



Full wwPDB NMR Structure Validation Report ⓘ

Apr 27, 2016 – 02:08 AM BST

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.;
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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
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

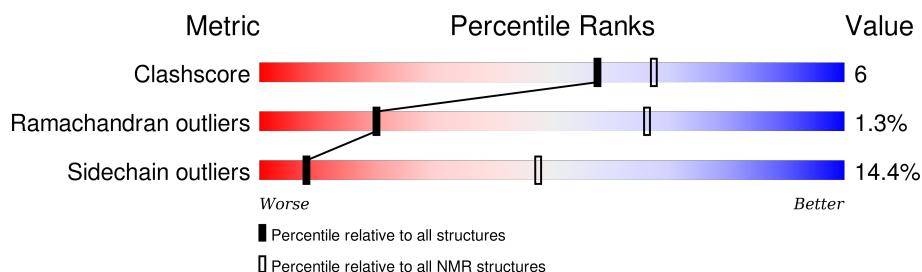
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment 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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	163	
2	B	131	

2 Ensemble composition and analysis

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)	0.47	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

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
1	A	163	Total	C	H	N	O	S	0
			1511	772	278	208	245	8	

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.

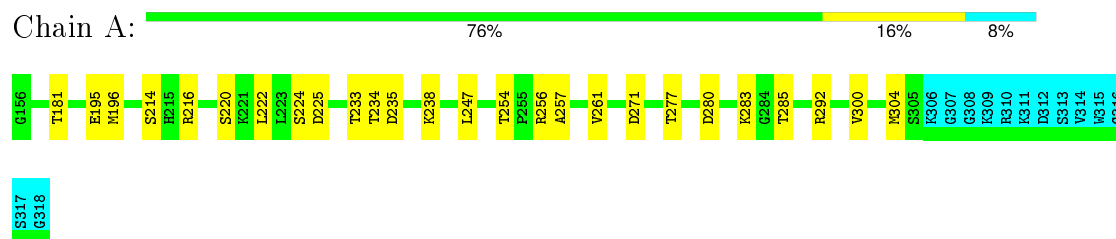
Mol	Chain	Residues	Atoms						Trace
2	B	131	Total	C	H	N	O	S	0
			1281	676	223	172	203	7	

4 Residue-property plots

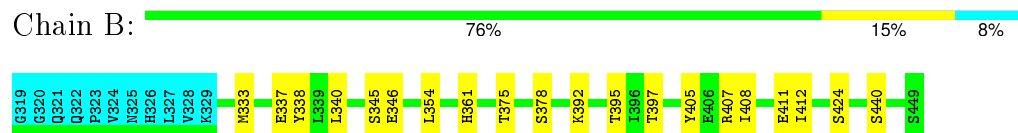
4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Programmed cell death protein 4



- Molecule 2: Programmed cell death protein 4

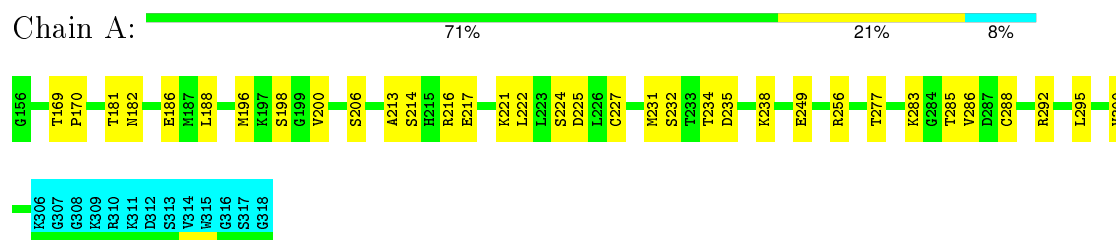


4.2 Scores per residue for each member of the ensemble

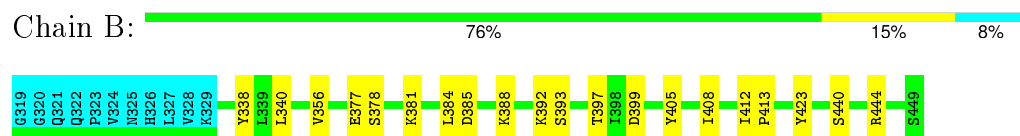
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Programmed cell death protein 4

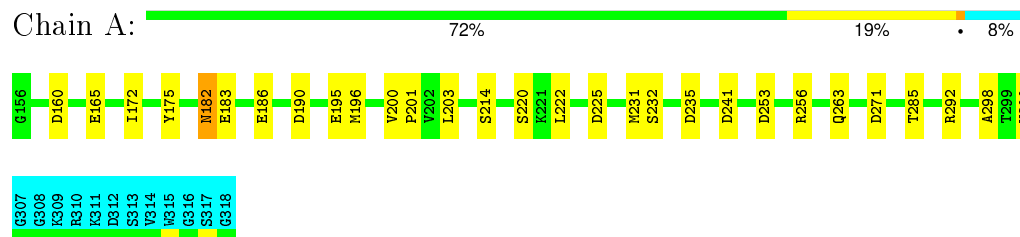


- Molecule 2: Programmed cell death protein 4

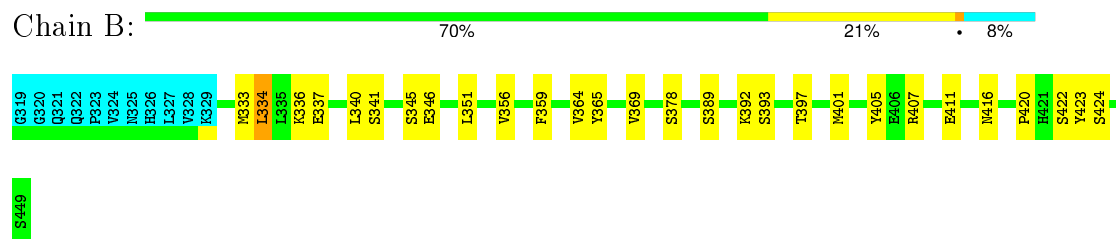


4.2.2 Score per residue for model 2

- Molecule 1: Programmed cell death protein 4

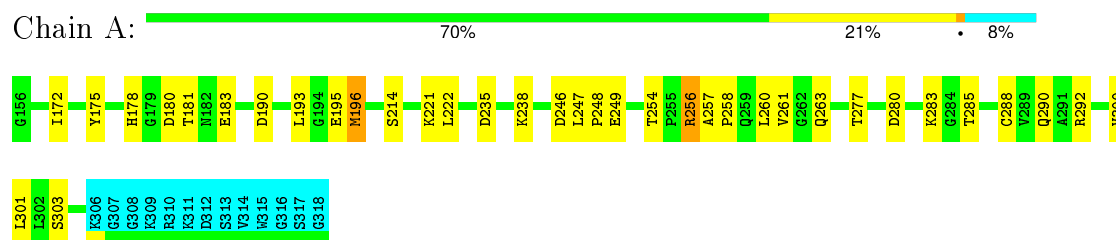


- Molecule 2: Programmed cell death protein 4

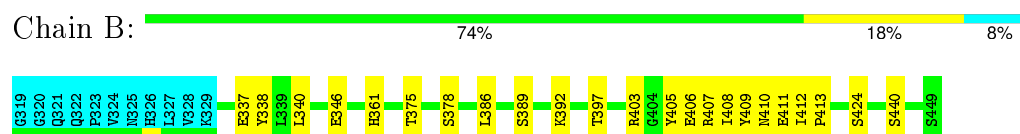


4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: Programmed cell death protein 4

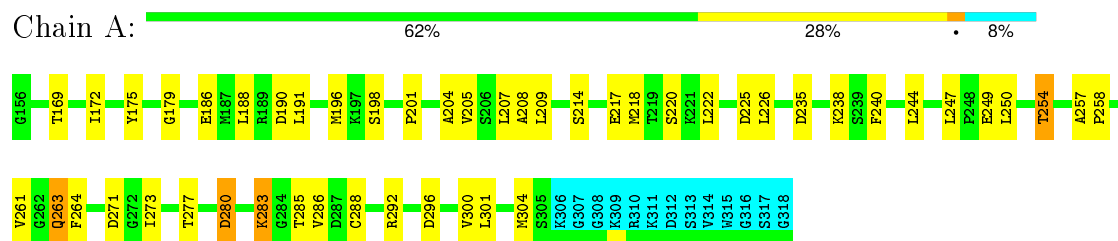


- Molecule 2: Programmed cell death protein 4

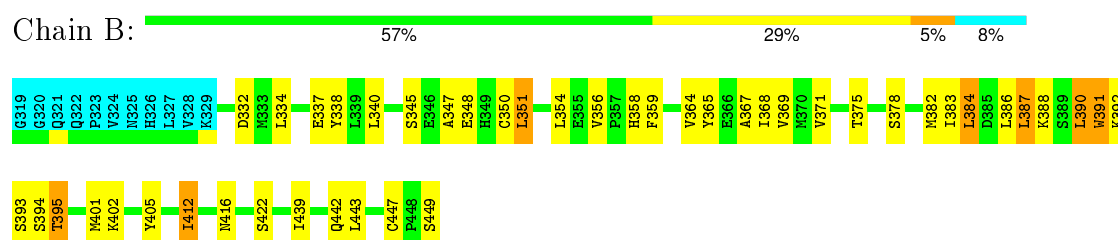


4.2.4 Score per residue for model 4

- Molecule 1: Programmed cell death protein 4

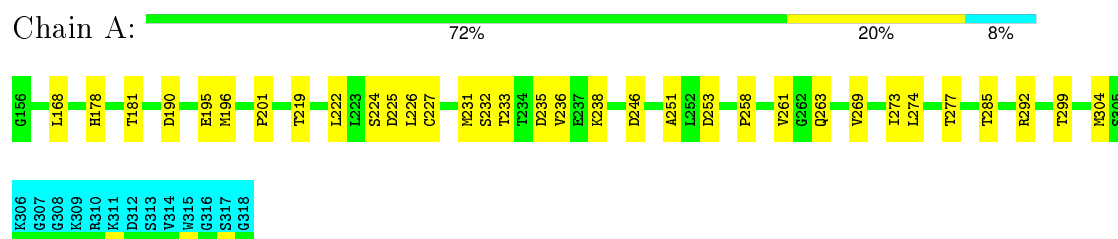


- Molecule 2: Programmed cell death protein 4

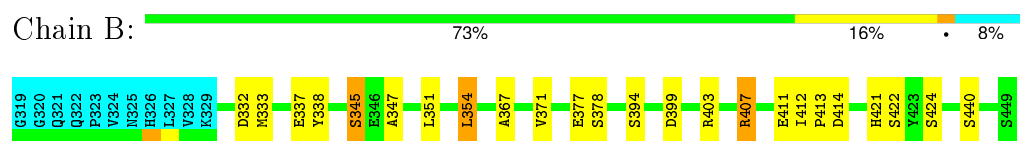


4.2.5 Score per residue for model 5

- Molecule 1: Programmed cell death protein 4



- Molecule 2: Programmed cell death protein 4



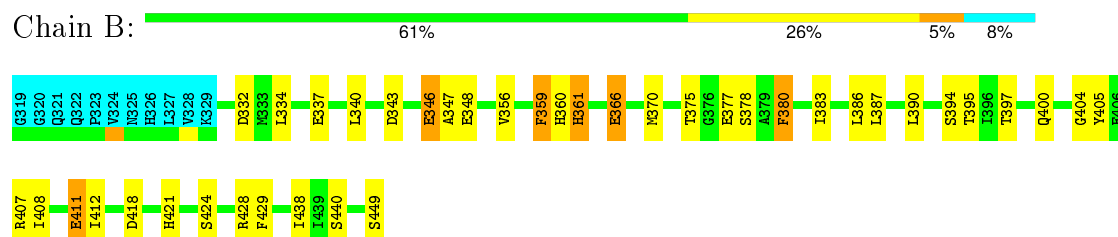
4.2.6 Score per residue for model 6

- Molecule 1: Programmed cell death protein 4



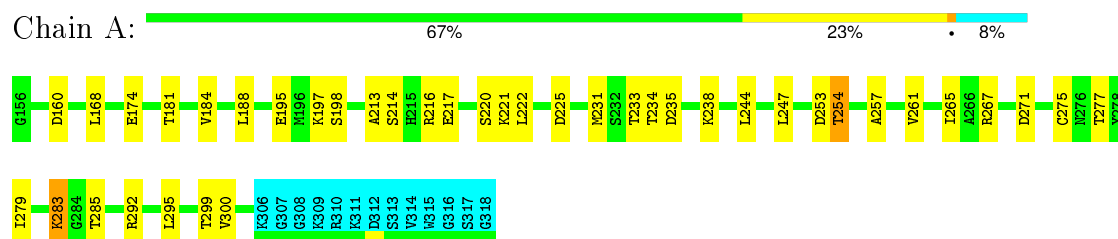


- Molecule 2: Programmed cell death protein 4

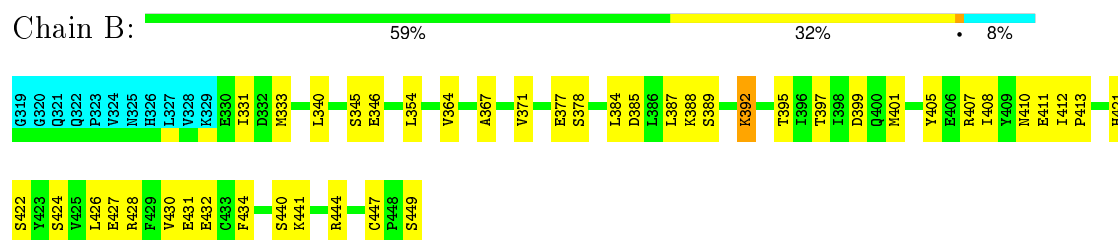


4.2.7 Score per residue for model 7

- Molecule 1: Programmed cell death protein 4

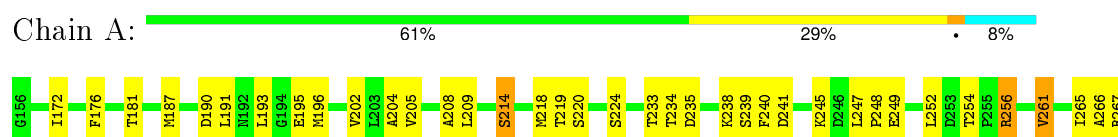


- Molecule 2: Programmed cell death protein 4



4.2.8 Score per residue for model 8

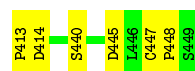
- Molecule 1: Programmed cell death protein 4





- Molecule 2: Programmed cell death protein 4

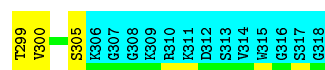
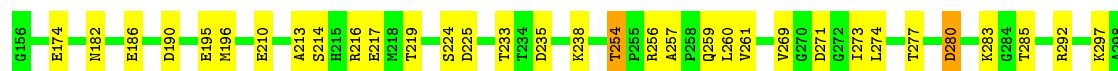
Chain B: 64% 23% 8%



4.2.9 Score per residue for model 9

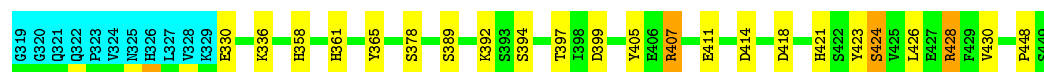
- Molecule 1: Programmed cell death protein 4

Chain A: 70% 21% 8%



- Molecule 2: Programmed cell death protein 4

Chain B: 74% 15% 8%



4.2.10 Score per residue for model 10

- Molecule 1: Programmed cell death protein 4

Chain A: 71% 21% 8%



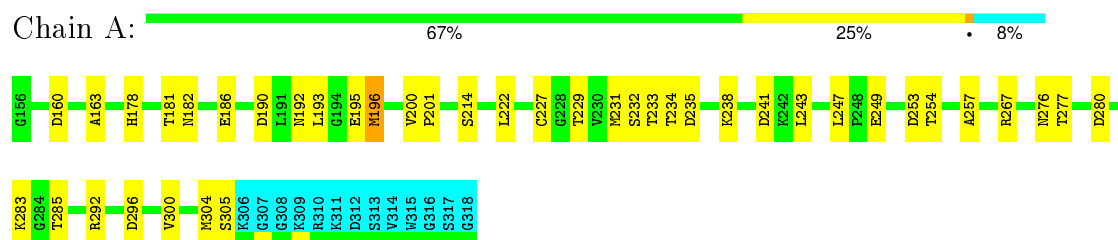
- Molecule 2: Programmed cell death protein 4

