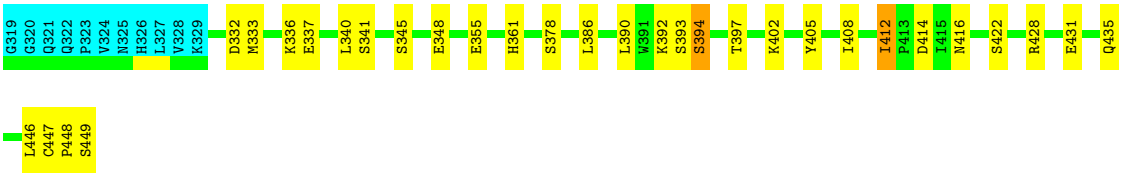
4.2.51 Score per residue for model 51

- Molecule 1: Programmed cell death protein 4

Chain A: 66% 26% • 8%

- Molecule 2: Programmed cell death protein 4

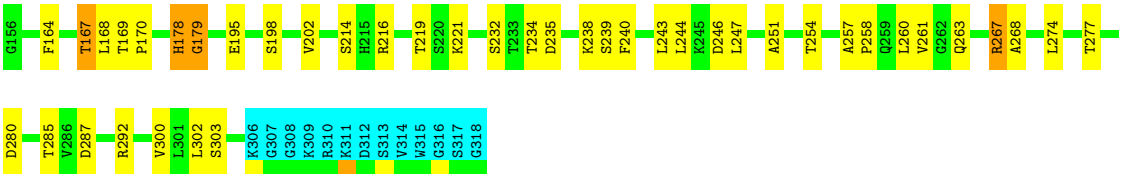
Chain B: 68% 22% • 8%



4.2.52 Score per residue for model 52

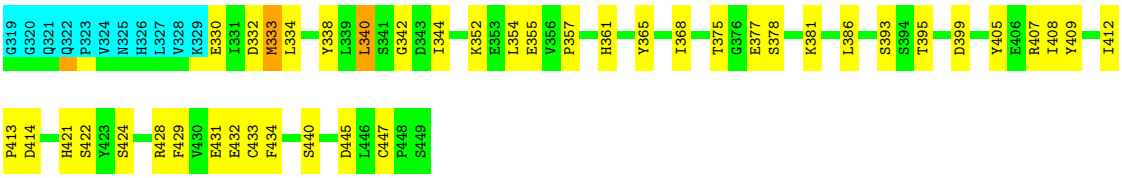
- Molecule 1: Programmed cell death protein 4

Chain A: 66% 23% • 8%



- Molecule 2: Programmed cell death protein 4

Chain B: 60% 31% • 8%



4.2.53 Score per residue for model 53

- Molecule 1: Programmed cell death protein 4

Chain A: 60% 31% • 8%

G156 E165 T169 P170 N182 E186 E195 M196 V200 P201 V202 L203 A204 V205 S206 L207 A208 L209 E210 S214 H215 R216 S220 K221 S224 D225 L226 C227 M231 S232 T233 T234 D235 K238 L243 L247 P248 E249 L250 A251 L252 D253 T254 V261 G262 Q263

F264 A268 D271 G272 I273 L274 T277 T285 V286 D287 C288 V289 Q290 A291 R292 K297 A298 T299 V300 L301 L302 S303 M304 S305 K306 G307 G308 K309 R310 K311 D312 S313 V314 W315 G316 S317 G318

• Molecule 2: Programmed cell death protein 4

Chain B: 65% 25% • 8%

G319 G320 Q321 Q322 P323 V324 N325 H326 L327 V328 K329 E330 I331 D332 M333 L334 E337 S341 I344 S345 E346 A347 E348 H349 C350 L354 H361 E362 L363 E373 S378 S389 K392 S393 S394 T397 Q400 M401 K402 Y405 E406 R407 I408 E411 T412 P413 D414

I415 N416 H421 S422 Y423 S424 F429 Q442 S449

4.2.54 Score per residue for model 54

• Molecule 1: Programmed cell death protein 4

Chain A: 65% 25% • 8%

G156 L157 P158 E161 L168 T181 D190 E195 M196 P201 V205 S206 L207 E210 S214 H215 R216 T219 S220 T229 T233 V236 E237 K238 S239 F240 K245 D246 L247 P248 L252 D253 T254 P255 R256 A257 P258 Q259 L260 V261 I265 D271 G272

I273 L274 C275 N276 T277 T285 R292 D296 K297 A298 T299 V300 K306 G307 G308 K309 R310 K311 D312 S313 V314 W315 G316 S317 G318

• Molecule 2: Programmed cell death protein 4

Chain B: 60% 29% • 8%

G319 G320 Q321 Q322 P323 V324 N325 H326 L327 V328 K329 L334 L335 K336 E337 Y338 L339 L340 I344 S345 E348 H349 C350 L351 K352 E353 L354 E355 V356 P357 H358 H361 E362 L363 V364 Y365 E366 A367 I368 T375 S378 M382 L387 K388 S389 L390 W391 K392 D399 Q400

Y405 E406 R407 I408 Y409 N410 E411 R428 F429 V430 E431 F434 I438 I439 S440 K441 R444 S449

4.2.55 Score per residue for model 55

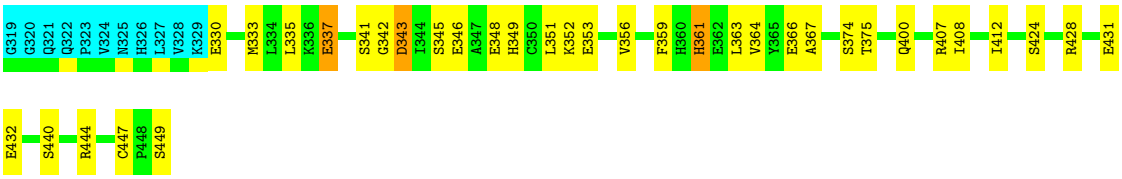
• Molecule 1: Programmed cell death protein 4

Chain A: 74% 15% • 8%

G156 D160 A163 T167 T181 E195 M196 L207 S214 H215 K221 L222 L223 S224 C227 M231 S232 T233 T234 D235 K238 R256 I273 Y278 T285 V286 D287 D296 K297 L301 M304 S305 K306 G307 G308 K309 R310 K311 D312 S313 V314 W315

• Molecule 2: Programmed cell death protein 4

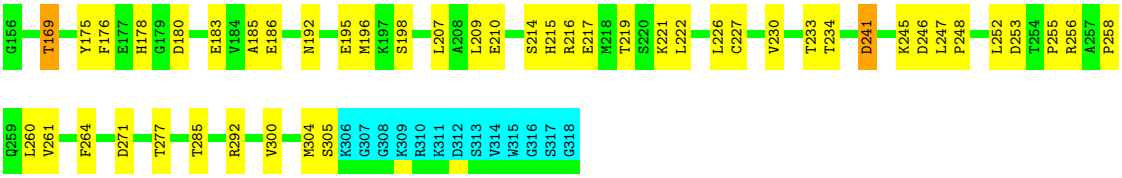
Chain B:



4.2.56 Score per residue for model 56

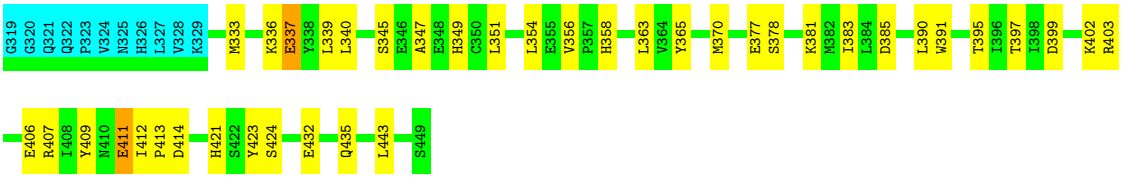
• Molecule 1: Programmed cell death protein 4

Chain A:



• Molecule 2: Programmed cell death protein 4

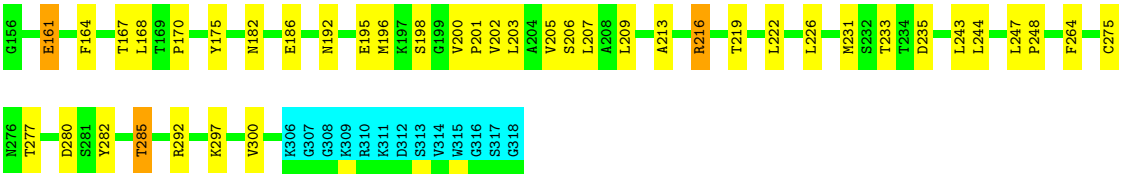
Chain B:



4.2.57 Score per residue for model 57

• Molecule 1: Programmed cell death protein 4

Chain A:



• Molecule 2: Programmed cell death protein 4

Chain B: 58% 29% 5% 8%

G319 G320 Q321 Q322 P323 V324 N325 H326 L327 V328 K329 E330 I331 D332 M333 L334 E337 L340 S341 G342 D343 I344 A347 E348 H349 C350 E353 V356 P357 H358 F359 H360 H361 T375 S378 K381 D385 K388 S393 S394 T395 I398 Y405 E406 R407 I408 Y409

I412 P413 D414 S422 Y423 S424 E427 R428 F429 V430 E431 E432 C433 F434 I438 I439 Q442 C447 P448 S449

4.2.58 Score per residue for model 58

- Molecule 1: Programmed cell death protein 4

Chain A: 75% 17% • 8%

G156 D160 D190 L191 N192 L193 G194 E195 M196 E210 S214 S224 D225 T233 T234 D235 V236 E237 K238 D246 L247 P248 E249 T254 D271 T277 D280 K283 G284 T285 R292 V300 L301 M304 S305 K306 G307 G308 K309 R310 K311 D312 S313 V314 W315

G316 S317 G318

- Molecule 2: Programmed cell death protein 4

Chain B: 69% 21% • 8%

G319 G320 Q321 Q322 P323 V324 N325 H326 L327 V328 K329 E330 I331 K336 L340 E348 E353 L354 F359 L363 V364 Y365 T375 A379 I383 L386 L390 T395 I396 T397 Y405 E406 R407 I408 Y409 N410 E411 I412 H421 S422 Y423 S424 V425 L426 E427

V430 C447 P448 S449

4.2.59 Score per residue for model 59

- Molecule 1: Programmed cell death protein 4

Chain A: 64% 27% • 8%

G156 L159 D160 E161 F164 E174 H178 T181 E195 S198 G199 V200 P201 E210 S214 T219 S220 K221 L222 T233 T234 E237 F240 L244 K245 D246 L247 L250 T254 A257 V261 F264 A268 D271 L274 T277 Y278

I279 D280 S281 Y282 K283 G284 T285 V286 D287 C288 A291 R292 L295 V300 L301 L302 S303 M304 S305 K306 G307 G308 K309 R310 K311 D312 S313 V314 W315 G316 S317 G318

- Molecule 2: Programmed cell death protein 4

Chain B: 68% 21% • 8%

G319 G320 Q321 Q322 P323 V324 N325 H326 L327 V328 K329 D332 M333 L334 L335 K336 E337 Y338 L339 L340 I344 F359 H360 H361 E362 E373 S378 L384 L387 K388 S389 L390 W391 K392 S393 Q400 G404 Y405 E406 Y409 N416 Y423 S424 E427 S440

S449

4.2.60 Score per residue for model 60

- Molecule 1: Programmed cell death protein 4

Chain A: 67% 25% • 8%

G156 D160 A163 H178 T181 N182 E186 N192 E195 M196 K197 P201 V205 A213 S214 H215 R216 L222 D225 M231 S232 T233 T234 D235 K238 D246 E249 L250 A251 P255 R256 A257 P258 Q259 L260 V261 F264 R267 T277

T285 V286 D287 C288 A291 R292 L295 D296 V300 M304 S305 K306 G307 G308 K309 R310 K311 D312 S313 V314 W315 G316 S317 G318

- Molecule 2: Programmed cell death protein 4

Chain B: 71% 19% • 8%

G319 G320 Q321 Q322 P323 V324 N325 H326 L327 V328 K329 E330 I331 D332 M333 E337 L340 S345 E346 E353 L363 V371 S374 L386 L387 K388 S389 L390 W391 K392 S393 I398 D399 G404 I408 I412 P413 H421 S422 Y423 S424 S440 R444 S449

4.2.61 Score per residue for model 61

- Molecule 1: Programmed cell death protein 4

Chain A: 63% 28% • 8%

G156 T167 L168 T169 P170 I171 I172 Q173 E174 Y175 H178 G179 D180 T181 A185 R189 D190 L191 N192 L193 G194 E195 K196 K197 V200 P201 S214 T219 S220 K221 D225 L226 C227 V230 M231 S232 T233 T234 D235 K238 S239 F240 D241 K245 T254 P255 R256 A257

P258 I265 A266 R267 A268 V269 G270 D271 L274 C275 N276 T277 T285 C288 V289 M304 S305 K306 G307 G308 K309 R310 K311 D312 S313 V314 W315 G316 S317 G318