Chain B: 65% 27% 8%

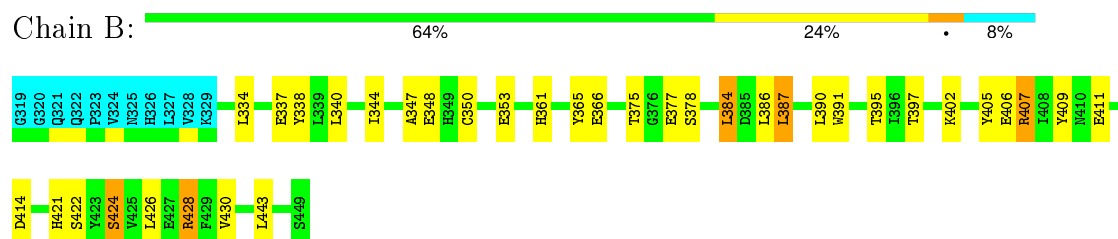


4.2.11 Score per residue for model 11

- Molecule 1: Programmed cell death protein 4

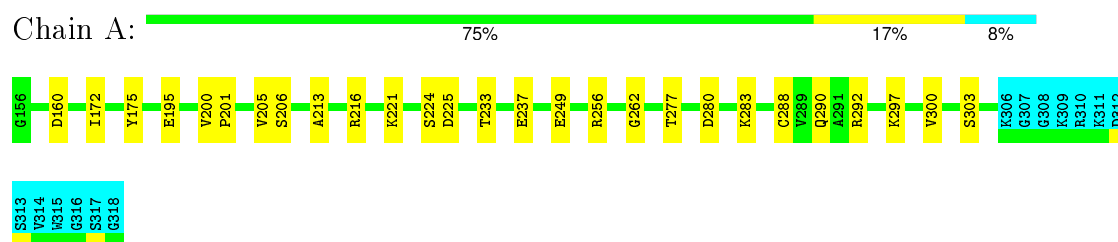


- Molecule 2: Programmed cell death protein 4

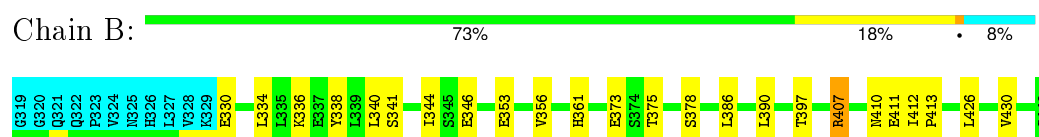


4.2.12 Score per residue for model 12

- Molecule 1: Programmed cell death protein 4

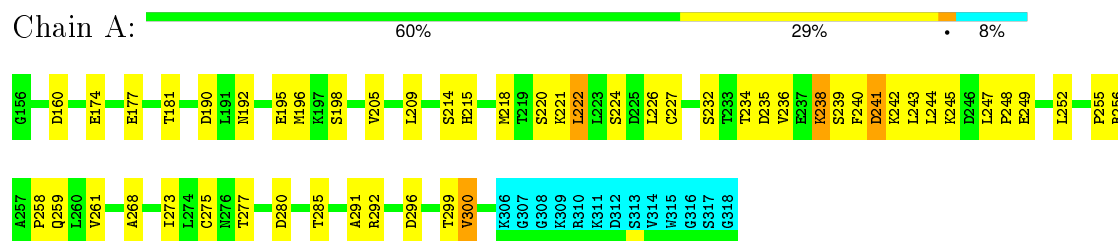


- Molecule 2: Programmed cell death protein 4

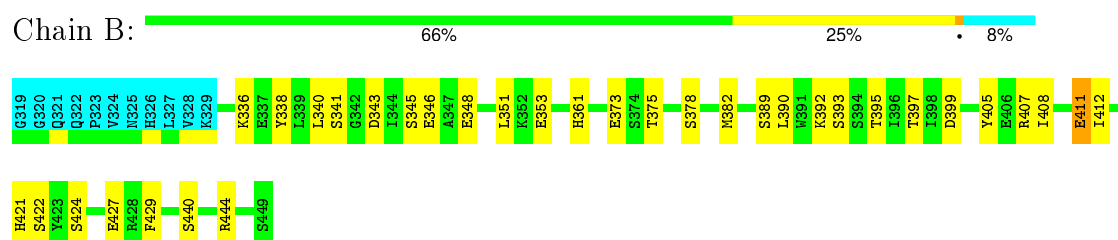


4.2.13 Score per residue for model 13

- Molecule 1: Programmed cell death protein 4

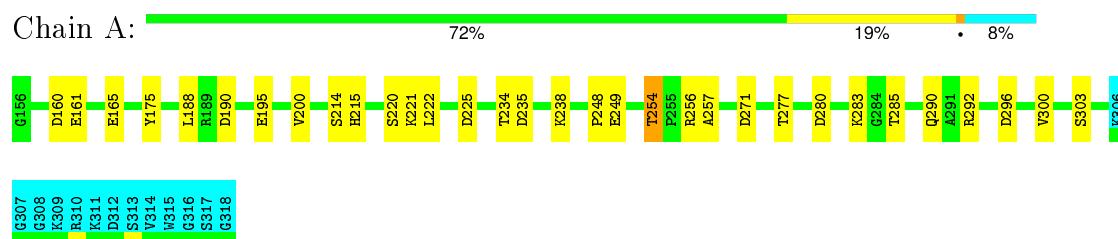


- Molecule 2: Programmed cell death protein 4

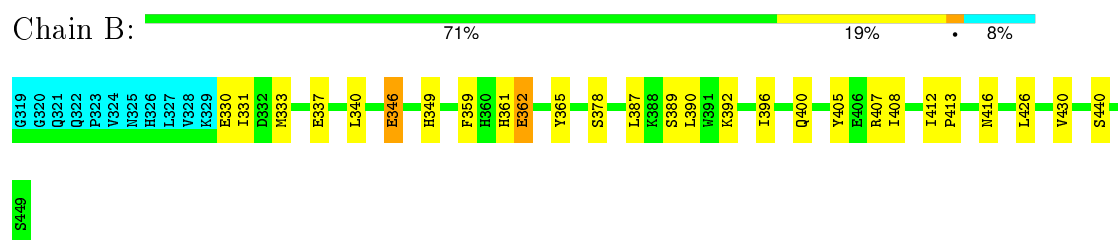


4.2.14 Score per residue for model 14

- Molecule 1: Programmed cell death protein 4

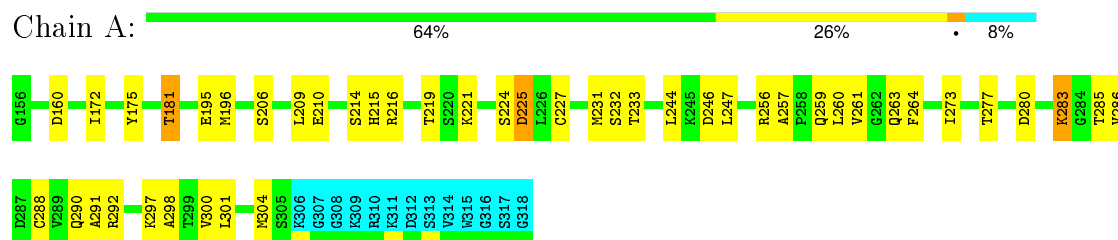


- Molecule 2: Programmed cell death protein 4

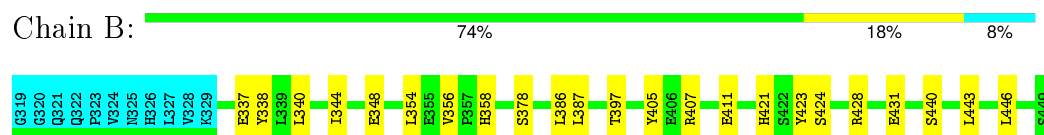


4.2.15 Score per residue for model 15

- Molecule 1: Programmed cell death protein 4

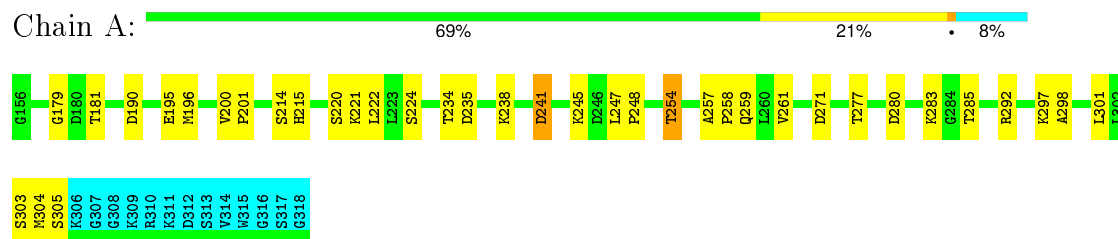


- Molecule 2: Programmed cell death protein 4

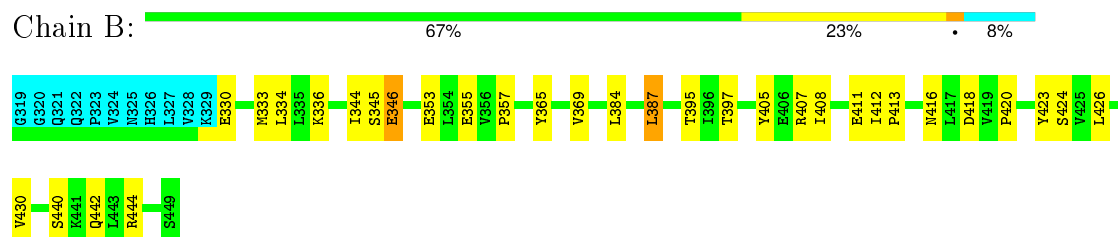


4.2.16 Score per residue for model 16

- Molecule 1: Programmed cell death protein 4

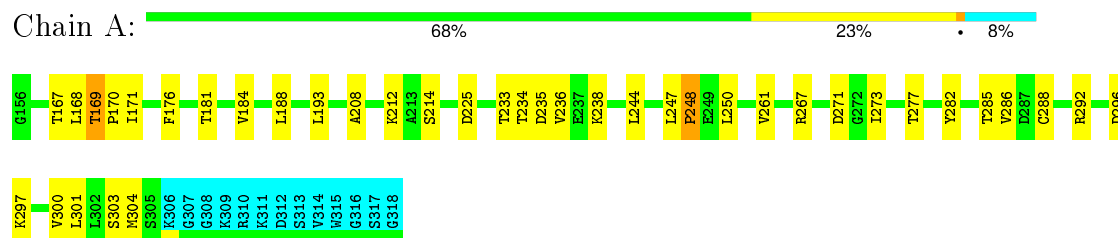


- Molecule 2: Programmed cell death protein 4

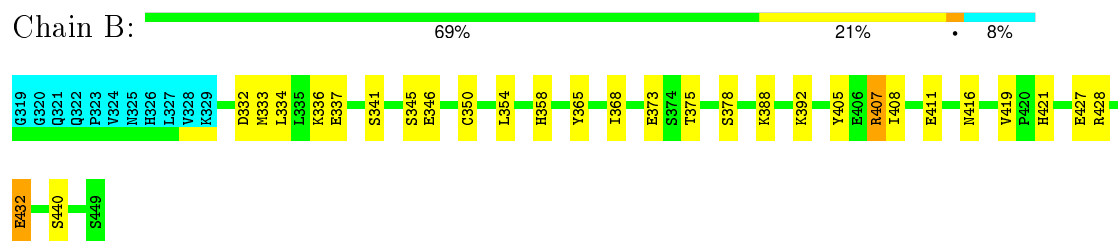


4.2.17 Score per residue for model 17

- Molecule 1: Programmed cell death protein 4

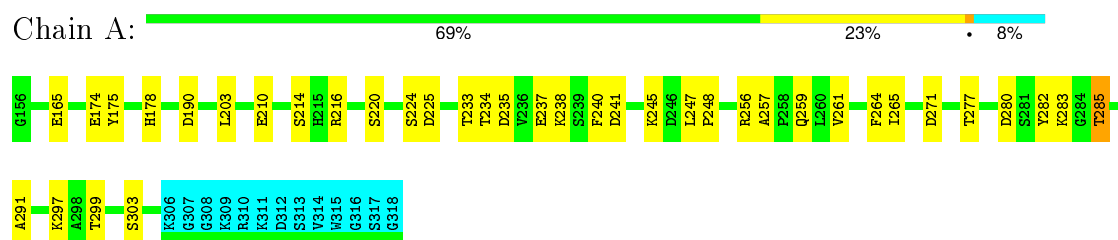


- Molecule 2: Programmed cell death protein 4

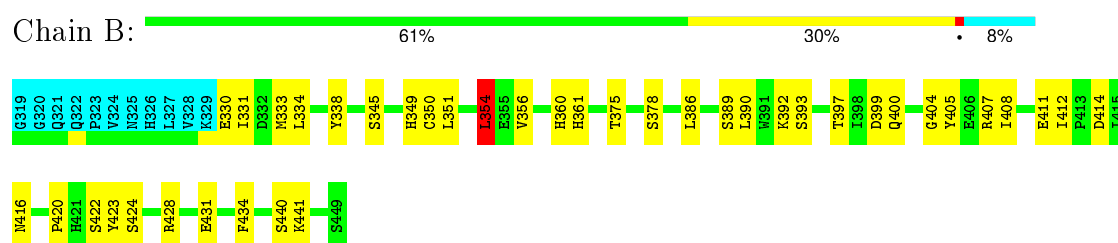


4.2.18 Score per residue for model 18

- Molecule 1: Programmed cell death protein 4

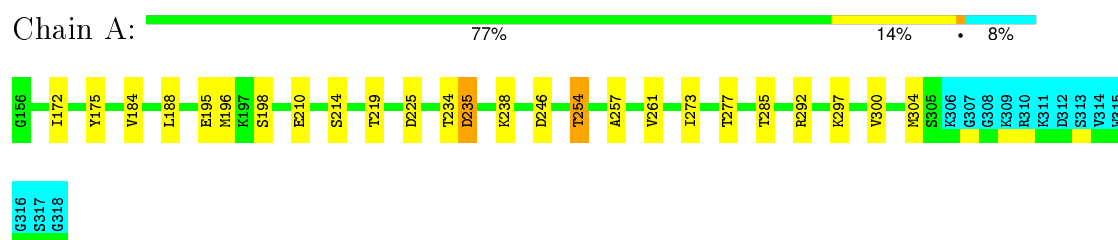


- Molecule 2: Programmed cell death protein 4

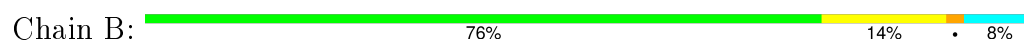


4.2.19 Score per residue for model 19

- Molecule 1: Programmed cell death protein 4



- Molecule 2: Programmed cell death protein 4

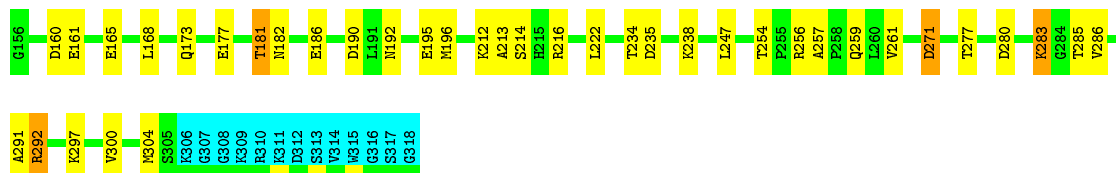




4.2.20 Score per residue for model 20

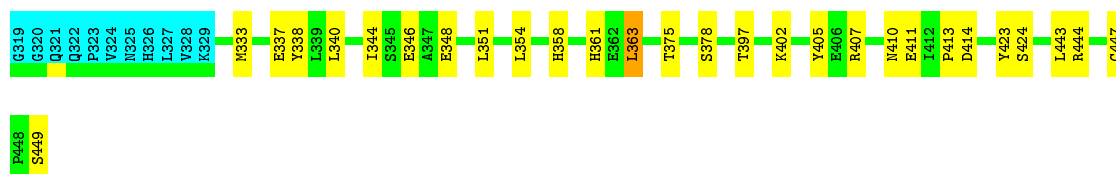
- Molecule 1: Programmed cell death protein 4

Chain A: 69% 21% 8%



- Molecule 2: Programmed cell death protein 4

Chain B: 70% 21% 8%



4.2.21 Score per residue for model 21

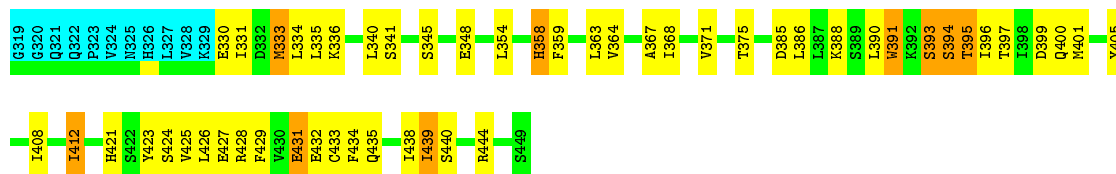
- Molecule 1: Programmed cell death protein 4

Chain A: 60% 31% 8%



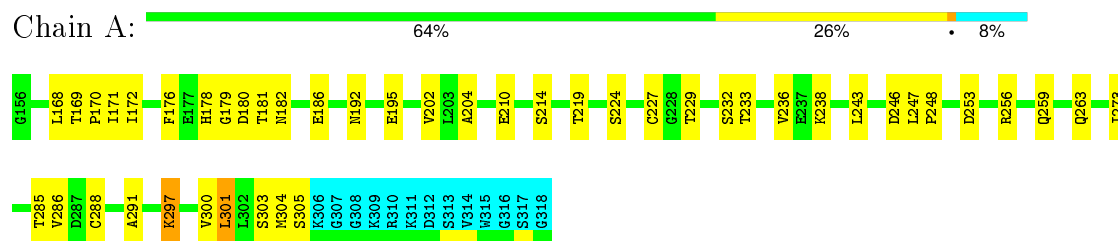
- Molecule 2: Programmed cell death protein 4

Chain B: 52% 33% 7% 8%

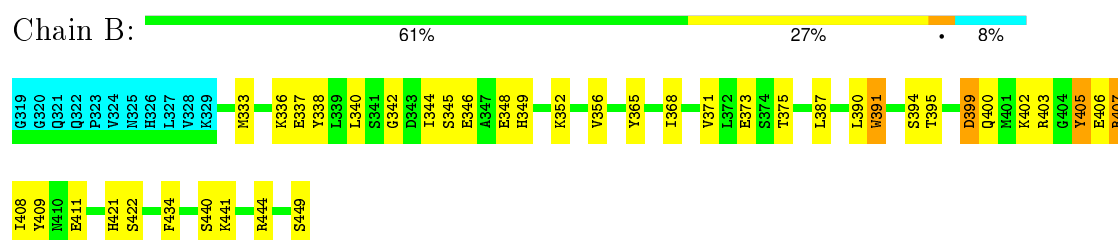


4.2.22 Score per residue for model 22

- Molecule 1: Programmed cell death protein 4

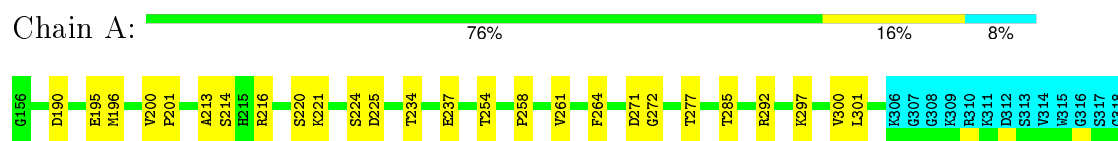


- Molecule 2: Programmed cell death protein 4

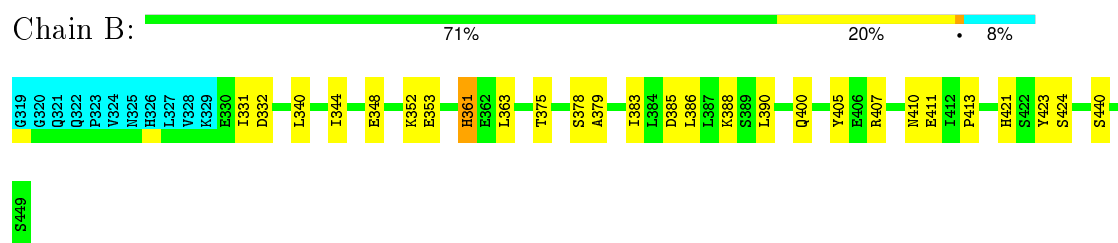


4.2.23 Score per residue for model 23

- Molecule 1: Programmed cell death protein 4



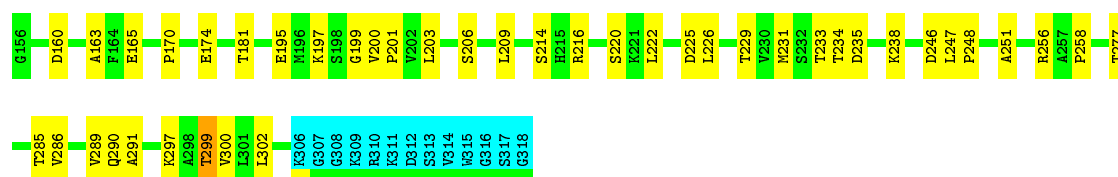
- Molecule 2: Programmed cell death protein 4



4.2.24 Score per residue for model 24

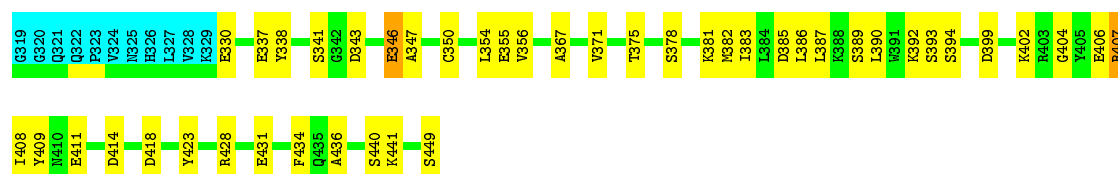
- Molecule 1: Programmed cell death protein 4





- Molecule 2: Programmed cell death protein 4

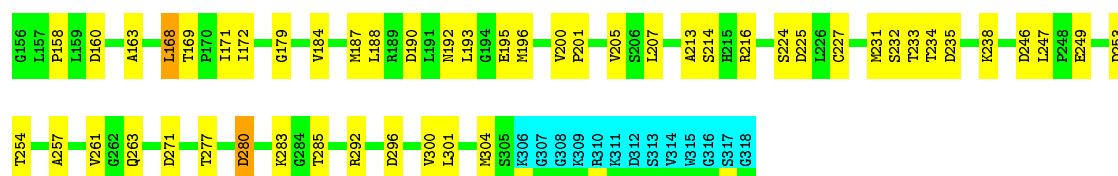
Chain B: 58% 32% 8%



4.2.25 Score per residue for model 25

- Molecule 1: Programmed cell death protein 4

Chain A: 61% 29% 8%



- Molecule 2: Programmed cell death protein 4

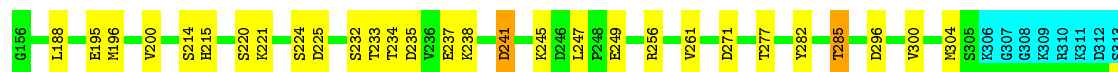
Chain B: 67% 24% 8%



4.2.26 Score per residue for model 26

- Molecule 1: Programmed cell death protein 4

Chain A: 74% 17% 8%



V314
W315
G316
S317
G318

- Molecule 2: Programmed cell death protein 4

Chain B: 

G319 G320 Q321 Q322 P323 V324 W325 H326 L327 V328 K329 E330 L331 L334 L335 K336 L340 S341 G342 D343 E346 E353 H358 E362 T375 S378 K381 D385 S389 K392 S393 S394 T397 I398 D399 Y405 E406 R407 E411 I412 P413 D414 V419 P420

H421 S422 Y423 S424 S440 L443 L446 S449

4.2.27 Score per residue for model 27

- Molecule 1: Programmed cell death protein 4

Chain A: 

G156 D160 T167 L168 T181 V184 L188 E195 M196 V200 P201 S214 S224 C227 S232 T233 T234 D235 V236 E237 K238 S239 L243 P248 L252 D253 T254 A257 V261 G262 Q263 I273 L274 T277 D280 K283 G284 T285 V286

A291 D296 K297 A298 T299 V300 S303 K304 S305 K306 G307 G308 K309 R310 D311 K312 S313 V314 W315 G316 S317 G318

- Molecule 2: Programmed cell death protein 4

Chain B: 

G319 G320 Q321 Q322 P323 V324 W325 H326 L327 V328 K329 E330 L331 D332 K336 H349 C350 L351 L354 E355 V356 H360 A367 V371 L372 E373 S374 T375 S378 L386 S389 L390 W391 K392 S393 S394 T395 D399 K402 E406 R407 I408 Y409 W410 E411 I412 P413

H421 S422 E427 R428 E431 E432 C433 I438 I439 S440 K441 Q442 D445 S449

4.2.28 Score per residue for model 28

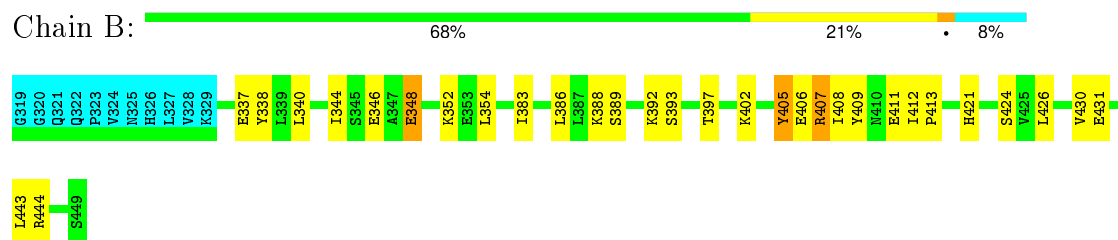
- Molecule 1: Programmed cell death protein 4

Chain A: 

G156 D160 T167 L168 T169 P170 I171 G179 D180 T181 L193 G194 E195 M196 E210 T219 S224 D225 T233 T234 E237 D241 L247 P248 E249 D253 T254 P255 R256 A257 P258 Q259 L260 V261 G262 Q263 I273 L274 T277 D280 K283 G284 T285 P413 V286

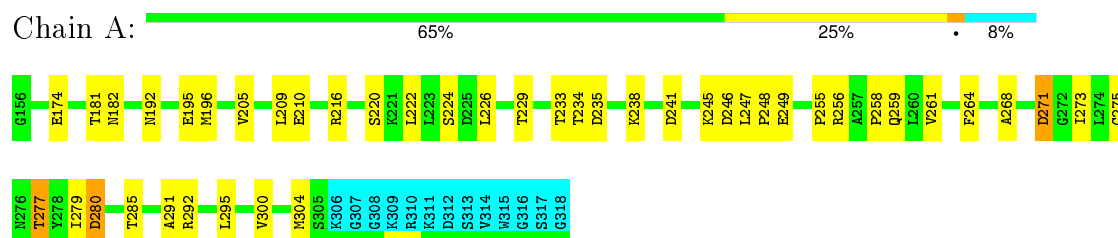
D287 C288 R292 V300 L301 L302 S303 K306 G307 G308 K309 R310 K311 D312 S313 V314 W315 G316 S317 G318

- Molecule 2: Programmed cell death protein 4

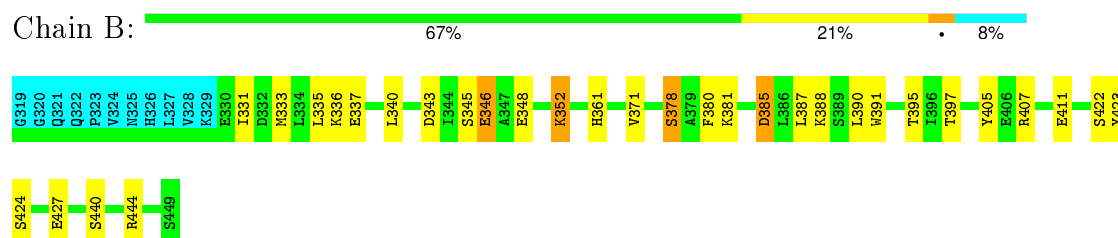


4.2.29 Score per residue for model 29

- Molecule 1: Programmed cell death protein 4

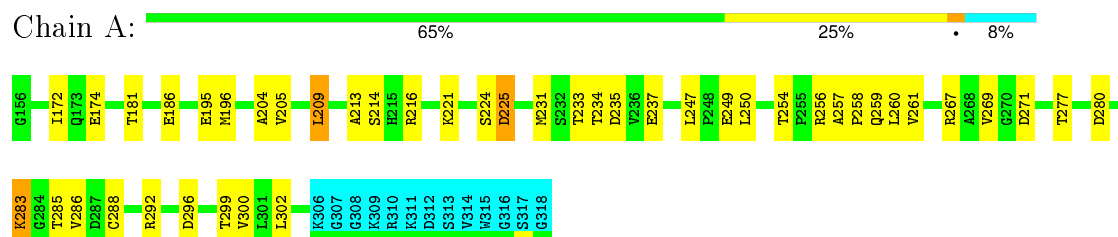


- Molecule 2: Programmed cell death protein 4

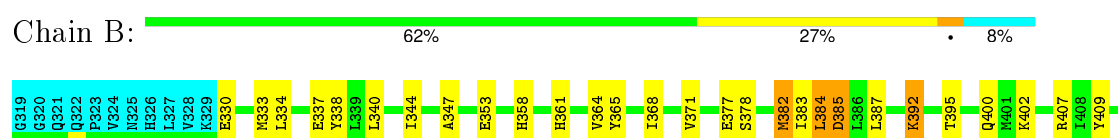


4.2.30 Score per residue for model 30

- Molecule 1: Programmed cell death protein 4



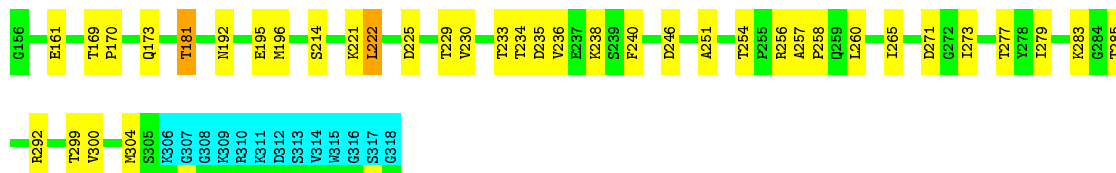
- Molecule 2: Programmed cell death protein 4



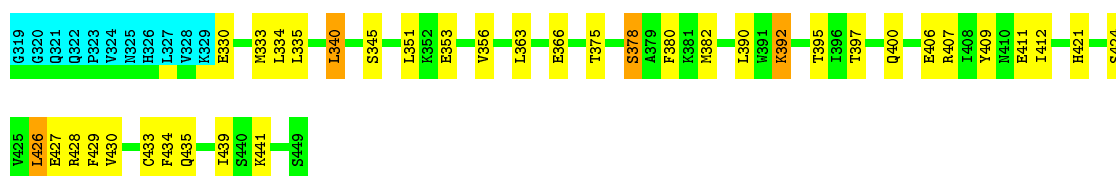


4.2.31 Score per residue for model 31

- Molecule 1: Programmed cell death protein 4

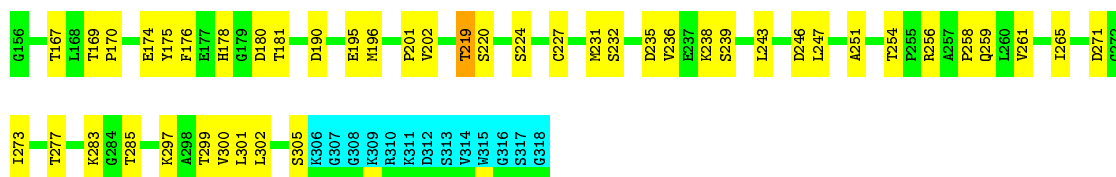


- Molecule 2: Programmed cell death protein 4

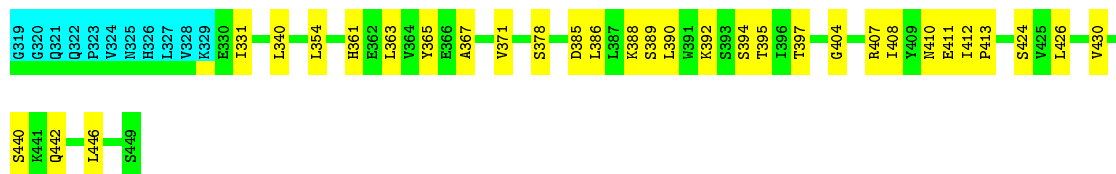


4.2.32 Score per residue for model 32

- Molecule 1: Programmed cell death protein 4

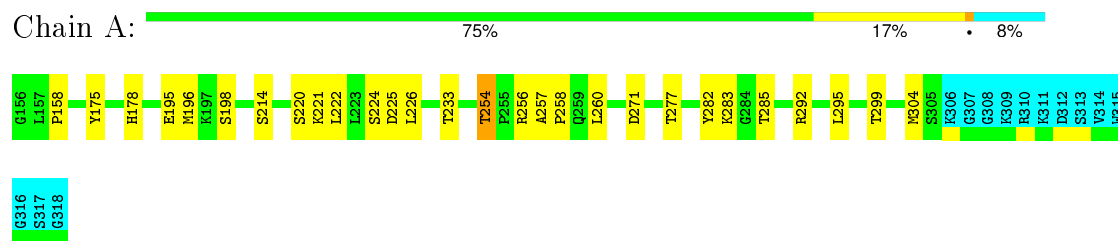


- Molecule 2: Programmed cell death protein 4

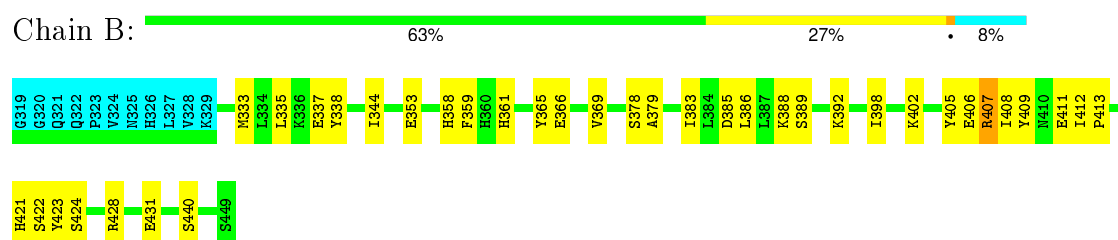


4.2.33 Score per residue for model 33

- Molecule 1: Programmed cell death protein 4

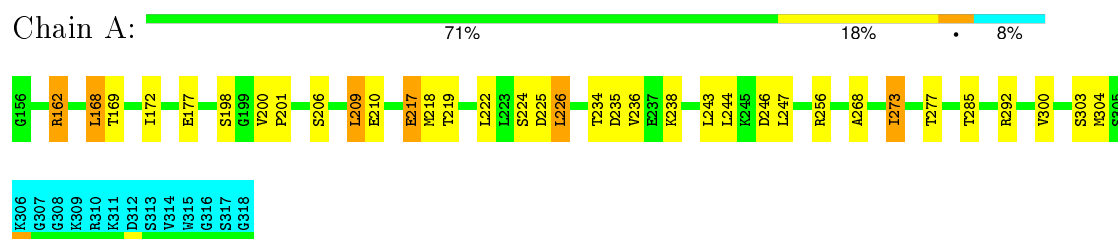


- Molecule 2: Programmed cell death protein 4

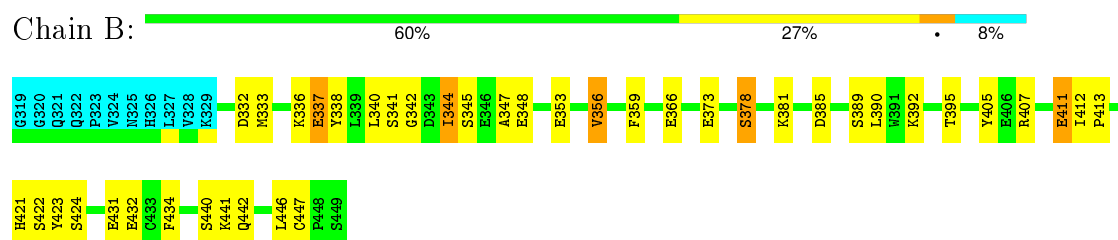


4.2.34 Score per residue for model 34

- Molecule 1: Programmed cell death protein 4

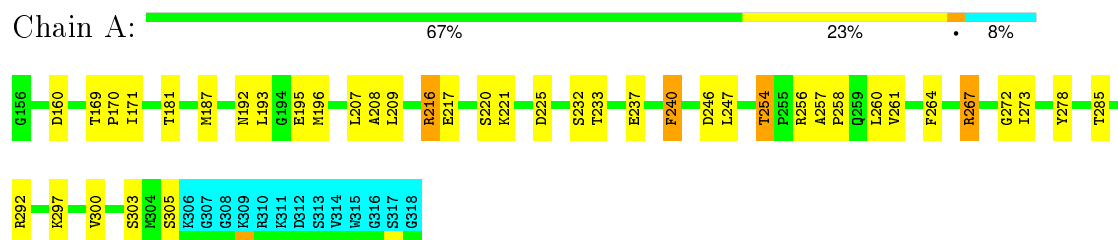


- Molecule 2: Programmed cell death protein 4

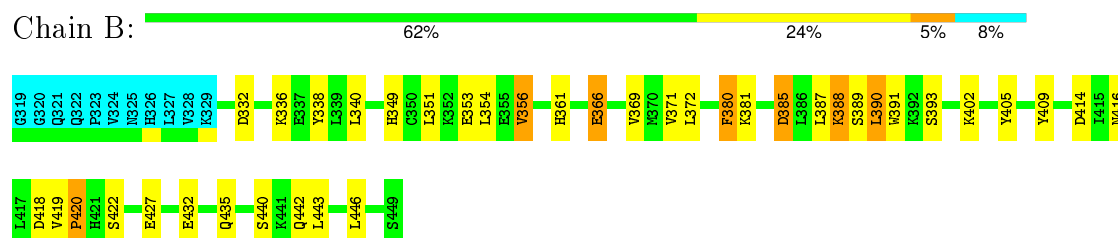


4.2.35 Score per residue for model 35

- Molecule 1: Programmed cell death protein 4

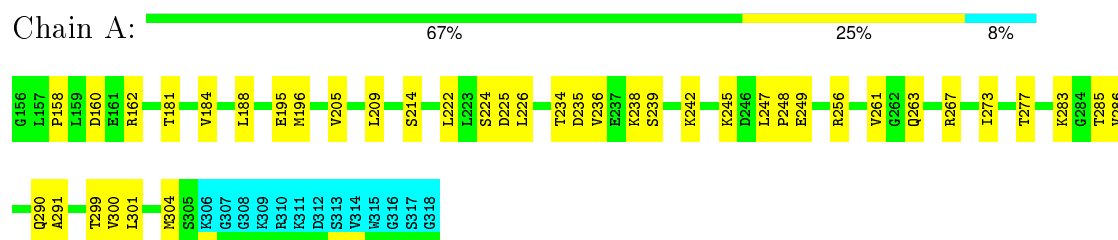


- Molecule 2: Programmed cell death protein 4

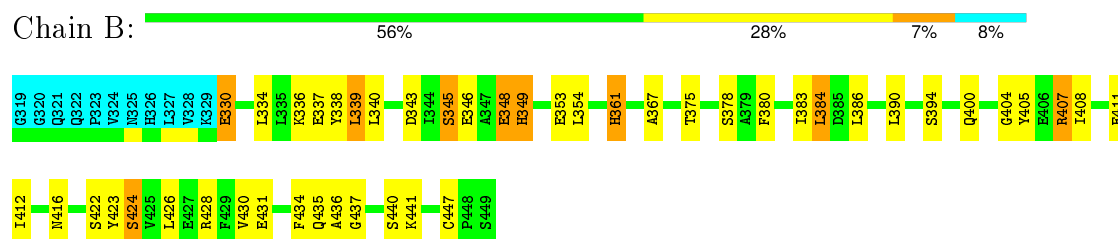


4.2.36 Score per residue for model 36

- Molecule 1: Programmed cell death protein 4

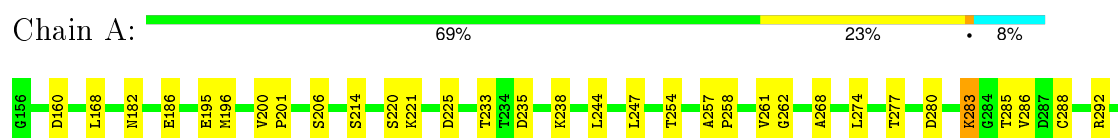


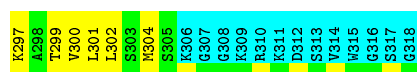
- Molecule 2: Programmed cell death protein 4



4.2.37 Score per residue for model 37

- Molecule 1: Programmed cell death protein 4





- Molecule 2: Programmed cell death protein 4

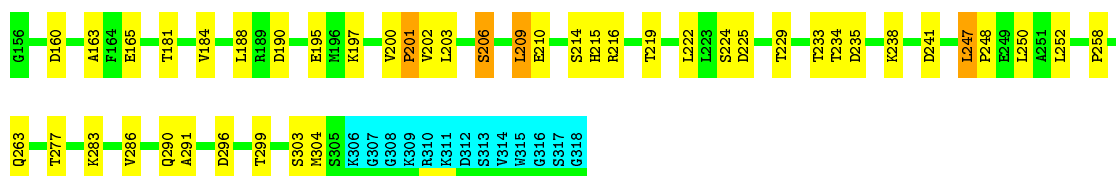
Chain B: 71% 17% 8%



4.2.38 Score per residue for model 38

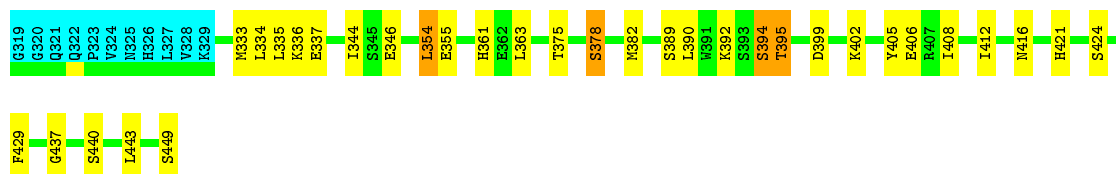
- Molecule 1: Programmed cell death protein 4