- Molecule 2: Programmed cell death protein 4

Chain B: 60% 30% • 8%

G319 G320 Q321 Q322 P323 V324 N325 H326 L327 V328 K329 M333 L340 S345 E346 A347 E348 H349 C350 L351 K352 E353 L354 E355 V356 F359 H360 H361 E362 L363 I368 V369 M370 T375 S378 A379 F380 L384 L387 W391 K392 S393 S394 T395 I396 T397 R403 G404

I408 I412 P413 D414 I415 N416 P420 H421 S422 Y423 S424 E427 Q435 S440 S449

4.2.62 Score per residue for model 62

- Molecule 1: Programmed cell death protein 4

Chain A: 66% 26% • 8%

G156 L157 P158 L159 D160 A163 F164 T169 E174 E177 H178 G179 D190 L193 G194 E195 M196 V200 L203 L207 A208 L209 S214 T219 S220 K221 D225 T233 T234 L247 P248 E249 T254 P255 R256 A257 P258 Q259 G262 Q263 R267 L274

C275 T285 R292 K297 V300 L301 L302 S303 M304 S305 K306 G307 G308 K309 R310 K311 D312 S313 V314 W315 G316 S317 G318

• Molecule 2: Programmed cell death protein 4

Chain B: 64% 25% • 8%

G319 G320 Q321 Q322 P323 V324 N325 H326 L327 V328 K329 E330 M333 L334 L335 K336 E337 L340 S341 G342 S345 H349 C350 L354 E355 V356 F359 H360 H361 V364 A367 T375 S378 L387 L390 T395 Y405 E406 R407 I408 E411 I412 H421 S422

Y423 S424 R428 F429 V430 E431 S440 L446 S449

4.2.63 Score per residue for model 63

• Molecule 1: Programmed cell death protein 4

Chain A: 66% 23% • 8%

G156 E161 E165 L168 T169 P170 I171 I172 T181 N182 E186 M196 V200 L203 S214 H215 R216 S220 K221 S224 D225 T233 T234 D235 V236 E237 K238 K242 L243 L244 K245 D246 L247 P248 R256 Q259 L260 V261 R267 D271 G272 I273

T277 D280 K283 G284 T285 R292 V300 S303 M304 S305 K306 G307 G308 K309 R310 K311 D312 S313 V314 W315 G316 S317 G318

• Molecule 2: Programmed cell death protein 4

Chain B: 66% 24% • 8%

G319 G320 Q321 Q322 P323 V324 N325 H326 L327 V328 K329 E330 I331 D332 M333 L334 E337 Y338 L339 L340 S345 C350 V356 H361 E362 L363 V364 I368 E373 S374 T375 S378 L386 S389 K392 S393 S394 T397 E406 R407 I408 Y409 I412 P413 Y423

S424 S440 K441 Q442 L446 S449

4.2.64 Score per residue for model 64

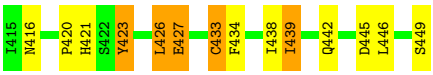
• Molecule 1: Programmed cell death protein 4

Chain A: 61% 27% • 8%

G156 R162 T167 L168 T169 P170 I171 I172 Q173 E177 H178 E183 D190 L191 N192 E195 S198 G199 V200 L203 S206 L207 A208 L209 E210 A213 S214 H215 R216 T219 S220 K221 V230 T233 E237 D241 D246 L247 P248 E249 D253 A257

• Molecule 2: Programmed cell death protein 4

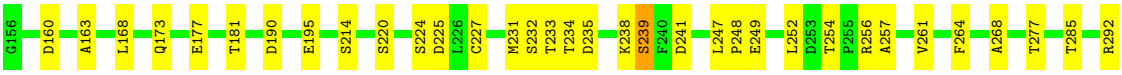
Chain B:

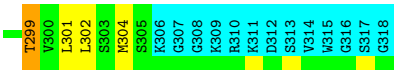


4.2.65 Score per residue for model 65

• Molecule 1: Programmed cell death protein 4

Chain A:





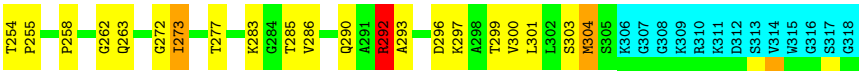
• Molecule 2: Programmed cell death protein 4

Chain B:

4.2.66 Score per residue for model 66

• Molecule 1: Programmed cell death protein 4

Chain A:



• Molecule 2: Programmed cell death protein 4

Chain B: 63% 25% • 8%

G319 G320 Q321 Q322 P323 V324 N325 H326 L327 V328 K329 D332 L335 K336 L340 S345 E355 H360 A367 I368 T375 G376 E377 S378 A379 F380 I383 L384 L387 K388 S389 K392 D399 K402 Y405 E406 R407 I408 Y409 N410 E411 I412 N416 S422

F429 V430 A436 I439 L443 C447 P448 S449

4.2.67 Score per residue for model 67

• Molecule 1: Programmed cell death protein 4

Chain A: 69% 21% • 8%

G156 D160 A163 T169 P170 E174 V184 D190 L193 G194 E195 M196 K197 S198 G199 L209 S214 H215 R216 L222 L223 S224 D225 D235 V236 E237 K238 S239 F240 P248 T254 P255 R256 D271 T277 D280 K283 G284 T285 Q290 D296

K297 A298 T299 V300 L301 M304 S305 K306 G307 G308 K309 R310 K311 D312 S313 V314 W315 G316 S317 G318

• Molecule 2: Programmed cell death protein 4

Chain B: 70% 18% • 8%

G319 G320 Q321 Q322 P323 V324 N325 H326 L327 V328 K329 E330 Y338 L339 L340 S341 I344 S345 E346 L354 H361 E377 S378 K381 L387 K388 S389 K392 D399 Q400 E406 R407 I408 Y409 N410 E411 I412 P413 D414 H421 S422 Y423 C433 F434 K441 S449

4.2.68 Score per residue for model 68

• Molecule 1: Programmed cell death protein 4

Chain A: 60% 29% • 8%

G156 L157 P158 L159 D160 E161 E165 K166 T167 L168 T169 P170 I171 Y175 F176 E177 H178 T181 N182 E186 M187 L188 L191 N192 E195 M196 K197 S198 G199 V200 P201 K212 A213 S214 H215 L222 D225 L226 C227 S232 T233 T234 D235 K238 D241 E249

T254 A257 P258 Q259 Q263 R267 D271 T277 Y278 I279 D280 K283 G284 T285 A291 R292 L295 D296 K297 K306 G307 G308 K309 R310 K311 D312 S313 V314 W315 G316 S317 G318

• Molecule 2: Programmed cell death protein 4

Chain B: 60% 24% 7% 8%

G319 G320 Q321 Q322 P323 V324 N325 H326 L327 V328 K329 E330 G342 E348 H349 C350 L351 K352 E353 L354 E355 V356 P357 H358 F359 H360 H361 S378 M382 I383 L384 D385 L386 L387 K388 S389 L390 W391 K392 S393 S394 T395 D399 Q400 M401 K402 R407 E411 D414 D418

S424 R428 F429 V430 E431 I438 I439 Q442 L443 C447 P448 S449

4.2.69 Score per residue for model 69

- Molecule 1: Programmed cell death protein 4

Chain A: 71% 21% 8%

G156 D160 I171 E174 Y175 T181 N182 E183 E186 M187 N192 E195 M196 S214 H215 T219 S220 K221 S224 T233 T234 D235 V236 E237 K238 D241 D253 R256 A257 P258 Q259 L260 D271 T277 T285 R292 V300 L301 M304 S305

K306 G307 G308 K309 R310 K311 D312 S313 V314 W315 G316 S317 G318

- Molecule 2: Programmed cell death protein 4

Chain B: 59% 31% • 8%

G319 G320 Q321 Q322 P323 V324 N325 H326 L327 V328 K329 L334 E337 Y338 L339 L340 S341 G342 D343 I344 S345 E346 C350 F359 H360 H361 I368 V371 S378 K381 M382 I383 L384 D385 L386 L387 K388 S389 K392 T397 Y405 E406 R407 I408 Y409 N410 E411 I412 P413

D414 D418 H421 S422 Y423 C433 F434 Q435 I438 I439 R444 S449

4.2.70 Score per residue for model 70

- Molecule 1: Programmed cell death protein 4

Chain A: 66% 25% • 8%

G156 L157 P158 L159 D160 A163 P170 E174 T181 E195 M196 V200 P201 K212 A213 S214 H215 R216 E217 S224 M231 S232 T233 T234 D235 V236 E237 K238 S239 L243 L247 P248 A251 R256 A257 P258 V261 F264 I265 A266 R267 A268 I273

T277 T285 D296 T299 V300 L301 L302 S303 M304 S305 K306 G307 G308 K309 R310 K311 D312 S313 V314 W315 G316 S317 G318

- Molecule 2: Programmed cell death protein 4

Chain B: 61% 27% • 8%

G319 G320 Q321 Q322 P323 V324 N325 H326 L327 V328 K329 E330 M333 L334 L335 K336 E337 Y338 L339 L340 S341 G342 D343 I344 S345 E346 A347 E348 H349 C350 E353 L354 E355 V356 F359 H360 H361 S378 I383 L386 L390 S394 T395 D399 R407 I408 E411 I412

N416 P420 H421 S422 Y423 S424 R428 E431 F434 I439 S440 D445 S449

4.2.71 Score per residue for model 71

- Molecule 1: Programmed cell death protein 4

Chain A: 67% 23% • 8%

G156 T169 G179 D180 T181 L188 L191 E195 M196 V200 P201 S214 S220 K221 L222 L226 C227 S232 T233 T234 D235 D241 D246 T254 P255 R256 A257 P258 Q259 L260 Q263 N276 T277 Y278 I279 D280 K283 G284 T285 V286 D287 A291 R292

L295 V300 L301 S305 K306 G307 G308 K309 R310 K311 D312 S313 V314 W315 G316 S317 G318

• Molecule 2: Programmed cell death protein 4

Chain B: 66% 24% • 8%

G319 G320 Q321 Q322 P323 V324 N325 H326 L327 V328 K329 Y338 L339 L340 S341 G342 S345 K352 E353 L354 H361 I368 V369 M370 E377 S378 A379 F380 L384 D385 L386 S389 L390 W391 K392 I398 K402 I408 D414 D418 S422 Y423 S424 E427

E432 Q435 S440 K441 Q442 L443 R444 D445 L446 S449

4.2.72 Score per residue for model 72

• Molecule 1: Programmed cell death protein 4

Chain A: 59% 27% 6% 8%

G156 F164 L168 F176 N182 E186 L193 G194 E195 M196 V200 L203 A204 V205 S206 L207 E210 S214 H215 R216 T219 S220 K221 L222 L223 S224 D225 L226 T229 T233 T234 D235 K238 D241 K242 K245 D246 E249 L250 A251 L252 D253 T254

Q263 A268 V269 I273 L274 T277 Y282 T285 V286 D287 C288 V289 Q290 D296 T299 V300 L301 S305 K306 G307 G308 K309 R310 K311 D312 S313 V314 W315 G316 S317 G318

• Molecule 2: Programmed cell death protein 4

Chain B: 60% 29% • 8%

G319 G320 Q321 Q322 P323 V324 N325 H326 L327 V328 K329 E330 I331 D332 M333 L334 E337 L340 E348 H349 C350 L351 K352 E353 L354 E355 H358 F359 H360 H361 E362 L363 E366 V369 E373 S374 T375 S378 K381 M382 L387 K388 S389 K392 T395 I396 T397

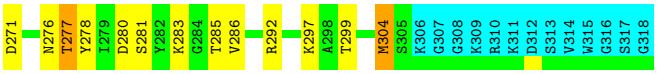
Q400 I408 I412 P413 D414 I415 N416 L426 V430 F434 Q435 A436 I439 S440 L443 S449

4.2.73 Score per residue for model 73

• Molecule 1: Programmed cell death protein 4

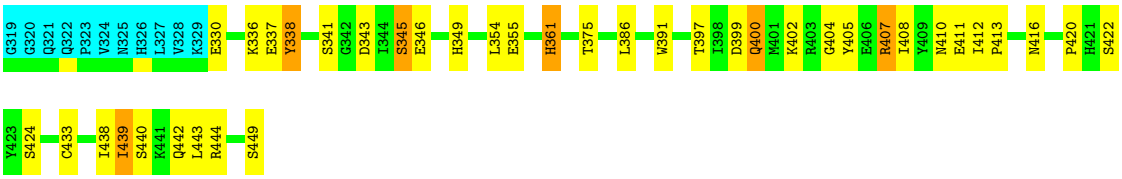
Chain A: 62% 28% • 8%

G156 D160 A163 T167 L168 T169 I172 G179 V184 L188 E195 M196 V200 P201 V202 L203 A204 V205 S206 E210 S214 H215 R216 K221 S224 V230 T233 L244 K245 D246 L247 P248 E249 L250 A251 L252 A257 P258 Q259 L260 R267



• Molecule 2: Programmed cell death protein 4

Chain B:



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *HADDOCK*.

Of the 200 calculated structures, 73 were deposited, based on the following criterion: *acceptable RMSD to lowest HADDOCK score structure*.

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

Software name	Classification	Version
HADDOCK	refinement	2.0
X-PLOR NIH	refinement	

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) 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	0.31±0.02	0±0/1152 (0.0± 0.0%)	0.49±0.04	0±0/1560 (0.0± 0.0%)
2	B	0.30±0.02	0±0/995 (0.0± 0.0%)	0.48±0.05	0±0/1342 (0.0± 0.0%)
All	All	0.30	0/156731 (0.0%)	0.49	1/211846 (0.0%)

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

Mol	Chain	Chirality	Planarity
2	B	0.0±0.1	0.0±0.0
All	All	1	0

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	385	ASP	N-CA-CB	5.01	119.61	110.60	47	1

All unique chiral outliers are listed below.

Mol	Chain	Res	Type	Atoms	Models (Total)
2	B	371	VAL	CA	1

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	1137	248	1155	15±4
2	B	976	200	970	13±4
All	All	154249	32704	155125	1872

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 6.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:304:MET:HG2	2:B:333:MET:HA	0.96	1.37	53	1
1:A:160:ASP:HB3	1:A:163:ALA:HB3	0.89	1.45	73	14
1:A:254:THR:HB	1:A:257:ALA:HB2	0.86	1.45	59	26
1:A:304:MET:SD	2:B:333:MET:HA	0.86	2.11	50	20
2:B:389:SER:HA	2:B:392:LYS:HE2	0.83	1.49	53	13
1:A:300:VAL:HG11	2:B:337:GLU:HA	0.82	1.50	63	16
1:A:280:ASP:HA	1:A:283:LYS:HD3	0.82	1.51	16	7
1:A:300:VAL:HB	2:B:336:LYS:HB3	0.82	1.51	35	4
1:A:300:VAL:HG13	2:B:340:LEU:HB2	0.82	1.52	66	14
1:A:300:VAL:HG21	2:B:337:GLU:HA	0.81	1.51	34	1
1:A:236:VAL:HG11	1:A:273:ILE:HB	0.81	1.50	63	6
1:A:247:LEU:HD23	1:A:291:ALA:HA	0.80	1.52	18	1
2:B:389:SER:HA	2:B:392:LYS:HE3	0.80	1.51	7	13
1:A:235:ASP:HA	1:A:238:LYS:HE2	0.80	1.53	34	5
2:B:334:LEU:HD21	2:B:350:CYS:HB2	0.78	1.55	4	11
2:B:402:LYS:HG3	2:B:443:LEU:HD13	0.78	1.55	56	12
1:A:300:VAL:HG22	2:B:340:LEU:HB3	0.78	1.55	36	7
1:A:193:LEU:HB3	1:A:196:MET:HB3	0.77	1.55	67	4
2:B:361:HIS:HB3	2:B:400:GLN:HA	0.76	1.58	64	1
1:A:268:ALA:HB1	1:A:274:LEU:HB3	0.76	1.56	53	3
1:A:235:ASP:HA	1:A:238:LYS:HE3	0.76	1.58	55	43
1:A:247:LEU:HD21	1:A:258:PRO:HA	0.76	1.58	35	5
1:A:300:VAL:HG13	2:B:340:LEU:HD12	0.76	1.57	30	14
2:B:428:ARG:HA	2:B:431:GLU:HG2	0.75	1.58	70	13
1:A:243:LEU:O	1:A:247:LEU:HB2	0.75	1.82	63	2
1:A:256:ARG:HH21	2:B:346:GLU:HA	0.74	1.41	55	3
2:B:434:PHE:HA	2:B:439:ILE:HD11	0.74	1.56	70	9
1:A:304:MET:HB3	2:B:333:MET:HG2	0.73	1.59	53	3
2:B:349:HIS:O	2:B:353:GLU:HG3	0.73	1.84	55	2
2:B:430:VAL:O	2:B:434:PHE:HB2	0.72	1.85	41	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:434:PHE:HA	2:B:439:ILE:HG12	0.72	1.59	72	1
2:B:360:HIS:HB2	2:B:400:GLN:HG3	0.71	1.60	65	1
1:A:188:LEU:HD21	1:A:200:VAL:HG21	0.71	1.61	1	5
2:B:385:ASP:HA	2:B:388:LYS:HE3	0.71	1.61	21	8
1:A:200:VAL:HB	1:A:201:PRO:HD3	0.70	1.62	47	12
1:A:247:LEU:HD11	1:A:261:VAL:HG21	0.70	1.62	26	10
2:B:423:TYR:O	2:B:427:GLU:HB2	0.70	1.86	64	2
1:A:263:GLN:HA	1:A:301:LEU:HD13	0.70	1.63	22	8
1:A:248:PRO:HG3	1:A:290:GLN:HG3	0.70	1.64	67	1
2:B:335:LEU:HD22	2:B:367:ALA:HB2	0.69	1.63	62	5
1:A:221:LYS:HA	1:A:221:LYS:HE2	0.69	1.64	48	3
2:B:427:GLU:O	2:B:431:GLU:HG2	0.69	1.88	57	2
1:A:286:VAL:HG11	1:A:291:ALA:HB3	0.69	1.65	40	10
2:B:399:ASP:O	2:B:403:ARG:HD3	0.69	1.88	65	4
2:B:366:GLU:O	2:B:370:MET:HG2	0.68	1.89	6	1
2:B:384:LEU:HG	2:B:429:PHE:HE1	0.68	1.46	30	1
1:A:172:ILE:HG21	1:A:204:ALA:HA	0.68	1.66	22	3
1:A:203:LEU:HG	1:A:207:LEU:HG	0.67	1.65	66	1
2:B:351:LEU:HD23	2:B:390:LEU:HD11	0.67	1.66	68	1
1:A:266:ALA:HB1	1:A:302:LEU:HG	0.67	1.66	70	1
1:A:247:LEU:HD11	1:A:258:PRO:HA	0.66	1.68	62	4
1:A:236:VAL:HG11	1:A:273:ILE:HG22	0.66	1.68	17	4
2:B:439:ILE:HB	2:B:443:LEU:HD23	0.66	1.66	72	3
2:B:390:LEU:HB3	2:B:395:THR:HB	0.65	1.69	38	8
1:A:169:THR:HB	1:A:170:PRO:HD3	0.65	1.68	52	11
1:A:286:VAL:HG21	1:A:292:ARG:HG3	0.65	1.68	66	1
2:B:366:GLU:HA	2:B:369:VAL:HG22	0.65	1.67	35	1
1:A:222:LEU:HA	1:A:225:ASP:HB2	0.65	1.69	66	1
1:A:203:LEU:O	1:A:207:LEU:HB2	0.65	1.92	57	2
1:A:256:ARG:NH2	2:B:346:GLU:HA	0.64	2.05	55	1
2:B:384:LEU:O	2:B:388:LYS:HG3	0.64	1.93	47	1
1:A:300:VAL:HG11	2:B:337:GLU:HG2	0.64	1.70	34	1
2:B:378:SER:HA	2:B:381:LYS:HE2	0.64	1.70	67	6
2:B:361:HIS:HB3	2:B:400:GLN:HG3	0.64	1.69	18	1
1:A:296:ASP:HB3	2:B:340:LEU:HD21	0.64	1.70	54	1
1:A:304:MET:SD	2:B:336:LYS:HG3	0.63	2.34	73	1
1:A:255:PRO:O	1:A:258:PRO:HD2	0.63	1.94	13	5
1:A:261:VAL:HA	1:A:264:PHE:HD2	0.63	1.52	53	5
2:B:350:CYS:HA	2:B:353:GLU:HB2	0.63	1.70	68	1
1:A:300:VAL:HG22	2:B:340:LEU:HD12	0.63	1.71	4	2
1:A:251:ALA:HB2	1:A:258:PRO:HD3	0.63	1.71	32	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:300:VAL:HG22	2:B:340:LEU:HD23	0.63	1.70	60	1
2:B:361:HIS:HB3	2:B:400:GLN:HB3	0.63	1.70	72	1
1:A:250:LEU:H	1:A:250:LEU:HD23	0.63	1.54	53	2
2:B:391:TRP:HZ2	2:B:398:ILE:HB	0.63	1.53	60	1
1:A:289:VAL:HG13	1:A:290:GLN:H	0.63	1.53	72	1
2:B:337:GLU:O	2:B:341:SER:HB2	0.63	1.94	62	6
1:A:262:GLY:HA3	1:A:297:LYS:HB3	0.63	1.69	66	4
2:B:377:GLU:HA	2:B:380:PHE:CB	0.63	2.24	66	1
2:B:407:ARG:O	2:B:411:GLU:HG2	0.63	1.92	69	51
1:A:231:MET:HG3	1:A:235:ASP:HB3	0.63	1.70	6	2
2:B:334:LEU:HD22	2:B:347:ALA:HA	0.62	1.69	53	8
2:B:405:TYR:HE2	2:B:430:VAL:HG22	0.62	1.53	46	1
1:A:259:GLN:HG2	2:B:346:GLU:HG2	0.62	1.70	40	1
2:B:356:VAL:HB	2:B:359:PHE:HB2	0.62	1.70	34	3
2:B:434:PHE:HE1	2:B:441:LYS:HA	0.61	1.55	36	6
2:B:364:VAL:HG11	2:B:401:MET:HG3	0.61	1.72	21	6
1:A:256:ARG:O	1:A:260:LEU:HG	0.61	1.95	30	12
1:A:205:VAL:HG13	1:A:209:LEU:HD12	0.61	1.72	47	1
1:A:237:GLU:HG3	1:A:274:LEU:HD12	0.61	1.72	10	3
1:A:213:ALA:HA	1:A:216:ARG:HD2	0.61	1.71	9	13
1:A:227:CYS:HA	1:A:231:MET:O	0.61	1.96	55	12
1:A:247:LEU:N	1:A:248:PRO:HD2	0.61	2.11	63	17
1:A:257:ALA:O	1:A:261:VAL:HG23	0.61	1.96	51	13
2:B:333:MET:O	2:B:337:GLU:HB2	0.61	1.96	55	7
2:B:388:LYS:HA	2:B:391:TRP:HB2	0.60	1.71	4	1
1:A:249:GLU:O	1:A:252:LEU:HG	0.60	1.95	21	1
1:A:206:SER:O	1:A:209:LEU:HB3	0.60	1.96	34	1
2:B:432:GLU:HA	2:B:435:GLN:HE21	0.60	1.55	35	3
1:A:259:GLN:NE2	2:B:346:GLU:HA	0.60	2.12	41	2
1:A:282:TYR:HD2	1:A:286:VAL:HG22	0.60	1.56	17	1
1:A:164:PHE:HZ	1:A:200:VAL:HG22	0.60	1.57	40	3
2:B:331:ILE:HG23	2:B:363:LEU:HA	0.60	1.73	21	6
2:B:361:HIS:HB2	2:B:400:GLN:HG3	0.60	1.73	44	5
2:B:365:TYR:HE1	2:B:411:GLU:HG3	0.60	1.56	56	8
1:A:216:ARG:HB3	1:A:264:PHE:HZ	0.60	1.56	18	4
2:B:438:ILE:HG13	2:B:439:ILE:H	0.60	1.56	21	5
2:B:330:GLU:O	2:B:334:LEU:HG	0.60	1.97	45	11
2:B:338:TYR:CE1	2:B:344:ILE:HG12	0.60	2.32	20	3
2:B:338:TYR:HA	2:B:342:GLY:HA2	0.60	1.74	34	2
1:A:300:VAL:CG1	2:B:337:GLU:HA	0.60	2.27	63	4
1:A:235:ASP:HA	1:A:238:LYS:CE	0.59	2.26	18	13