Chain A: 65% 25% 8%



- Molecule 2: Programmed cell death protein 4

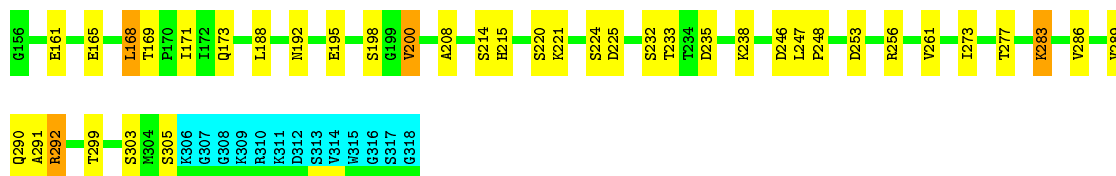
Chain B: 66% 22% 8%



4.2.39 Score per residue for model 39

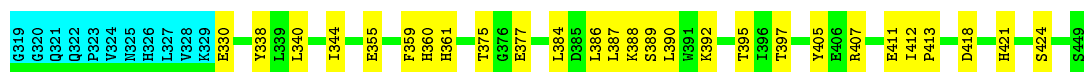
- Molecule 1: Programmed cell death protein 4

Chain A: 68% 21% 8%



- Molecule 2: Programmed cell death protein 4

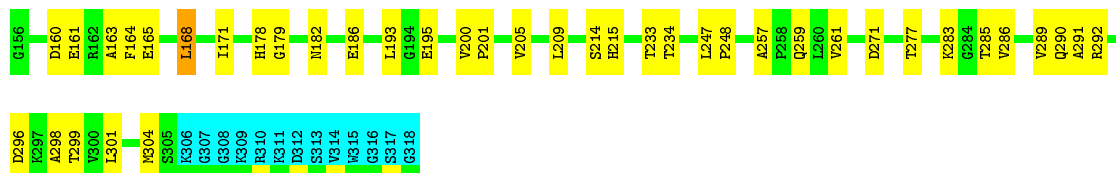
Chain B: 71% 21% 8%



4.2.40 Score per residue for model 40

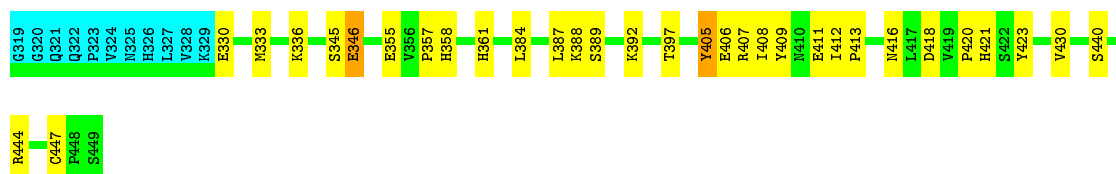
- Molecule 1: Programmed cell death protein 4

Chain A: 67% 24% 8%



- Molecule 2: Programmed cell death protein 4

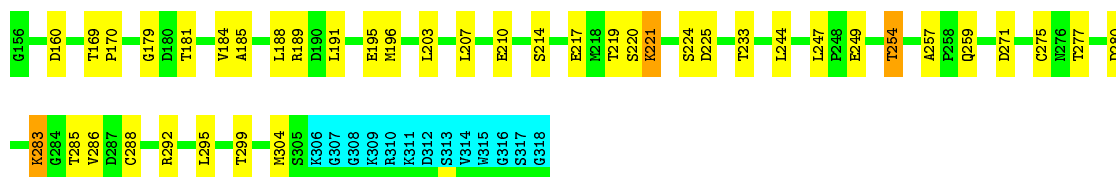
Chain B: 67% 23% 8%



4.2.41 Score per residue for model 41

- Molecule 1: Programmed cell death protein 4

Chain A: 67% 23% 8%



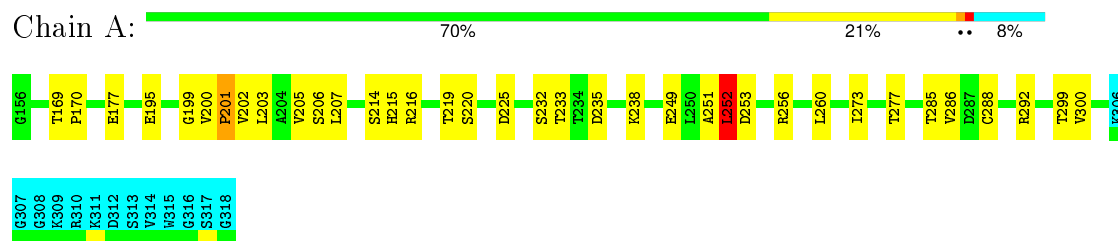
- Molecule 2: Programmed cell death protein 4

Chain B: 64% 26% 8%

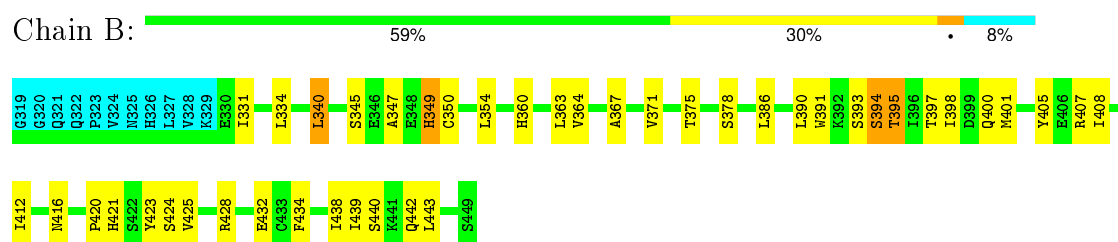


4.2.42 Score per residue for model 42

- Molecule 1: Programmed cell death protein 4

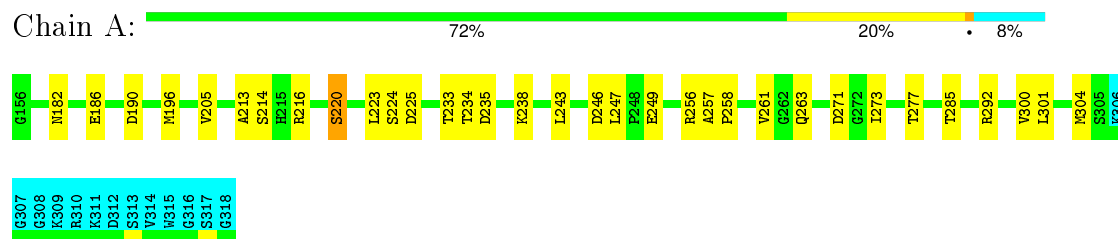


- Molecule 2: Programmed cell death protein 4

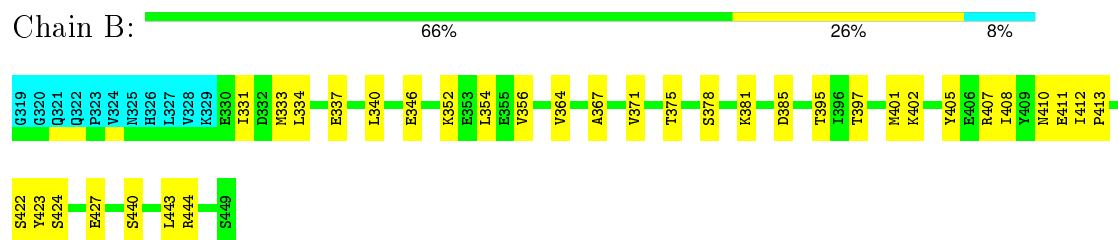


4.2.43 Score per residue for model 43

- Molecule 1: Programmed cell death protein 4

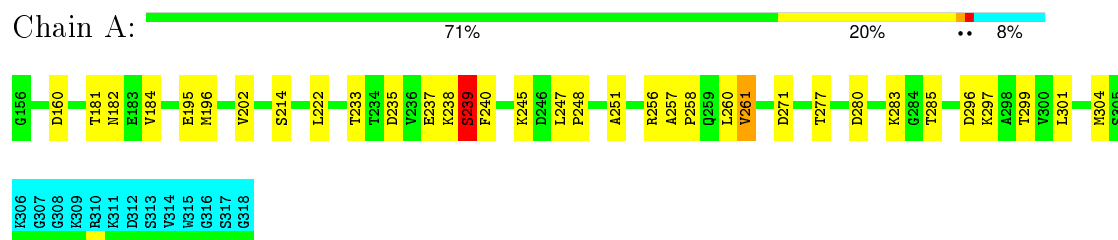


- Molecule 2: Programmed cell death protein 4

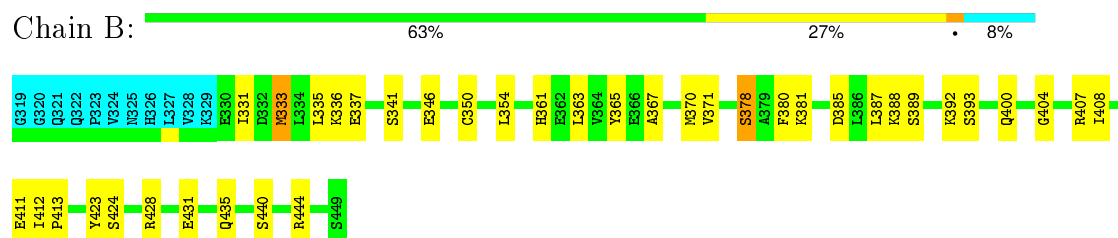


4.2.44 Score per residue for model 44

- Molecule 1: Programmed cell death protein 4

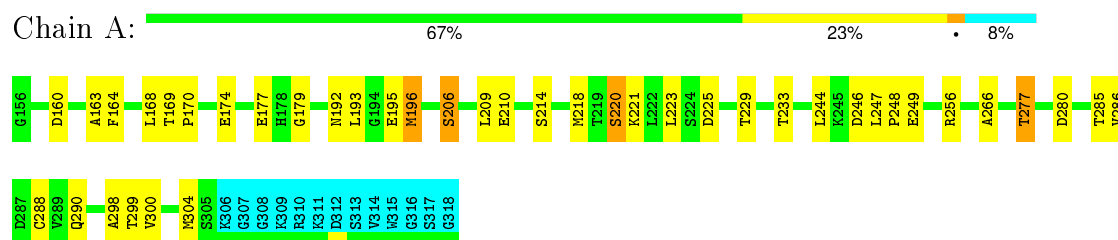


• Molecule 2: Programmed cell death protein 4

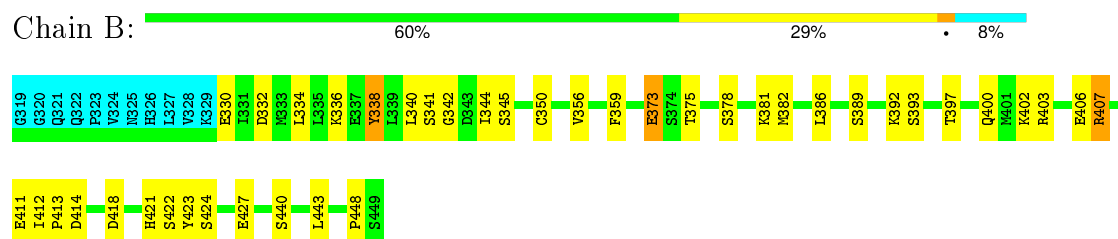


4.2.45 Score per residue for model 45

• Molecule 1: Programmed cell death protein 4

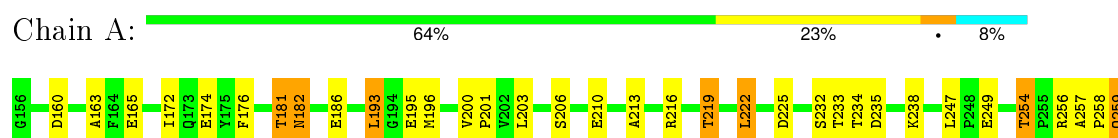


• Molecule 2: Programmed cell death protein 4



4.2.46 Score per residue for model 46

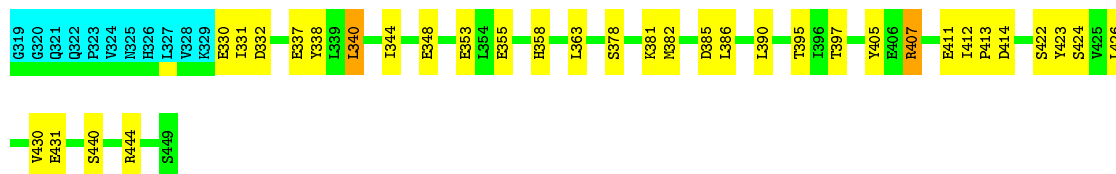
• Molecule 1: Programmed cell death protein 4





- Molecule 2: Programmed cell death protein 4

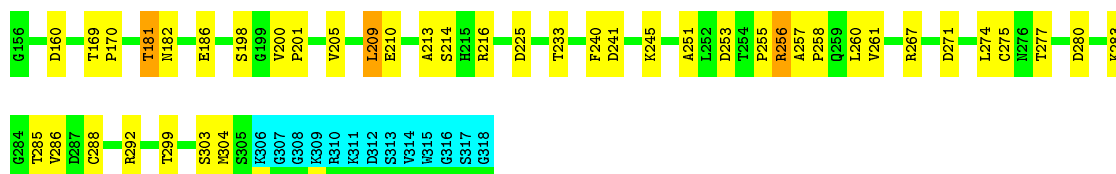
Chain B: 66% 24% 8%



4.2.47 Score per residue for model 47

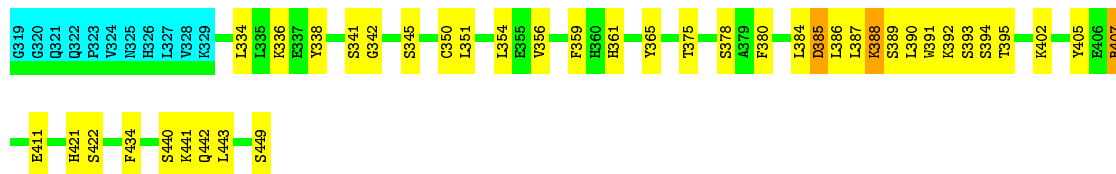
- Molecule 1: Programmed cell death protein 4

Chain A: 66% 24% 8%



- Molecule 2: Programmed cell death protein 4

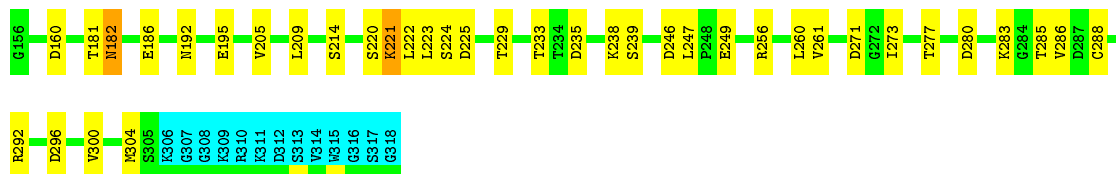
Chain B: 61% 28% 8%



4.2.48 Score per residue for model 48

- Molecule 1: Programmed cell death protein 4

Chain A: 69% 22% 8%



- Molecule 2: Programmed cell death protein 4

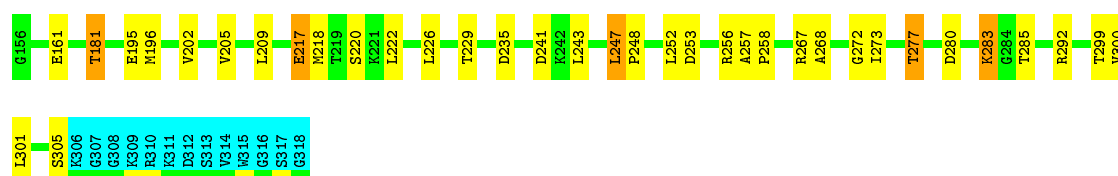
Chain B: 



4.2.49 Score per residue for model 49

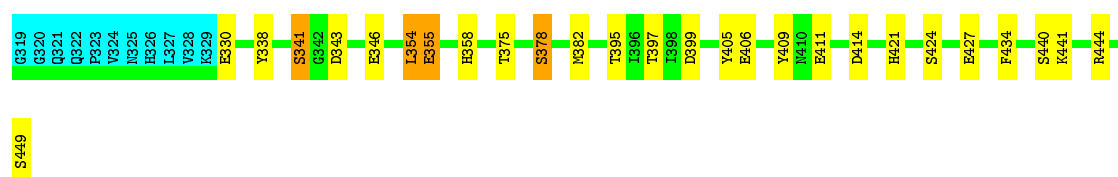
- Molecule 1: Programmed cell death protein 4

Chain A: 



- Molecule 2: Programmed cell death protein 4

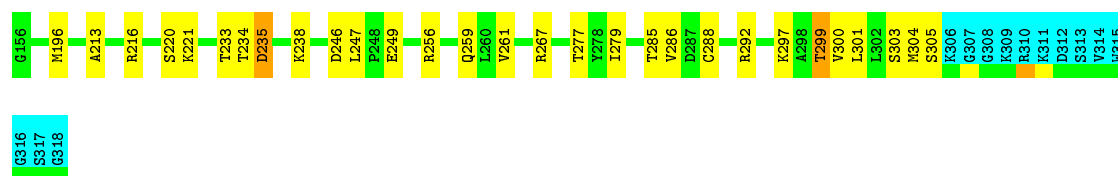
Chain B: 



4.2.50 Score per residue for model 50

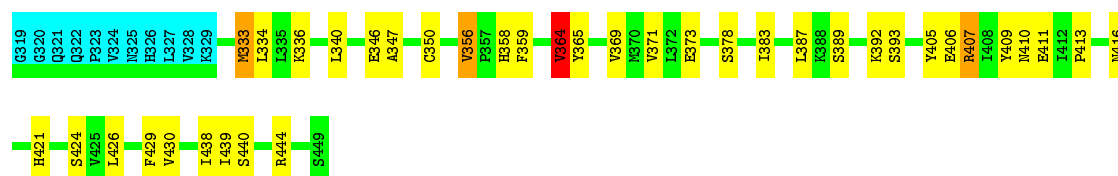
- Molecule 1: Programmed cell death protein 4

Chain A: 



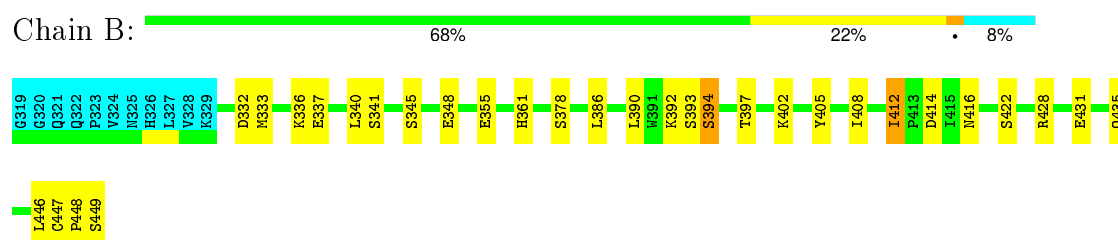
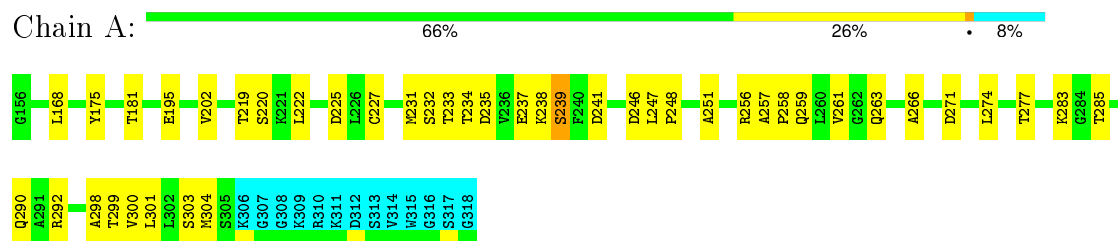
- Molecule 2: Programmed cell death protein 4

Chain B: 