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:331:ILE:HG23	2:B:363:LEU:HG	0.59	1.73	72	1
1:A:245:LYS:O	1:A:248:PRO:HD2	0.59	1.96	54	6
2:B:390:LEU:H	2:B:390:LEU:HD23	0.59	1.57	68	1
1:A:169:THR:HA	1:A:172:ILE:HD12	0.59	1.74	34	1
1:A:205:VAL:HG23	1:A:206:SER:H	0.59	1.57	42	1
1:A:298:ALA:HA	1:A:301:LEU:HD12	0.59	1.74	16	6
2:B:345:SER:HA	2:B:348:GLU:HB3	0.59	1.72	13	3
2:B:337:GLU:HG2	2:B:347:ALA:HB2	0.59	1.74	24	2
1:A:158:PRO:HB3	1:A:196:MET:SD	0.59	2.38	68	3
1:A:240:PHE:HE1	1:A:265:ILE:HG12	0.59	1.58	31	1
2:B:385:ASP:O	2:B:389:SER:HB2	0.59	1.97	48	3
1:A:251:ALA:HB1	1:A:258:PRO:HD3	0.59	1.71	66	1
2:B:343:ASP:HB3	2:B:346:GLU:HB2	0.59	1.74	24	6
1:A:304:MET:SD	2:B:336:LYS:HB2	0.59	2.37	70	7
1:A:172:ILE:O	1:A:175:TYR:HB3	0.59	1.98	61	7
2:B:389:SER:HA	2:B:392:LYS:HD2	0.59	1.75	8	3
1:A:193:LEU:HD13	1:A:196:MET:HB3	0.58	1.75	3	5
2:B:432:GLU:HA	2:B:435:GLN:NE2	0.58	2.13	71	1
1:A:247:LEU:HD12	1:A:250:LEU:HD12	0.58	1.75	73	1
1:A:268:ALA:HA	1:A:273:ILE:HD12	0.58	1.74	72	2
2:B:444:ARG:HD2	2:B:447:CYS:SG	0.58	2.37	20	1
1:A:198:SER:O	1:A:201:PRO:HD2	0.58	1.99	57	4
1:A:304:MET:SD	2:B:337:GLU:HG3	0.58	2.38	15	1
2:B:371:VAL:HG11	2:B:380:PHE:CD1	0.58	2.34	29	1
1:A:304:MET:SD	2:B:336:LYS:HE2	0.58	2.38	44	2
2:B:377:GLU:HA	2:B:380:PHE:HB3	0.58	1.76	66	1
2:B:338:TYR:CE2	2:B:386:LEU:HB2	0.58	2.34	63	8
1:A:251:ALA:HB2	1:A:258:PRO:HG3	0.58	1.76	24	7
1:A:291:ALA:O	1:A:295:LEU:HG	0.58	1.98	59	5
2:B:362:GLU:O	2:B:366:GLU:HB2	0.58	1.99	8	1
1:A:182:ASN:O	1:A:186:GLU:HG2	0.58	1.99	43	21
2:B:386:LEU:O	2:B:390:LEU:HG	0.58	1.99	24	17
2:B:364:VAL:HG11	2:B:401:MET:HA	0.58	1.76	25	2
2:B:338:TYR:HD2	2:B:386:LEU:HB2	0.58	1.58	73	2
1:A:301:LEU:HA	1:A:304:MET:SD	0.58	2.39	69	3
2:B:349:HIS:O	2:B:353:GLU:HG2	0.57	1.99	36	1
1:A:300:VAL:HG21	2:B:337:GLU:HG2	0.57	1.76	6	1
2:B:348:GLU:HA	2:B:390:LEU:HD23	0.57	1.76	4	1
1:A:282:TYR:HB3	1:A:295:LEU:HD13	0.57	1.75	33	1
1:A:188:LEU:HD21	1:A:200:VAL:HG11	0.57	1.75	39	1
1:A:304:MET:HG2	2:B:336:LYS:HE2	0.57	1.77	50	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:160:ASP:HB3	1:A:163:ALA:CB	0.57	2.28	73	2
1:A:168:LEU:HB3	1:A:203:LEU:HD23	0.57	1.77	73	1
1:A:247:LEU:HD13	1:A:261:VAL:HG21	0.57	1.77	3	8
2:B:368:ILE:HD12	2:B:408:ILE:HG13	0.57	1.77	61	1
1:A:256:ARG:HD2	2:B:349:HIS:CB	0.57	2.28	36	1
2:B:412:ILE:HB	2:B:413:PRO:HD3	0.56	1.76	5	23
1:A:283:LYS:HB3	1:A:283:LYS:NZ	0.56	2.16	7	4
2:B:368:ILE:O	2:B:371:VAL:HG23	0.56	1.99	22	1
1:A:175:TYR:HE2	1:A:219:THR:HA	0.56	1.61	69	1
2:B:384:LEU:O	2:B:387:LEU:HG	0.56	2.01	11	5
2:B:371:VAL:HG22	2:B:383:ILE:HG13	0.56	1.78	50	2
2:B:412:ILE:HG13	2:B:426:LEU:HD11	0.56	1.78	31	2
1:A:263:GLN:HA	1:A:301:LEU:HD11	0.56	1.77	64	1
2:B:408:ILE:O	2:B:412:ILE:HG12	0.56	2.01	44	31
2:B:425:VAL:O	2:B:429:PHE:HB3	0.56	2.00	21	1
1:A:297:LYS:O	1:A:300:VAL:HB	0.56	2.01	24	3
2:B:388:LYS:O	2:B:391:TRP:HB2	0.56	2.01	68	2
2:B:447:CYS:HB2	2:B:448:PRO:HD2	0.56	1.78	57	2
2:B:345:SER:O	2:B:348:GLU:HB2	0.56	2.01	36	1
2:B:378:SER:O	2:B:382:MET:HB2	0.56	2.00	46	5
2:B:384:LEU:HD21	2:B:432:GLU:HG2	0.56	1.76	7	1
1:A:268:ALA:HB1	1:A:273:ILE:HB	0.56	1.76	13	2
2:B:371:VAL:HG11	2:B:380:PHE:HA	0.56	1.77	44	1
2:B:347:ALA:HA	2:B:350:CYS:SG	0.56	2.41	57	1
1:A:296:ASP:HB3	2:B:340:LEU:CD1	0.56	2.31	67	1
2:B:384:LEU:HG	2:B:429:PHE:CE1	0.56	2.32	30	1
1:A:178:HIS:N	1:A:178:HIS:CD2	0.56	2.74	66	1
1:A:293:ALA:O	1:A:297:LYS:HB2	0.55	2.00	21	1
1:A:205:VAL:HG12	1:A:219:THR:CG2	0.55	2.32	42	1
2:B:378:SER:O	2:B:381:LYS:HG2	0.55	2.01	44	2
2:B:443:LEU:HA	2:B:446:LEU:HD12	0.55	1.79	15	1
1:A:209:LEU:HA	1:A:216:ARG:HD3	0.55	1.77	21	1
2:B:387:LEU:O	2:B:391:TRP:HB2	0.55	2.01	22	3
1:A:168:LEU:HD13	1:A:171:ILE:HD12	0.55	1.79	22	1
1:A:181:THR:HG21	1:A:225:ASP:HB2	0.55	1.78	47	2
2:B:356:VAL:HB	2:B:359:PHE:CB	0.55	2.31	6	1
2:B:361:HIS:H	2:B:400:GLN:HG3	0.55	1.62	36	2
1:A:193:LEU:HB3	1:A:196:MET:HB2	0.55	1.77	66	1
1:A:248:PRO:HA	1:A:290:GLN:HG3	0.55	1.77	3	4
1:A:204:ALA:O	1:A:208:ALA:HB2	0.55	2.02	53	1
1:A:185:ALA:HB2	1:A:226:LEU:HD22	0.55	1.77	56	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:356:VAL:HG23	2:B:359:PHE:HB2	0.55	1.79	62	1
2:B:439:ILE:HG21	2:B:443:LEU:HD22	0.55	1.77	73	1
1:A:263:GLN:HA	1:A:301:LEU:CD1	0.54	2.32	15	4
1:A:297:LYS:O	1:A:301:LEU:HG	0.54	2.02	32	5
2:B:332:ASP:O	2:B:336:LYS:HG2	0.54	2.01	59	4
1:A:236:VAL:HG21	1:A:273:ILE:HB	0.54	1.77	21	1
1:A:297:LYS:NZ	2:B:346:GLU:HG3	0.54	2.18	22	1
1:A:298:ALA:O	1:A:302:LEU:HG	0.54	2.02	53	1
2:B:447:CYS:SG	2:B:448:PRO:HD2	0.54	2.42	68	3
2:B:365:TYR:CE1	2:B:411:GLU:HG3	0.54	2.37	11	5
1:A:286:VAL:HG12	1:A:288:CYS:H	0.54	1.62	30	18
2:B:365:TYR:O	2:B:369:VAL:HG23	0.54	2.01	2	7
1:A:265:ILE:HG21	1:A:279:ILE:HD11	0.54	1.78	31	3
2:B:404:GLY:O	2:B:408:ILE:HG12	0.54	2.03	24	10
1:A:259:GLN:O	1:A:297:LYS:HG2	0.54	2.03	68	5
1:A:263:GLN:O	1:A:267:ARG:HB2	0.54	2.02	62	3
1:A:280:ASP:HA	1:A:283:LYS:HB2	0.54	1.77	48	9
2:B:358:HIS:HA	2:B:400:GLN:NE2	0.54	2.18	68	2
2:B:433:CYS:HB2	2:B:438:ILE:HD11	0.54	1.79	64	3
1:A:197:LYS:HE3	1:A:231:MET:SD	0.54	2.42	61	2
2:B:378:SER:O	2:B:382:MET:HG2	0.54	2.02	38	3
1:A:212:LYS:HG2	1:A:213:ALA:H	0.54	1.63	20	1
1:A:168:LEU:HD22	1:A:171:ILE:HD12	0.54	1.78	39	3
1:A:252:LEU:H	1:A:252:LEU:HD23	0.54	1.62	42	1
2:B:334:LEU:HD11	2:B:347:ALA:HA	0.54	1.80	30	1
2:B:332:ASP:OD2	2:B:336:LYS:HG3	0.54	2.03	51	1
1:A:300:VAL:HA	2:B:340:LEU:HD12	0.54	1.78	34	1
1:A:219:THR:O	1:A:222:LEU:HB3	0.54	2.03	46	1
2:B:331:ILE:HG23	2:B:363:LEU:HD12	0.53	1.80	23	3
1:A:209:LEU:HA	1:A:216:ARG:HG2	0.53	1.79	47	1
2:B:416:ASN:OD1	2:B:420:PRO:HA	0.53	2.02	70	10
2:B:351:LEU:HD13	2:B:390:LEU:HD21	0.53	1.79	4	2
1:A:261:VAL:O	1:A:265:ILE:HG13	0.53	2.03	32	2
1:A:170:PRO:O	1:A:174:GLU:HG3	0.53	2.02	32	2
1:A:256:ARG:HA	1:A:259:GLN:OE1	0.53	2.03	51	3
1:A:300:VAL:HG12	2:B:340:LEU:HB2	0.53	1.80	6	1
2:B:335:LEU:HD13	2:B:366:GLU:HB3	0.53	1.81	31	1
1:A:216:ARG:HA	1:A:219:THR:OG1	0.53	2.02	54	3
2:B:348:GLU:HG3	2:B:352:LYS:HD2	0.53	1.80	55	1
2:B:406:GLU:HA	2:B:409:TYR:CZ	0.53	2.38	57	1
1:A:288:CYS:SG	1:A:290:GLN:HB2	0.53	2.44	15	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:226:LEU:HB3	1:A:230:VAL:HB	0.53	1.81	56	1
2:B:402:LYS:HG2	2:B:443:LEU:HD13	0.53	1.81	68	1
1:A:205:VAL:O	1:A:209:LEU:HG	0.53	2.03	13	7
1:A:251:ALA:HA	1:A:257:ALA:HB3	0.53	1.81	31	1
2:B:331:ILE:HA	2:B:334:LEU:HD12	0.53	1.80	43	1
2:B:444:ARG:O	2:B:447:CYS:HB3	0.52	2.04	55	1
1:A:183:GLU:HA	1:A:186:GLU:CG	0.52	2.35	56	1
2:B:388:LYS:O	2:B:392:LYS:HG3	0.52	2.04	28	4
2:B:406:GLU:HA	2:B:409:TYR:CD2	0.52	2.39	11	15
1:A:248:PRO:O	1:A:252:LEU:HG	0.52	2.04	27	6
1:A:292:ARG:NE	1:A:292:ARG:HA	0.52	2.18	23	1
1:A:258:PRO:HA	1:A:261:VAL:HG23	0.52	1.79	5	2
1:A:167:THR:O	1:A:170:PRO:HD2	0.52	2.05	52	6
2:B:389:SER:O	2:B:392:LYS:HB2	0.52	2.05	54	2
2:B:399:ASP:O	2:B:403:ARG:HB2	0.52	2.05	56	1
1:A:300:VAL:CB	2:B:336:LYS:HB3	0.52	2.31	35	1
1:A:279:ILE:HG21	1:A:299:THR:HG23	0.52	1.80	50	1
1:A:164:PHE:O	1:A:168:LEU:HB2	0.52	2.04	52	2
2:B:426:LEU:O	2:B:430:VAL:HG23	0.52	2.04	12	14
1:A:261:VAL:HB	1:A:294:ALA:HB1	0.52	1.80	8	1
1:A:231:MET:HE3	1:A:235:ASP:HB3	0.52	1.81	2	1
1:A:202:VAL:CG2	1:A:239:SER:HB3	0.52	2.35	8	1
1:A:198:SER:HB3	1:A:239:SER:HA	0.52	1.81	13	1
1:A:283:LYS:NZ	1:A:283:LYS:HB3	0.52	2.17	49	2
1:A:209:LEU:HD13	1:A:261:VAL:HG22	0.52	1.80	47	1
2:B:372:LEU:HD21	2:B:426:LEU:HB3	0.52	1.81	64	1
1:A:242:LYS:HD2	1:A:242:LYS:H	0.52	1.64	13	1
2:B:333:MET:O	2:B:337:GLU:HG2	0.52	2.05	51	1
1:A:258:PRO:HA	1:A:261:VAL:CG2	0.52	2.34	5	1
1:A:304:MET:HG3	2:B:332:ASP:OD1	0.52	2.04	6	2
1:A:304:MET:SD	2:B:333:MET:HG2	0.52	2.45	61	3
1:A:209:LEU:HD23	1:A:216:ARG:HG2	0.52	1.82	57	2
2:B:383:ILE:HG23	2:B:386:LEU:HD23	0.52	1.81	4	1
1:A:304:MET:HA	2:B:336:LYS:CE	0.52	2.35	21	1
1:A:202:VAL:HG13	1:A:243:LEU:HD12	0.52	1.80	53	1
1:A:259:GLN:CG	1:A:297:LYS:HE3	0.52	2.35	9	1
2:B:344:ILE:HG22	2:B:348:GLU:HG3	0.52	1.81	34	2
2:B:338:TYR:CD2	2:B:386:LEU:HB2	0.52	2.39	52	3
2:B:392:LYS:C	2:B:394:SER:H	0.52	2.09	51	2
1:A:175:TYR:CZ	1:A:222:LEU:HB2	0.51	2.39	68	5
2:B:338:TYR:HE2	2:B:344:ILE:HA	0.51	1.65	30	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:202:VAL:HG13	1:A:243:LEU:HD13	0.51	1.82	57	4
2:B:389:SER:HA	2:B:392:LYS:CE	0.51	2.33	54	9
1:A:165:GLU:HA	1:A:203:LEU:HD21	0.51	1.82	24	5
1:A:231:MET:HG3	1:A:235:ASP:HB2	0.51	1.82	57	8
1:A:241:ASP:O	1:A:245:LYS:HG2	0.51	2.05	8	6
1:A:172:ILE:HG21	1:A:204:ALA:HB2	0.51	1.83	30	1
1:A:168:LEU:HD21	1:A:200:VAL:HG22	0.51	1.82	34	1
2:B:434:PHE:CZ	2:B:441:LYS:HG2	0.51	2.40	54	3
1:A:223:LEU:HB3	1:A:273:ILE:CD1	0.51	2.36	48	1
1:A:292:ARG:HD2	1:A:295:LEU:HD12	0.51	1.81	1	1
1:A:259:GLN:HG2	1:A:297:LYS:HE3	0.51	1.81	9	1
2:B:355:GLU:O	2:B:357:PRO:HD3	0.51	2.05	40	3
1:A:169:THR:O	1:A:173:GLN:HG3	0.51	2.06	31	2
1:A:205:VAL:HG12	1:A:219:THR:HG21	0.51	1.82	42	1
2:B:410:ASN:O	2:B:413:PRO:HD2	0.51	2.06	27	12
1:A:251:ALA:CB	1:A:258:PRO:HD3	0.51	2.34	32	1
1:A:217:GLU:HG3	1:A:218:MET:N	0.51	2.21	34	1
1:A:242:LYS:O	1:A:245:LYS:HB2	0.51	2.06	36	2
1:A:191:LEU:O	1:A:193:LEU:HG	0.51	2.06	61	1
1:A:264:PHE:O	1:A:268:ALA:HB2	0.51	2.06	65	2
1:A:220:SER:HA	1:A:223:LEU:HG	0.51	1.81	66	2
1:A:175:TYR:HE2	1:A:222:LEU:HD22	0.51	1.66	66	1
2:B:335:LEU:HD13	2:B:366:GLU:HG2	0.51	1.82	33	2
1:A:299:THR:HA	1:A:302:LEU:HD12	0.51	1.83	32	2
1:A:202:VAL:HA	1:A:205:VAL:HG22	0.51	1.83	42	1
2:B:335:LEU:HD21	2:B:363:LEU:HG	0.50	1.83	37	3
2:B:381:LYS:HG3	2:B:382:MET:N	0.50	2.20	72	2
1:A:244:LEU:O	1:A:247:LEU:HB2	0.50	2.06	73	3
2:B:338:TYR:CZ	2:B:386:LEU:HB2	0.50	2.41	3	1
1:A:183:GLU:HA	1:A:186:GLU:HG3	0.50	1.82	56	1
1:A:277:THR:HA	1:A:280:ASP:HB2	0.50	1.82	29	1
1:A:169:THR:HG22	1:A:207:LEU:HD21	0.50	1.83	56	1
2:B:434:PHE:HZ	2:B:441:LYS:HG2	0.50	1.66	49	3
1:A:256:ARG:HD2	2:B:349:HIS:HB2	0.50	1.82	36	1
1:A:200:VAL:N	1:A:201:PRO:HD2	0.50	2.21	61	3
2:B:368:ILE:HG23	2:B:429:PHE:CE2	0.50	2.41	54	2
2:B:430:VAL:HG11	2:B:447:CYS:SG	0.50	2.46	10	1
2:B:428:ARG:O	2:B:432:GLU:HB2	0.50	2.07	17	3
1:A:248:PRO:HB3	1:A:290:GLN:HG3	0.50	1.84	38	4
1:A:300:VAL:HG22	1:A:304:MET:HE1	0.50	1.84	37	1
1:A:261:VAL:HA	1:A:264:PHE:CD2	0.50	2.40	53	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:262:GLY:HA3	1:A:297:LYS:HG2	0.50	1.84	53	1
1:A:199:GLY:O	1:A:203:LEU:HB2	0.50	2.06	42	1
1:A:226:LEU:O	1:A:231:MET:HB3	0.50	2.07	57	1
1:A:222:LEU:O	1:A:226:LEU:HG	0.49	2.06	49	10
1:A:300:VAL:HG13	2:B:340:LEU:HB3	0.49	1.83	15	1
1:A:247:LEU:N	1:A:248:PRO:CD	0.49	2.74	17	3
1:A:220:SER:HA	1:A:223:LEU:HD12	0.49	1.83	45	1
1:A:299:THR:HA	1:A:302:LEU:HB3	0.49	1.83	24	1
1:A:176:PHE:HB3	1:A:215:HIS:CD2	0.49	2.42	56	2
1:A:173:GLN:O	1:A:177:GLU:HG2	0.49	2.07	65	2
1:A:304:MET:HE1	2:B:337:GLU:HB2	0.49	1.84	33	1
1:A:185:ALA:O	1:A:189:ARG:HG3	0.49	2.08	41	2
1:A:178:HIS:CG	1:A:179:GLY:H	0.49	2.26	52	1
2:B:365:TYR:HB2	2:B:408:ILE:HD11	0.49	1.85	54	1
2:B:348:GLU:HG2	2:B:390:LEU:HD22	0.49	1.85	11	1
1:A:221:LYS:O	1:A:225:ASP:HB2	0.49	2.07	15	2
1:A:171:ILE:HG23	1:A:187:MET:SD	0.49	2.47	69	2
2:B:360:HIS:HB2	2:B:400:GLN:CG	0.49	2.36	65	2
1:A:300:VAL:HA	2:B:340:LEU:HD22	0.49	1.83	21	1
1:A:269:VAL:HB	1:A:302:LEU:HD11	0.49	1.85	30	1
2:B:384:LEU:HG	2:B:388:LYS:HE2	0.49	1.84	39	1
1:A:266:ALA:HB2	1:A:298:ALA:HB1	0.49	1.84	51	1
2:B:343:ASP:HB2	2:B:346:GLU:HG2	0.49	1.82	55	1
2:B:346:GLU:HA	2:B:346:GLU:OE1	0.49	2.07	55	3
2:B:377:GLU:HA	2:B:380:PHE:HB2	0.49	1.84	6	2
2:B:423:TYR:HA	2:B:426:LEU:HB3	0.49	1.84	21	1
1:A:178:HIS:CE1	1:A:180:ASP:HB2	0.49	2.43	32	1
2:B:344:ILE:HA	2:B:347:ALA:HB3	0.49	1.84	34	1
1:A:266:ALA:HB2	1:A:298:ALA:HA	0.49	1.83	45	1
2:B:361:HIS:CD2	2:B:403:ARG:HB3	0.49	2.43	61	1
2:B:368:ILE:HG21	2:B:408:ILE:HG13	0.49	1.84	66	4
1:A:172:ILE:HD12	1:A:207:LEU:HD12	0.49	1.85	25	1
1:A:253:ASP:O	1:A:255:PRO:HD3	0.49	2.08	66	1
1:A:184:VAL:O	1:A:188:LEU:HG	0.48	2.08	27	8
1:A:237:GLU:HG2	1:A:274:LEU:HD12	0.48	1.84	27	2
2:B:346:GLU:O	2:B:350:CYS:SG	0.48	2.71	44	1
2:B:360:HIS:HB2	2:B:400:GLN:HG2	0.48	1.85	59	1
1:A:175:TYR:OH	1:A:222:LEU:HB2	0.48	2.08	14	2
1:A:184:VAL:O	1:A:188:LEU:HB2	0.48	2.07	41	1
1:A:240:PHE:O	1:A:244:LEU:HG	0.48	2.08	4	2
1:A:214:SER:O	1:A:218:MET:HG2	0.48	2.09	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:240:PHE:HE2	1:A:265:ILE:HA	0.48	1.68	18	1
1:A:240:PHE:HE2	1:A:265:ILE:HG12	0.48	1.68	54	1
2:B:332:ASP:CG	2:B:336:LYS:HZ1	0.48	2.11	17	1
2:B:366:GLU:HA	2:B:369:VAL:CG2	0.48	2.38	35	1
1:A:223:LEU:HB3	1:A:273:ILE:HD13	0.48	1.83	48	1
1:A:286:VAL:HB	1:A:292:ARG:NH1	0.48	2.22	73	1
1:A:201:PRO:O	1:A:205:VAL:HB	0.48	2.08	4	2
2:B:338:TYR:HE1	2:B:344:ILE:HG12	0.48	1.68	12	3
1:A:168:LEU:HD11	1:A:200:VAL:HG13	0.48	1.86	25	2
2:B:334:LEU:HD11	2:B:350:CYS:HB3	0.48	1.84	72	1
2:B:419:VAL:HG12	2:B:421:HIS:CD2	0.48	2.44	17	1
2:B:424:SER:O	2:B:428:ARG:HB2	0.48	2.09	57	4
2:B:377:GLU:O	2:B:381:LYS:HG2	0.48	2.09	8	3
1:A:257:ALA:N	1:A:258:PRO:HD2	0.48	2.23	4	14
2:B:380:PHE:O	2:B:384:LEU:HB2	0.48	2.09	47	3
1:A:244:LEU:O	1:A:248:PRO:HD3	0.48	2.09	17	1
2:B:419:VAL:HG12	2:B:421:HIS:HD2	0.48	1.67	17	1
1:A:304:MET:HG3	2:B:332:ASP:OD2	0.48	2.09	34	1
1:A:220:SER:O	1:A:223:LEU:HB2	0.48	2.09	66	2
1:A:286:VAL:HB	1:A:292:ARG:HG3	0.48	1.86	8	1
1:A:303:SER:HB3	2:B:336:LYS:HD2	0.48	1.86	27	1
1:A:304:MET:CE	2:B:333:MET:HA	0.48	2.39	31	1
2:B:367:ALA:O	2:B:371:VAL:HG23	0.48	2.07	24	10
2:B:368:ILE:HG23	2:B:429:PHE:HE2	0.48	1.69	54	2
1:A:300:VAL:HG13	2:B:340:LEU:CB	0.48	2.39	59	2
2:B:434:PHE:CE1	2:B:441:LYS:HA	0.48	2.43	7	8
1:A:168:LEU:HD12	1:A:171:ILE:HD12	0.48	1.86	17	1
1:A:206:SER:HA	1:A:209:LEU:HD12	0.48	1.86	24	1
2:B:381:LYS:O	2:B:385:ASP:HB2	0.48	2.09	43	3
2:B:442:GLN:O	2:B:446:LEU:HG	0.48	2.08	63	3
2:B:387:LEU:HD11	2:B:433:CYS:SG	0.48	2.49	67	1
1:A:172:ILE:CD1	1:A:207:LEU:HD12	0.47	2.39	25	1
1:A:268:ALA:HB1	1:A:273:ILE:HG13	0.47	1.86	29	1
2:B:343:ASP:HB3	2:B:346:GLU:HG3	0.47	1.84	36	2
2:B:351:LEU:HD23	2:B:390:LEU:HD22	0.47	1.85	35	1
1:A:268:ALA:HB1	1:A:274:LEU:HB2	0.47	1.85	59	2
1:A:181:THR:CG2	1:A:222:LEU:HA	0.47	2.39	60	3
2:B:428:ARG:O	2:B:432:GLU:N	0.47	2.47	27	3
1:A:206:SER:HA	1:A:209:LEU:HG	0.47	1.86	45	1
2:B:350:CYS:HA	2:B:353:GLU:HG3	0.47	1.85	70	1
1:A:205:VAL:O	1:A:219:THR:HB	0.47	2.09	72	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:412:ILE:HG23	2:B:416:ASN:ND2	0.47	2.24	66	2
2:B:393:SER:O	2:B:394:SER:CB	0.47	2.62	21	2
2:B:383:ILE:O	2:B:386:LEU:HB3	0.47	2.09	28	2
1:A:300:VAL:HG21	2:B:341:SER:OG	0.47	2.09	57	3
1:A:197:LYS:C	1:A:199:GLY:H	0.47	2.12	67	2
1:A:301:LEU:HA	1:A:304:MET:HE3	0.47	1.85	55	1
1:A:248:PRO:HG3	1:A:288:CYS:SG	0.47	2.49	3	1
2:B:419:VAL:N	2:B:420:PRO:HD3	0.47	2.25	26	2
1:A:304:MET:HG3	2:B:336:LYS:HE2	0.47	1.86	56	1
1:A:256:ARG:NH1	2:B:349:HIS:HB3	0.47	2.24	61	1
1:A:181:THR:HG21	1:A:225:ASP:CB	0.47	2.39	46	2
2:B:391:TRP:HH2	2:B:398:ILE:HA	0.47	1.70	42	1
1:A:266:ALA:HB3	1:A:301:LEU:HD23	0.47	1.85	6	1
1:A:205:VAL:O	1:A:209:LEU:HB2	0.47	2.09	30	1
2:B:434:PHE:HA	2:B:439:ILE:CD1	0.47	2.33	70	3
1:A:176:PHE:HZ	1:A:219:THR:HG23	0.47	1.70	32	1
2:B:430:VAL:HG21	2:B:447:CYS:SG	0.47	2.50	66	2
1:A:300:VAL:HG21	2:B:341:SER:HA	0.47	1.86	51	1
1:A:158:PRO:HB2	1:A:161:GLU:HG2	0.47	1.86	54	1
2:B:379:ALA:O	2:B:383:ILE:HG13	0.47	2.10	58	1
1:A:277:THR:O	1:A:280:ASP:N	0.47	2.45	68	3
1:A:232:SER:O	1:A:235:ASP:HB2	0.47	2.10	2	1
1:A:259:GLN:HA	1:A:297:LYS:CD	0.47	2.40	9	1
1:A:184:VAL:HG11	1:A:222:LEU:HD11	0.47	1.85	67	2
2:B:409:TYR:HA	2:B:412:ILE:CG1	0.47	2.40	57	1
1:A:304:MET:HG2	2:B:336:LYS:HB3	0.47	1.87	58	1
1:A:283:LYS:HB3	1:A:283:LYS:HZ3	0.47	1.69	7	2
1:A:200:VAL:H	1:A:201:PRO:HD2	0.47	1.70	37	2
2:B:406:GLU:HG2	2:B:446:LEU:HD22	0.47	1.86	62	1
1:A:172:ILE:HD12	1:A:203:LEU:HD23	0.47	1.87	63	1
1:A:164:PHE:CE1	1:A:200:VAL:HG22	0.47	2.45	72	1
1:A:263:GLN:HG3	1:A:301:LEU:HG	0.47	1.84	72	1
1:A:304:MET:HG2	2:B:332:ASP:OD2	0.47	2.10	5	3
2:B:405:TYR:HE1	2:B:430:VAL:HG22	0.47	1.69	28	2
2:B:366:GLU:O	2:B:369:VAL:HB	0.46	2.10	72	1
2:B:402:LYS:HD2	2:B:443:LEU:HD13	0.46	1.88	20	1
1:A:185:ALA:CB	1:A:226:LEU:HD22	0.46	2.40	56	1
2:B:367:ALA:O	2:B:383:ILE:HG21	0.46	2.10	66	1
1:A:207:LEU:C	1:A:209:LEU:H	0.46	2.13	4	2
1:A:263:GLN:HA	1:A:301:LEU:HD22	0.46	1.87	4	1
1:A:269:VAL:HA	1:A:274:LEU:O	0.46	2.10	72	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:249:GLU:O	1:A:252:LEU:HB2	0.46	2.11	73	2
1:A:247:LEU:HD11	1:A:261:VAL:HG11	0.46	1.87	20	2
2:B:433:CYS:HB3	2:B:438:ILE:HD11	0.46	1.87	73	4
1:A:217:GLU:HG3	1:A:267:ARG:HH22	0.46	1.71	35	2
2:B:402:LYS:HG2	2:B:406:GLU:OE2	0.46	2.10	45	1
1:A:174:GLU:O	1:A:177:GLU:HB2	0.46	2.11	62	2
1:A:209:LEU:HA	1:A:216:ARG:HE	0.46	1.70	24	2
1:A:300:VAL:HA	2:B:340:LEU:CD1	0.46	2.41	45	1
2:B:345:SER:O	2:B:349:HIS:HB2	0.46	2.10	42	2
1:A:256:ARG:HA	1:A:259:GLN:NE2	0.46	2.25	46	1
1:A:201:PRO:O	1:A:205:VAL:HG23	0.46	2.10	12	7
1:A:161:GLU:O	1:A:165:GLU:HG3	0.46	2.10	14	4
1:A:162:ARG:N	1:A:162:ARG:HD2	0.46	2.25	34	1
1:A:257:ALA:HB3	1:A:258:PRO:HD3	0.46	1.88	54	2
2:B:444:ARG:O	2:B:447:CYS:HB2	0.46	2.11	10	1
1:A:168:LEU:HA	1:A:171:ILE:HD12	0.46	1.88	28	1
1:A:240:PHE:CE1	1:A:265:ILE:HG12	0.46	2.44	31	1
2:B:380:PHE:CE1	2:B:429:PHE:HB3	0.46	2.45	31	1
1:A:222:LEU:O	1:A:226:LEU:HB2	0.46	2.10	34	1
1:A:240:PHE:HE2	1:A:265:ILE:HG23	0.46	1.71	61	1
1:A:203:LEU:O	1:A:207:LEU:N	0.46	2.49	72	2
1:A:236:VAL:HG11	1:A:273:ILE:O	0.46	2.11	13	2
2:B:402:LYS:O	2:B:406:GLU:HG3	0.46	2.10	22	1
2:B:389:SER:HA	2:B:392:LYS:CD	0.46	2.40	8	1
2:B:335:LEU:CD1	2:B:366:GLU:HB3	0.46	2.41	31	2
1:A:263:GLN:HE21	1:A:301:LEU:HD22	0.46	1.70	36	1
2:B:338:TYR:CZ	2:B:344:ILE:HG23	0.46	2.46	54	1
1:A:268:ALA:HA	1:A:271:ASP:OD1	0.46	2.11	29	1
2:B:368:ILE:O	2:B:371:VAL:HG12	0.46	2.11	48	3
1:A:172:ILE:HG13	1:A:173:GLN:N	0.46	2.26	64	1
1:A:240:PHE:O	1:A:243:LEU:HB2	0.45	2.10	13	1
1:A:300:VAL:CG2	2:B:340:LEU:HB3	0.45	2.41	46	2
2:B:398:ILE:O	2:B:402:LYS:HG3	0.45	2.10	33	1
1:A:193:LEU:HD22	1:A:196:MET:HB3	0.45	1.88	58	1
2:B:351:LEU:HD21	2:B:363:LEU:HD13	0.45	1.87	20	1
1:A:209:LEU:HD21	1:A:264:PHE:HE2	0.45	1.72	53	1
2:B:384:LEU:HB2	2:B:429:PHE:CE1	0.45	2.45	66	1
1:A:265:ILE:HD13	1:A:295:LEU:HD23	0.45	1.87	8	1
1:A:304:MET:SD	2:B:333:MET:HG3	0.45	2.51	41	2
1:A:249:GLU:HA	1:A:252:LEU:HG	0.45	1.88	65	1
1:A:282:TYR:HA	1:A:285:THR:OG1	0.45	2.10	57	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:333:MET:O	2:B:337:GLU:HG3	0.45	2.11	29	1
2:B:424:SER:O	2:B:428:ARG:HG2	0.45	2.12	36	1
1:A:300:VAL:HG11	2:B:337:GLU:CA	0.45	2.38	48	1
2:B:348:GLU:O	2:B:352:LYS:HD2	0.45	2.12	8	1
1:A:300:VAL:CG1	2:B:340:LEU:HB2	0.45	2.42	23	4
2:B:371:VAL:HG11	2:B:380:PHE:HD1	0.45	1.70	29	1
2:B:434:PHE:HD1	2:B:439:ILE:HD11	0.45	1.71	30	1
2:B:429:PHE:O	2:B:432:GLU:HB3	0.45	2.11	57	1
1:A:225:ASP:C	1:A:227:CYS:H	0.45	2.14	68	1
1:A:249:GLU:O	1:A:251:ALA:N	0.45	2.50	72	1
2:B:334:LEU:HD21	2:B:351:LEU:HB2	0.45	1.88	2	1
2:B:338:TYR:CD2	2:B:386:LEU:HD13	0.45	2.47	4	1
1:A:201:PRO:HG3	1:A:231:MET:SD	0.45	2.52	32	2
1:A:266:ALA:HA	1:A:269:VAL:HG23	0.45	1.87	8	1
1:A:268:ALA:CB	1:A:273:ILE:HB	0.45	2.42	13	1
1:A:169:THR:N	1:A:170:PRO:HD2	0.45	2.27	63	4
2:B:338:TYR:O	2:B:342:GLY:HA2	0.45	2.11	69	2
2:B:382:MET:O	2:B:386:LEU:HB2	0.45	2.11	68	1
1:A:187:MET:O	1:A:191:LEU:HG	0.45	2.12	8	2
1:A:171:ILE:HG12	1:A:187:MET:SD	0.45	2.52	25	1
1:A:240:PHE:HB3	1:A:278:TYR:OH	0.45	2.12	35	1
2:B:368:ILE:CD1	2:B:408:ILE:HG13	0.45	2.40	61	2
1:A:258:PRO:HB2	1:A:293:ALA:HB1	0.45	1.87	66	1
1:A:176:PHE:CZ	1:A:208:ALA:HB2	0.45	2.46	17	2
1:A:296:ASP:O	1:A:300:VAL:HG23	0.45	2.10	70	3
1:A:304:MET:HG2	2:B:336:LYS:HG3	0.45	1.89	22	1
1:A:217:GLU:HA	1:A:267:ARG:NH2	0.45	2.26	49	1
2:B:384:LEU:HB2	2:B:429:PHE:HE1	0.45	1.71	66	1
2:B:334:LEU:CD2	2:B:347:ALA:HA	0.45	2.42	11	2
2:B:405:TYR:CE1	2:B:430:VAL:HG22	0.45	2.47	40	2
1:A:208:ALA:HA	1:A:215:HIS:ND1	0.45	2.27	39	1
2:B:442:GLN:HB3	2:B:446:LEU:HD12	0.45	1.88	64	1
1:A:244:LEU:HA	1:A:247:LEU:HD13	0.45	1.89	59	4
1:A:300:VAL:HB	2:B:340:LEU:CB	0.45	2.41	21	1
2:B:331:ILE:O	2:B:335:LEU:HG	0.45	2.12	29	1
2:B:354:LEU:O	2:B:355:GLU:HB2	0.45	2.11	49	1
2:B:334:LEU:HD21	2:B:350:CYS:CB	0.44	2.42	50	1