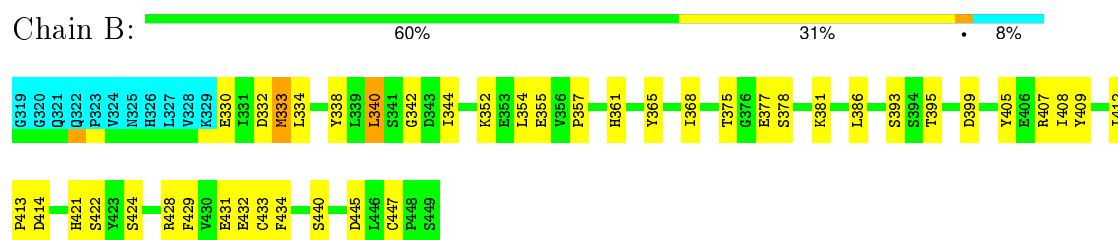
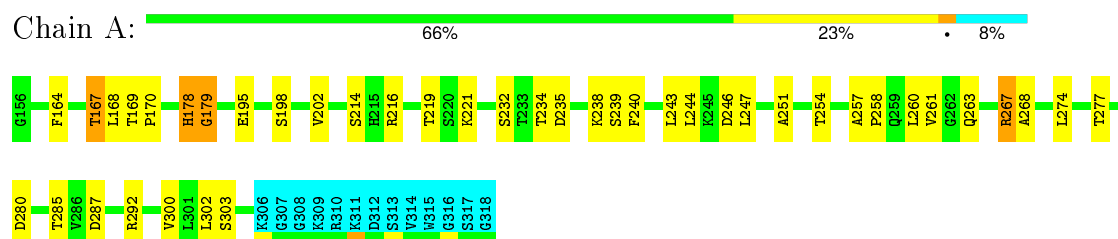


4.2.51 Score per residue for model 51

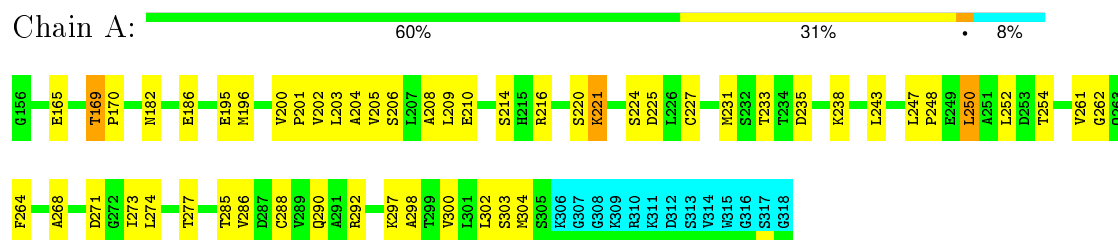
- Molecule 1: Programmed cell death protein 4



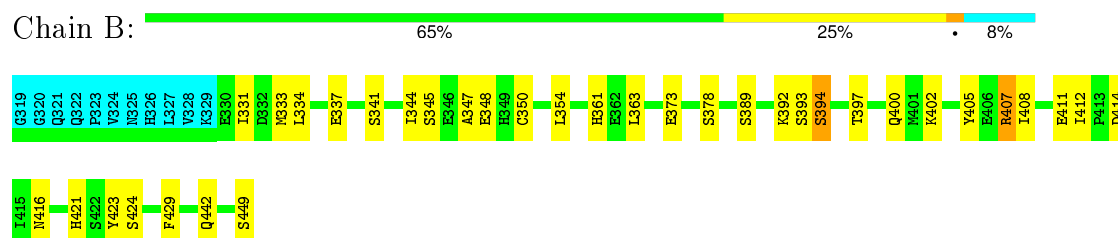
- Molecule 1: Programmed cell death protein 4



- Molecule 1: Programmed cell death protein 4

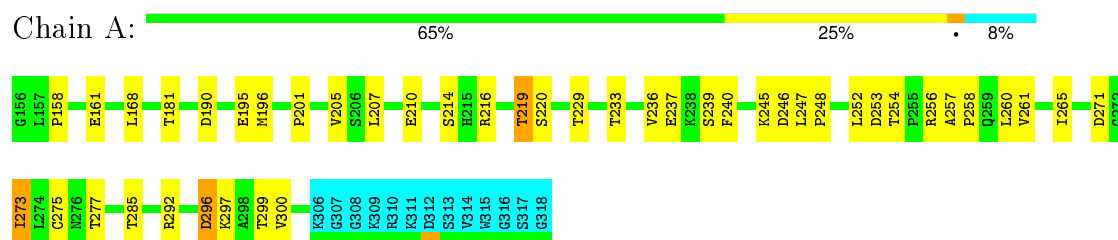


- Molecule 2: Programmed cell death protein 4

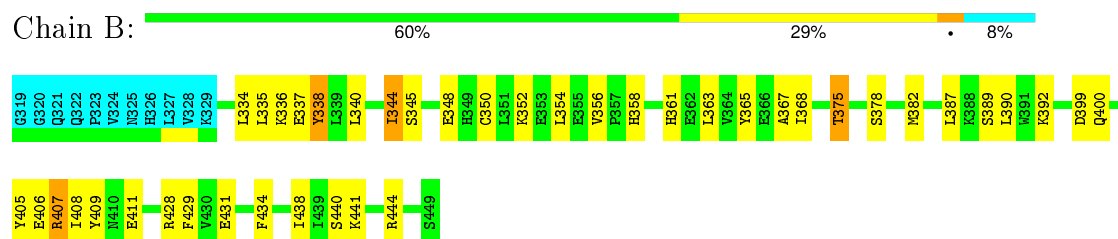


4.2.54 Score per residue for model 54

- Molecule 1: Programmed cell death protein 4

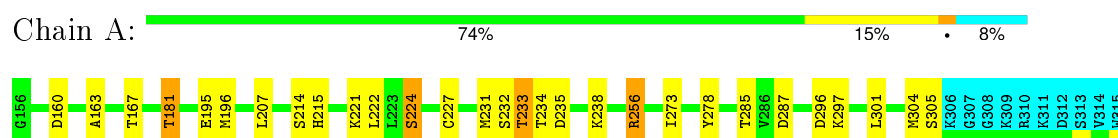


- Molecule 2: Programmed cell death protein 4



4.2.55 Score per residue for model 55

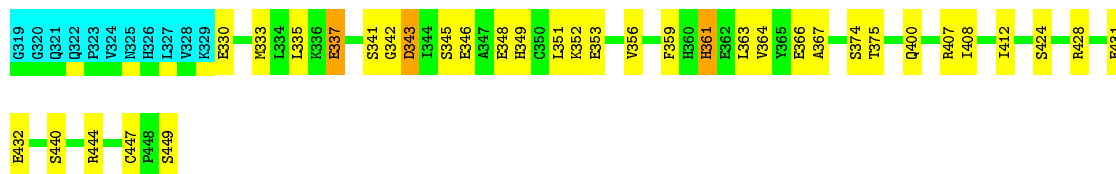
- Molecule 1: Programmed cell death protein 4





- Molecule 2: Programmed cell death protein 4

Chain B: 65% 24% 8%



4.2.56 Score per residue for model 56

- Molecule 1: Programmed cell death protein 4

Chain A: 63% 28% 8%



- Molecule 2: Programmed cell death protein 4

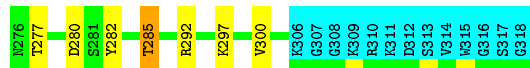
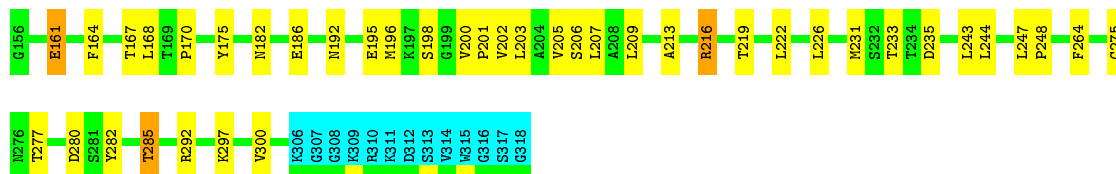
Chain B: 61% 29% 8%



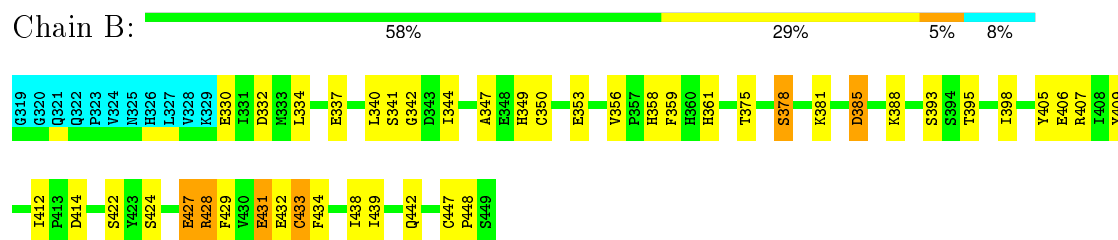
4.2.57 Score per residue for model 57

- Molecule 1: Programmed cell death protein 4

Chain A: 67% 23% 8%

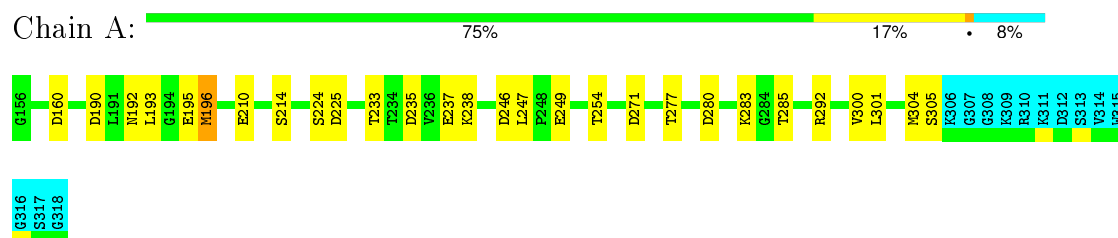


- Molecule 2: Programmed cell death protein 4

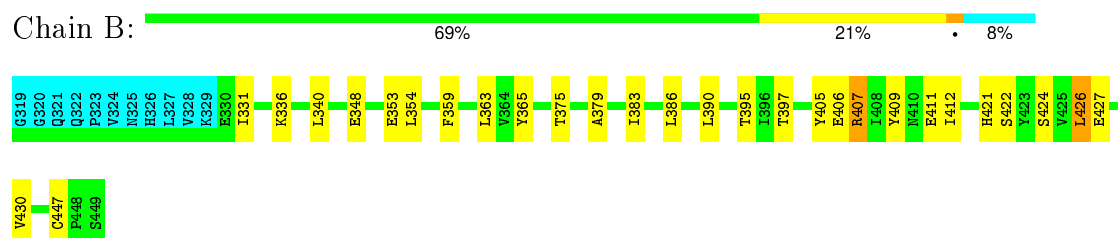


4.2.58 Score per residue for model 58

- Molecule 1: Programmed cell death protein 4

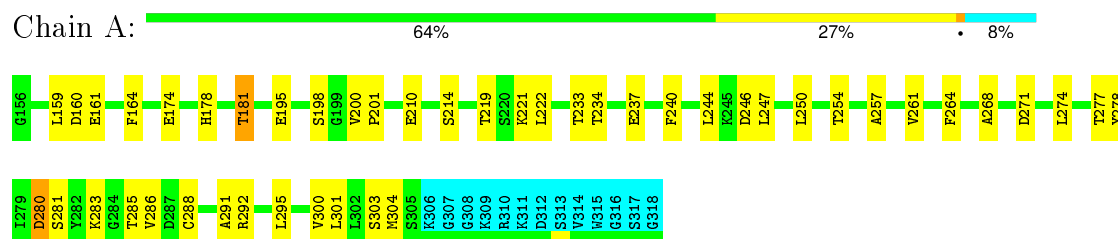


- Molecule 2: Programmed cell death protein 4

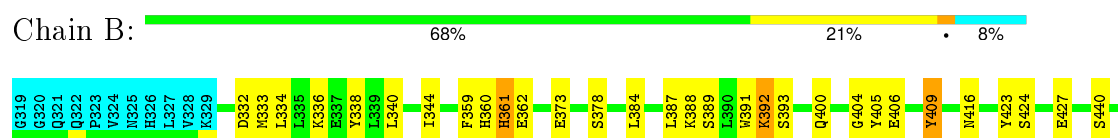


4.2.59 Score per residue for model 59

- Molecule 1: Programmed cell death protein 4



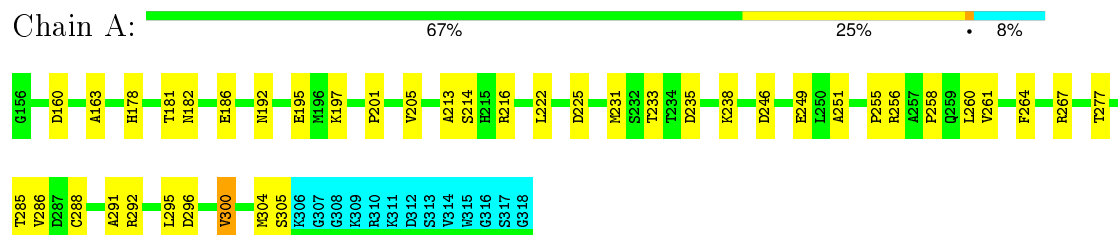
- Molecule 2: Programmed cell death protein 4



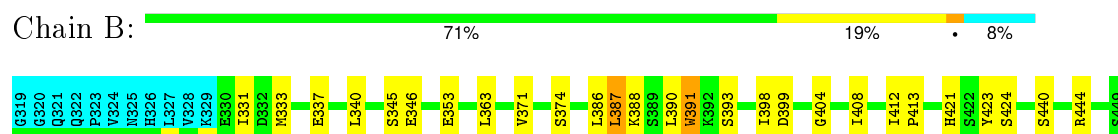
S449

4.2.60 Score per residue for model 60

- Molecule 1: Programmed cell death protein 4

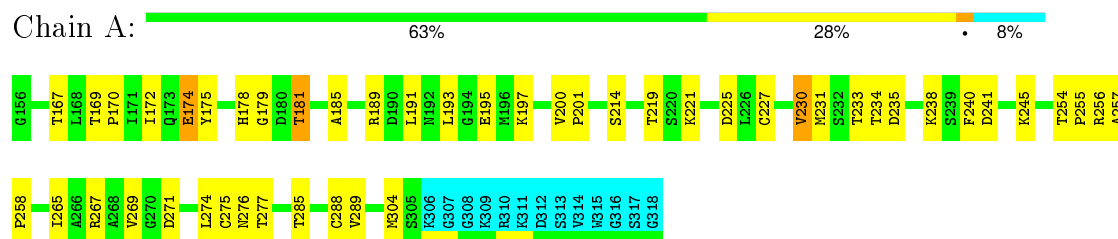


- Molecule 2: Programmed cell death protein 4

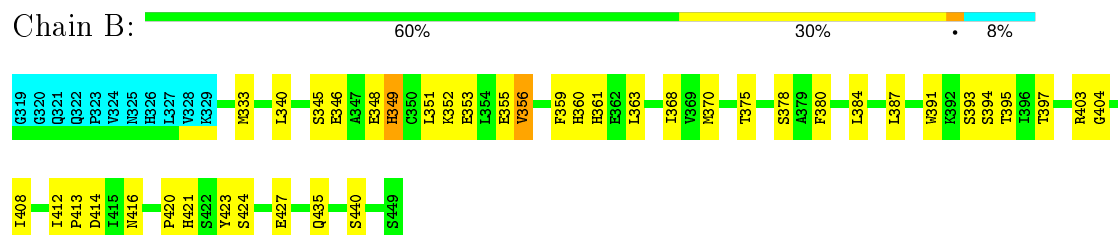


4.2.61 Score per residue for model 61

- Molecule 1: Programmed cell death protein 4

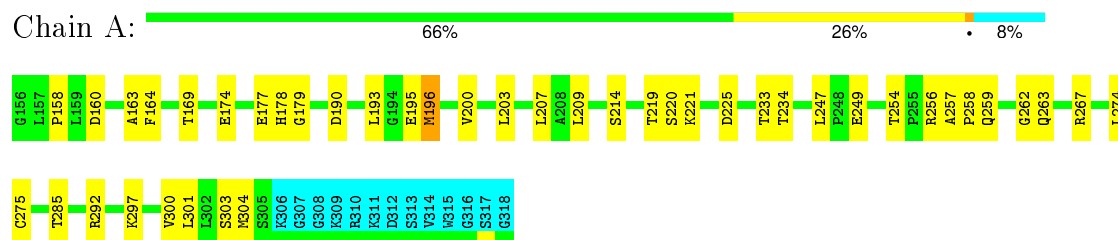


- Molecule 2: Programmed cell death protein 4

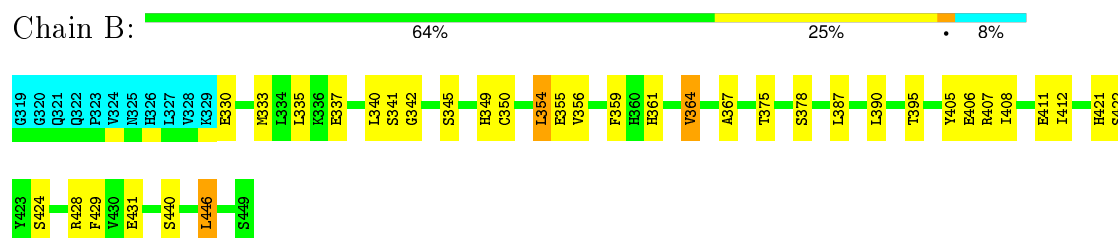


4.2.62 Score per residue for model 62

- Molecule 1: Programmed cell death protein 4

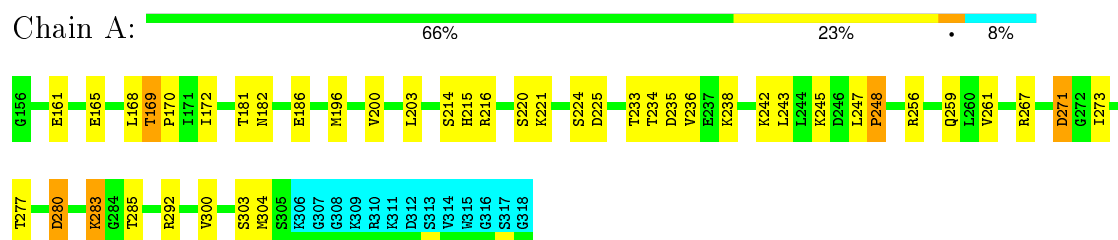


- Molecule 2: Programmed cell death protein 4

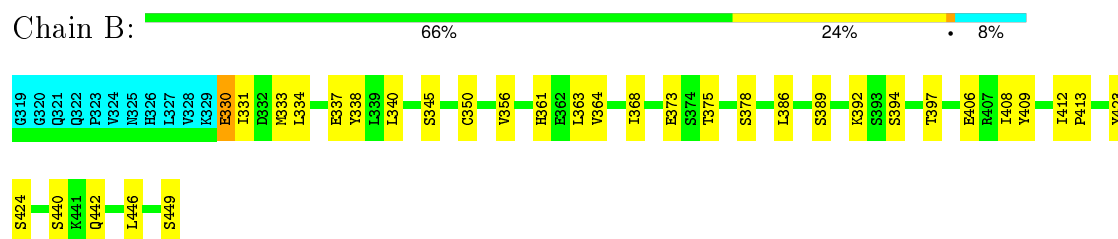


4.2.63 Score per residue for model 63

- Molecule 1: Programmed cell death protein 4

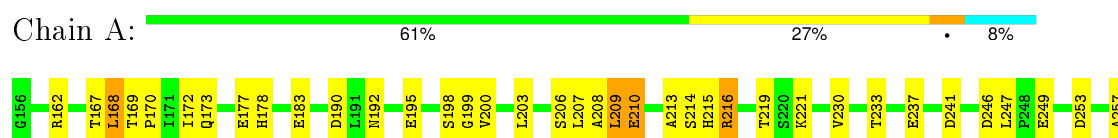


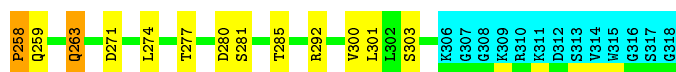
- Molecule 2: Programmed cell death protein 4