1:A:289:VAL:HA	1:A:292:ARG:HB2	0.44	1.89	21	2
2:B:367:ALA:HB1	2:B:383:ILE:HD12	0.44	1.87	36	1
1:A:301:LEU:HD23	1:A:304:MET:HE3	0.44	1.87	37	2
2:B:348:GLU:O	2:B:352:LYS:HG2	0.44	2.12	61	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:398:ILE:O	2:B:402:LYS:HB2	0.44	2.11	71	1
2:B:330:GLU:HG3	2:B:331:ILE:N	0.44	2.27	18	1
1:A:304:MET:HE1	2:B:333:MET:HG3	0.44	1.89	29	2
1:A:205:VAL:HG22	1:A:219:THR:CG2	0.44	2.42	54	1
2:B:338:TYR:CE2	2:B:344:ILE:HA	0.44	2.47	30	1
1:A:267:ARG:O	1:A:271:ASP:HB2	0.44	2.12	73	2
1:A:181:THR:HG22	1:A:222:LEU:HD12	0.44	1.89	71	3
1:A:193:LEU:O	1:A:197:LYS:HB2	0.44	2.12	21	1
1:A:240:PHE:HA	1:A:243:LEU:HB3	0.44	1.88	52	1
2:B:402:LYS:HE3	2:B:442:GLN:OE1	0.44	2.12	53	1
2:B:361:HIS:HB2	2:B:400:GLN:HA	0.44	1.88	73	1
2:B:338:TYR:CD1	2:B:382:MET:HB3	0.44	2.47	45	1
1:A:274:LEU:HG	1:A:275:CYS:N	0.44	2.28	62	2
1:A:169:THR:H	1:A:170:PRO:HD2	0.44	1.73	66	1
2:B:361:HIS:HB3	2:B:400:GLN:CB	0.44	2.41	72	1
1:A:202:VAL:HG23	1:A:239:SER:HB3	0.44	1.90	8	3
1:A:257:ALA:HA	1:A:260:LEU:HD12	0.44	1.90	44	2
2:B:406:GLU:HA	2:B:409:TYR:CE2	0.44	2.48	59	4
2:B:424:SER:O	2:B:428:ARG:HB3	0.44	2.13	9	2
2:B:402:LYS:HG2	2:B:443:LEU:HD22	0.44	1.88	66	1
2:B:331:ILE:HD13	2:B:362:GLU:HB3	0.44	1.89	14	1
1:A:227:CYS:SG	1:A:273:ILE:HG22	0.44	2.53	27	2
2:B:379:ALA:O	2:B:383:ILE:HG12	0.44	2.13	33	3
2:B:352:LYS:HD2	2:B:352:LYS:N	0.44	2.27	29	1
2:B:371:VAL:HB	2:B:383:ILE:HG21	0.44	1.89	69	2
2:B:347:ALA:O	2:B:351:LEU:HB2	0.44	2.13	56	1
2:B:384:LEU:O	2:B:388:LYS:HE3	0.44	2.13	59	1
1:A:168:LEU:HD21	1:A:200:VAL:HG13	0.44	1.88	63	1
2:B:399:ASP:HA	2:B:402:LYS:HG3	0.44	1.90	73	1
1:A:244:LEU:HD11	1:A:295:LEU:HD21	0.43	1.89	41	2
1:A:259:GLN:HB3	2:B:346:GLU:OE1	0.43	2.13	50	1
1:A:247:LEU:HD23	1:A:290:GLN:HB3	0.43	1.88	53	1
1:A:300:VAL:HG22	2:B:340:LEU:HB2	0.43	1.90	1	1
1:A:304:MET:HA	2:B:336:LYS:NZ	0.43	2.28	2	1
2:B:373:GLU:HA	2:B:373:GLU:OE1	0.43	2.13	13	1
2:B:338:TYR:OH	2:B:385:ASP:HB3	0.43	2.14	30	1
1:A:203:LEU:O	1:A:207:LEU:HG	0.43	2.13	41	2
1:A:174:GLU:HA	1:A:177:GLU:HG2	0.43	1.89	45	1
1:A:304:MET:HE3	2:B:337:GLU:HB2	0.43	1.88	53	1
1:A:269:VAL:HG11	1:A:276:ASN:HB3	0.43	1.90	61	1
1:A:216:ARG:NH1	1:A:260:LEU:HD13	0.43	2.28	73	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:297:LYS:HZ3	2:B:346:GLU:CD	0.43	2.17	8	1
2:B:348:GLU:O	2:B:352:LYS:HG3	0.43	2.13	28	1
1:A:256:ARG:HG2	1:A:260:LEU:HG	0.43	1.90	42	1
2:B:391:TRP:CZ2	2:B:398:ILE:HB	0.43	2.42	60	1
1:A:280:ASP:O	1:A:283:LYS:HB2	0.43	2.14	9	2
2:B:391:TRP:HA	2:B:396:ILE:HB	0.43	1.89	21	1
1:A:172:ILE:HG22	1:A:176:PHE:CZ	0.43	2.49	46	2
1:A:224:SER:HA	1:A:273:ILE:HG21	0.43	1.89	22	2
2:B:402:LYS:O	2:B:406:GLU:HB2	0.43	2.12	27	2
1:A:240:PHE:CZ	1:A:274:LEU:HD22	0.43	2.48	47	1
1:A:263:GLN:HB2	1:A:301:LEU:HD13	0.43	1.90	51	1
2:B:334:LEU:HD22	2:B:350:CYS:SG	0.43	2.53	57	1
1:A:178:HIS:O	1:A:180:ASP:N	0.43	2.51	22	1
2:B:405:TYR:O	2:B:408:ILE:HB	0.43	2.12	22	1
2:B:352:LYS:HD2	2:B:352:LYS:H	0.43	1.73	29	1
1:A:158:PRO:HB3	1:A:196:MET:HG2	0.43	1.90	62	1
1:A:300:VAL:HG13	2:B:336:LYS:HB3	0.43	1.89	54	1
2:B:351:LEU:HD23	2:B:395:THR:HG21	0.43	1.91	61	1
1:A:232:SER:H	1:A:235:ASP:HB3	0.43	1.74	71	1
1:A:204:ALA:HA	1:A:207:LEU:HD12	0.43	1.89	4	1
2:B:358:HIS:HA	2:B:400:GLN:HE22	0.43	1.74	21	1
1:A:304:MET:HE2	2:B:333:MET:HG2	0.43	1.91	34	1
2:B:364:VAL:HG23	2:B:365:TYR:H	0.43	1.74	50	1
2:B:412:ILE:N	2:B:413:PRO:HD2	0.43	2.28	72	1
1:A:181:THR:HG22	1:A:222:LEU:HA	0.43	1.89	7	3
1:A:300:VAL:HG11	2:B:337:GLU:HG3	0.43	1.91	4	1
2:B:343:ASP:HB3	2:B:346:GLU:CG	0.43	2.42	13	1
2:B:331:ILE:HD13	2:B:362:GLU:HB2	0.43	1.90	26	1
1:A:200:VAL:HB	1:A:201:PRO:CD	0.43	2.44	34	8
1:A:292:ARG:HD2	1:A:292:ARG:HA	0.43	1.63	20	1
1:A:247:LEU:HA	1:A:250:LEU:HB2	0.43	1.89	21	1
2:B:431:GLU:HG3	2:B:432:GLU:N	0.43	2.29	55	3
2:B:440:SER:OG	2:B:443:LEU:HB2	0.43	2.14	42	1
2:B:331:ILE:CG2	2:B:363:LEU:HA	0.43	2.44	58	1
1:A:277:THR:O	1:A:280:ASP:HB2	0.43	2.14	59	1
2:B:380:PHE:O	2:B:384:LEU:HB3	0.43	2.13	61	1
2:B:360:HIS:CB	2:B:400:GLN:HG3	0.43	2.38	65	1
1:A:197:LYS:O	1:A:200:VAL:HG23	0.43	2.13	38	1
1:A:258:PRO:HG2	1:A:259:GLN:OE1	0.43	2.13	46	1
2:B:371:VAL:O	2:B:374:SER:HB2	0.43	2.14	60	1
2:B:361:HIS:HB2	2:B:400:GLN:O	0.42	2.14	23	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:351:LEU:HD11	2:B:363:LEU:HD11	0.42	1.90	56	1
1:A:195:GLU:HA	1:A:238:LYS:NZ	0.42	2.29	70	1
1:A:251:ALA:CB	1:A:258:PRO:HG3	0.42	2.44	70	2
2:B:364:VAL:O	2:B:368:ILE:HG13	0.42	2.14	63	2
2:B:336:LYS:O	2:B:339:LEU:HB3	0.42	2.14	36	1
1:A:286:VAL:CG1	1:A:291:ALA:HB3	0.42	2.43	38	1
1:A:292:ARG:O	1:A:296:ASP:HB2	0.42	2.15	66	2
1:A:300:VAL:HG21	2:B:341:SER:CA	0.42	2.44	51	1
2:B:348:GLU:HG2	2:B:390:LEU:HD23	0.42	1.90	54	1
2:B:368:ILE:O	2:B:371:VAL:HB	0.42	2.13	4	1
1:A:216:ARG:HB3	1:A:264:PHE:CE1	0.42	2.49	15	1
1:A:181:THR:HG21	1:A:225:ASP:HB3	0.42	1.90	28	1
2:B:380:PHE:HE1	2:B:429:PHE:HB3	0.42	1.74	31	1
2:B:335:LEU:HD11	2:B:366:GLU:HB3	0.42	1.90	65	1
1:A:158:PRO:HA	1:A:196:MET:SD	0.42	2.53	66	1
1:A:283:LYS:O	1:A:283:LYS:HG2	0.42	2.13	7	1
2:B:390:LEU:HD12	2:B:396:ILE:HD11	0.42	1.90	14	1
2:B:416:ASN:HB3	2:B:420:PRO:HB3	0.42	1.91	35	1
1:A:244:LEU:HB3	1:A:291:ALA:CB	0.42	2.45	13	1
2:B:443:LEU:HD12	2:B:446:LEU:HD12	0.42	1.91	26	1
1:A:279:ILE:HG23	1:A:295:LEU:HD22	0.42	1.90	29	1
1:A:300:VAL:HG23	2:B:340:LEU:HD12	0.42	1.89	2	1
2:B:397:THR:OG1	2:B:400:GLN:HG2	0.42	2.14	10	1
2:B:346:GLU:OE1	2:B:346:GLU:HA	0.42	2.15	14	1
1:A:216:ARG:HB3	1:A:264:PHE:CZ	0.42	2.44	18	1
2:B:344:ILE:O	2:B:348:GLU:HB2	0.42	2.15	22	2
1:A:236:VAL:HG21	1:A:273:ILE:HG21	0.42	1.90	66	1
2:B:424:SER:O	2:B:428:ARG:HD3	0.42	2.15	70	1
2:B:348:GLU:O	2:B:352:LYS:HD3	0.42	2.14	23	1
2:B:351:LEU:HD22	2:B:390:LEU:HD13	0.42	1.91	27	1
2:B:354:LEU:HB3	2:B:355:GLU:H	0.42	1.57	64	2
1:A:172:ILE:HD13	1:A:204:ALA:HB2	0.42	1.92	30	1
1:A:251:ALA:O	1:A:253:ASP:N	0.42	2.53	42	1
1:A:300:VAL:HA	2:B:340:LEU:HD13	0.42	1.92	64	2
2:B:348:GLU:HB3	2:B:352:LYS:HE2	0.42	1.90	54	1
1:A:297:LYS:HE3	2:B:346:GLU:OE2	0.42	2.15	55	1
2:B:360:HIS:O	2:B:363:LEU:HB3	0.42	2.15	61	1
1:A:206:SER:O	1:A:209:LEU:HB2	0.42	2.15	15	1
2:B:409:TYR:CZ	2:B:447:CYS:HB3	0.42	2.49	52	1
2:B:338:TYR:CD1	2:B:386:LEU:HD13	0.42	2.50	8	1
1:A:178:HIS:H	1:A:178:HIS:CD2	0.41	2.32	52	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:212:LYS:O	1:A:216:ARG:HG3	0.41	2.15	70	1
1:A:188:LEU:HA	1:A:191:LEU:HD12	0.41	1.91	71	1
2:B:412:ILE:HD13	2:B:412:ILE:HA	0.41	1.81	21	1
2:B:435:GLN:C	2:B:437:GLY:H	0.41	2.18	36	1
2:B:339:LEU:HB2	2:B:383:ILE:HD11	0.41	1.91	56	1
1:A:208:ALA:C	1:A:210:GLU:H	0.41	2.19	64	1
1:A:180:ASP:HB3	1:A:183:GLU:HB2	0.41	1.91	3	1
1:A:206:SER:HA	1:A:209:LEU:HB2	0.41	1.91	38	1
2:B:388:LYS:HG3	2:B:438:ILE:HD13	0.41	1.91	48	1
1:A:216:ARG:HD3	1:A:260:LEU:HD22	0.41	1.92	56	1
1:A:259:GLN:NE2	2:B:346:GLU:HB3	0.41	2.30	73	1
2:B:412:ILE:O	2:B:416:ASN:HB2	0.41	2.16	25	1
2:B:431:GLU:HA	2:B:434:PHE:HB3	0.41	1.93	52	1
1:A:213:ALA:HA	1:A:216:ARG:CZ	0.41	2.46	64	1
1:A:170:PRO:O	1:A:174:GLU:HG2	0.41	2.14	70	1
2:B:338:TYR:O	2:B:341:SER:O	0.41	2.37	73	1
1:A:254:THR:HG22	1:A:256:ARG:H	0.41	1.76	8	1
1:A:247:LEU:HD21	1:A:258:PRO:CA	0.41	2.42	13	1
2:B:438:ILE:HG13	2:B:439:ILE:N	0.41	2.30	41	1
2:B:351:LEU:HD13	2:B:363:LEU:HD13	0.41	1.93	55	1
1:A:247:LEU:HA	1:A:250:LEU:HD12	0.41	1.91	59	1
2:B:356:VAL:HB	2:B:359:PHE:HB3	0.41	1.90	61	1
1:A:253:ASP:O	1:A:254:THR:CB	0.41	2.68	72	1
1:A:215:HIS:HD2	1:A:218:MET:SD	0.41	2.38	13	1
2:B:351:LEU:HD22	2:B:390:LEU:HD22	0.41	1.93	31	2
1:A:304:MET:HE2	2:B:336:LYS:HB2	0.41	1.91	22	1
1:A:258:PRO:O	1:A:261:VAL:HB	0.41	2.16	23	1
1:A:181:THR:HG21	1:A:222:LEU:HA	0.41	1.93	31	1
1:A:259:GLN:HG2	2:B:346:GLU:CG	0.41	2.44	40	1
2:B:438:ILE:HG13	2:B:439:ILE:HG12	0.41	1.92	50	1
1:A:176:PHE:CE1	1:A:219:THR:HA	0.41	2.50	66	1
2:B:365:TYR:CE1	2:B:407:ARG:HG2	0.41	2.50	17	1
1:A:239:SER:O	1:A:243:LEU:HB2	0.41	2.15	70	2
2:B:367:ALA:HA	2:B:370:MET:HB2	0.41	1.92	44	1
1:A:219:THR:HB	1:A:264:PHE:HE1	0.41	1.74	56	2
1:A:213:ALA:HA	1:A:216:ARG:NH1	0.41	2.30	57	1
2:B:388:LYS:O	2:B:391:TRP:N	0.41	2.37	68	1
1:A:188:LEU:HD23	1:A:191:LEU:HD12	0.41	1.93	4	1
1:A:206:SER:OG	1:A:243:LEU:HD11	0.41	2.15	34	1
2:B:431:GLU:O	2:B:435:GLN:HG3	0.41	2.16	44	1
1:A:297:LYS:NZ	2:B:337:GLU:OE1	0.41	2.52	57	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:409:TYR:CE1	2:B:447:CYS:HB3	0.41	2.51	57	1
1:A:198:SER:C	1:A:200:VAL:H	0.41	2.19	64	1
1:A:168:LEU:HG	1:A:200:VAL:HG22	0.41	1.93	66	1
1:A:175:TYR:O	1:A:177:GLU:N	0.41	2.54	66	1
1:A:170:PRO:O	1:A:174:GLU:HB2	0.41	2.16	67	1
1:A:301:LEU:HA	1:A:304:MET:CE	0.41	2.46	67	1
1:A:161:GLU:O	1:A:165:GLU:HB2	0.41	2.16	68	1
1:A:225:ASP:C	1:A:227:CYS:N	0.41	2.74	68	1
1:A:276:ASN:C	1:A:278:TYR:H	0.41	2.19	73	1
1:A:237:GLU:HG3	1:A:274:LEU:CD1	0.41	2.46	28	1
1:A:300:VAL:HG11	2:B:336:LYS:O	0.41	2.16	35	1
1:A:283:LYS:HZ3	1:A:283:LYS:HB3	0.40	1.76	15	1
2:B:402:LYS:HE3	2:B:443:LEU:HD13	0.40	1.91	37	1
2:B:397:THR:O	2:B:400:GLN:HB2	0.40	2.16	42	1
1:A:248:PRO:O	1:A:252:LEU:HD12	0.40	2.16	53	1
1:A:301:LEU:HD23	1:A:304:MET:CE	0.40	2.47	66	1
2:B:344:ILE:H	2:B:344:ILE:HD12	0.40	1.76	10	1
2:B:434:PHE:CD1	2:B:439:ILE:HD11	0.40	2.51	30	1
1:A:297:LYS:HE3	1:A:301:LEU:HD21	0.40	1.93	44	1
2:B:334:LEU:HD11	2:B:350:CYS:HB2	0.40	1.91	17	1
2:B:354:LEU:HD22	2:B:354:LEU:HA	0.40	1.80	18	1
1:A:169:THR:HB	1:A:170:PRO:CD	0.40	2.46	21	1
1:A:216:ARG:NH1	1:A:260:LEU:HD12	0.40	2.31	52	1
2:B:361:HIS:CE1	2:B:404:GLY:HA2	0.40	2.51	59	1
2:B:396:ILE:HG23	2:B:400:GLN:HB3	0.40	1.94	65	1
1:A:205:VAL:HG11	1:A:243:LEU:HD21	0.40	1.92	43	1
1:A:304:MET:HB3	2:B:333:MET:SD	0.40	2.56	21	1
2:B:367:ALA:HB1	2:B:383:ILE:HG23	0.40	1.93	66	1
1:A:158:PRO:HB2	1:A:196:MET:HE2	0.40	1.94	70	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	149/163 (91%)	135±5 (91±3%)	12±4 (8±3%)	2±2 (1±1%)	16 63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	119/131 (91%)	105±5 (88±4%)	13±4 (11±3%)	2±2 (1±1%)	16 63
All	All	19564/21462 (91%)	17506 (89%)	1805 (9%)	253 (1%)	16 63

All 79 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	354	LEU	22
2	B	394	SER	22
1	A	283	LYS	20
1	A	192	ASN	16
1	A	179	GLY	13
1	A	273	ILE	10
2	B	355	GLU	9
1	A	261	VAL	7
2	B	342	GLY	7
2	B	393	SER	6
2	B	395	THR	5
2	B	439	ILE	5
2	B	436	ALA	4
2	B	392	LYS	4
2	B	361	HIS	4
1	A	289	VAL	3
1	A	168	LEU	3
2	B	373	GLU	3
1	A	272	GLY	3
1	A	239	SER	3
1	A	277	THR	3
1	A	278	TYR	3
1	A	208	ALA	2
2	B	345	SER	2
2	B	438	ILE	2
2	B	448	PRO	2
1	A	245	LYS	2
1	A	248	PRO	2
1	A	202	VAL	2
1	A	238	LYS	2
1	A	230	VAL	2
2	B	353	GLU	2
2	B	356	VAL	2
1	A	201	PRO	2
1	A	305	SER	2

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Mol	Chain	Res	Type	Models (Total)
1	A	209	LEU	2
2	B	364	VAL	2
1	A	254	THR	2
1	A	227	CYS	2
1	A	247	LEU	2
1	A	255	PRO	2
1	A	199	GLY	2
1	A	216	ARG	2
1	A	190	ASP	1
2	B	360	HIS	1
2	B	362	GLU	1
1	A	241	ASP	1
1	A	175	TYR	1
1	A	181	THR	1
1	A	229	THR	1
2	B	357	PRO	1
2	B	380	PHE	1
2	B	420	PRO	1
1	A	219	THR	1
1	A	222	LEU	1
2	B	437	GLY	1
1	A	200	VAL	1
1	A	252	LEU	1
2	B	403	ARG	1
2	B	386	LEU	1
2	B	375	THR	1
1	A	233	THR	1
2	B	374	SER	1
1	A	180	ASP	1
1	A	256	ARG	1
1	A	161	GLU	1
1	A	244	LEU	1
2	B	344	ILE	1
1	A	174	GLU	1
1	A	288	CYS	1
1	A	258	PRO	1
1	A	176	PHE	1
1	A	223	LEU	1
1	A	292	ARG	1
1	A	212	LYS	1
1	A	226	LEU	1
2	B	389	SER	1