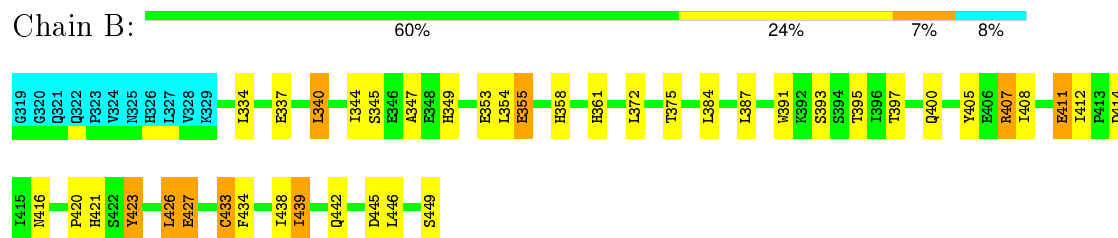
4.2.64 Score per residue for model 64

- Molecule 1: Programmed cell death protein 4



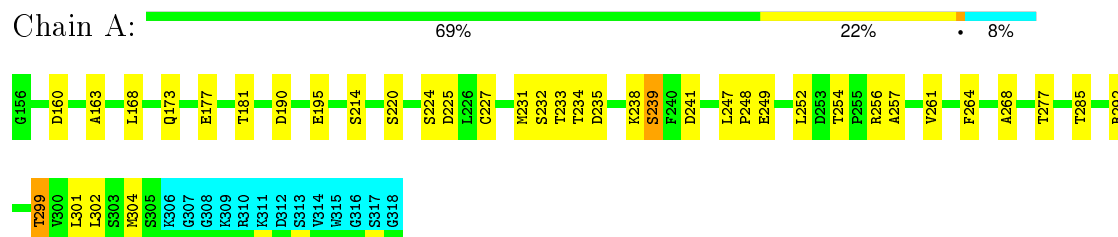


- Molecule 2: Programmed cell death protein 4

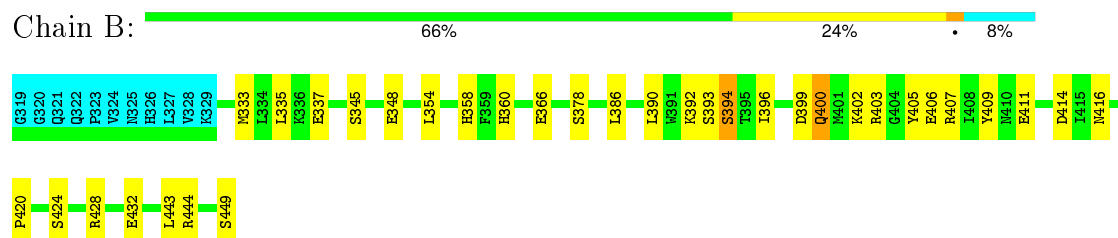


4.2.65 Score per residue for model 65

- Molecule 1: Programmed cell death protein 4

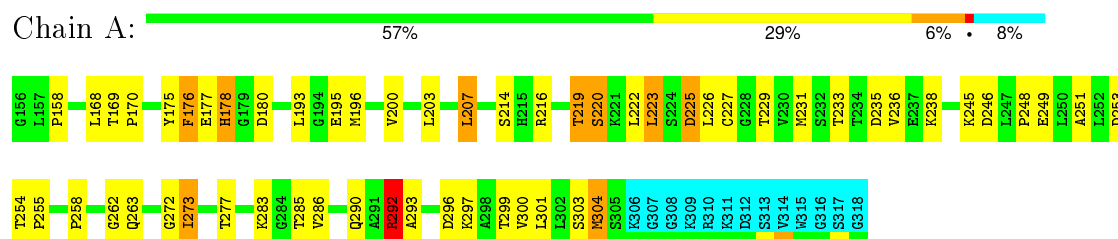


- Molecule 2: Programmed cell death protein 4

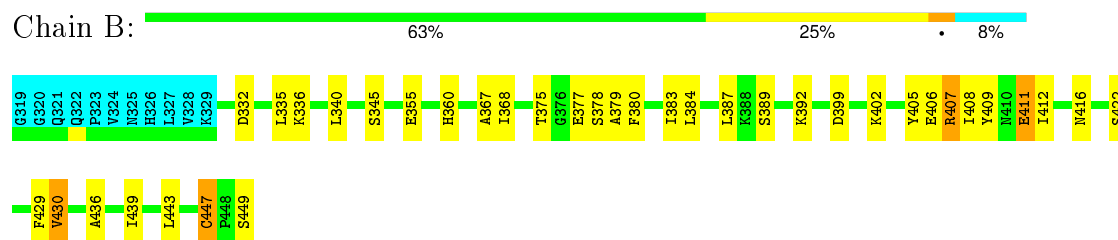


4.2.66 Score per residue for model 66

- Molecule 1: Programmed cell death protein 4

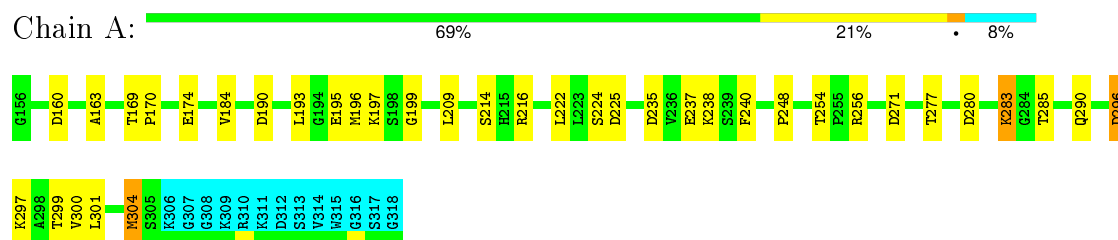


- Molecule 2: Programmed cell death protein 4

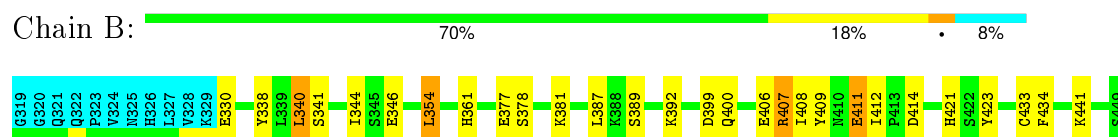


4.2.67 Score per residue for model 67

- Molecule 1: Programmed cell death protein 4

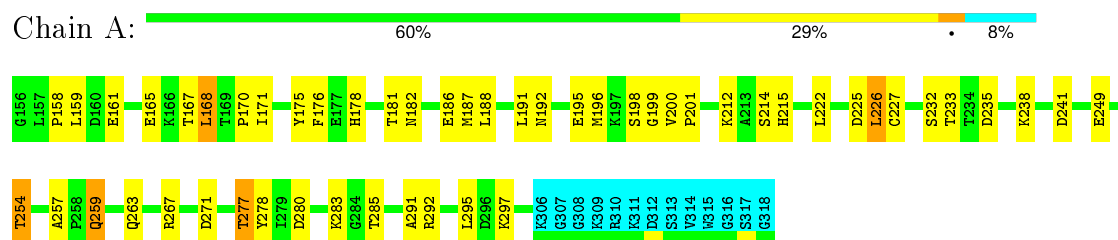


- Molecule 2: Programmed cell death protein 4

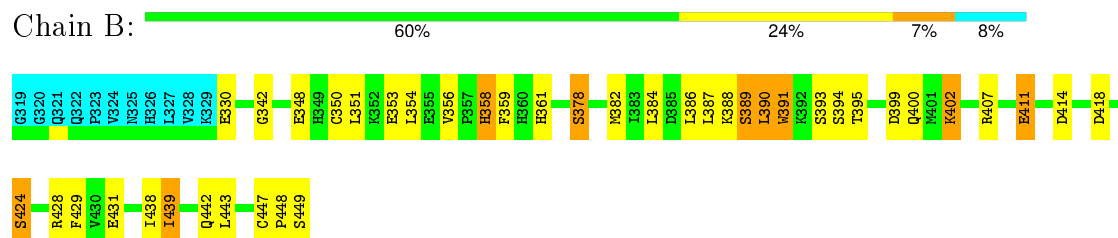


4.2.68 Score per residue for model 68

- Molecule 1: Programmed cell death protein 4

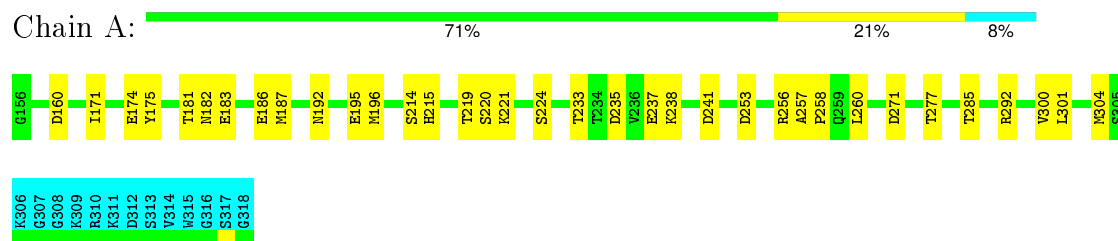


- Molecule 2: Programmed cell death protein 4

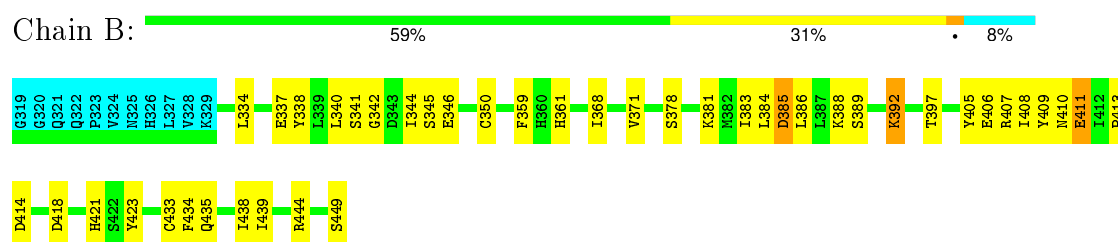


4.2.69 Score per residue for model 69

- Molecule 1: Programmed cell death protein 4

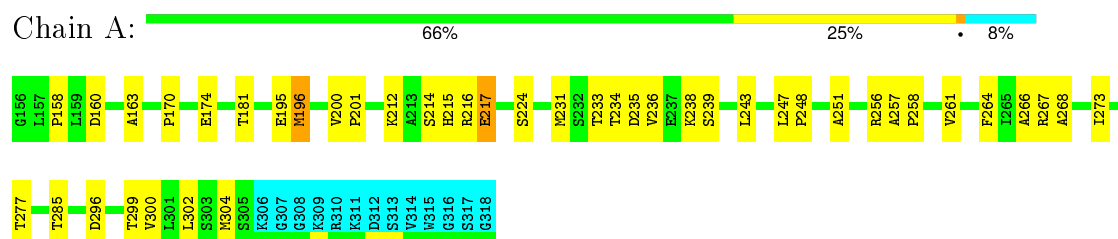


- Molecule 2: Programmed cell death protein 4

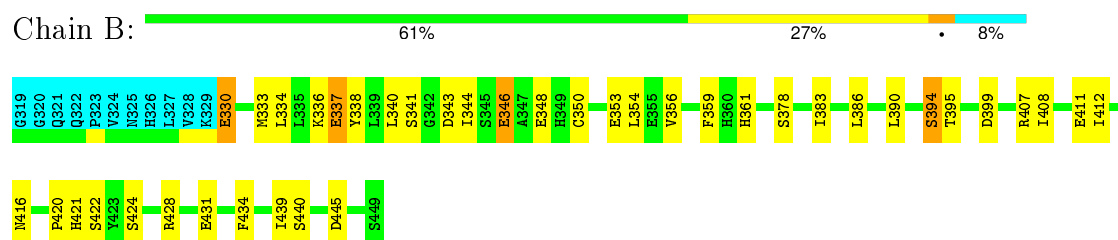


4.2.70 Score per residue for model 70

- Molecule 1: Programmed cell death protein 4

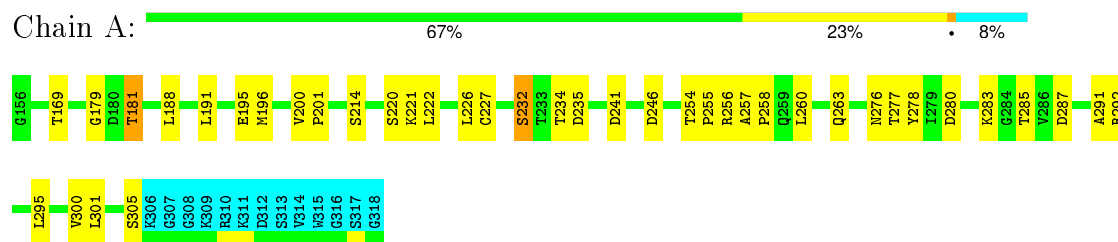


- Molecule 2: Programmed cell death protein 4

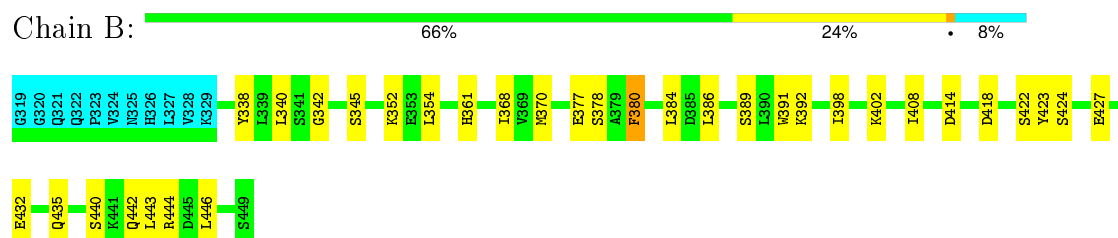


4.2.71 Score per residue for model 71

- Molecule 1: Programmed cell death protein 4

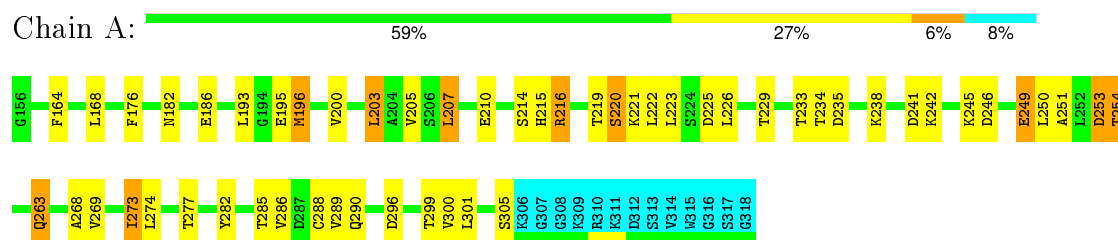


- Molecule 2: Programmed cell death protein 4

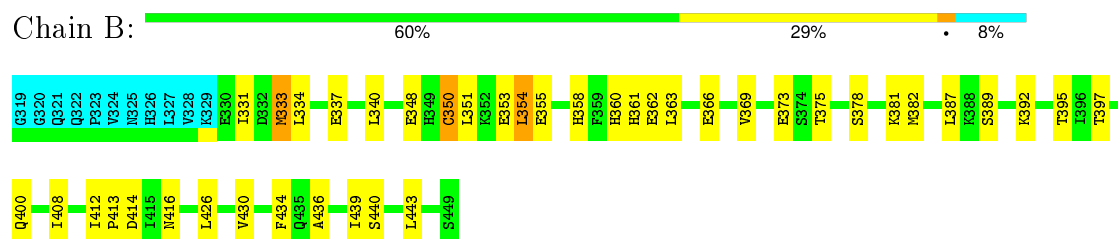


4.2.72 Score per residue for model 72

- Molecule 1: Programmed cell death protein 4

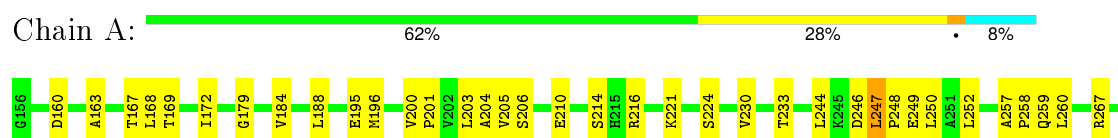


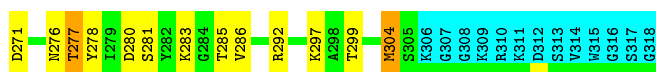
- Molecule 2: Programmed cell death protein 4



4.2.73 Score per residue for model 73

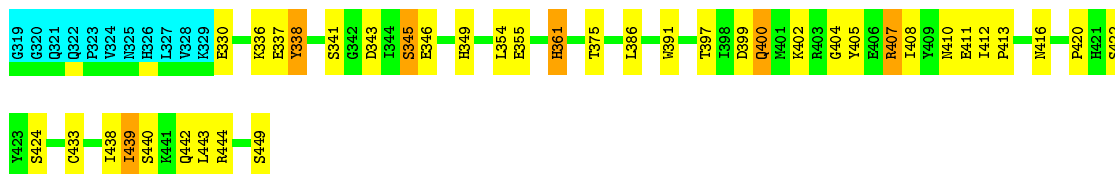
- Molecule 1: Programmed cell death protein 4





● Molecule 2: Programmed cell death protein 4

Chain B: 62% 25% 5% 8%



5 Refinement protocol and experimental data overview

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

6 Model quality

6.1 Standard geometry

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(°)	Ideal(°)	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