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Mol	Chain	Res	Type	Models (Total)
2	B	402	LYS	1
1	A	250	LEU	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	127/136 (93%)	109±3 (86±3%)	18±3 (14±3%)	6 45
2	B	112/121 (93%)	96±4 (86±3%)	16±4 (14±3%)	6 46
All	All	17447/18761 (93%)	14942 (86%)	2505 (14%)	6 45

All 190 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	285	THR	69
1	A	277	THR	66
1	A	195	GLU	61
1	A	214	SER	60
1	A	233	THR	56
2	B	378	SER	52
1	A	292	ARG	52
2	B	405	TYR	50
2	B	440	SER	46
2	B	424	SER	46
1	A	225	ASP	44
1	A	196	MET	43
1	A	234	THR	42
2	B	375	THR	40
2	B	397	THR	38
1	A	181	THR	38
1	A	271	ASP	37
1	A	224	SER	36
1	A	220	SER	36
2	B	421	HIS	35
2	B	407	ARG	34
2	B	345	SER	32

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Mol	Chain	Res	Type	Models (Total)
1	A	299	THR	32
1	A	221	LYS	31
2	B	422	SER	31
1	A	246	ASP	30
2	B	423	TYR	29
2	B	361	HIS	29
1	A	256	ARG	28
1	A	249	GLU	27
2	B	414	ASP	27
2	B	387	LEU	25
2	B	395	THR	25
2	B	356	VAL	24
1	A	190	ASP	24
2	B	449	SER	24
1	A	280	ASP	23
2	B	444	ARG	22
1	A	232	SER	21
2	B	399	ASP	21
2	B	346	GLU	21
2	B	358	HIS	21
1	A	219	THR	21
2	B	354	LEU	21
1	A	210	GLU	21
1	A	303	SER	21
1	A	160	ASP	20
1	A	254	THR	20
2	B	393	SER	19
1	A	241	ASP	19
1	A	296	ASP	18
2	B	359	PHE	17
2	B	330	GLU	17
2	B	353	GLU	17
2	B	338	TYR	16
1	A	253	ASP	16
2	B	391	TRP	16
2	B	344	ILE	16
2	B	341	SER	15
1	A	178	HIS	15
1	A	168	LEU	15
2	B	427	GLU	15
2	B	385	ASP	14
2	B	337	GLU	14

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Mol	Chain	Res	Type	Models (Total)
2	B	442	GLN	14
2	B	418	ASP	14
1	A	305	SER	14
1	A	237	GLU	13
1	A	215	HIS	13
1	A	169	THR	12
2	B	348	GLU	12
1	A	267	ARG	12
2	B	411	GLU	11
1	A	229	THR	11
2	B	349	HIS	11
1	A	198	SER	10
1	A	206	SER	10
1	A	283	LYS	10
2	B	429	PHE	10
1	A	174	GLU	10
2	B	373	GLU	10
2	B	416	ASN	10
2	B	384	LEU	9
2	B	340	LEU	9
1	A	217	GLU	8
1	A	222	LEU	8
1	A	263	GLN	8
2	B	392	LYS	8
2	B	333	MET	8
2	B	377	GLU	8
2	B	360	HIS	8
1	A	275	CYS	8
1	A	239	SER	8
1	A	259	GLN	8
2	B	447	CYS	7
2	B	431	GLU	7
2	B	435	GLN	7
2	B	352	LYS	6
2	B	400	GLN	6
1	A	167	THR	6
2	B	394	SER	6
2	B	363	LEU	6
1	A	216	ARG	6
1	A	182	ASN	5
1	A	273	ILE	5
2	B	351	LEU	5

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Mol	Chain	Res	Type	Models (Total)
2	B	428	ARG	5
2	B	445	ASP	5
1	A	304	MET	5
1	A	193	LEU	5
1	A	297	LYS	5
1	A	209	LEU	5
1	A	161	GLU	5
2	B	433	CYS	5
1	A	247	LEU	5
1	A	207	LEU	5
2	B	390	LEU	4
2	B	412	ILE	4
2	B	366	GLU	4
2	B	380	PHE	4
1	A	240	PHE	4
2	B	362	GLU	4
2	B	365	TYR	4
2	B	336	LYS	4
1	A	250	LEU	4
1	A	235	ASP	4
1	A	287	ASP	4
2	B	409	TYR	4
2	B	350	CYS	4
1	A	226	LEU	4
2	B	388	LYS	4
2	B	446	LEU	4
2	B	355	GLU	4
1	A	183	GLU	3
2	B	334	LEU	3
1	A	264	PHE	3
1	A	192	ASN	3
1	A	301	LEU	3
2	B	402	LYS	3
2	B	426	LEU	3
1	A	162	ARG	3
1	A	177	GLU	3
1	A	252	LEU	3
2	B	364	VAL	3
2	B	370	MET	3
1	A	281	SER	3
1	A	230	VAL	3
1	A	186	GLU	2

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Mol	Chain	Res	Type	Models (Total)
1	A	276	ASN	2
1	A	227	CYS	2
1	A	300	VAL	2
1	A	248	PRO	2
2	B	332	ASP	2
2	B	382	MET	2
1	A	175	TYR	2
2	B	381	LYS	2
1	A	218	MET	2
1	A	165	GLU	2
1	A	203	LEU	2
2	B	343	ASP	2
1	A	159	LEU	2
2	B	403	ARG	1
2	B	383	ILE	1
1	A	197	LYS	1
1	A	238	LYS	1
1	A	212	LYS	1
2	B	432	GLU	1
1	A	243	LEU	1
2	B	371	VAL	1
2	B	372	LEU	1
1	A	158	PRO	1
2	B	339	LEU	1
1	A	289	VAL	1
1	A	191	LEU	1
2	B	425	VAL	1
1	A	164	PHE	1
2	B	331	ILE	1
1	A	278	TYR	1
2	B	398	ILE	1
1	A	274	LEU	1
1	A	242	LYS	1
2	B	408	ILE	1
1	A	180	ASP	1
1	A	290	GLN	1
2	B	335	LEU	1
2	B	430	VAL	1
1	A	188	LEU	1
2	B	389	SER	1
2	B	386	LEU	1
1	A	176	PHE	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 monosaccharides 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 (i)

No chemical shift data were provided