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:300:VAL:HB	2:B:336:LYS:HB3	0.82	1.51	35	4
1:A:280:ASP:HA	1:A:283:LYS:HD3	0.82	1.51	16	7
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	2
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	1
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: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
1:A:247:LEU:N	1:A:248:PRO:HD2	0.61	2.11	63	17
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
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: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:365:TYR:HE1	2:B:411:GLU:HG3	0.60	1.56	56	8
2:B:361:HIS:HB2	2:B:400:GLN:HG3	0.60	1.73	44	5
2:B:438:ILE:HG13	2:B:439:ILE:H	0.60	1.56	21	5
1:A:216:ARG:HB3	1:A:264:PHE:HZ	0.60	1.56	18	4
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
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
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
2:B:390:LEU:HD23	2:B:390:LEU:H	0.59	1.57	68	1
1:A:245:LYS:O	1:A:248:PRO:HD2	0.59	1.96	54	6
1:A:205:VAL:HG23	1:A:206:SER:H	0.59	1.57	42	1
1:A:169:THR:HA	1:A:172:ILE:HD12	0.59	1.74	34	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
1:A:247:LEU:HD12	1:A:250:LEU:HD12	0.58	1.75	73	1
2:B:432:GLU:HA	2:B:435:GLN:NE2	0.58	2.13	71	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
1:A:304:MET:SD	2:B:336:LYS:HE2	0.58	2.38	44	2
2:B:371:VAL:HG11	2:B:380:PHE:CD1	0.58	2.34	29	1
2:B:377:GLU:HA	2:B:380:PHE:HB3	0.58	1.76	66	1
1:A:291:ALA:O	1:A:295:LEU:HG	0.58	1.98	59	5
1:A:251:ALA:HB2	1:A:258:PRO:HG3	0.58	1.76	24	7
2:B:338:TYR:CE2	2:B:386:LEU:HB2	0.58	2.34	63	8
2:B:362:GLU:O	2:B:366:GLU:HB2	0.58	1.99	8	1
2:B:386:LEU:O	2:B:390:LEU:HG	0.58	1.99	24	17
1:A:182:ASN:O	1:A:186:GLU:HG2	0.58	1.99	43	21
2:B:364:VAL:HG11	2:B:401:MET:HA	0.58	1.76	25	2
1:A:301:LEU:HA	1:A:304:MET:SD	0.58	2.39	69	3
2:B:338:TYR:HD2	2:B:386:LEU:HB2	0.58	1.58	73	2
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:175:TYR:HE2	1:A:219:THR:HA	0.56	1.61	69	1
1:A:283:LYS:NZ	1:A:283:LYS:HB3	0.56	2.16	7	4
2:B:368:ILE:O	2:B:371:VAL:HG23	0.56	1.99	22	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
1:A:263:GLN:HA	1:A:301:LEU:HD11	0.56	1.77	64	1
2:B:412:ILE:HG13	2:B:426:LEU:HD11	0.56	1.78	31	2
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
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
1:A:297:LYS:O	1:A:300:VAL:HB	0.56	2.01	24	3
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:371:VAL:HG11	2:B:380:PHE:HA	0.56	1.77	44	1
1:A:296:ASP:HB3	2:B:340:LEU:CD1	0.56	2.31	67	1
1:A:268:ALA:HB1	1:A:273:ILE:HB	0.56	1.76	13	2
2:B:384:LEU:HD21	2:B:432:GLU:HG2	0.56	1.76	7	1
2:B:347:ALA:HA	2:B:350:CYS:SG	0.56	2.41	57	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:205:VAL:HG12	1:A:219:THR:CG2	0.55	2.32	42	1
1:A:293:ALA:O	1:A:297:LYS:HB2	0.55	2.00	21	1
2:B:378:SER:O	2:B:381:LYS:HG2	0.55	2.01	44	2
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
2:B:443:LEU:HA	2:B:446:LEU:HD12	0.55	1.79	15	1
1:A:181:THR:HG21	1:A:225:ASP:HB2	0.55	1.78	47	2
1:A:168:LEU:HD13	1:A:171:ILE:HD12	0.55	1.79	22	1
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:185:ALA:HB2	1:A:226:LEU:HD22	0.55	1.77	56	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

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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:297:LYS:O	1:A:301:LEU:HG	0.54	2.02	32	5
1:A:263:GLN:HA	1:A:301:LEU:CD1	0.54	2.32	15	4
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
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
2:B:404:GLY:O	2:B:408:ILE:HG12	0.54	2.03	24	10
2:B:358:HIS:HA	2:B:400:GLN:NE2	0.54	2.18	68	2
1:A:280:ASP:HA	1:A:283:LYS:HB2	0.54	1.77	48	9
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
1:A:252:LEU:HD23	1:A:252:LEU:H	0.54	1.62	42	1
1:A:168:LEU:HD22	1:A:171:ILE:HD12	0.54	1.78	39	3
1:A:212:LYS:HG2	1:A:213:ALA:H	0.54	1.63	20	1
2:B:378:SER:O	2:B:382:MET:HG2	0.54	2.02	38	3
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
1:A:209:LEU:HA	1:A:216:ARG:HG2	0.53	1.79	47	1
2:B:331:ILE:HG23	2:B:363:LEU:HD12	0.53	1.80	23	3
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:216:ARG:HA	1:A:219:THR:OG1	0.53	2.02	54	3
2:B:406:GLU:HA	2:B:409:TYR:CZ	0.53	2.38	57	1
2:B:335:LEU:HD13	2:B:366:GLU:HB3	0.53	1.81	31	1
1:A:300:VAL:HG12	2:B:340:LEU:HB2	0.53	1.80	6	1
2:B:348:GLU:HG3	2:B:352:LYS:HD2	0.53	1.80	55	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
2:B:402:LYS:HG2	2:B:443:LEU:HD13	0.53	1.81	68	1
1:A:226:LEU:HB3	1:A:230:VAL:HB	0.53	1.81	56	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
1:A:183:GLU:HA	1:A:186:GLU:CG	0.52	2.35	56	1
2:B:444:ARG:O	2:B:447:CYS:HB3	0.52	2.04	55	1
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:HA	1:A:292:ARG:NE	0.52	2.18	23	1
2:B:388:LYS:O	2:B:392:LYS:HG3	0.52	2.04	28	4
1:A:167:THR:O	1:A:170:PRO:HD2	0.52	2.05	52	6
2:B:399:ASP:O	2:B:403:ARG:HB2	0.52	2.05	56	1
2:B:389:SER:O	2:B:392:LYS:HB2	0.52	2.05	54	2
1:A:258:PRO:HA	1:A:261:VAL:HG23	0.52	1.79	5	2
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
1:A:300:VAL:CB	2:B:336:LYS:HB3	0.52	2.31	35	1
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:209:LEU:HD13	1:A:261:VAL:HG22	0.52	1.80	47	1
1:A:231:MET:HE3	1:A:235:ASP:HB3	0.52	1.81	2	1
1:A:198:SER:HB3	1:A:239:SER:HA	0.52	1.81	13	1
2:B:372:LEU:HD21	2:B:426:LEU:HB3	0.52	1.81	64	1
1:A:202:VAL:CG2	1:A:239:SER:HB3	0.52	2.35	8	1
2:B:333:MET:O	2:B:337:GLU:HG2	0.52	2.05	51	1
1:A:242:LYS:H	1:A:242:LYS:HD2	0.52	1.64	13	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
1:A:258:PRO:HA	1:A:261:VAL:CG2	0.52	2.34	5	1
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
1:A:202:VAL:HG13	1:A:243:LEU:HD13	0.51	1.82	57	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:389:SER:HA	2:B:392:LYS:CE	0.51	2.33	54	9
1:A:168:LEU:HD21	1:A:200:VAL:HG22	0.51	1.82	34	1
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:231:MET:HG3	1:A:235:ASP:HB2	0.51	1.82	57	8
1:A:165:GLU:HA	1:A:203:LEU:HD21	0.51	1.82	24	5
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:217:GLU:HG3	1:A:218:MET:N	0.51	2.21	34	1
1:A:264:PHE:O	1:A:268:ALA:HB2	0.51	2.06	65	2
1:A:251:ALA:CB	1:A:258:PRO:HD3	0.51	2.34	32	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:175:TYR:HE2	1:A:222:LEU:HD22	0.51	1.66	66	1
1:A:220:SER:HA	1:A:223:LEU:HG	0.51	1.81	66	2
1:A:202:VAL:HA	1:A:205:VAL:HG22	0.51	1.83	42	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
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
1:A:183:GLU:HA	1:A:186:GLU:HG3	0.50	1.82	56	1
2:B:338:TYR:CZ	2:B:386:LEU:HB2	0.50	2.41	3	1
1:A:169:THR:HG22	1:A:207:LEU:HD21	0.50	1.83	56	1
1:A:277:THR:HA	1:A:280:ASP:HB2	0.50	1.82	29	1
1:A:200:VAL:N	1:A:201:PRO:HD2	0.50	2.21	61	3
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
2:B:368:ILE:HG23	2:B:429:PHE:CE2	0.50	2.41	54	2
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
2:B:430:VAL:HG11	2:B:447:CYS:SG	0.50	2.46	10	1
1:A:261:VAL:HA	1:A:264:PHE:CD2	0.50	2.40	53	1
1:A:262:GLY:HA3	1:A:297:LYS:HG2	0.50	1.84	53	1
1:A:300:VAL:HG22	1:A:304:MET:HE1	0.50	1.84	37	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:220:SER:HA	1:A:223:LEU:HD12	0.49	1.83	45	1
1:A:247:LEU:N	1:A:248:PRO:CD	0.49	2.74	17	3
1:A:300:VAL:HG13	2:B:340:LEU:HB3	0.49	1.83	15	1
1:A:176:PHE:HB3	1:A:215:HIS:CD2	0.49	2.42	56	2
1:A:299:THR:HA	1:A:302:LEU:HB3	0.49	1.83	24	1
1:A:304:MET:HE1	2:B:337:GLU:HB2	0.49	1.84	33	1
1:A:173:GLN:O	1:A:177:GLU:HG2	0.49	2.07	65	2
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
1:A:221:LYS:HE2	1:A:221:LYS:HA	0.49	1.83	53	1
2:B:365:TYR:HB2	2:B:408:ILE:HD11	0.49	1.85	54	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:348:GLU:HG2	2:B:390:LEU:HD22	0.49	1.85	11	1
2:B:360:HIS:HB2	2:B:400:GLN:CG	0.49	2.36	65	2
1:A:269:VAL:HB	1:A:302:LEU:HD11	0.49	1.85	30	1
1:A:266:ALA:HB2	1:A:298:ALA:HB1	0.49	1.84	51	1
1:A:300:VAL:HA	2:B:340:LEU:HD22	0.49	1.83	21	1
2:B:384:LEU:HG	2:B:388:LYS:HE2	0.49	1.84	39	1
2:B:343:ASP:HB2	2:B:346:GLU:HG2	0.49	1.82	55	1
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:377:GLU:HA	2:B:380:PHE:HB2	0.49	1.84	6	2
2:B:346:GLU:OE1	2:B:346:GLU:HA	0.49	2.07	55	3
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
1:A:172:ILE:HD12	1:A:207:LEU:HD12	0.49	1.85	25	1
2:B:368:ILE:HG21	2:B:408:ILE:HG13	0.49	1.84	66	4
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
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:237:GLU:HG2	1:A:274:LEU:HD12	0.48	1.84	27	2
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:240:PHE:HE2	1:A:265:ILE:HA	0.48	1.68	18	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:HG12	0.48	1.68	54	1
1:A:214:SER:O	1:A:218:MET:HG2	0.48	2.09	8	1
1:A:286:VAL:HB	1:A:292:ARG:NH1	0.48	2.22	73	1
1:A:223:LEU:HB3	1:A:273:ILE:HD13	0.48	1.83	48	1
2:B:366:GLU:HA	2:B:369:VAL:CG2	0.48	2.38	35	1
1:A:283:LYS:HB3	1:A:283:LYS:NZ	0.48	2.23	11	2
2:B:332:ASP:CG	2:B:336:LYS:HZ1	0.48	2.11	17	1
1:A:168:LEU:HD11	1:A:200:VAL:HG13	0.48	1.86	25	2
2:B:338:TYR:HE1	2:B:344:ILE:HG12	0.48	1.68	12	3
1:A:201:PRO:O	1:A:205:VAL:HB	0.48	2.08	4	2
2:B:334:LEU:HD11	2:B:350:CYS:HB3	0.48	1.84	72	1
2:B:424:SER:O	2:B:428:ARG:HB2	0.48	2.09	57	4
2:B:419:VAL:HG12	2:B:421:HIS:CD2	0.48	2.44	17	1
1:A:304:MET:HG3	2:B:332:ASP:OD2	0.48	2.09	34	1
2:B:380:PHE:O	2:B:384:LEU:HB2	0.48	2.09	47	3
1:A:257:ALA:N	1:A:258:PRO:HD2	0.48	2.23	4	14
2:B:377:GLU:O	2:B:381:LYS:HG2	0.48	2.09	8	3
1:A:220:SER:O	1:A:223:LEU:HB2	0.48	2.09	66	2
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:CE	2:B:333:MET:HA	0.48	2.39	31	1
1:A:303:SER:HB3	2:B:336:LYS:HD2	0.48	1.86	27	1
1:A:286:VAL:HB	1:A:292:ARG:HG3	0.48	1.86	8	1
2:B:367:ALA:O	2:B:371:VAL:HG23	0.48	2.07	24	10
1:A:300:VAL:HG13	2:B:340:LEU:CB	0.48	2.39	59	2
2:B:368:ILE:HG23	2:B:429:PHE:HE2	0.48	1.69	54	2
2:B:434:PHE:CE1	2:B:441:LYS:HA	0.48	2.43	7	8
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
2:B:381:LYS:O	2:B:385:ASP:HB2	0.48	2.09	43	3
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
1:A:172:ILE:CD1	1:A:207:LEU:HD12	0.47	2.39	25	1
1:A:181:THR:CG2	1:A:222:LEU:HA	0.47	2.39	60	3
2:B:351:LEU:HD23	2:B:390:LEU:HD22	0.47	1.85	35	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
1:A:268:ALA:HB1	1:A:274:LEU:HB2	0.47	1.85	59	2
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:205:VAL:O	1:A:219:THR:HB	0.47	2.09	72	1
2:B:393:SER:O	2:B:394:SER:CB	0.47	2.62	21	2
1:A:300:VAL:HG21	2:B:341:SER:OG	0.47	2.09	57	3
2:B:412:ILE:HG23	2:B:416:ASN:ND2	0.47	2.24	66	2
2:B:383:ILE:O	2:B:386:LEU:HB3	0.47	2.09	28	2
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:304:MET:HG3	2:B:336:LYS:HE2	0.47	1.86	56	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:256:ARG:NH1	2:B:349:HIS:HB3	0.47	2.24	61	1
2:B:391:TRP:HH2	2:B:398:ILE:HA	0.47	1.70	42	1
1:A:181:THR:HG21	1:A:225:ASP:CB	0.47	2.39	46	2
1:A:277:THR:O	1:A:280:ASP:N	0.47	2.45	68	3
2:B:434:PHE:HA	2:B:439:ILE:CD1	0.47	2.33	70	3
1:A:205:VAL:O	1:A:209:LEU:HB2	0.47	2.09	30	1
1:A:300:VAL:HG21	2:B:341:SER:HA	0.47	1.86	51	1
2:B:430:VAL:HG21	2:B:447:CYS:SG	0.47	2.50	66	2
1:A:176:PHE:HZ	1:A:219:THR:HG23	0.47	1.70	32	1
1:A:158:PRO:HB2	1:A:161:GLU:HG2	0.47	1.86	54	1
1:A:266:ALA:HB3	1:A:301:LEU:HD23	0.47	1.85	6	1
2:B:379:ALA:O	2:B:383:ILE:HG13	0.47	2.10	58	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:232:SER:O	1:A:235:ASP:HB2	0.47	2.10	2	1
1:A:304:MET:HG2	2:B:336:LYS:HB3	0.47	1.87	58	1
2:B:406:GLU:HG2	2:B:446:LEU:HD22	0.47	1.86	62	1
1:A:200:VAL:H	1:A:201:PRO:HD2	0.47	1.70	37	2
1:A:283:LYS:HZ3	1:A:283:LYS:HB3	0.47	1.69	7	3
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
1:A:185:ALA:CB	1:A:226:LEU:HD22	0.46	2.40	56	1
2:B:402:LYS:HD2	2:B:443:LEU:HD13	0.46	1.88	20	1
2:B:367:ALA:O	2:B:383:ILE:HG21	0.46	2.10	66	1
1:A:269:VAL:HA	1:A:274:LEU:O	0.46	2.10	72	3
2:B:433:CYS:HB3	2:B:438:ILE:HD11	0.46	1.87	73	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:263:GLN:HA	1:A:301:LEU:HD22	0.46	1.87	4	1
1:A:207:LEU:C	1:A:209:LEU:H	0.46	2.13	4	2
2:B:402:LYS:HG2	2:B:406:GLU:OE2	0.46	2.10	45	1
1:A:249:GLU:O	1:A:252:LEU:HB2	0.46	2.11	73	2
1:A:217:GLU:HG3	1:A:267:ARG:HH22	0.46	1.71	35	2
1:A:247:LEU:HD11	1:A:261:VAL:HG11	0.46	1.87	20	2
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:162:ARG:N	1:A:162:ARG:HD2	0.46	2.25	34	1
1:A:161:GLU:O	1:A:165:GLU:HG3	0.46	2.10	14	4
1:A:257:ALA:HB3	1:A:258:PRO:HD3	0.46	1.88	54	2
1:A:222:LEU:O	1:A:226:LEU:HB2	0.46	2.10	34	1
2:B:444:ARG:O	2:B:447:CYS:HB2	0.46	2.11	10	1
1:A:203:LEU:O	1:A:207:LEU:N	0.46	2.49	72	2
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:168:LEU:HA	1:A:171:ILE:HD12	0.46	1.88	28	1
1:A:240:PHE:HE2	1:A:265:ILE:HG23	0.46	1.71	61	1
2:B:402:LYS:O	2:B:406:GLU:HG3	0.46	2.10	22	1
1:A:236:VAL:HG11	1:A:273:ILE:O	0.46	2.11	13	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
2:B:335:LEU:CD1	2:B:366:GLU:HB3	0.46	2.41	31	2
2:B:389:SER:HA	2:B:392:LYS:CD	0.46	2.40	8	1
2:B:368:ILE:O	2:B:371:VAL:HG12	0.46	2.11	48	3
1:A:268:ALA:HA	1:A:271:ASP:OD1	0.46	2.11	29	1
1:A:172:ILE:HG13	1:A:173:GLN:N	0.46	2.26	64	1
2:B:398:ILE:O	2:B:402:LYS:HG3	0.45	2.10	33	1
1:A:300:VAL:CG2	2:B:340:LEU:HB3	0.45	2.41	46	2
1:A:240:PHE:O	1:A:243:LEU:HB2	0.45	2.10	13	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
2:B:384:LEU:HB2	2:B:429:PHE:CE1	0.45	2.45	66	1
1:A:209:LEU:HD21	1:A:264:PHE:HE2	0.45	1.72	53	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:265:ILE:HD13	1:A:295:LEU:HD23	0.45	1.87	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:282:TYR:HA	1:A:285:THR:OG1	0.45	2.10	57	4
1:A:300:VAL:HG11	2:B:337:GLU:CA	0.45	2.38	48	1
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:225:ASP:C	1:A:227:CYS:H	0.45	2.14	68	1
1:A:300:VAL:CG1	2:B:340:LEU:HB2	0.45	2.42	23	4
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
2:B:371:VAL:HG11	2:B:380:PHE:HD1	0.45	1.70	29	1
2:B:348:GLU:O	2:B:352:LYS:HD2	0.45	2.12	8	1
1:A:249:GLU:O	1:A:251:ALA:N	0.45	2.50	72	1
2:B:382:MET:O	2:B:386:LEU:HB2	0.45	2.11	68	1
2:B:338:TYR:O	2:B:342:GLY:HA2	0.45	2.11	69	2
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:169:THR:N	1:A:170:PRO:HD2	0.45	2.27	63	4
2:B:334:LEU:HD21	2:B:351:LEU:HB2	0.45	1.88	2	1
1:A:268:ALA:CB	1:A:273:ILE:HB	0.45	2.42	13	1
1:A:266:ALA:HA	1:A:269:VAL:HG23	0.45	1.87	8	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
2:B:368:ILE:CD1	2:B:408:ILE:HG13	0.45	2.40	61	2
1:A:240:PHE:HB3	1:A:278:TYR:OH	0.45	2.12	35	1
1:A:258:PRO:HB2	1:A:293:ALA:HB1	0.45	1.87	66	1
1:A:296:ASP:O	1:A:300:VAL:HG23	0.45	2.10	70	3
1:A:217:GLU:HA	1:A:267:ARG:NH2	0.45	2.26	49	1
1:A:304:MET:HG2	2:B:336:LYS:HG3	0.45	1.89	22	1
2:B:384:LEU:HB2	2:B:429:PHE:HE1	0.45	1.71	66	1
1:A:176:PHE:CZ	1:A:208:ALA:HB2	0.45	2.46	17	2
2:B:405:TYR:CE1	2:B:430:VAL:HG22	0.45	2.47	40	2
2:B:334:LEU:CD2	2:B:347:ALA:HA	0.45	2.42	11	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:354:LEU:O	2:B:355:GLU:HB2	0.45	2.11	49	1
2:B:331:ILE:O	2:B:335:LEU:HG	0.45	2.12	29	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:398:ILE:O	2:B:402:LYS:HB2	0.44	2.11	71	1
2:B:367:ALA:HB1	2:B:383:ILE:HD12	0.44	1.87	36	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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
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:240:PHE:HA	1:A:243:LEU:HB3	0.44	1.88	52	1
1:A:193:LEU:O	1:A:197:LYS:HB2	0.44	2.12	21	1
2:B:361:HIS:HB2	2:B:400:GLN:HA	0.44	1.88	73	1
1:A:181:THR:HG22	1:A:222:LEU:HD12	0.44	1.89	71	3
2:B:402:LYS:HE3	2:B:442:GLN:OE1	0.44	2.12	53	1
1:A:274:LEU:HG	1:A:275:CYS:N	0.44	2.28	62	2
2:B:338:TYR:CD1	2:B:382:MET:HB3	0.44	2.47	45	1
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
2:B:406:GLU:HA	2:B:409:TYR:CE2	0.44	2.48	59	4
1:A:257:ALA:HA	1:A:260:LEU:HD12	0.44	1.90	44	2
1:A:202:VAL:HG23	1:A:239:SER:HB3	0.44	1.90	8	3
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: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:379:ALA:O	2:B:383:ILE:HG12	0.44	2.13	33	3
2:B:399:ASP:HA	2:B:402:LYS:HG3	0.44	1.90	73	1
1:A:227:CYS:SG	1:A:273:ILE:HG22	0.44	2.53	27	2
2:B:352:LYS:N	2:B:352:LYS:HD2	0.44	2.27	29	1
1:A:168:LEU:HD21	1:A:200:VAL:HG13	0.44	1.88	63	1
2:B:331:ILE:HD13	2:B:362:GLU:HB3	0.44	1.89	14	1
2:B:384:LEU:O	2:B:388:LYS:HE3	0.44	2.13	59	1
1:A:259:GLN:HB3	2:B:346:GLU:OE1	0.43	2.13	50	1
1:A:244:LEU:HD11	1:A:295:LEU:HD21	0.43	1.89	41	2
1:A:247:LEU:HD23	1:A:290:GLN:HB3	0.43	1.88	53	1
1:A:203:LEU:O	1:A:207:LEU:HG	0.43	2.13	41	2
2:B:338:TYR:OH	2:B:385:ASP:HB3	0.43	2.14	30	1
1:A:250:LEU:HD23	1:A:250:LEU:H	0.43	1.73	4	1
1:A:174:GLU:HA	1:A:177:GLU:HG2	0.43	1.89	45	1
1:A:216:ARG:NH1	1:A:260:LEU:HD13	0.43	2.28	73	1
1:A:304:MET:HE3	2:B:337:GLU:HB2	0.43	1.88	53	1
1:A:304:MET:HA	2:B:336:LYS:NZ	0.43	2.28	2	1
2:B:373:GLU:OE1	2:B:373:GLU:HA	0.43	2.13	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:300:VAL:HG22	2:B:340:LEU:HB2	0.43	1.90	1	1
1:A:269:VAL:HG11	1:A:276:ASN:HB3	0.43	1.90	61	1
1:A:256:ARG:HG2	1:A:260:LEU:HG	0.43	1.90	42	1
2:B:346:GLU:HA	2:B:346:GLU:OE1	0.43	2.13	16	1
2:B:391:TRP:CZ2	2:B:398:ILE:HB	0.43	2.42	60	1
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:280:ASP:O	1:A:283:LYS:HB2	0.43	2.14	9	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: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:334:LEU:HD22	2:B:350:CYS:SG	0.43	2.53	57	1
2:B:402:LYS:O	2:B:406:GLU:HB2	0.43	2.12	27	2
1:A:158:PRO:HB3	1:A:196:MET:HG2	0.43	1.90	62	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:H	2:B:352:LYS:HD2	0.43	1.73	29	1
1:A:232:SER:H	1:A:235:ASP:HB3	0.43	1.74	71	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: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
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
2:B:412:ILE:N	2:B:413:PRO:HD2	0.43	2.28	72	1
1:A:300:VAL:HG11	2:B:337:GLU:HG3	0.43	1.91	4	1
1:A:181:THR:HG22	1:A:222:LEU:HA	0.43	1.89	7	3
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
2:B:440:SER:OG	2:B:443:LEU:HB2	0.43	2.14	42	1
1:A:200:VAL:HB	1:A:201:PRO:CD	0.43	2.44	34	8
2:B:431:GLU:HG3	2:B:432:GLU:N	0.43	2.29	55	3
1:A:247:LEU:HA	1:A:250:LEU:HB2	0.43	1.89	21	1
1:A:292:ARG:HD2	1:A:292:ARG:HA	0.43	1.63	20	1
2:B:360:HIS:CB	2:B:400:GLN:HG3	0.43	2.38	65	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:331:ILE:CG2	2:B:363:LEU:HA	0.43	2.44	58	1
1:A:258:PRO:HG2	1:A:259:GLN:OE1	0.43	2.13	46	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:371:VAL:O	2:B:374:SER:HB2	0.43	2.14	60	1
1:A:197:LYS:O	1:A:200:VAL:HG23	0.43	2.13	38	1
2:B:351:LEU:HD11	2:B:363:LEU:HD11	0.42	1.90	56	1
2:B:361:HIS:HB2	2:B:400:GLN:O	0.42	2.14	23	1
1:A:195:GLU:HA	1:A:238:LYS:NZ	0.42	2.29	70	1
2:B:364:VAL:O	2:B:368:ILE:HG13	0.42	2.14	63	2
1:A:300:VAL:HG21	2:B:341:SER:CA	0.42	2.44	51	1
1:A:292:ARG:O	1:A:296:ASP:HB2	0.42	2.15	66	2
1:A:251:ALA:CB	1:A:258:PRO:HG3	0.42	2.44	70	2
2:B:336:LYS:O	2:B:339:LEU:HB3	0.42	2.14	36	1
2:B:348:GLU:HG2	2:B:390:LEU:HD23	0.42	1.90	54	1
1:A:286:VAL:CG1	1:A:291:ALA:HB3	0.42	2.43	38	1
2:B:368:ILE:O	2:B:371:VAL:HB	0.42	2.13	4	1
1:A:158:PRO:HA	1:A:196:MET:SD	0.42	2.53	66	1
2:B:335:LEU:HD11	2:B:366:GLU:HB3	0.42	1.90	65	1
1:A:216:ARG:HB3	1:A:264:PHE:CE1	0.42	2.49	15	1
2:B:380:PHE:HE1	2:B:429:PHE:HB3	0.42	1.74	31	1
1:A:181:THR:HG21	1:A:225:ASP:HB3	0.42	1.90	28	1
1:A:283:LYS:O	1:A:283:LYS:HG2	0.42	2.13	7	1
2:B:416:ASN:HB3	2:B:420:PRO:HB3	0.42	1.91	35	1
2:B:390:LEU:HD12	2:B:396:ILE:HD11	0.42	1.90	14	1
1:A:279:ILE:HG23	1:A:295:LEU:HD22	0.42	1.90	29	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:216:ARG:HB3	1:A:264:PHE:CZ	0.42	2.44	18	1
2:B:424:SER:O	2:B:428:ARG:HD3	0.42	2.15	70	1
2:B:397:THR:OG1	2:B:400:GLN:HG2	0.42	2.14	10	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
1:A:300:VAL:HG23	2:B:340:LEU:HD12	0.42	1.89	2	1
1:A:172:ILE:HD13	1:A:204:ALA:HB2	0.42	1.92	30	1
2:B:348:GLU:O	2:B:352:LYS:HD3	0.42	2.14	23	1
2:B:354:LEU:HB3	2:B:355:GLU:H	0.42	1.57	64	2
2:B:351:LEU:HD22	2:B:390:LEU:HD13	0.42	1.91	27	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
2:B:409:TYR:CZ	2:B:447:CYS:HB3	0.42	2.49	52	1
1:A:206:SER:O	1:A:209:LEU:HB2	0.42	2.15	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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
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:339:LEU:HB2	2:B:383:ILE:HD11	0.41	1.91	56	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
1:A:208:ALA:C	1:A:210:GLU:H	0.41	2.19	64	1
1:A:216:ARG:HD3	1:A:260:LEU:HD22	0.41	1.92	56	1
1:A:180:ASP:HB3	1:A:183:GLU:HB2	0.41	1.91	3	1
1:A:259:GLN:NE2	2:B:346:GLU:HB3	0.41	2.30	73	1
2:B:388:LYS:HG3	2:B:438:ILE:HD13	0.41	1.91	48	1
1:A:206:SER:HA	1:A:209:LEU:HB2	0.41	1.91	38	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
2:B:338:TYR:O	2:B:341:SER:O	0.41	2.37	73	1
1:A:170:PRO:O	1:A:174:GLU:HG2	0.41	2.14	70	1
1:A:213:ALA:HA	1:A:216:ARG:CZ	0.41	2.46	64	1
2:B:438:ILE:HG13	2:B:439:ILE:N	0.41	2.30	41	1
1:A:247:LEU:HD21	1:A:258:PRO:CA	0.41	2.42	13	1
1:A:247:LEU:HA	1:A:250:LEU:HD12	0.41	1.91	59	1
1:A:254:THR:HG22	1:A:256:ARG:H	0.41	1.76	8	1
1:A:253:ASP:O	1:A:254:THR:CB	0.41	2.68	72	1
2:B:351:LEU:HD13	2:B:363:LEU:HD13	0.41	1.93	55	1
2:B:356:VAL:HB	2:B:359:PHE:HB3	0.41	1.90	61	1
1:A:258:PRO:O	1:A:261:VAL:HB	0.41	2.16	23	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:215:HIS:HD2	1:A:218:MET:SD	0.41	2.38	13	1
1:A:181:THR:HG21	1:A:222:LEU:HA	0.41	1.93	31	1
2:B:438:ILE:HG13	2:B:439:ILE:HG12	0.41	1.92	50	1
1:A:259:GLN:HG2	2:B:346:GLU:CG	0.41	2.44	40	1
1:A:176:PHE:CE1	1:A:219:THR:HA	0.41	2.50	66	1
2:B:388:LYS:O	2:B:391:TRP:N	0.41	2.37	68	1
1:A:219:THR:HB	1:A:264:PHE:HE1	0.41	1.74	56	2
2:B:367:ALA:HA	2:B:370:MET:HB2	0.41	1.92	44	1
1:A:239:SER:O	1:A:243:LEU:HB2	0.41	2.15	70	2
1:A:213:ALA:HA	1:A:216:ARG:NH1	0.41	2.30	57	1
2:B:365:TYR:CE1	2:B:407:ARG:HG2	0.41	2.50	17	1
1:A:225:ASP:C	1:A:227:CYS:N	0.41	2.74	68	1
1:A:161:GLU:O	1:A:165:GLU:HB2	0.41	2.16	68	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:301:LEU:HA	1:A:304:MET:CE	0.41	2.46	67	1
1:A:170:PRO:O	1:A:174:GLU:HB2	0.41	2.16	67	1
1:A:188:LEU:HD23	1:A:191:LEU:HD12	0.41	1.93	4	1
1:A:276:ASN:C	1:A:278:TYR:H	0.41	2.19	73	1
1:A:175:TYR:O	1:A:177:GLU:N	0.41	2.54	66	1
1:A:168:LEU:HG	1:A:200:VAL:HG22	0.41	1.93	66	1
2:B:409:TYR:CE1	2:B:447:CYS:HB3	0.41	2.51	57	1
1:A:297:LYS:NZ	2:B:337:GLU:OE1	0.41	2.52	57	1
1:A:198:SER:C	1:A:200:VAL:H	0.41	2.19	64	1
1:A:300:VAL:HG11	2:B:336:LYS:O	0.41	2.16	35	1
1:A:237:GLU:HG3	1:A:274:LEU:CD1	0.41	2.46	28	1
2:B:397:THR:O	2:B:400:GLN:HB2	0.40	2.16	42	1
1:A:301:LEU:HD23	1:A:304:MET:CE	0.40	2.47	66	1
1:A:248:PRO:O	1:A:252:LEU:HD12	0.40	2.16	53	1
2:B:402:LYS:HE3	2:B:443:LEU:HD13	0.40	1.91	37	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:344:ILE:HD12	2:B:344:ILE:H	0.40	1.76	10	1
1:A:216:ARG:NH1	1:A:260:LEU:HD12	0.40	2.31	52	1
1:A:169:THR:HB	1:A:170:PRO:CD	0.40	2.46	21	1
2:B:354:LEU:HD22	2:B:354:LEU:HA	0.40	1.80	18	1
2:B:334:LEU:HD11	2:B:350:CYS:HB2	0.40	1.91	17	1
2:B:396:ILE:HG23	2:B:400:GLN:HB3	0.40	1.94	65	1
2:B:361:HIS:CE1	2:B:404:GLY:HA2	0.40	2.51	59	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
1:A:158:PRO:HB2	1:A:196:MET:HE2	0.40	1.94	70	1
2:B:367:ALA:HB1	2:B:383:ILE:HG23	0.40	1.93	66	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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%)	20	66
2	B	119/131 (91%)	105±5 (88±4%)	13±4 (11±3%)	2±2 (1±1%)	20	66
All	All	19564/21462 (91%)	17506 (89%)	1805 (9%)	253 (1%)	20	66

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	361	HIS	4
2	B	436	ALA	4
2	B	392	LYS	4
1	A	277	THR	3
1	A	168	LEU	3
1	A	272	GLY	3
1	A	239	SER	3
1	A	289	VAL	3
2	B	373	GLU	3
1	A	278	TYR	3
2	B	345	SER	2
1	A	245	LYS	2
2	B	356	VAL	2
1	A	227	CYS	2
1	A	208	ALA	2
1	A	247	LEU	2
2	B	353	GLU	2
1	A	305	SER	2
2	B	364	VAL	2
1	A	238	LYS	2
1	A	230	VAL	2
1	A	216	ARG	2
1	A	248	PRO	2

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Mol	Chain	Res	Type	Models (Total)
2	B	438	ILE	2
1	A	255	PRO	2
1	A	201	PRO	2
1	A	199	GLY	2
2	B	448	PRO	2
1	A	202	VAL	2
1	A	254	THR	2
1	A	209	LEU	2
1	A	226	LEU	1
2	B	402	LYS	1
1	A	252	LEU	1
1	A	190	ASP	1
1	A	176	PHE	1
1	A	256	ARG	1
1	A	161	GLU	1
2	B	389	SER	1
2	B	386	LEU	1
2	B	357	PRO	1
1	A	223	LEU	1
1	A	229	THR	1
2	B	374	SER	1
2	B	362	GLU	1
1	A	212	LYS	1
1	A	244	LEU	1
1	A	292	ARG	1
2	B	437	GLY	1
1	A	241	ASP	1
1	A	181	THR	1
2	B	344	ILE	1
1	A	219	THR	1
2	B	375	THR	1
1	A	180	ASP	1
2	B	420	PRO	1
2	B	360	HIS	1
1	A	222	LEU	1
2	B	380	PHE	1
1	A	174	GLU	1
1	A	258	PRO	1
1	A	288	CYS	1
1	A	200	VAL	1
1	A	250	LEU	1
2	B	403	ARG	1

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Mol	Chain	Res	Type	Models (Total)
1	A	233	THR	1
1	A	175	TYR	1

6.3.2 Protein sidechains ⓘ

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%)	8	47
2	B	112/121 (93%)	96±4 (86±3%)	16±4 (14±3%)	8	48
All	All	17447/18761 (93%)	14942 (86%)	2505 (14%)	8	47

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	220	SER	36
1	A	224	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
2	B	422	SER	31
1	A	221	LYS	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
1	A	190	ASP	24
2	B	449	SER	24
2	B	356	VAL	24
1	A	280	ASP	23
2	B	444	ARG	22
2	B	354	LEU	21
2	B	346	GLU	21
1	A	232	SER	21
1	A	219	THR	21
1	A	303	SER	21
2	B	399	ASP	21
2	B	358	HIS	21
1	A	210	GLU	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	330	GLU	17
2	B	353	GLU	17
2	B	359	PHE	17
1	A	253	ASP	16
2	B	338	TYR	16
2	B	391	TRP	16
2	B	344	ILE	16
2	B	427	GLU	15
1	A	168	LEU	15
2	B	341	SER	15
1	A	178	HIS	15
1	A	305	SER	14
2	B	442	GLN	14

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Mol	Chain	Res	Type	Models (Total)
2	B	385	ASP	14
2	B	418	ASP	14
2	B	337	GLU	14
1	A	237	GLU	13
1	A	215	HIS	13
2	B	348	GLU	12
1	A	267	ARG	12
1	A	169	THR	12
1	A	229	THR	11
2	B	411	GLU	11
2	B	349	HIS	11
2	B	416	ASN	10
1	A	206	SER	10
2	B	373	GLU	10
2	B	429	PHE	10
1	A	174	GLU	10
1	A	198	SER	10
1	A	283	LYS	10
2	B	340	LEU	9
2	B	384	LEU	9
1	A	275	CYS	8
1	A	259	GLN	8
2	B	377	GLU	8
1	A	222	LEU	8
2	B	333	MET	8
1	A	239	SER	8
1	A	217	GLU	8
2	B	360	HIS	8
1	A	263	GLN	8
2	B	392	LYS	8
2	B	435	GLN	7
2	B	431	GLU	7
2	B	447	CYS	7
2	B	352	LYS	6
2	B	363	LEU	6
1	A	216	ARG	6
1	A	167	THR	6
2	B	394	SER	6
2	B	400	GLN	6
1	A	207	LEU	5
1	A	304	MET	5
2	B	433	CYS	5

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Mol	Chain	Res	Type	Models (Total)
2	B	351	LEU	5
2	B	445	ASP	5
1	A	247	LEU	5
1	A	193	LEU	5
1	A	182	ASN	5
1	A	297	LYS	5
1	A	209	LEU	5
2	B	428	ARG	5
1	A	161	GLU	5
1	A	273	ILE	5
2	B	365	TYR	4
2	B	366	GLU	4
1	A	287	ASP	4
2	B	409	TYR	4
1	A	226	LEU	4
1	A	240	PHE	4
2	B	362	GLU	4
1	A	235	ASP	4
2	B	336	LYS	4
2	B	446	LEU	4
1	A	250	LEU	4
2	B	355	GLU	4
2	B	388	LYS	4
2	B	350	CYS	4
2	B	390	LEU	4
2	B	412	ILE	4
2	B	380	PHE	4
2	B	334	LEU	3
2	B	364	VAL	3
1	A	177	GLU	3
2	B	370	MET	3
1	A	192	ASN	3
1	A	162	ARG	3
2	B	426	LEU	3
1	A	264	PHE	3
1	A	252	LEU	3
1	A	230	VAL	3
1	A	183	GLU	3
1	A	281	SER	3
2	B	402	LYS	3
1	A	301	LEU	3
1	A	227	CYS	2

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Mol	Chain	Res	Type	Models (Total)
2	B	382	MET	2
2	B	332	ASP	2
1	A	300	VAL	2
1	A	165	GLU	2
1	A	203	LEU	2
1	A	186	GLU	2
1	A	175	TYR	2
1	A	248	PRO	2
1	A	159	LEU	2
1	A	218	MET	2
2	B	381	LYS	2
2	B	343	ASP	2
1	A	276	ASN	2
1	A	188	LEU	1
2	B	383	ILE	1
1	A	164	PHE	1
2	B	372	LEU	1
1	A	212	LYS	1
2	B	425	VAL	1
1	A	274	LEU	1
2	B	398	ILE	1
2	B	386	LEU	1
1	A	191	LEU	1
1	A	289	VAL	1
2	B	430	VAL	1
2	B	408	ILE	1
1	A	197	LYS	1
1	A	180	ASP	1
1	A	242	LYS	1
2	B	389	SER	1
1	A	176	PHE	1
2	B	339	LEU	1
1	A	290	GLN	1
2	B	335	LEU	1
2	B	371	VAL	1
2	B	432	GLU	1
1	A	158	PRO	1
2	B	331	ILE	1
1	A	278	TYR	1
1	A	238	LYS	1
1	A	243	LEU	1
2	B	403	ARG	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided