



Full wwPDB NMR Structure Validation Report ⓘ

Mar 26, 2026 – 10:02 AM UTC

PDB ID : 2KZT / pdb_00002kzt
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

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

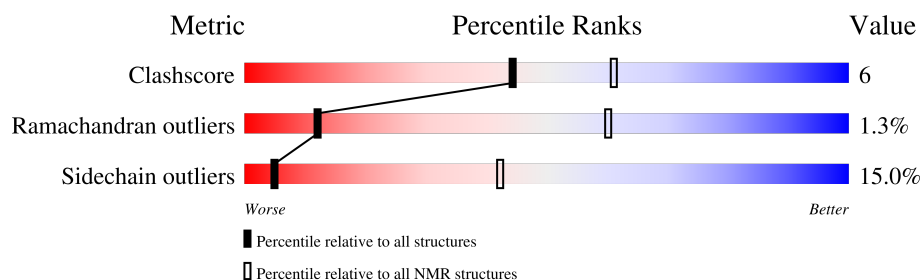
1 Overall quality at a glance

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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)	0.81	3

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

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

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

Cluster number	Models
1	1, 2, 3, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 16, 17, 18, 22, 24, 26, 27, 29, 32, 33, 34, 37, 38, 39, 40, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 57, 60, 61, 62, 63, 64, 65, 67, 68, 70, 71, 73
2	15, 20, 21, 23, 25, 28, 30, 31, 41, 42, 58, 66, 69, 72
3	4, 35
4	56, 59
Single-model clusters	19; 36

3 Entry composition

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.

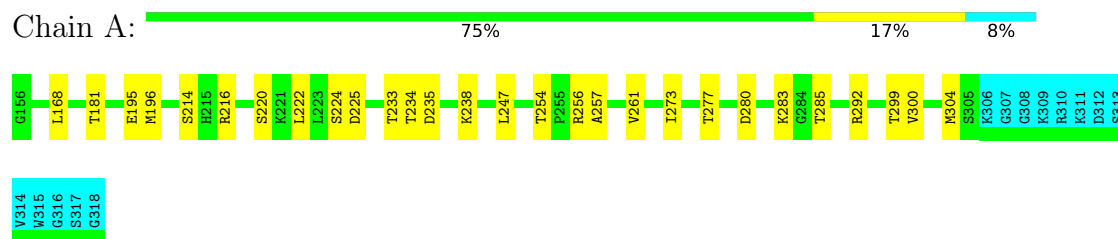
Mol	Chain	Residues	Atoms						Trace
2	B	131	Total	C	H	N	O	S	0
			1281	676	223	172	203	7	

4 Residue-property plots [i](#)

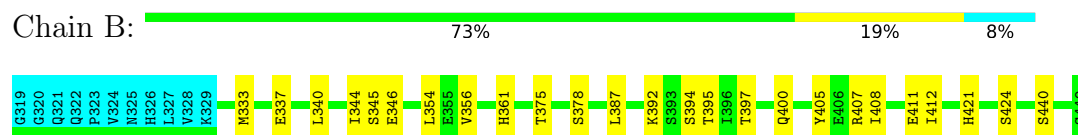
4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Programmed cell death protein 4



- Molecule 2: Programmed cell death protein 4

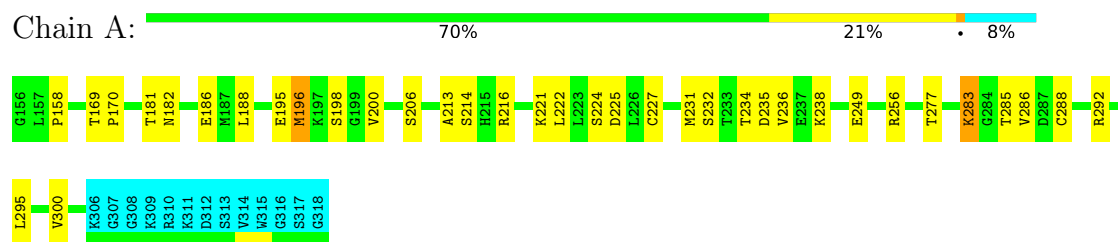


4.2 Scores per residue for each member of the ensemble

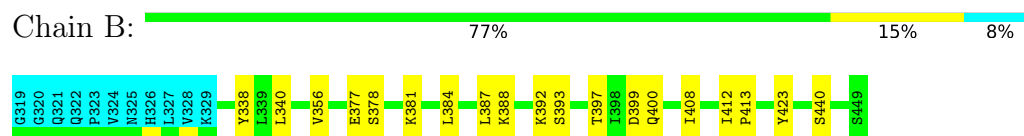
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Programmed cell death protein 4

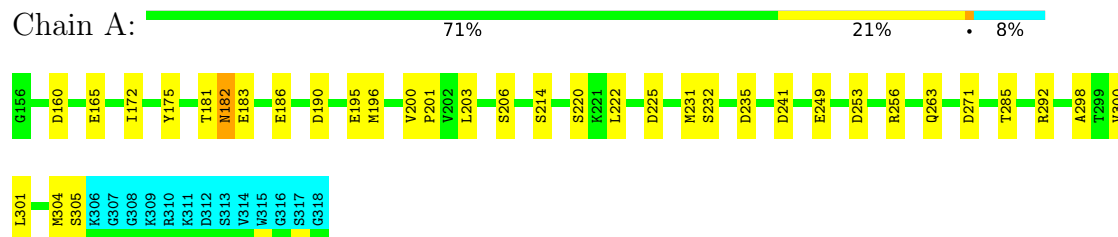


- Molecule 2: Programmed cell death protein 4

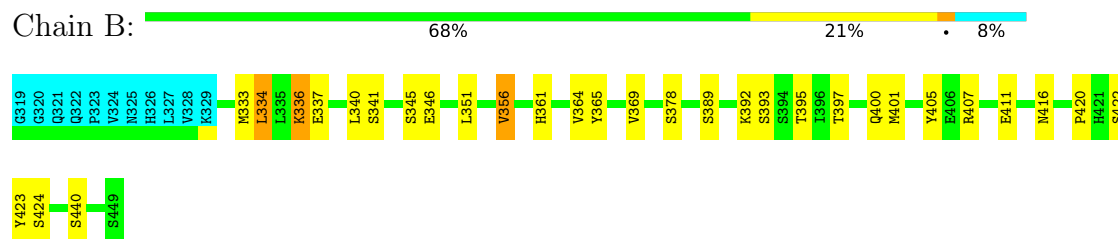


4.2.2 Score per residue for model 2

- Molecule 1: Programmed cell death protein 4

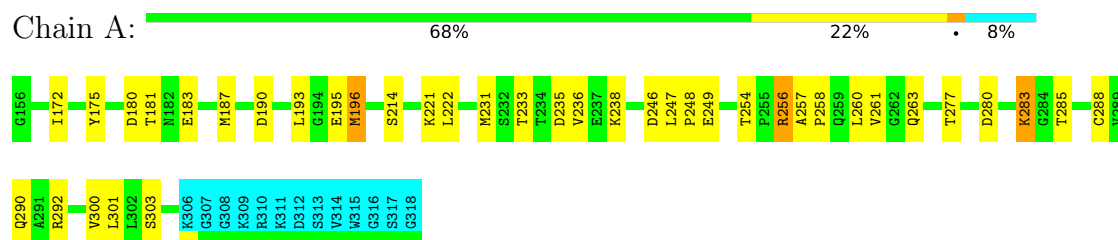


- Molecule 2: Programmed cell death protein 4

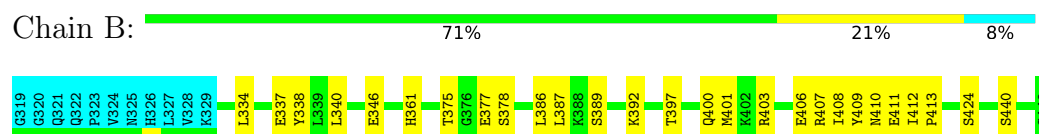


4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: Programmed cell death protein 4

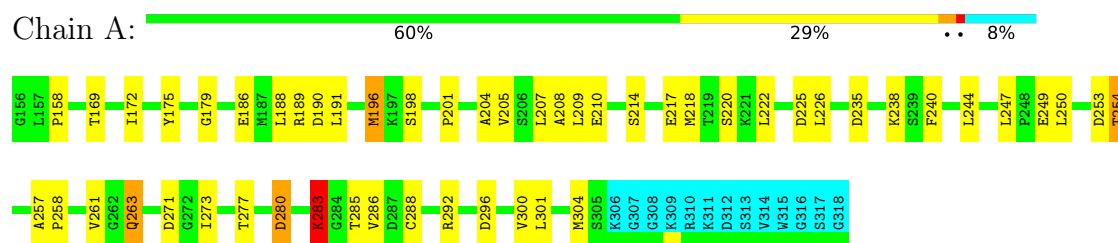


- Molecule 2: Programmed cell death protein 4

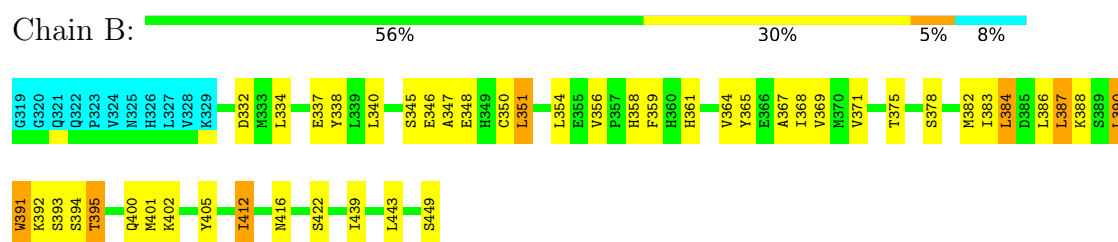


4.2.4 Score per residue for model 4

- Molecule 1: Programmed cell death protein 4

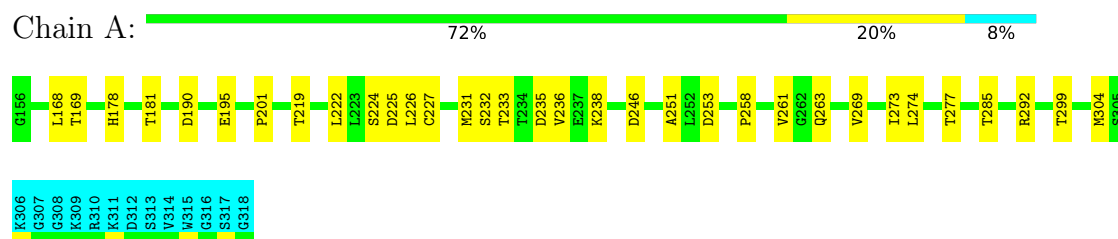


- Molecule 2: Programmed cell death protein 4

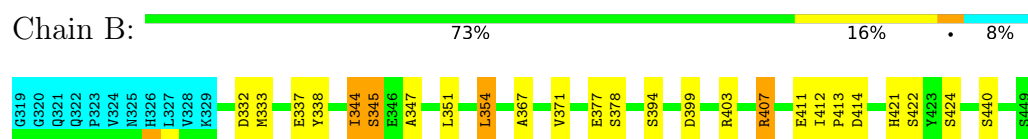


4.2.5 Score per residue for model 5

- Molecule 1: Programmed cell death protein 4



- Molecule 2: Programmed cell death protein 4



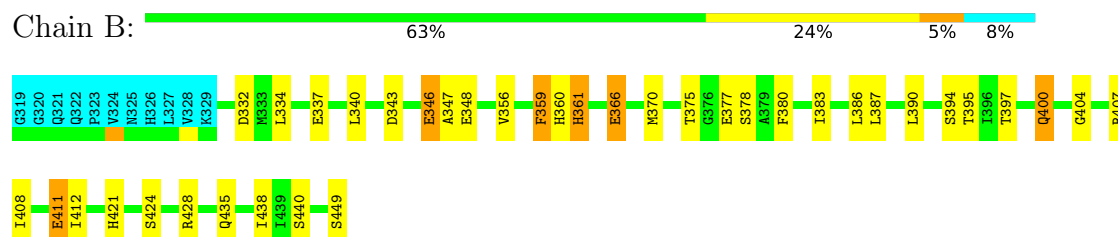
4.2.6 Score per residue for model 6

- Molecule 1: Programmed cell death protein 4



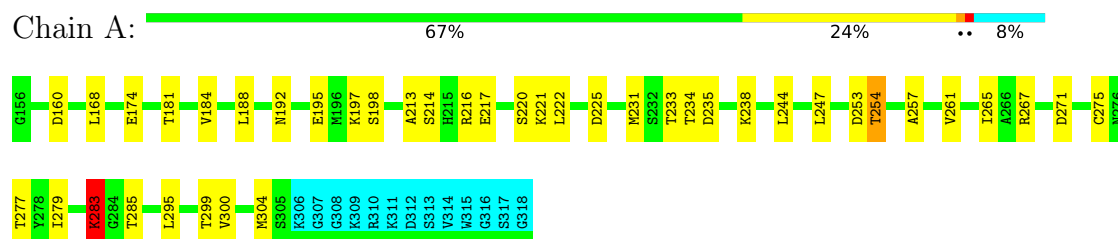


- Molecule 2: Programmed cell death protein 4

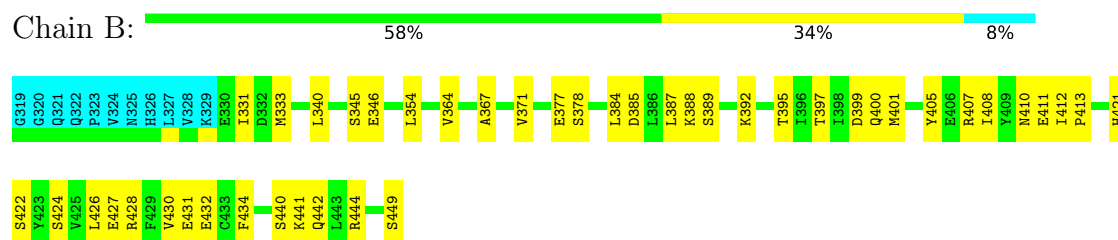


4.2.7 Score per residue for model 7

- Molecule 1: Programmed cell death protein 4

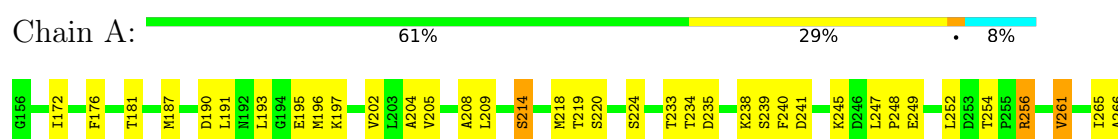


- Molecule 2: Programmed cell death protein 4



4.2.8 Score per residue for model 8

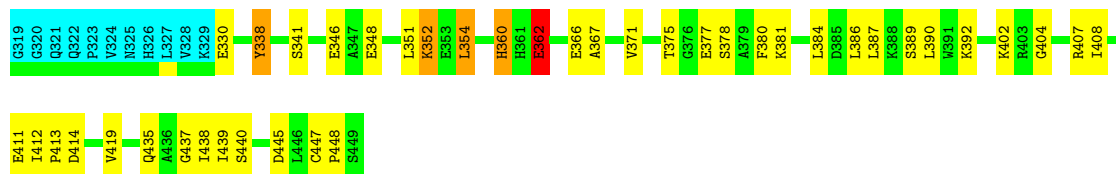
- Molecule 1: Programmed cell death protein 4





• Molecule 2: Programmed cell death protein 4

Chain B: 60% 27% 8%



4.2.9 Score per residue for model 9

• Molecule 1: Programmed cell death protein 4

Chain A: 66% 23% 8%



• Molecule 2: Programmed cell death protein 4

Chain B: 75% 15% 8%



4.2.10 Score per residue for model 10

• Molecule 1: Programmed cell death protein 4

Chain A: 69% 23% 8%



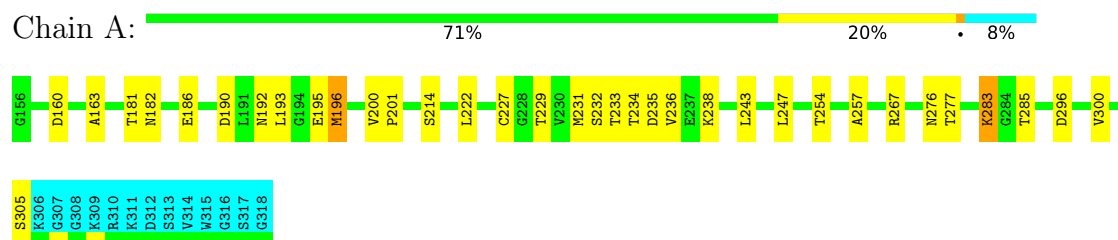
• Molecule 2: Programmed cell death protein 4

Chain B: 65% 26% 8%

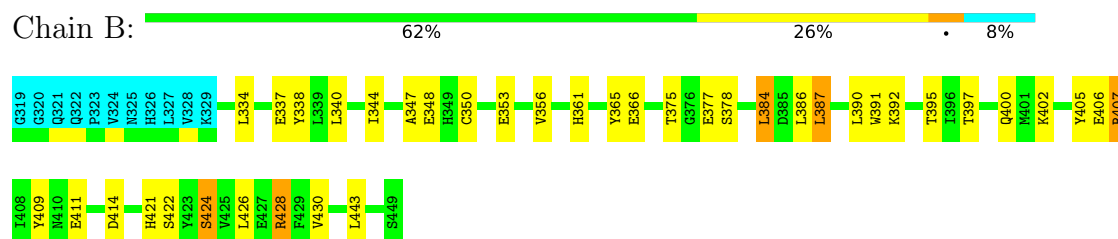


4.2.11 Score per residue for model 11

- Molecule 1: Programmed cell death protein 4

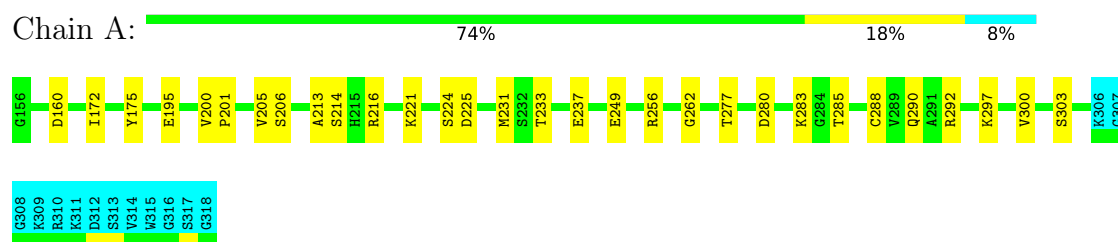


- Molecule 2: Programmed cell death protein 4

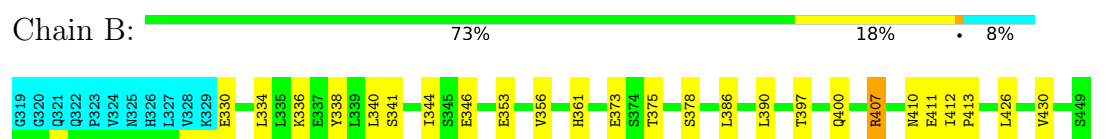


4.2.12 Score per residue for model 12

- Molecule 1: Programmed cell death protein 4

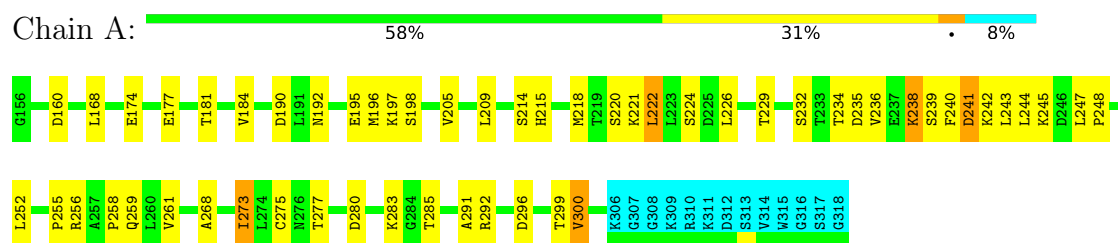


- Molecule 2: Programmed cell death protein 4

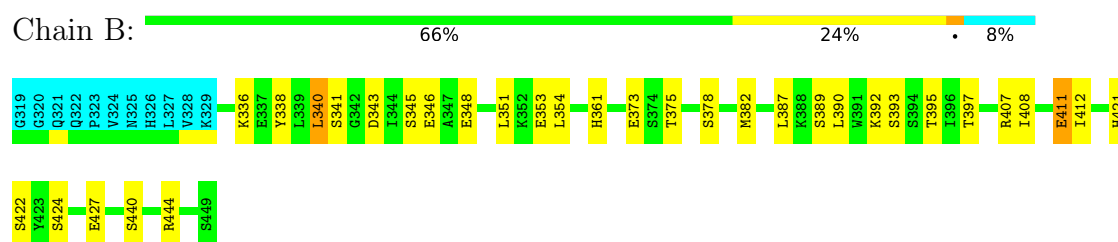


4.2.13 Score per residue for model 13

- Molecule 1: Programmed cell death protein 4

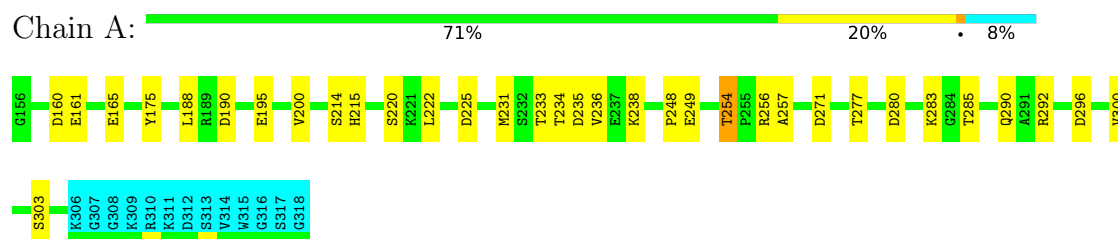


- Molecule 2: Programmed cell death protein 4

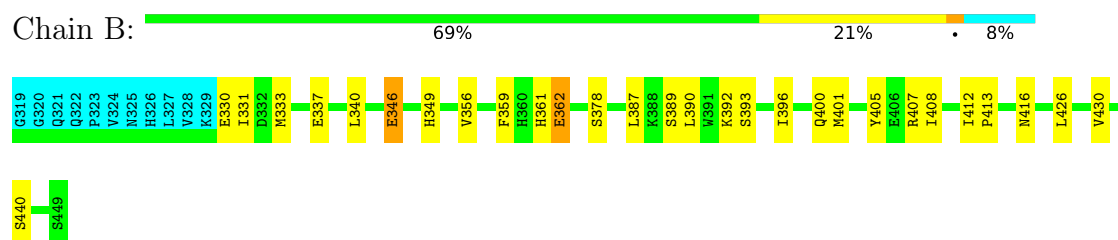


4.2.14 Score per residue for model 14

- Molecule 1: Programmed cell death protein 4

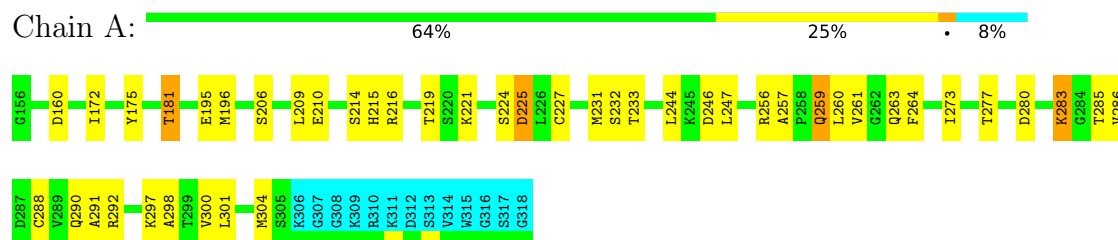


- Molecule 2: Programmed cell death protein 4

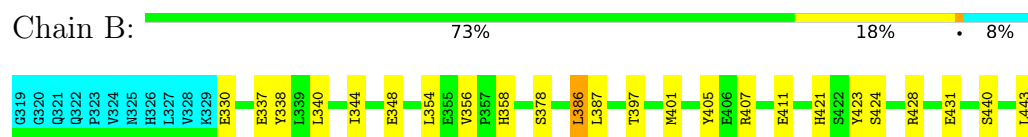


4.2.15 Score per residue for model 15

- Molecule 1: Programmed cell death protein 4

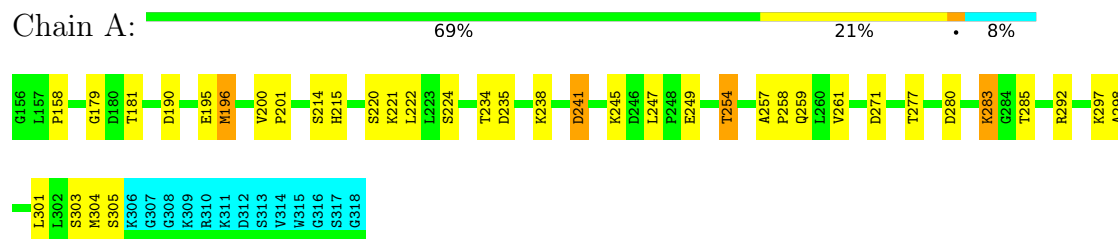


- Molecule 2: Programmed cell death protein 4

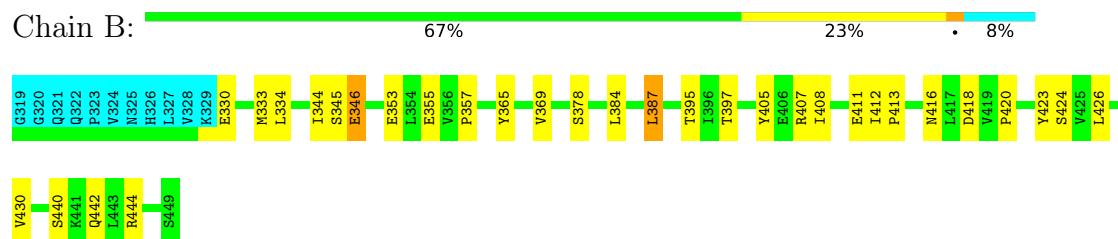


4.2.16 Score per residue for model 16

- Molecule 1: Programmed cell death protein 4

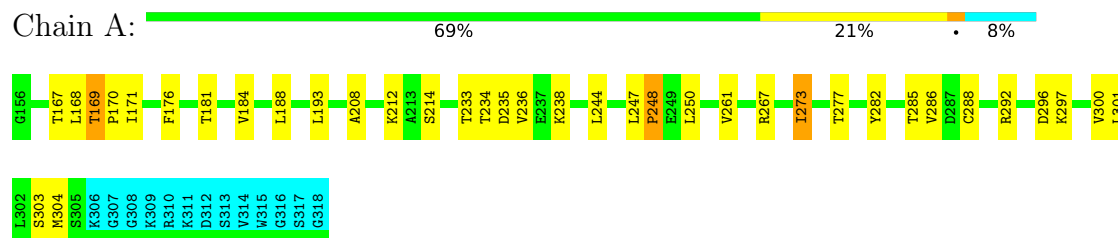


- Molecule 2: Programmed cell death protein 4



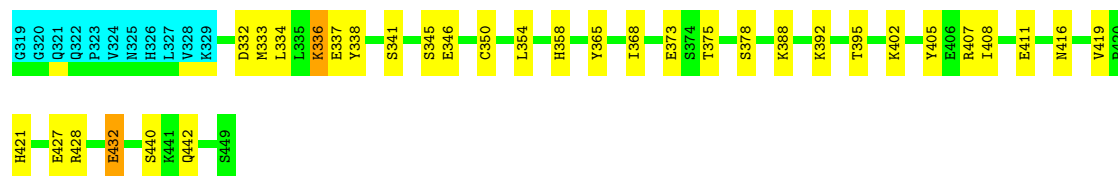
4.2.17 Score per residue for model 17

- Molecule 1: Programmed cell death protein 4



- Molecule 2: Programmed cell death protein 4

Chain B: 



4.2.18 Score per residue for model 18

- Molecule 1: Programmed cell death protein 4

Chain A: 



- Molecule 2: Programmed cell death protein 4

Chain B: 



4.2.19 Score per residue for model 19

- Molecule 1: Programmed cell death protein 4

Chain A: 



- Molecule 2: Programmed cell death protein 4

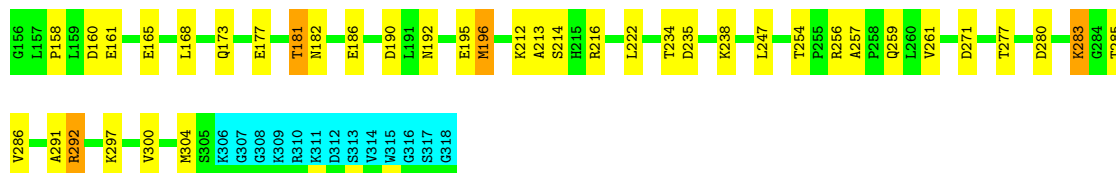
Chain B: 



4.2.20 Score per residue for model 20

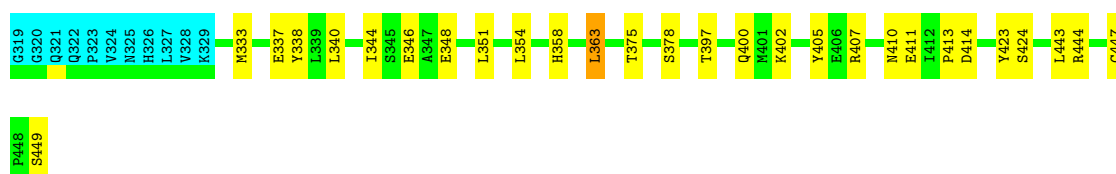
- Molecule 1: Programmed cell death protein 4

Chain A: 68% 21% 8%



- Molecule 2: Programmed cell death protein 4

Chain B: 70% 21% 8%



4.2.21 Score per residue for model 21

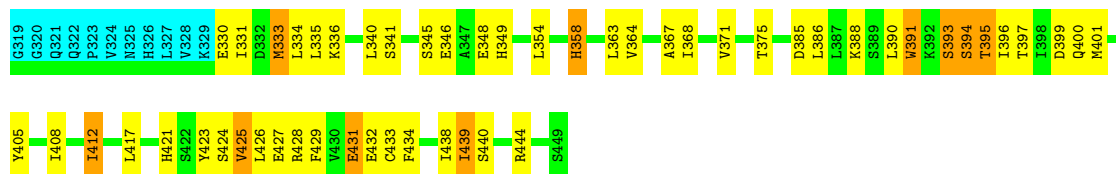
- Molecule 1: Programmed cell death protein 4

Chain A: 60% 31% 8%



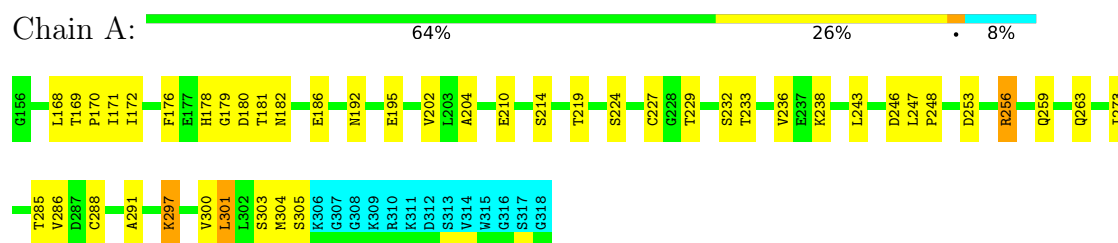
- Molecule 2: Programmed cell death protein 4

Chain B: 51% 33% 8%

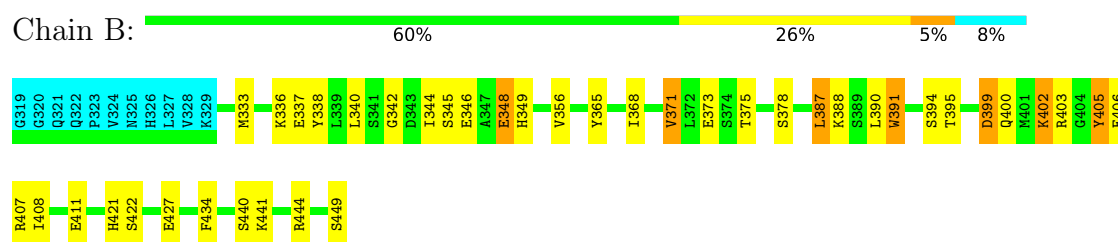


4.2.22 Score per residue for model 22

- Molecule 1: Programmed cell death protein 4

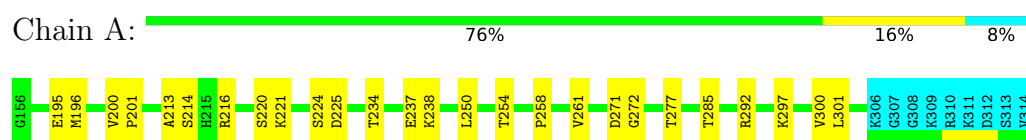


- Molecule 2: Programmed cell death protein 4

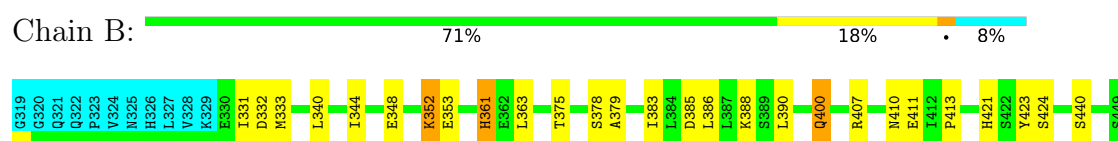


4.2.23 Score per residue for model 23

- Molecule 1: Programmed cell death protein 4

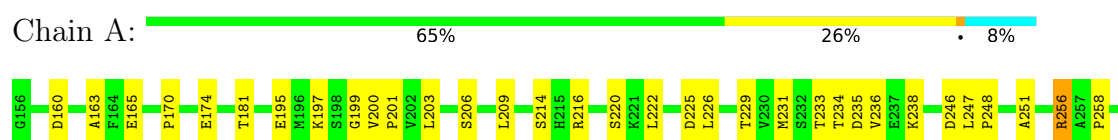


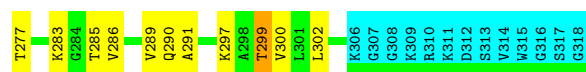
- Molecule 2: Programmed cell death protein 4



4.2.24 Score per residue for model 24

- Molecule 1: Programmed cell death protein 4





- Molecule 2: Programmed cell death protein 4

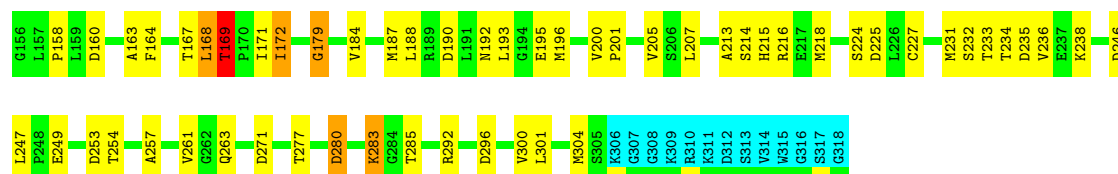
Chain B: 56% 34% 8%



4.2.25 Score per residue for model 25

- Molecule 1: Programmed cell death protein 4

Chain A: 58% 30% 8%



- Molecule 2: Programmed cell death protein 4

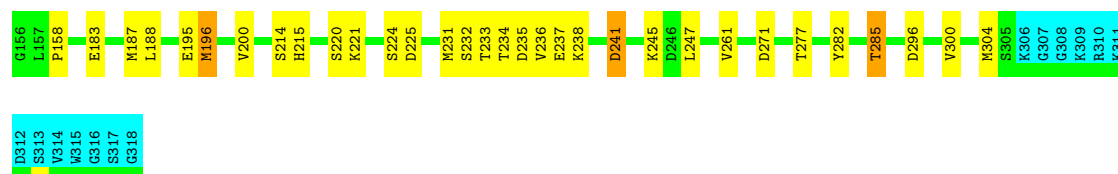
Chain B: 66% 25% 8%



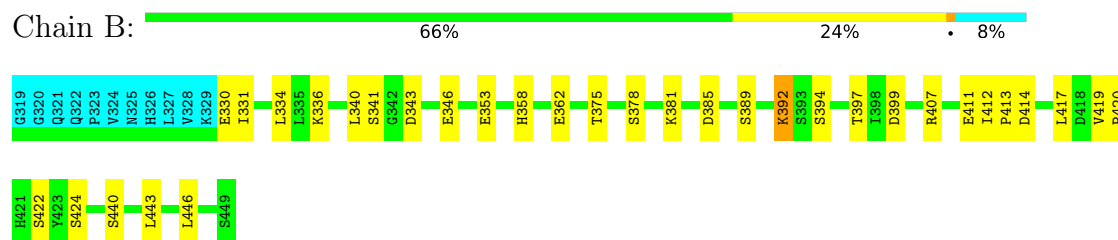
4.2.26 Score per residue for model 26

- Molecule 1: Programmed cell death protein 4

Chain A: 72% 18% 8%

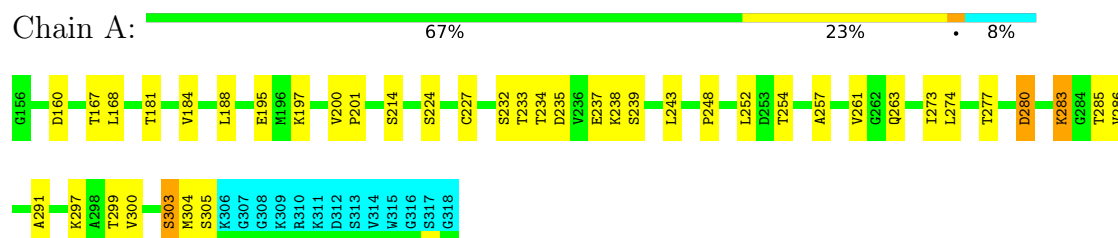


- Molecule 2: Programmed cell death protein 4

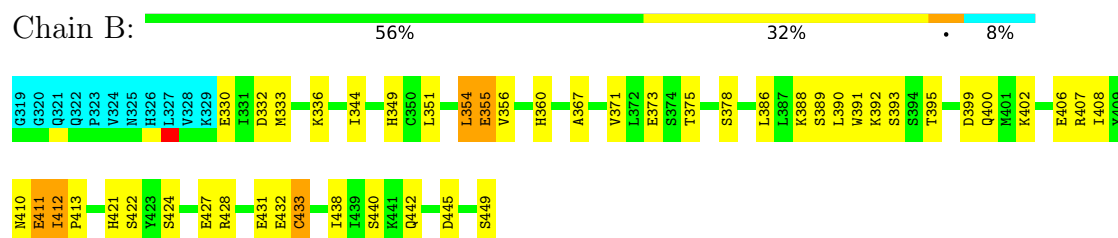


4.2.27 Score per residue for model 27

- Molecule 1: Programmed cell death protein 4

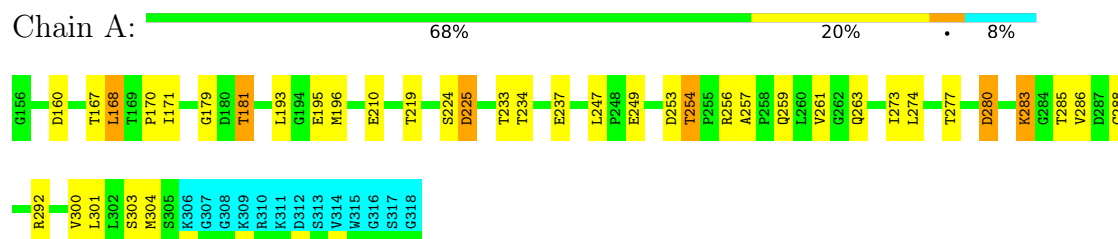


- Molecule 2: Programmed cell death protein 4



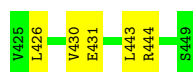
4.2.28 Score per residue for model 28

- Molecule 1: Programmed cell death protein 4



- Molecule 2: Programmed cell death protein 4

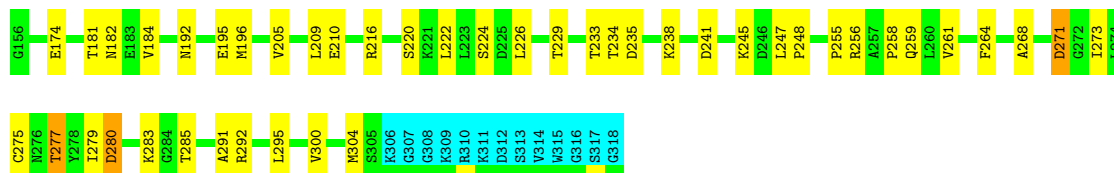




4.2.29 Score per residue for model 29

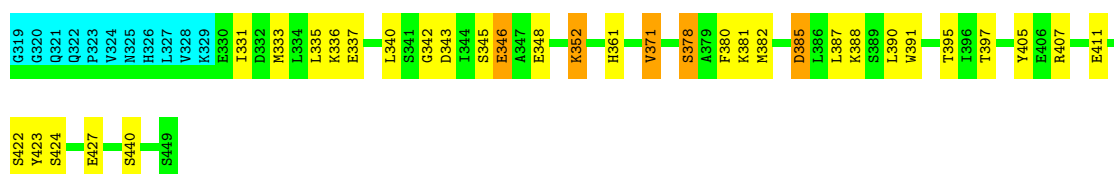
- Molecule 1: Programmed cell death protein 4

Chain A: 65% 25% 8%



- Molecule 2: Programmed cell death protein 4

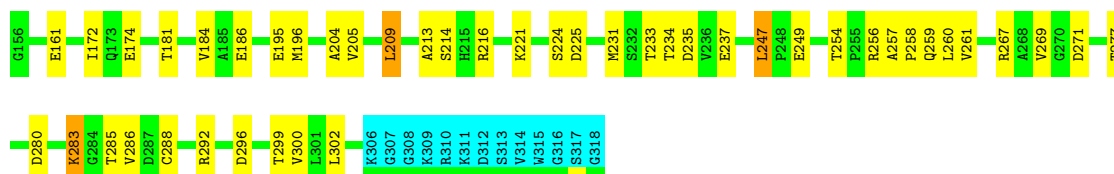
Chain B: 66% 21% 8%



4.2.30 Score per residue for model 30

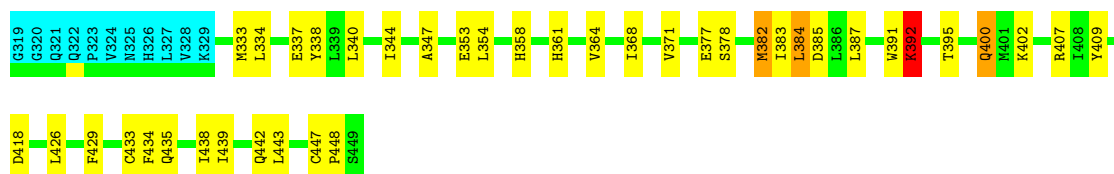
- Molecule 1: Programmed cell death protein 4

Chain A: 64% 26% 8%



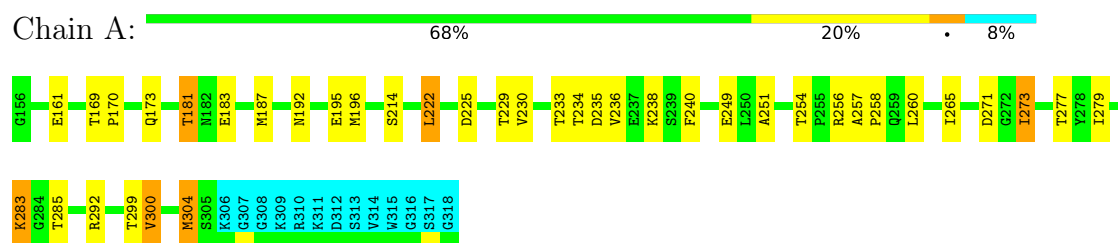
- Molecule 2: Programmed cell death protein 4

Chain B: 61% 27% 8%

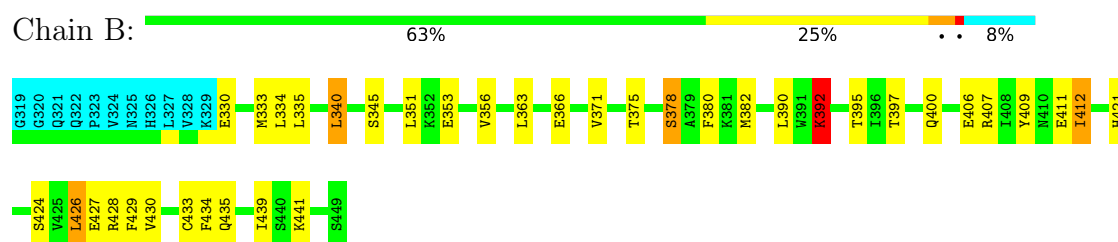


4.2.31 Score per residue for model 31

- Molecule 1: Programmed cell death protein 4

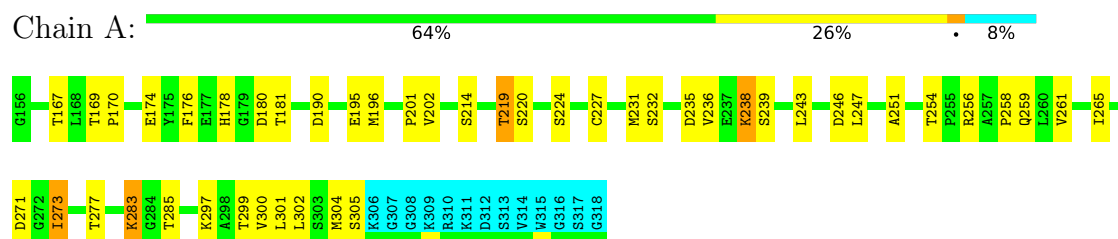


- Molecule 2: Programmed cell death protein 4

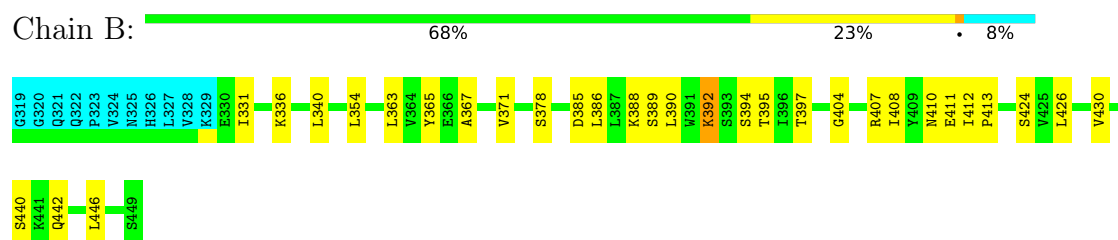


4.2.32 Score per residue for model 32

- Molecule 1: Programmed cell death protein 4

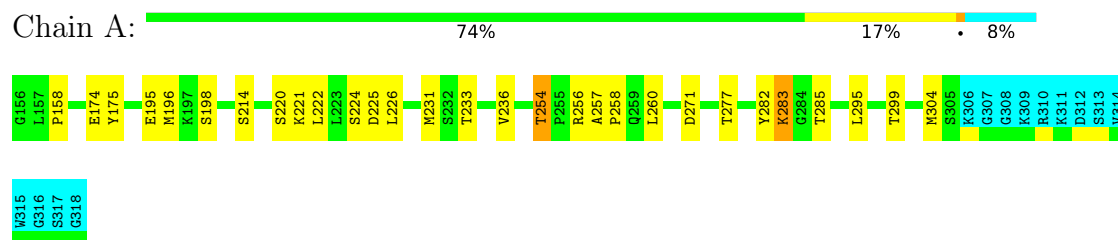


- Molecule 2: Programmed cell death protein 4

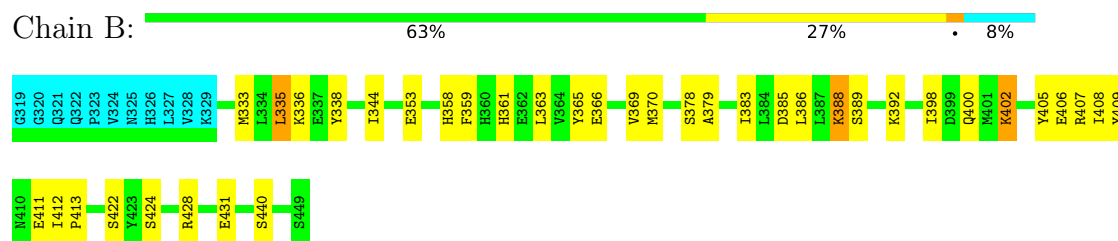


4.2.33 Score per residue for model 33

- Molecule 1: Programmed cell death protein 4

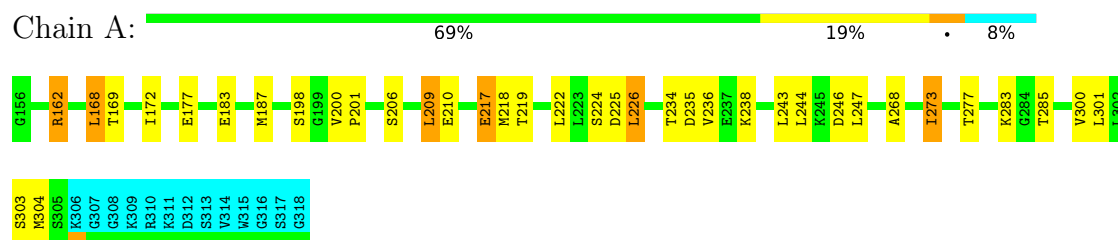


- Molecule 2: Programmed cell death protein 4

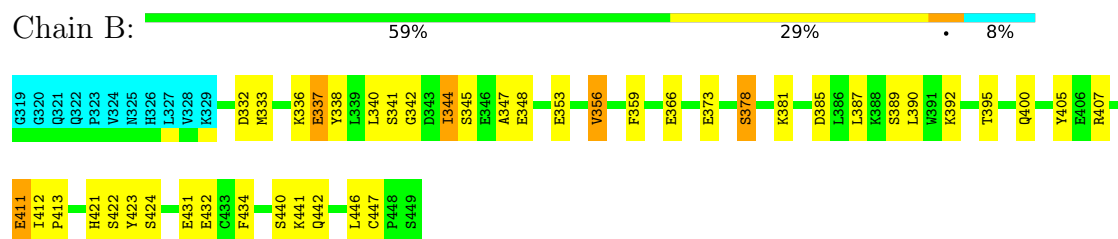


4.2.34 Score per residue for model 34

- Molecule 1: Programmed cell death protein 4



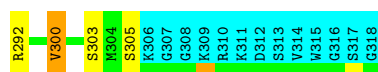
- Molecule 2: Programmed cell death protein 4



4.2.35 Score per residue for model 35

- Molecule 1: Programmed cell death protein 4





- Molecule 2: Programmed cell death protein 4

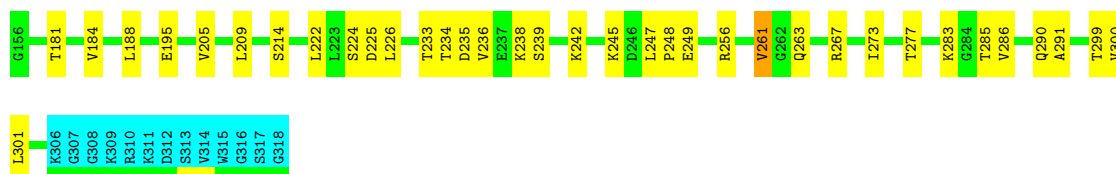
Chain B: 59% 28% 5% 8%



4.2.36 Score per residue for model 36

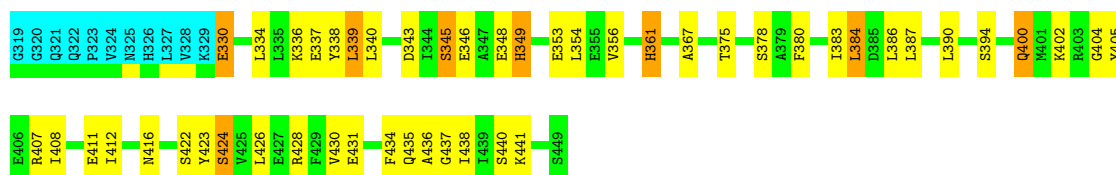
- Molecule 1: Programmed cell death protein 4

Chain A: 70% 21% 8%



- Molecule 2: Programmed cell death protein 4

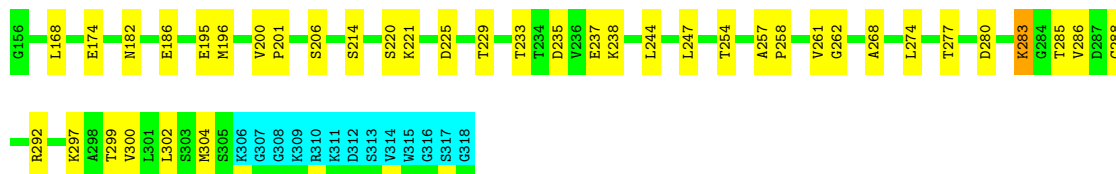
Chain B: 54% 31% 6% 8%



4.2.37 Score per residue for model 37

- Molecule 1: Programmed cell death protein 4

Chain A: 68% 23% 8%



- Molecule 2: Programmed cell death protein 4

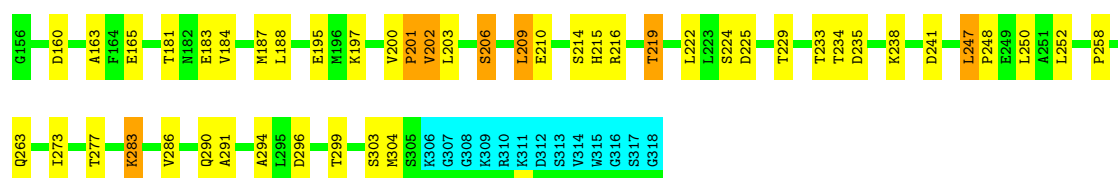
Chain B: 



4.2.38 Score per residue for model 38

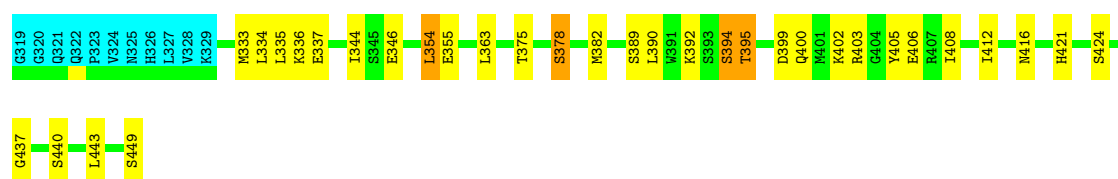
- Molecule 1: Programmed cell death protein 4

Chain A: 



- Molecule 2: Programmed cell death protein 4

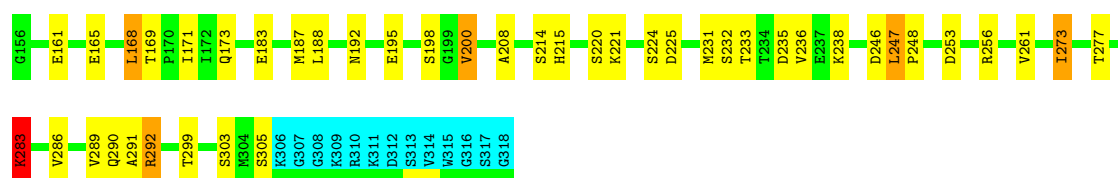
Chain B: 



4.2.39 Score per residue for model 39

- Molecule 1: Programmed cell death protein 4

Chain A: 



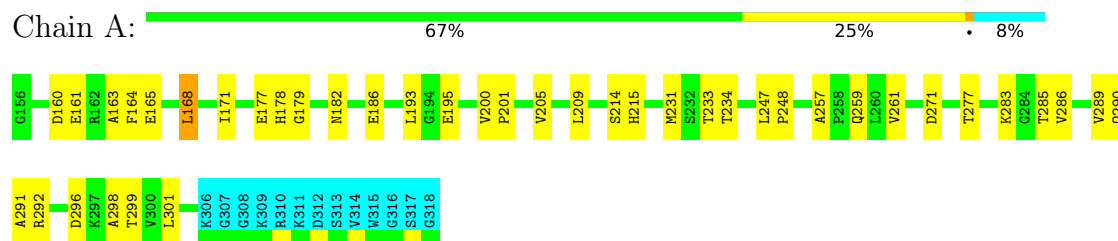
- Molecule 2: Programmed cell death protein 4

Chain B: 

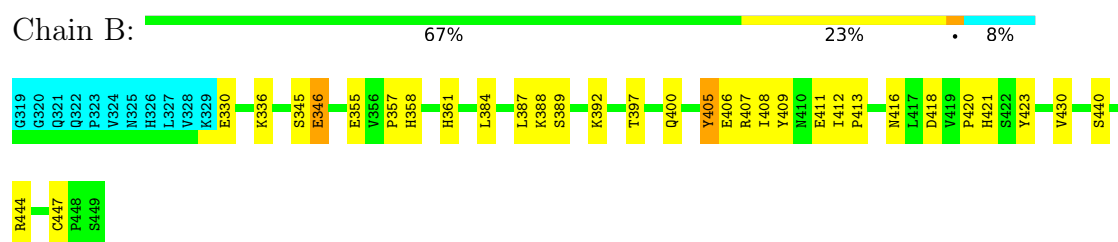


4.2.40 Score per residue for model 40

- Molecule 1: Programmed cell death protein 4

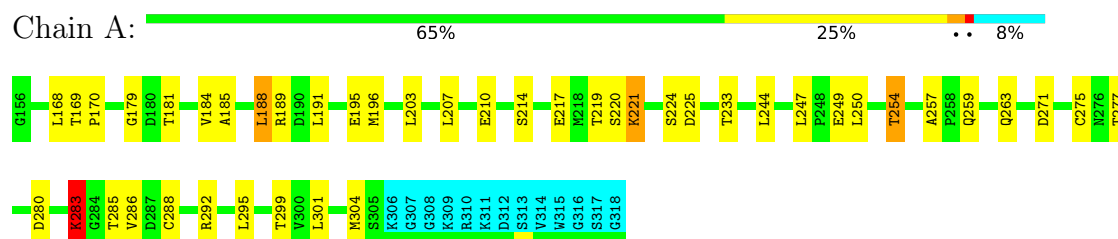


- Molecule 2: Programmed cell death protein 4

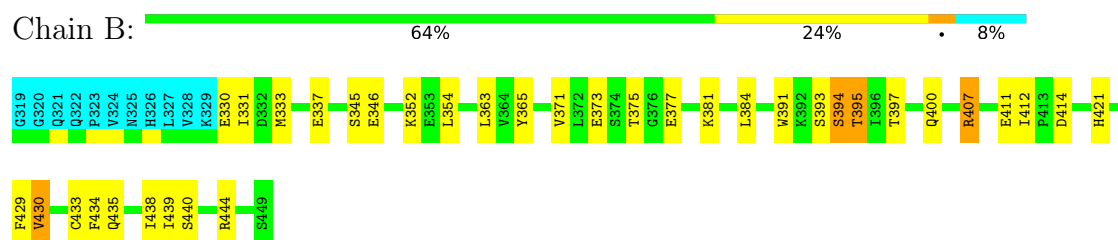


4.2.41 Score per residue for model 41

- Molecule 1: Programmed cell death protein 4

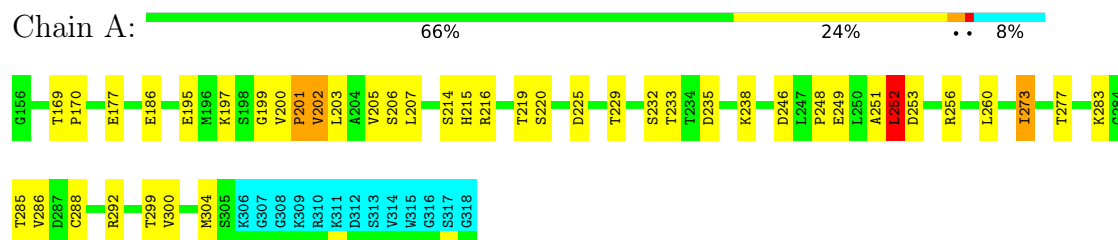


- Molecule 2: Programmed cell death protein 4

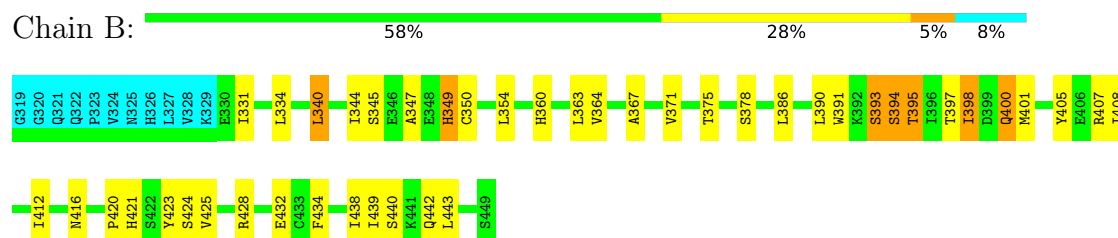


4.2.42 Score per residue for model 42

- Molecule 1: Programmed cell death protein 4

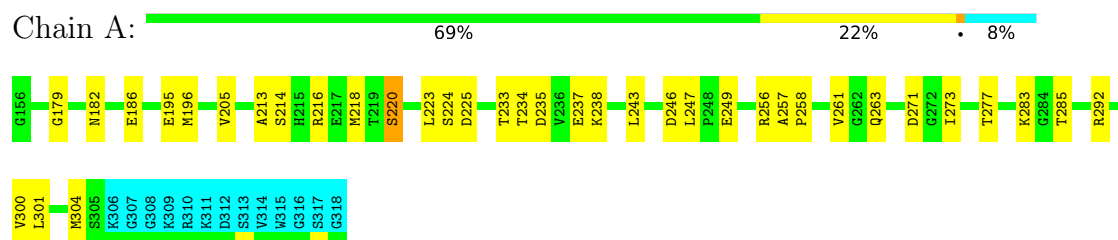


• Molecule 2: Programmed cell death protein 4

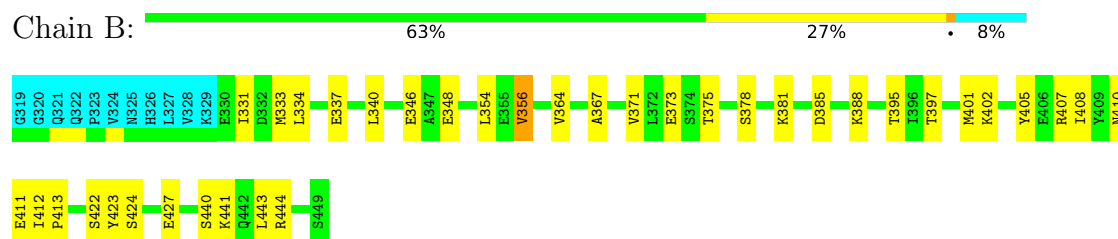


4.2.43 Score per residue for model 43

• Molecule 1: Programmed cell death protein 4

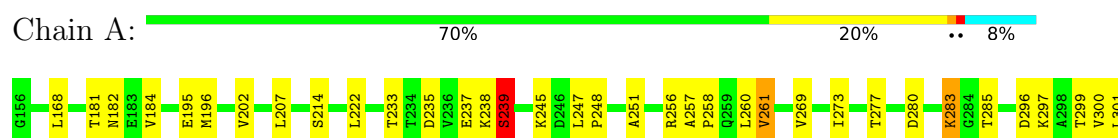


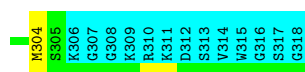
• Molecule 2: Programmed cell death protein 4



4.2.44 Score per residue for model 44

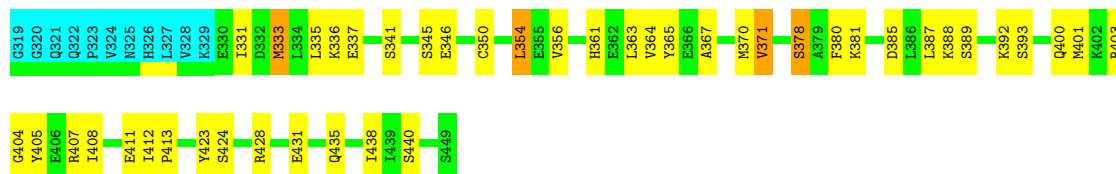
• Molecule 1: Programmed cell death protein 4





• Molecule 2: Programmed cell death protein 4

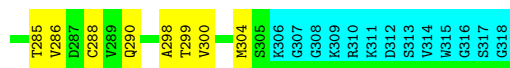
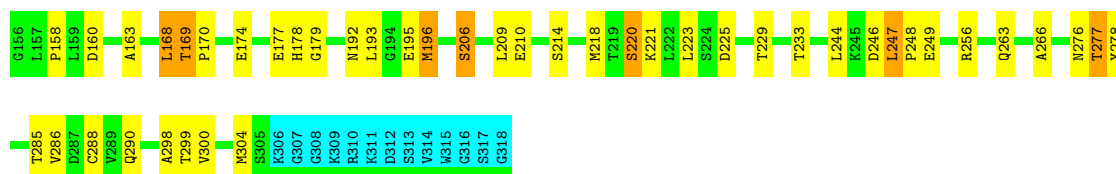
Chain B: 58% 31% 8%



4.2.45 Score per residue for model 45

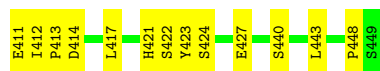
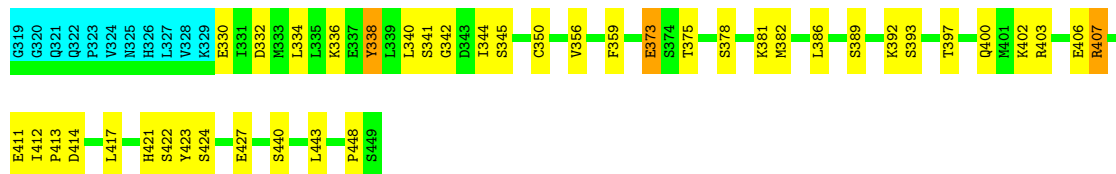
• Molecule 1: Programmed cell death protein 4

Chain A: 65% 23% 8%



• Molecule 2: Programmed cell death protein 4

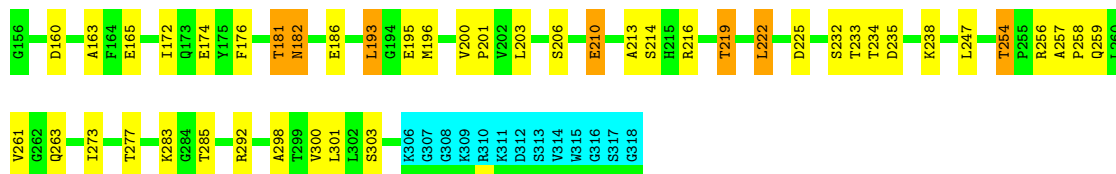
Chain B: 60% 29% 8%



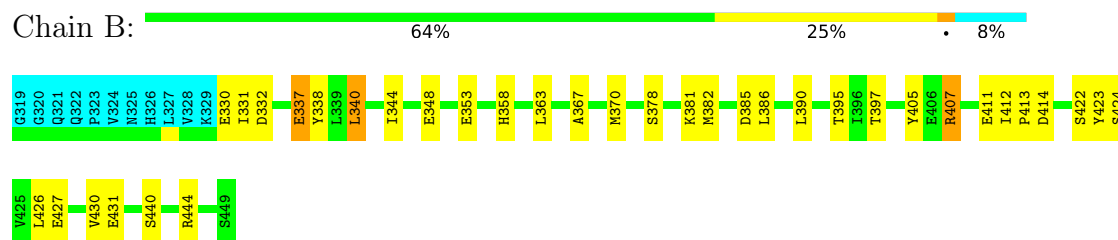
4.2.46 Score per residue for model 46

• Molecule 1: Programmed cell death protein 4

Chain A: 64% 23% 8%

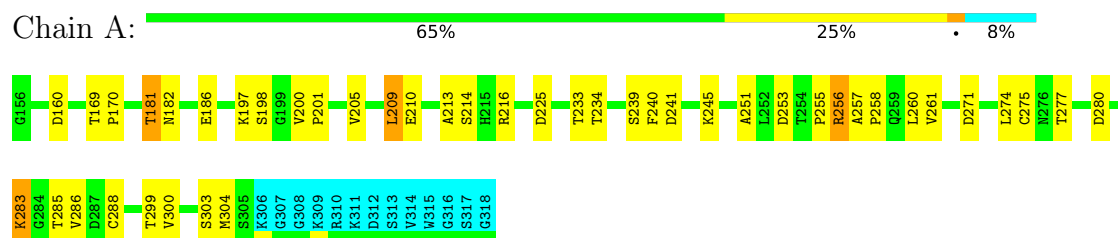


• Molecule 2: Programmed cell death protein 4

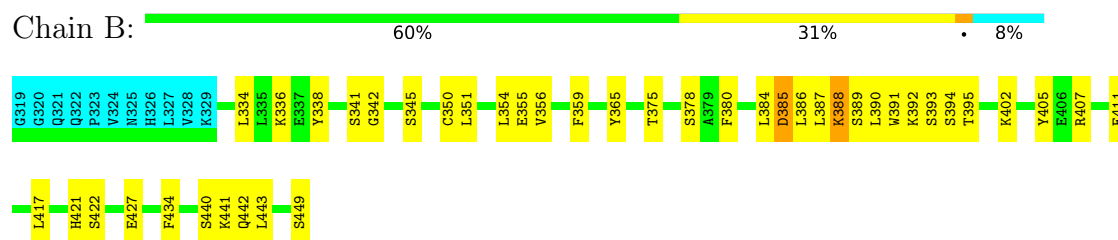


4.2.47 Score per residue for model 47

- Molecule 1: Programmed cell death protein 4

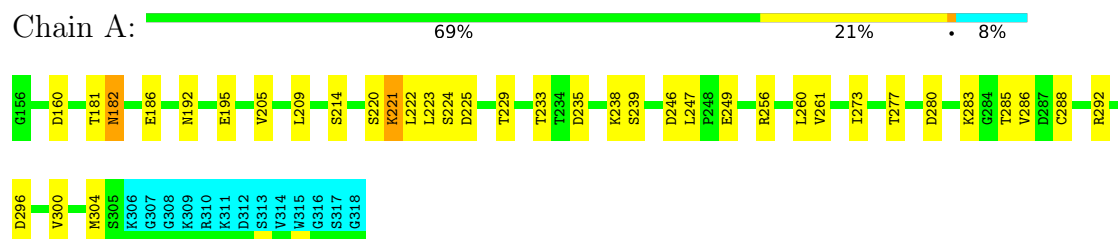


- Molecule 2: Programmed cell death protein 4

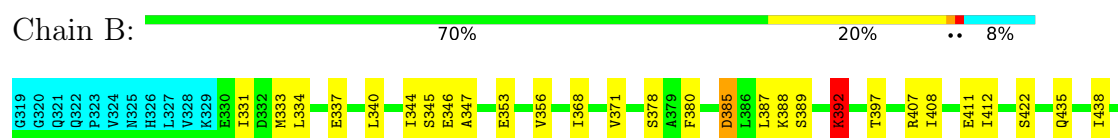


4.2.48 Score per residue for model 48

- Molecule 1: Programmed cell death protein 4



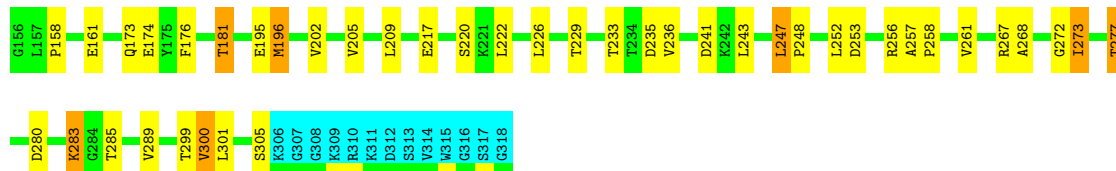
- Molecule 2: Programmed cell death protein 4



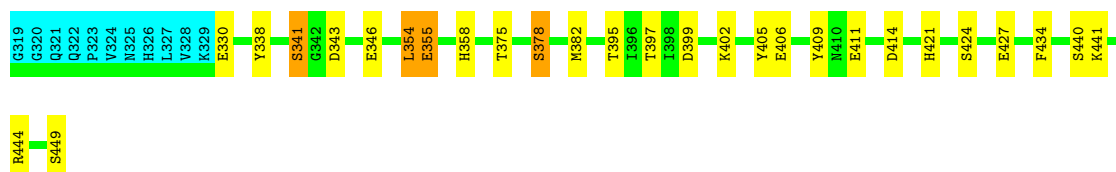
S449

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

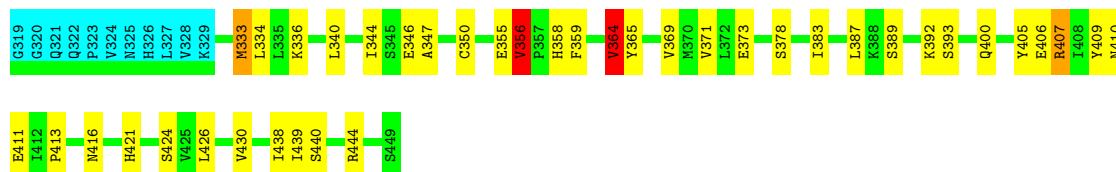
Chain B: 

4.2.50 Score per residue for model 50

- Molecule 1: Programmed cell death protein 4

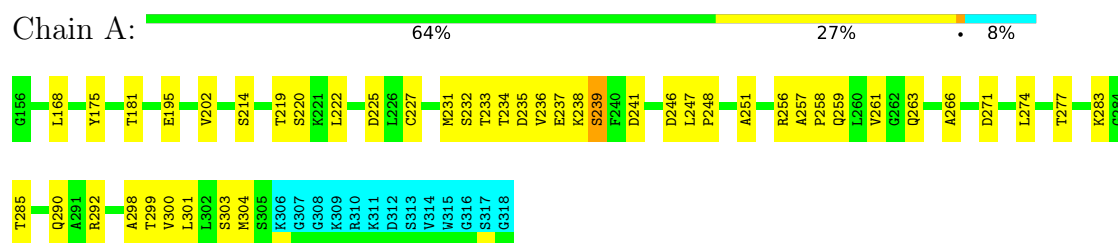
Chain A: 

- Molecule 2: Programmed cell death protein 4

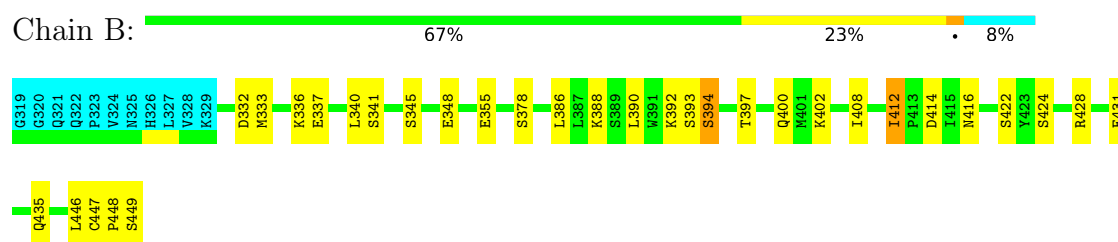
Chain B: 

4.2.51 Score per residue for model 51

- Molecule 1: Programmed cell death protein 4

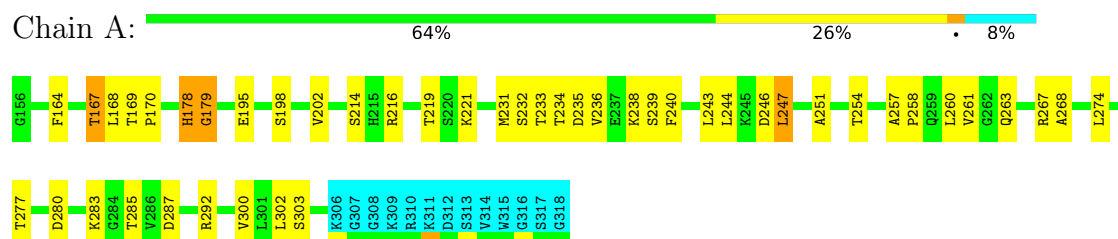


- Molecule 2: Programmed cell death protein 4

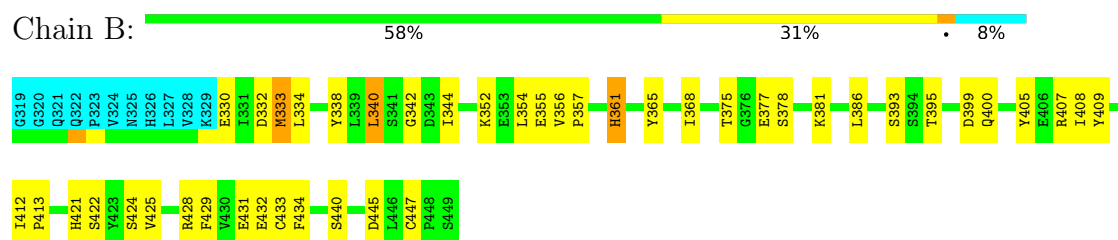


4.2.52 Score per residue for model 52

- Molecule 1: Programmed cell death protein 4

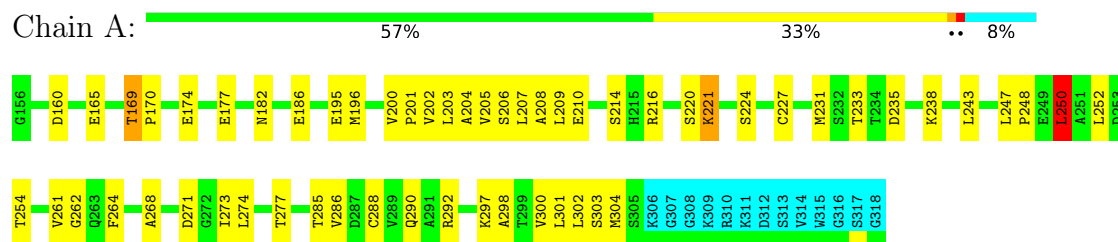


- Molecule 2: Programmed cell death protein 4

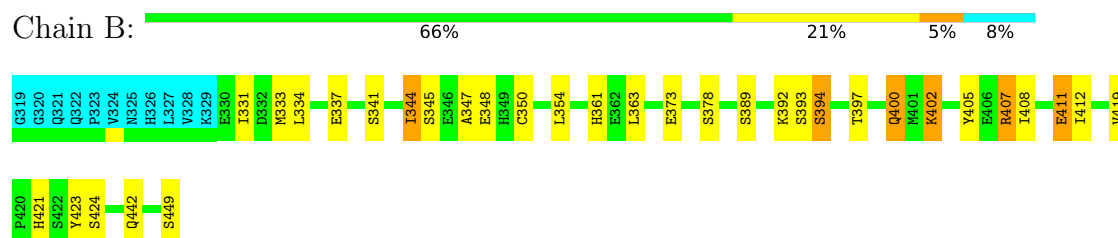


4.2.53 Score per residue for model 53

- Molecule 1: Programmed cell death protein 4

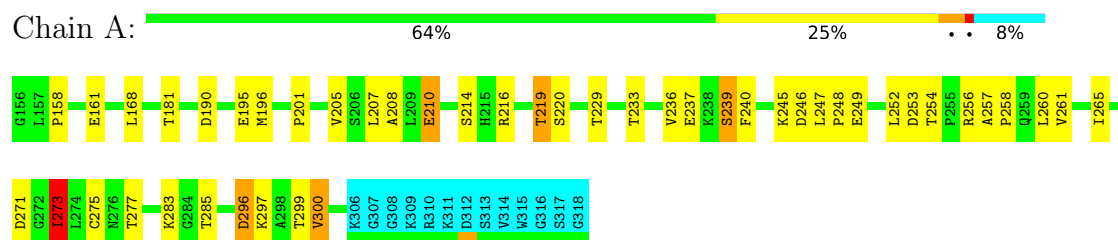


• Molecule 2: Programmed cell death protein 4

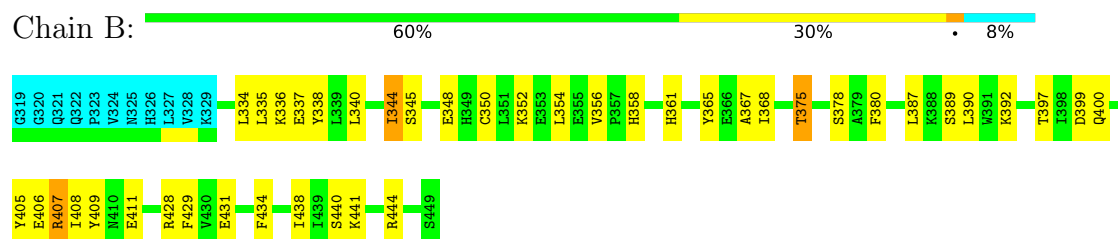


4.2.54 Score per residue for model 54

• Molecule 1: Programmed cell death protein 4

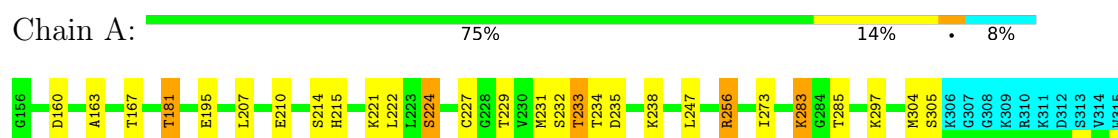


• Molecule 2: Programmed cell death protein 4



4.2.55 Score per residue for model 55

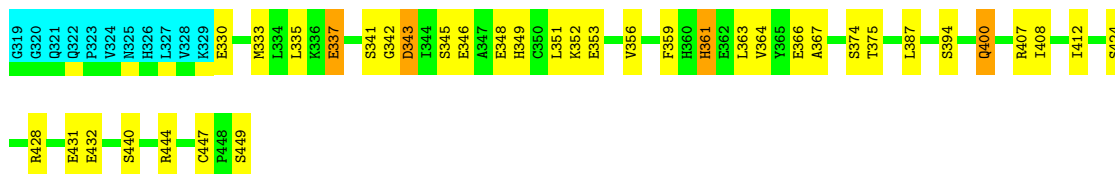
• Molecule 1: Programmed cell death protein 4





• Molecule 2: Programmed cell death protein 4

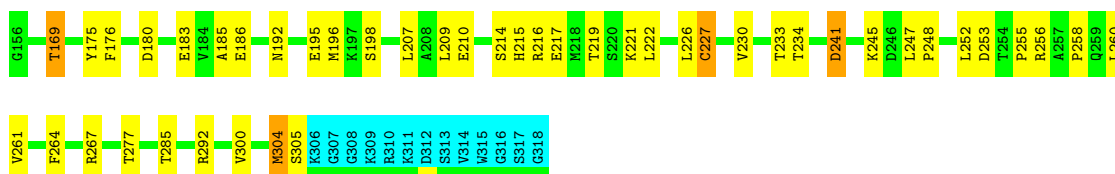
Chain B: 63% 25% 8%



4.2.56 Score per residue for model 56

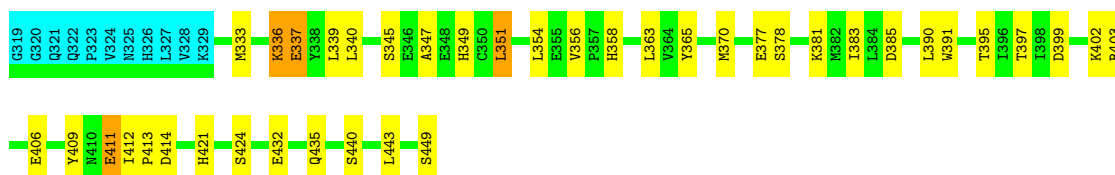
• Molecule 1: Programmed cell death protein 4

Chain A: 64% 25% 8%



• Molecule 2: Programmed cell death protein 4

Chain B: 61% 27% 8%



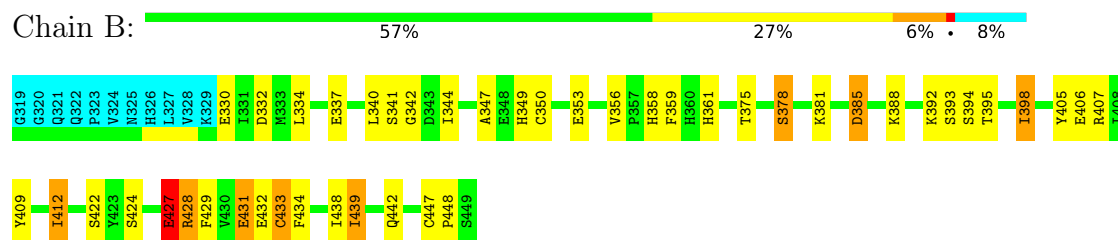
4.2.57 Score per residue for model 57

• Molecule 1: Programmed cell death protein 4

Chain A: 65% 24% 8%

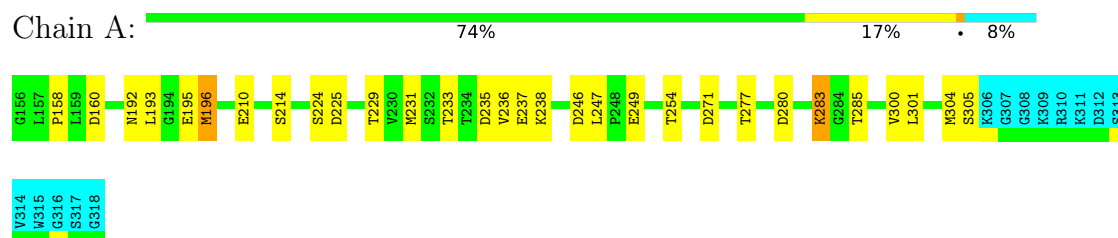


• Molecule 2: Programmed cell death protein 4

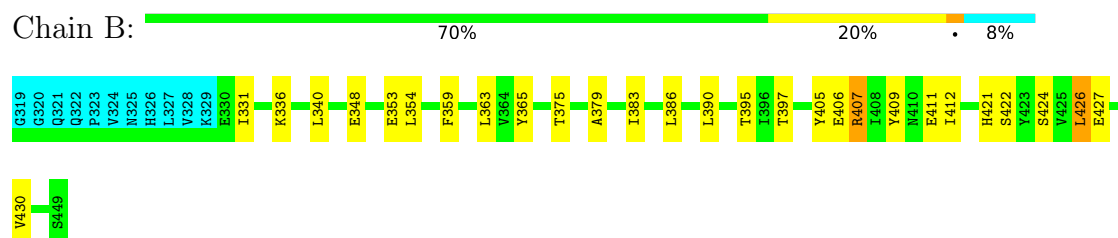


4.2.58 Score per residue for model 58

- Molecule 1: Programmed cell death protein 4

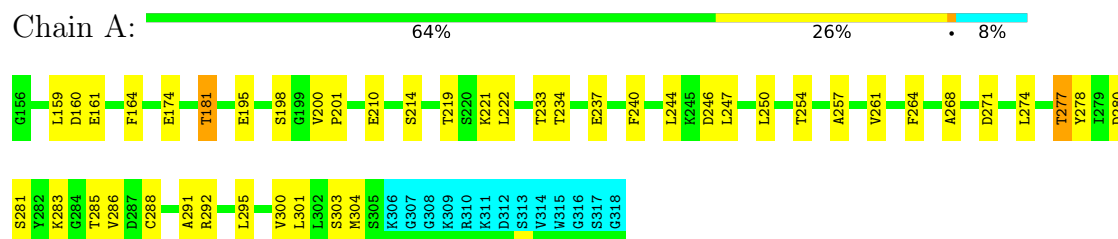


- Molecule 2: Programmed cell death protein 4

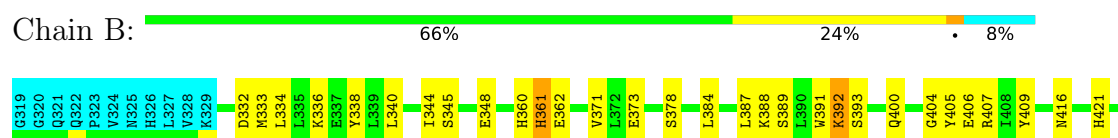


4.2.59 Score per residue for model 59

- Molecule 1: Programmed cell death protein 4



- Molecule 2: Programmed cell death protein 4

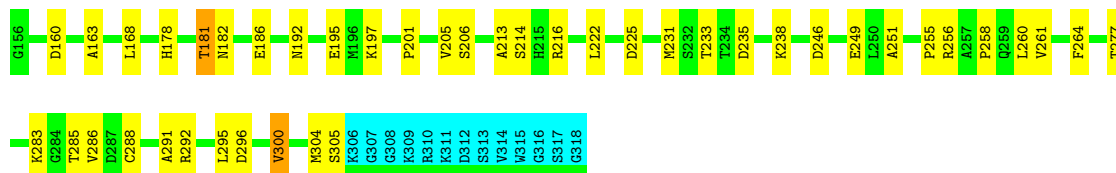




4.2.60 Score per residue for model 60

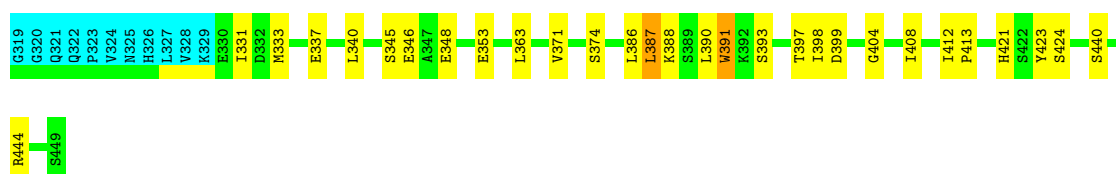
- Molecule 1: Programmed cell death protein 4

Chain A: 66% 25% 8%



- Molecule 2: Programmed cell death protein 4

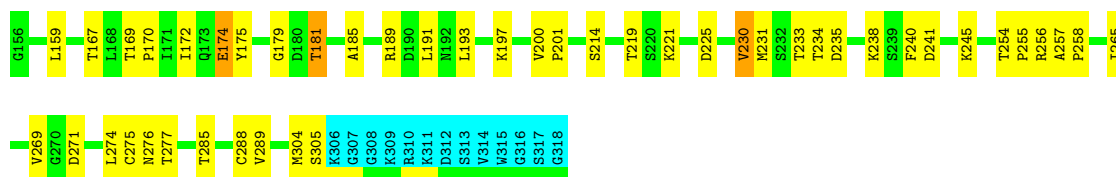
Chain B: 69% 21% 8%



4.2.61 Score per residue for model 61

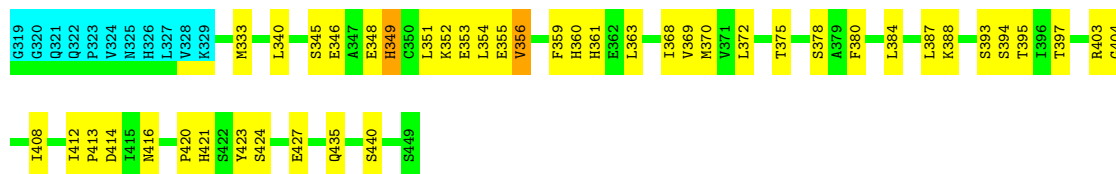
- Molecule 1: Programmed cell death protein 4

Chain A: 64% 26% 8%



- Molecule 2: Programmed cell death protein 4

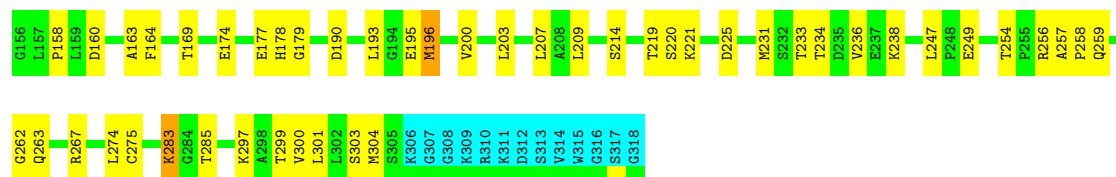
Chain B: 58% 32% 8%



4.2.62 Score per residue for model 62

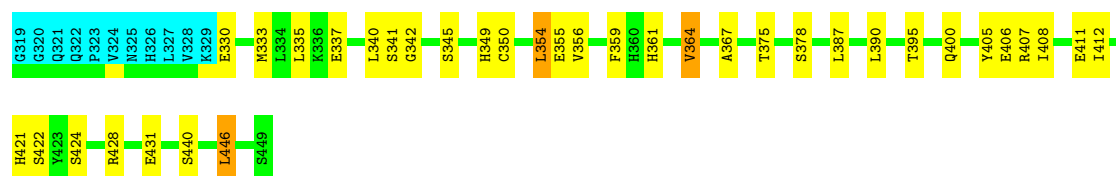
- Molecule 1: Programmed cell death protein 4

Chain A: 



- Molecule 2: Programmed cell death protein 4

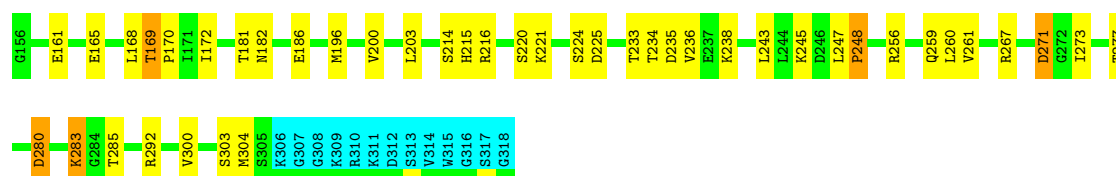
Chain B: 



4.2.63 Score per residue for model 63

- Molecule 1: Programmed cell death protein 4

Chain A: 



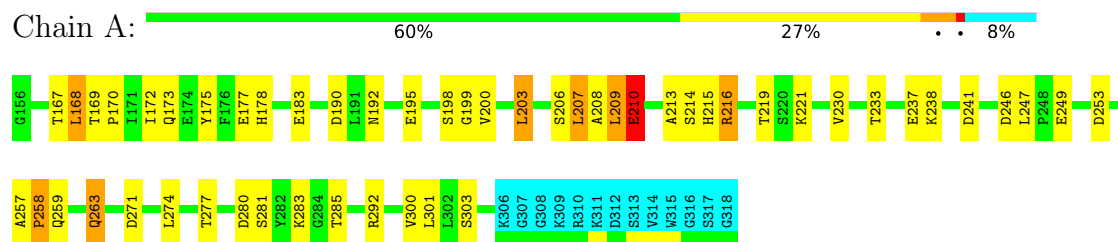
- Molecule 2: Programmed cell death protein 4

Chain B: 

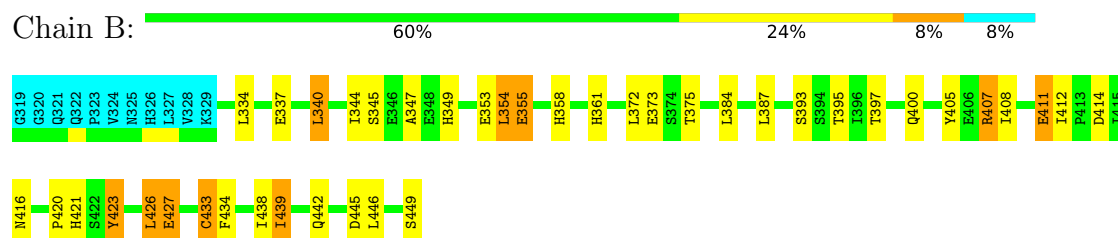


4.2.64 Score per residue for model 64

- Molecule 1: Programmed cell death protein 4

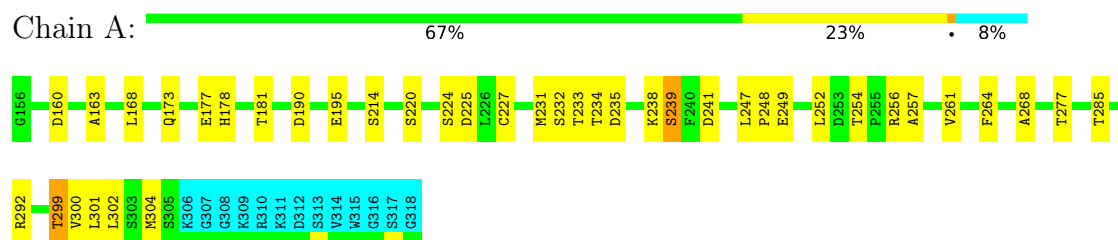


- Molecule 2: Programmed cell death protein 4

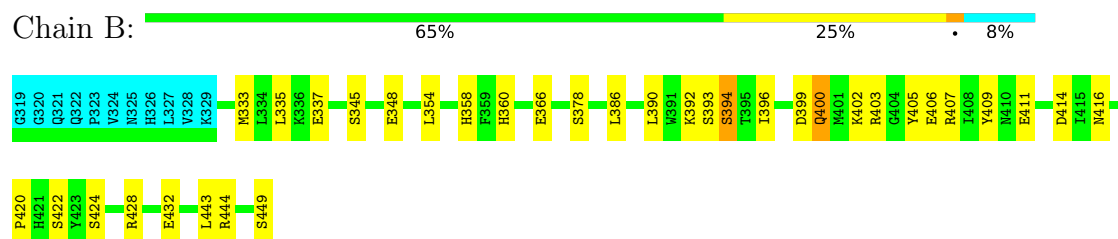


4.2.65 Score per residue for model 65

- Molecule 1: Programmed cell death protein 4

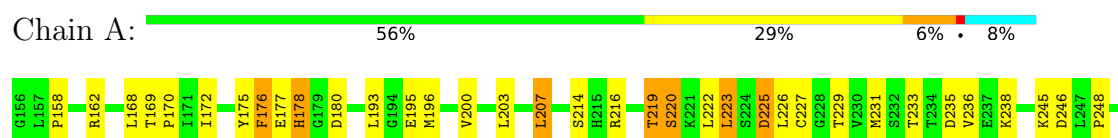


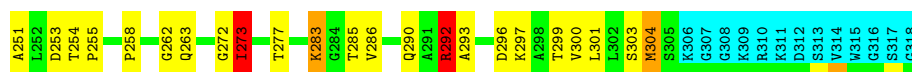
- Molecule 2: Programmed cell death protein 4



4.2.66 Score per residue for model 66

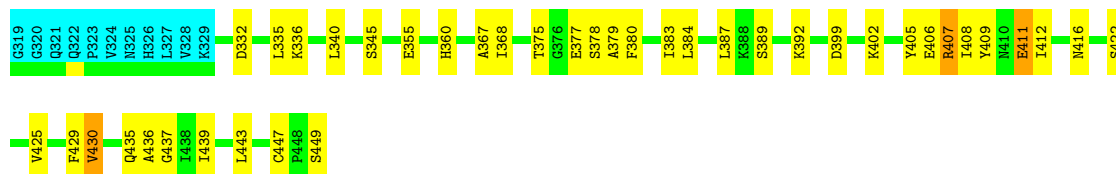
- Molecule 1: Programmed cell death protein 4





• Molecule 2: Programmed cell death protein 4

Chain B: 61% 28% 8%



4.2.67 Score per residue for model 67

• Molecule 1: Programmed cell death protein 4

Chain A: 69% 22% 8%



• Molecule 2: Programmed cell death protein 4

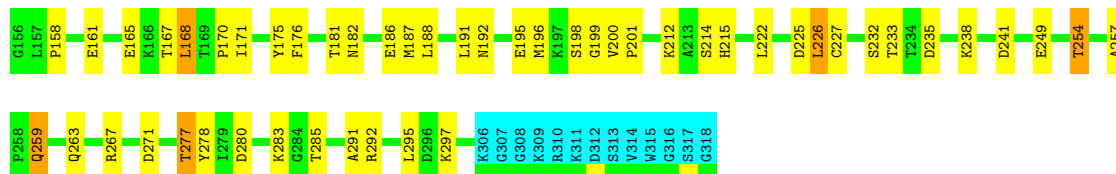
Chain B: 70% 18% 8%



4.2.68 Score per residue for model 68

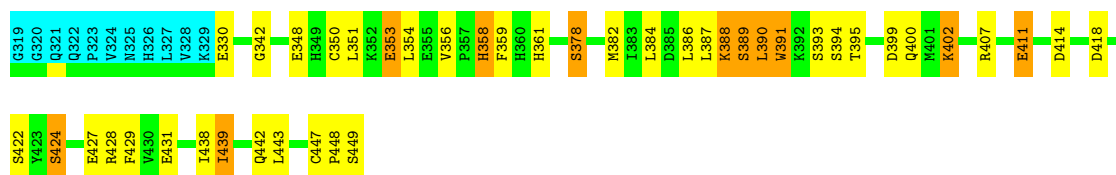
• Molecule 1: Programmed cell death protein 4

Chain A: 61% 28% 8%



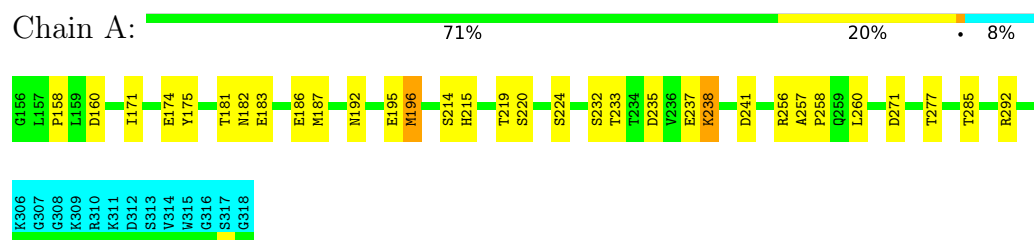
• Molecule 2: Programmed cell death protein 4

Chain B: 59% 24% 8% 8%

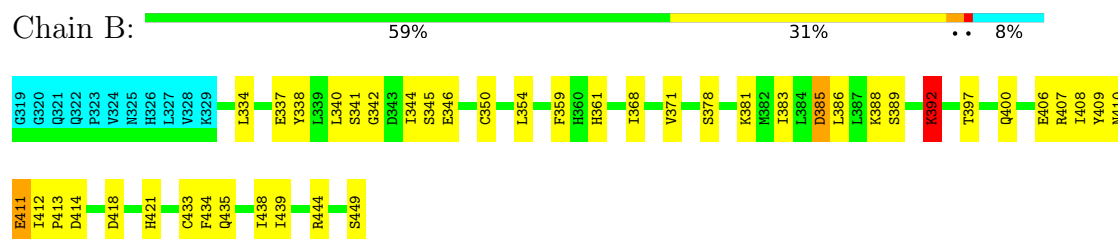


4.2.69 Score per residue for model 69

- Molecule 1: Programmed cell death protein 4

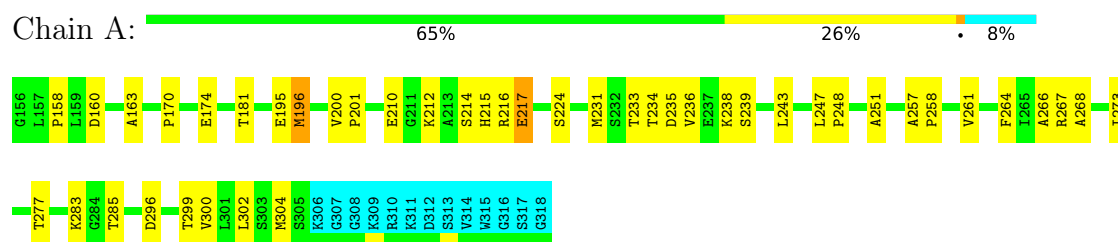


- Molecule 2: Programmed cell death protein 4

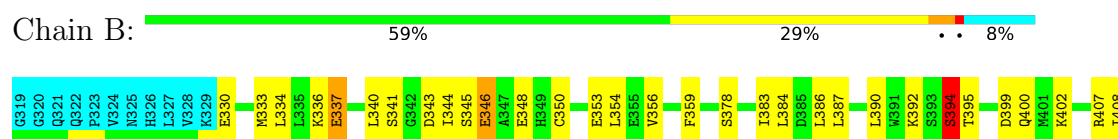


4.2.70 Score per residue for model 70

- Molecule 1: Programmed cell death protein 4



- Molecule 2: Programmed cell death protein 4





4.2.71 Score per residue for model 71

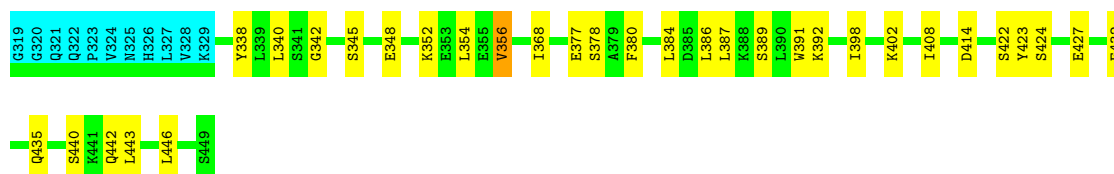
- Molecule 1: Programmed cell death protein 4

Chain A: 66% 23% 8%



- Molecule 2: Programmed cell death protein 4

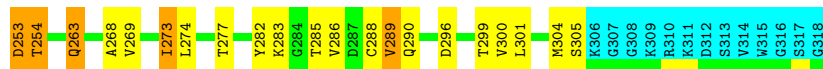
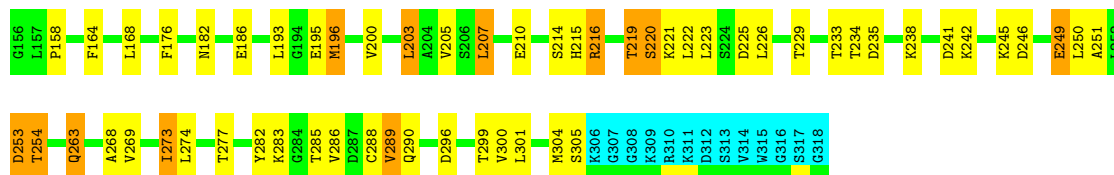
Chain B: 67% 24% 8%



4.2.72 Score per residue for model 72

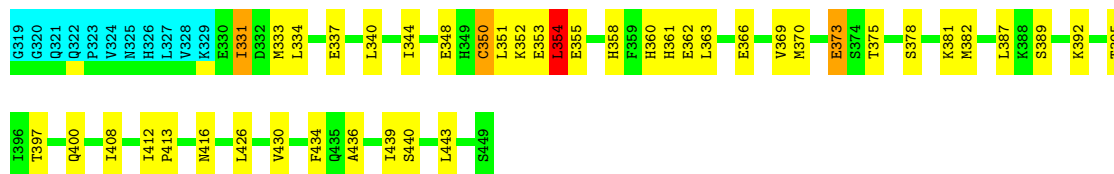
- Molecule 1: Programmed cell death protein 4

Chain A: 57% 28% 7% 8%



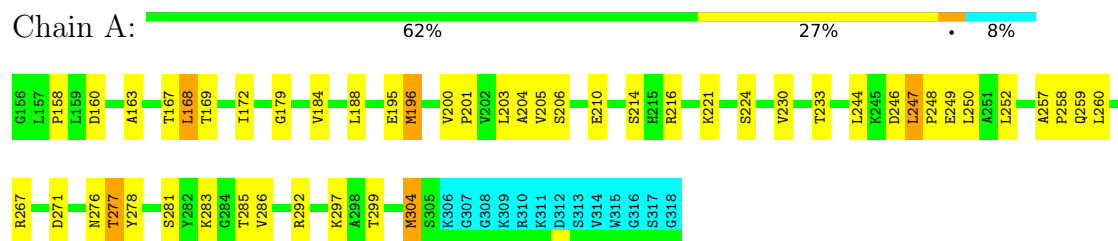
- Molecule 2: Programmed cell death protein 4

Chain B: 59% 30% 8%

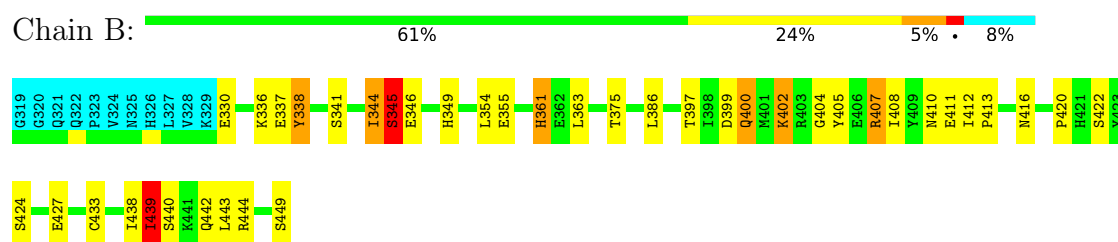


4.2.73 Score per residue for model 73

- Molecule 1: Programmed cell death protein 4



- Molecule 2: Programmed cell death protein 4



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.

6 Model quality i

6.1 Standard geometry i

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.45±0.04	0±0/1152 (0.0± 0.0%)	0.83±0.05	0±1/1560 (0.0± 0.1%)
2	B	0.43±0.04	0±0/995 (0.0± 0.0%)	0.82±0.06	1±1/1342 (0.0± 0.1%)
All	All	0.44	0/156731 (0.0%)	0.83	71/211846 (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. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	344	ILE	N-CA-C	13.00	122.64	110.42	5	2
2	B	371	VAL	N-CA-C	11.89	121.56	110.74	35	1
2	B	371	VAL	N-CA-CB	8.21	120.49	110.64	35	1
1	A	210	GLU	N-CA-C	7.47	122.57	111.81	64	3
1	A	283	LYS	N-CA-C	7.02	120.44	110.68	8	4
1	A	177	GLU	CA-C-N	-7.01	112.52	121.98	40	1
1	A	177	GLU	C-N-CA	-7.01	112.52	121.98	40	1
1	A	169	THR	N-CA-CB	6.83	116.88	110.39	25	2
2	B	356	VAL	N-CA-C	6.79	113.74	107.56	52	11
1	A	269	VAL	N-CA-C	6.79	116.80	110.42	44	1
2	B	380	PHE	N-CA-C	-6.64	104.65	112.89	54	1
2	B	345	SER	N-CA-C	6.54	120.85	112.34	70	2
1	A	256	ARG	N-CA-C	-6.38	106.71	114.75	22	1
1	A	277	THR	N-CA-C	6.17	118.01	111.28	59	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	438	ILE	N-CA-C	-6.06	107.08	112.90	44	3
2	B	412	ILE	N-CA-CB	6.06	114.32	110.50	10	1
2	B	370	MET	N-CA-C	-6.04	105.40	112.89	35	1
2	B	427	GLU	N-CA-C	-5.90	105.57	112.89	57	1
1	A	273	ILE	N-CA-C	-5.86	107.41	113.10	44	1
2	B	331	ILE	N-CA-C	5.79	116.00	110.74	72	1
2	B	386	LEU	N-CA-CB	5.77	118.67	110.13	35	1
1	A	250	LEU	N-CA-C	5.67	118.23	111.71	53	1
2	B	335	LEU	N-CA-C	5.66	120.23	111.56	33	1
2	B	435	GLN	N-CA-C	5.66	119.70	112.34	48	1
1	A	233	THR	N-CA-C	-5.64	106.24	113.23	36	1
1	A	160	ASP	CA-CB-CG	5.62	118.22	112.60	53	1
2	B	388	LYS	N-CA-C	5.60	119.83	112.89	35	2
1	A	209	LEU	N-CA-C	5.57	117.03	111.07	71	1
1	A	207	LEU	N-CA-C	5.53	119.77	113.19	53	2
2	B	385	ASP	N-CA-CB	5.48	119.61	110.41	47	1
1	A	203	LEU	N-CA-C	-5.47	106.44	113.23	64	1
2	B	373	GLU	N-CA-C	5.38	119.36	112.26	64	1
1	A	169	THR	N-CA-C	5.35	119.45	112.17	25	1
1	A	210	GLU	N-CA-CB	5.34	118.26	110.25	64	1
1	A	283	LYS	N-CA-CB	5.30	117.13	110.45	8	2
2	B	398	ILE	N-CA-C	5.26	120.29	109.34	57	1
2	B	403	ARG	N-CA-C	-5.26	106.71	113.23	38	1
2	B	373	GLU	N-CA-CB	5.24	119.34	110.49	72	1
1	A	294	ALA	N-CA-C	5.23	118.12	111.69	38	1
2	B	392	LYS	N-CA-C	5.22	121.92	110.80	69	4
2	B	393	SER	N-CA-C	5.19	118.39	111.75	42	1
2	B	338	TYR	N-CA-C	-5.07	106.26	112.90	17	1
2	B	385	ASP	N-CA-C	5.06	119.31	113.18	47	1
2	B	391	TRP	N-CA-C	5.06	116.87	111.36	30	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	16±4
2	B	976	200	970	14±4
All	All	154249	32704	155125	1980

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

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

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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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
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:301:LEU:HD22	2:B:333:MET:HE2	0.70	1.64	44	1
1:A:263:GLN:HA	1:A:301:LEU:HD13	0.70	1.63	22	8
1:A:248:PRO:HG3	1:A:290:GLN:HG3	0.70	1.64	67	1
2:B:335:LEU:HD22	2:B:367:ALA:HB2	0.69	1.63	62	5
1:A:221:LYS:HA	1:A:221:LYS:HE2	0.69	1.64	48	3
2:B:427:GLU:O	2:B:431:GLU:HG2	0.69	1.88	57	2
1:A:300:VAL:HG22	1:A:304:MET:HE3	0.69	1.65	65	1
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
1:A:300:VAL:HG12	1:A:304:MET:HE3	0.68	1.65	69	3
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:158:PRO:HB2	1:A:196:MET:HE2	0.65	1.68	50	18
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:361:HIS:HB3	2:B:400:GLN:HG3	0.64	1.69	18	1
1:A:300:VAL:HG12	1:A:304:MET:HE1	0.64	1.70	53	1
1:A:296:ASP:HB3	2:B:340:LEU:HD21	0.64	1.70	54	1
1:A:301:LEU:HD23	1:A:304:MET:HE1	0.63	1.67	66	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
1:A:300:VAL:HG22	2:B:340:LEU:HD23	0.63	1.70	60	1
2:B:361:HIS:HB3	2:B:400:GLN:HB3	0.63	1.70	72	1
1:A:250:LEU:H	1:A:250:LEU:HD23	0.63	1.54	53	2
2:B:391:TRP:HZ2	2:B:398:ILE:HB	0.63	1.53	60	1
1:A:289:VAL:HG13	1:A:290:GLN:H	0.63	1.53	72	1
2:B:337:GLU:O	2:B:341:SER:HB2	0.63	1.94	62	6
1:A:262:GLY:HA3	1:A:297:LYS:HB3	0.63	1.69	66	4
2:B:377:GLU:HA	2:B:380:PHE:CB	0.63	2.24	66	1
2:B:407:ARG:O	2:B:411:GLU:HG2	0.63	1.92	69	51
1:A:231:MET:HG3	1:A:235:ASP:HB3	0.63	1.70	6	2
2:B:334:LEU:HD22	2:B:347:ALA:HA	0.62	1.69	53	8
2:B:405:TYR:HE2	2:B:430:VAL:HG22	0.62	1.53	46	1
1:A:259:GLN:HG2	2:B:346:GLU:HG2	0.62	1.70	40	1
2:B:356:VAL:HB	2:B:359:PHE:HB2	0.62	1.70	34	3
2:B:434:PHE:HE1	2:B:441:LYS:HA	0.61	1.55	36	6
2:B:364:VAL:HG11	2:B:401:MET:HG3	0.61	1.72	21	6
1:A:256:ARG:O	1:A:260:LEU:HG	0.61	1.95	30	12
1:A:205:VAL:HG13	1:A:209:LEU:HD12	0.61	1.72	47	1
1:A:237:GLU:HG3	1:A:274:LEU:HD12	0.61	1.72	10	3
1:A:213:ALA:HA	1:A:216:ARG:HD2	0.61	1.71	9	13
1:A:227:CYS:HA	1:A:231:MET:O	0.61	1.96	55	12
1:A:247:LEU:N	1:A:248:PRO:HD2	0.61	2.11	63	17
1:A:257:ALA:O	1:A:261:VAL:HG23	0.61	1.96	51	13
2:B:333:MET:O	2:B:337:GLU:HB2	0.61	1.96	55	7
2:B:388:LYS:HA	2:B:391:TRP:HB2	0.60	1.71	4	1
1:A:249:GLU:O	1:A:252:LEU:HG	0.60	1.95	21	1
1:A:206:SER:O	1:A:209:LEU:HB3	0.60	1.96	34	1
2:B:432:GLU:HA	2:B:435:GLN:HE21	0.60	1.55	35	3
1:A:259:GLN:NE2	2:B:346:GLU:HA	0.60	2.12	41	2
1:A:282:TYR:HD2	1:A:286:VAL:HG22	0.60	1.56	17	1
1:A:183:GLU:HG3	1:A:187:MET:HE3	0.60	1.73	6	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:304:MET:HE1	2:B:337:GLU:HG2	0.60	1.72	55	2
1:A:164:PHE:HZ	1:A:200:VAL:HG22	0.60	1.57	40	3
2:B:331:ILE:HG23	2:B:363:LEU:HA	0.60	1.73	21	6
2:B:361:HIS:HB2	2:B:400:GLN:HG3	0.60	1.73	44	5
2:B:365:TYR:HE1	2:B:411:GLU:HG3	0.60	1.56	56	8
1:A:216:ARG:HB3	1:A:264:PHE:HZ	0.60	1.56	18	4
2:B:438:ILE:HG13	2:B:439:ILE:H	0.60	1.56	21	5
2:B:330:GLU:O	2:B:334:LEU:HG	0.60	1.97	45	11
2:B:338:TYR:CE1	2:B:344:ILE:HG12	0.60	2.32	20	3
2:B:338:TYR:HA	2:B:342:GLY:HA2	0.60	1.74	34	2
1:A:300:VAL:CG1	2:B:337:GLU:HA	0.60	2.27	63	4
1:A:300:VAL:HG12	1:A:304:MET:HE2	0.60	1.74	44	4
1:A:235:ASP:HA	1:A:238:LYS:CE	0.59	2.26	18	13
2:B:331:ILE:HG23	2:B:363:LEU:HG	0.59	1.73	72	1
1:A:245:LYS:O	1:A:248:PRO:HD2	0.59	1.96	54	6
2:B:390:LEU:H	2:B:390:LEU:HD23	0.59	1.57	68	1
1:A:169:THR:HA	1:A:172:ILE:HD12	0.59	1.74	34	1
1:A:205:VAL:HG23	1:A:206:SER:H	0.59	1.57	42	1
1:A:298:ALA:HA	1:A:301:LEU:HD12	0.59	1.74	16	6
2:B:345:SER:HA	2:B:348:GLU:HB3	0.59	1.72	13	3
2:B:337:GLU:HG2	2:B:347:ALA:HB2	0.59	1.74	24	2
1:A:158:PRO:HB3	1:A:196:MET:SD	0.59	2.38	68	3
1:A:240:PHE:HE1	1:A:265:ILE:HG12	0.59	1.58	31	1
1:A:301:LEU:HA	1:A:304:MET:HE3	0.59	1.74	67	3
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:183:GLU:HG3	1:A:187:MET:HE2	0.59	1.74	19	2
1:A:172:ILE:O	1:A:175:TYR:HB3	0.59	1.98	61	7
2:B:389:SER:HA	2:B:392:LYS:HD2	0.59	1.75	8	3
1:A:193:LEU:HD13	1:A:196:MET:HB3	0.58	1.75	3	5
2:B:432:GLU:HA	2:B:435:GLN:NE2	0.58	2.13	71	1
1:A:247:LEU:HD12	1:A:250:LEU:HD12	0.58	1.75	73	1
1:A:268:ALA:HA	1:A:273:ILE:HD12	0.58	1.74	72	2
2:B:444:ARG:HD2	2:B:447:CYS:SG	0.58	2.37	20	1
1:A:198:SER:O	1:A:201:PRO:HD2	0.58	1.99	57	4
1:A:304:MET:SD	2:B:337:GLU:HG3	0.58	2.38	15	1
1:A:263:GLN:HE22	2:B:333:MET:HE1	0.58	1.57	41	1
2:B:371:VAL:HG11	2:B:380:PHE:CD1	0.58	2.34	29	1
1:A:304:MET:SD	2:B:336:LYS:HE2	0.58	2.38	44	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:377:GLU:HA	2:B:380:PHE:HB3	0.58	1.76	66	1
2:B:338:TYR:CE2	2:B:386:LEU:HB2	0.58	2.34	63	8
1:A:251:ALA:HB2	1:A:258:PRO:HG3	0.58	1.76	24	7
1:A:291:ALA:O	1:A:295:LEU:HG	0.58	1.98	59	5
2:B:362:GLU:O	2:B:366:GLU:HB2	0.58	1.99	8	1
1:A:182:ASN:O	1:A:186:GLU:HG2	0.58	1.99	43	21
1:A:231:MET:HE3	1:A:236:VAL:HG22	0.58	1.73	24	15
2:B:386:LEU:O	2:B:390:LEU:HG	0.58	1.99	24	17
2:B:364:VAL:HG11	2:B:401:MET:HA	0.58	1.76	25	2
1:A:201:PRO:HG3	1:A:231:MET:HE1	0.58	1.75	40	5
2:B:338:TYR:HD2	2:B:386:LEU:HB2	0.58	1.58	73	2
1:A:301:LEU:HA	1:A:304:MET:SD	0.58	2.39	69	3
2:B:349:HIS:O	2:B:353:GLU:HG2	0.57	1.99	36	1
1:A:300:VAL:HG21	2:B:337:GLU:HG2	0.57	1.76	6	1
2:B:348:GLU:HA	2:B:390:LEU:HD23	0.57	1.76	4	1
1:A:282:TYR:HB3	1:A:295:LEU:HD13	0.57	1.75	33	1
1:A:188:LEU:HD21	1:A:200:VAL:HG11	0.57	1.75	39	1
1:A:304:MET:HG2	2:B:336:LYS:HE2	0.57	1.77	50	2
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
2:B:392:LYS:C	2:B:394:SER:H	0.56	2.09	51	6
1:A:283:LYS:HB3	1:A:283:LYS:NZ	0.56	2.16	7	4
2:B:368:ILE:O	2:B:371:VAL:HG23	0.56	1.99	22	1
1:A:175:TYR:HE2	1:A:219:THR:HA	0.56	1.61	69	1
2:B:384:LEU:O	2:B:387:LEU:HG	0.56	2.01	11	5
2:B:371:VAL:HG22	2:B:383:ILE:HG13	0.56	1.78	50	2
2:B:412:ILE:HG13	2:B:426:LEU:HD11	0.56	1.78	31	2
1:A:263:GLN:HA	1:A:301:LEU:HD11	0.56	1.77	64	1
2:B:408:ILE:O	2:B:412:ILE:HG12	0.56	2.01	44	31
2:B:425:VAL:O	2:B:429:PHE:HB3	0.56	2.00	21	1
1:A:297:LYS:O	1:A:300:VAL:HB	0.56	2.01	24	3
2:B:388:LYS:O	2:B:391:TRP:HB2	0.56	2.01	68	2
2:B:447:CYS:HB2	2:B:448:PRO:HD2	0.56	1.78	57	2
2:B:345:SER:O	2:B:348:GLU:HB2	0.56	2.01	36	1
2:B:378:SER:O	2:B:382:MET:HB2	0.56	2.00	46	5
2:B:384:LEU:HD21	2:B:432:GLU:HG2	0.56	1.76	7	1
1:A:268:ALA:HB1	1:A:273:ILE:HB	0.56	1.76	13	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:371:VAL:HG11	2:B:380:PHE:HA	0.56	1.77	44	1
2:B:347:ALA:HA	2:B:350:CYS:SG	0.56	2.41	57	1
1:A:296:ASP:HB3	2:B:340:LEU:CD1	0.56	2.31	67	1
2:B:384:LEU:HG	2:B:429:PHE:CE1	0.56	2.32	30	1
1:A:178:HIS:N	1:A:178:HIS:CD2	0.56	2.74	66	1
1:A:293:ALA:O	1:A:297:LYS:HB2	0.55	2.00	21	1
1:A:205:VAL:HG12	1:A:219:THR:CG2	0.55	2.32	42	1
2:B:378:SER:O	2:B:381:LYS:HG2	0.55	2.01	44	2
2:B:443:LEU:HA	2:B:446:LEU:HD12	0.55	1.79	15	1
1:A:209:LEU:HA	1:A:216:ARG:HD3	0.55	1.77	21	1
2:B:387:LEU:O	2:B:391:TRP:HB2	0.55	2.01	22	3
1:A:168:LEU:HD13	1:A:171:ILE:HD12	0.55	1.79	22	1
1:A:181:THR:HG21	1:A:225:ASP:HB2	0.55	1.78	47	2
2:B:356:VAL:HB	2:B:359:PHE:CB	0.55	2.31	6	1
2:B:361:HIS:H	2:B:400:GLN:HG3	0.55	1.62	36	2
1:A:193:LEU:HB3	1:A:196:MET:HB2	0.55	1.77	66	1
1:A:248:PRO:HA	1:A:290:GLN:HG3	0.55	1.77	3	4
1:A:204:ALA:O	1:A:208:ALA:HB2	0.55	2.02	53	1
1:A:185:ALA:HB2	1:A:226:LEU:HD22	0.55	1.77	56	1
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
2:B:387:LEU:HD22	2:B:401:MET:HE3	0.55	1.78	63	1
1:A:263:GLN:HA	1:A:301:LEU:CD1	0.54	2.32	15	4
1:A:297:LYS:O	1:A:301:LEU:HG	0.54	2.02	32	5
2:B:332:ASP:O	2:B:336:LYS:HG2	0.54	2.01	59	4
1:A:236:VAL:HG21	1:A:273:ILE:HB	0.54	1.77	21	1
1:A:297:LYS:NZ	2:B:346:GLU:HG3	0.54	2.18	22	1
1:A:298:ALA:O	1:A:302:LEU:HG	0.54	2.02	53	1
2:B:447:CYS:SG	2:B:448:PRO:HD2	0.54	2.42	68	3
2:B:365:TYR:CE1	2:B:411:GLU:HG3	0.54	2.37	11	5
1:A:286:VAL:HG12	1:A:288:CYS:H	0.54	1.62	30	18
2:B:365:TYR:O	2:B:369:VAL:HG23	0.54	2.01	2	7
1:A:265:ILE:HG21	1:A:279:ILE:HD11	0.54	1.78	31	3
2:B:404:GLY:O	2:B:408:ILE:HG12	0.54	2.03	24	10
1:A:259:GLN:O	1:A:297:LYS:HG2	0.54	2.03	68	5
1:A:263:GLN:O	1:A:267:ARG:HB2	0.54	2.02	62	3
1:A:280:ASP:HA	1:A:283:LYS:HB2	0.54	1.77	48	9
2:B:358:HIS:HA	2:B:400:GLN:NE2	0.54	2.18	68	2
2:B:433:CYS:HB2	2:B:438:ILE:HD11	0.54	1.79	64	3
1:A:197:LYS:HE3	1:A:231:MET:SD	0.54	2.42	61	2
2:B:378:SER:O	2:B:382:MET:HG2	0.54	2.02	38	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:212:LYS:HG2	1:A:213:ALA:H	0.54	1.63	20	1
1:A:168:LEU:HD22	1:A:171:ILE:HD12	0.54	1.78	39	3
1:A:252:LEU:H	1:A:252:LEU:HD23	0.54	1.62	42	1
2:B:332:ASP:CG	2:B:336:LYS:HZ1	0.54	2.10	17	1
2:B:334:LEU:HD11	2:B:347:ALA:HA	0.54	1.80	30	1
2:B:332:ASP:OD2	2:B:336:LYS:HG3	0.54	2.03	51	1
1:A:300:VAL:HA	2:B:340:LEU:HD12	0.54	1.78	34	1
1:A:219:THR:O	1:A:222:LEU:HB3	0.54	2.03	46	1
2:B:331:ILE:HG23	2:B:363:LEU:HD12	0.53	1.80	23	3
1:A:209:LEU:HA	1:A:216:ARG:HG2	0.53	1.79	47	1
2:B:416:ASN:OD1	2:B:420:PRO:HA	0.53	2.02	70	10
2:B:351:LEU:HD13	2:B:390:LEU:HD21	0.53	1.79	4	2
1:A:261:VAL:O	1:A:265:ILE:HG13	0.53	2.03	32	2
1:A:170:PRO:O	1:A:174:GLU:HG3	0.53	2.02	32	2
1:A:256:ARG:HA	1:A:259:GLN:OE1	0.53	2.03	51	3
1:A:300:VAL:HG12	2:B:340:LEU:HB2	0.53	1.80	6	1
2:B:335:LEU:HD13	2:B:366:GLU:HB3	0.53	1.81	31	1
1:A:216:ARG:HA	1:A:219:THR:OG1	0.53	2.02	54	3
2:B:348:GLU:HG3	2:B:352:LYS:HD2	0.53	1.80	55	1
2:B:406:GLU:HA	2:B:409:TYR:CZ	0.53	2.38	57	1
1:A:288:CYS:SG	1:A:290:GLN:HB2	0.53	2.44	15	4
1:A:226:LEU:HB3	1:A:230:VAL:HB	0.53	1.81	56	1
2:B:402:LYS:HG2	2:B:443:LEU:HD13	0.53	1.81	68	1
1:A:205:VAL:O	1:A:209:LEU:HG	0.53	2.03	13	7
1:A:251:ALA:HA	1:A:257:ALA:HB3	0.53	1.81	31	1
2:B:331:ILE:HA	2:B:334:LEU:HD12	0.53	1.80	43	1
2:B:444:ARG:O	2:B:447:CYS:HB3	0.52	2.04	55	1
1:A:183:GLU:HA	1:A:186:GLU:CG	0.52	2.35	56	1
2:B:388:LYS:O	2:B:392:LYS:HG3	0.52	2.04	28	4
2:B:406:GLU:HA	2:B:409:TYR:CD2	0.52	2.39	11	15
1:A:248:PRO:O	1:A:252:LEU:HG	0.52	2.04	27	6
1:A:292:ARG:NE	1:A:292:ARG:HA	0.52	2.18	23	1
1:A:258:PRO:HA	1:A:261:VAL:HG23	0.52	1.79	5	2
1:A:197:LYS:C	1:A:199:GLY:H	0.52	2.12	67	2
1:A:167:THR:O	1:A:170:PRO:HD2	0.52	2.05	52	6
2:B:389:SER:O	2:B:392:LYS:HB2	0.52	2.05	54	2
2:B:399:ASP:O	2:B:403:ARG:HB2	0.52	2.05	56	1
1:A:300:VAL:CB	2:B:336:LYS:HB3	0.52	2.31	35	1
1:A:279:ILE:HG21	1:A:299:THR:HG23	0.52	1.80	50	1
1:A:164:PHE:O	1:A:168:LEU:HB2	0.52	2.04	52	2
2:B:426:LEU:O	2:B:430:VAL:HG23	0.52	2.04	12	14

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:261:VAL:HB	1:A:294:ALA:HB1	0.52	1.80	8	1
1:A:202:VAL:CG2	1:A:239:SER:HB3	0.52	2.35	8	1
1:A:198:SER:HB3	1:A:239:SER:HA	0.52	1.81	13	1
1:A:283:LYS:NZ	1:A:283:LYS:HB3	0.52	2.17	49	2
1:A:209:LEU:HD13	1:A:261:VAL:HG22	0.52	1.80	47	1
2:B:401:MET:HE1	2:B:438:ILE:HD12	0.52	1.80	63	1
2:B:372:LEU:HD21	2:B:426:LEU:HB3	0.52	1.81	64	1
1:A:242:LYS:HD2	1:A:242:LYS:H	0.52	1.64	13	1
2:B:333:MET:O	2:B:337:GLU:HG2	0.52	2.05	51	1
1:A:267:ARG:HH21	2:B:333:MET:HE1	0.52	1.65	56	1
1:A:258:PRO:HA	1:A:261:VAL:CG2	0.52	2.34	5	1
1:A:304:MET:HG3	2:B:332:ASP:OD1	0.52	2.04	6	2
1:A:304:MET:SD	2:B:333:MET:HG2	0.52	2.45	61	3
1:A:301:LEU:HD23	1:A:304:MET:HE2	0.52	1.82	53	2
1:A:209:LEU:HD23	1:A:216:ARG:HG2	0.52	1.82	57	2
2:B:383:ILE:HG23	2:B:386:LEU:HD23	0.52	1.81	4	1
1:A:304:MET:HA	2:B:336:LYS:CE	0.52	2.35	21	1
1:A:202:VAL:HG13	1:A:243:LEU:HD12	0.52	1.80	53	1
1:A:259:GLN:CG	1:A:297:LYS:HE3	0.52	2.35	9	1
2:B:344:ILE:HG22	2:B:348:GLU:HG3	0.52	1.81	34	2
2:B:338:TYR:CD2	2:B:386:LEU:HB2	0.52	2.39	52	3
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
2:B:389:SER:HA	2:B:392:LYS:CE	0.51	2.33	54	9
1:A:165:GLU:HA	1:A:203:LEU:HD21	0.51	1.82	24	5
1:A:231:MET:HG3	1:A:235:ASP:HB2	0.51	1.82	57	8
1:A:241:ASP:O	1:A:245:LYS:HG2	0.51	2.05	8	6
1:A:172:ILE:HG21	1:A:204:ALA:HB2	0.51	1.83	30	1
1:A:168:LEU:HD21	1:A:200:VAL:HG22	0.51	1.82	34	1
2:B:434:PHE:CZ	2:B:441:LYS:HG2	0.51	2.40	54	3
1:A:223:LEU:HB3	1:A:273:ILE:CD1	0.51	2.36	48	1
1:A:292:ARG:HD2	1:A:295:LEU:HD12	0.51	1.81	1	1
1:A:207:LEU:C	1:A:209:LEU:H	0.51	2.13	4	2
1:A:259:GLN:HG2	1:A:297:LYS:HE3	0.51	1.81	9	1
2:B:355:GLU:O	2:B:357:PRO:HD3	0.51	2.05	40	3
1:A:169:THR:O	1:A:173:GLN:HG3	0.51	2.06	31	2
1:A:205:VAL:HG12	1:A:219:THR:HG21	0.51	1.82	42	1
2:B:410:ASN:O	2:B:413:PRO:HD2	0.51	2.06	27	12
1:A:251:ALA:CB	1:A:258:PRO:HD3	0.51	2.34	32	1
1:A:217:GLU:HG3	1:A:218:MET:N	0.51	2.21	34	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:242:LYS:O	1:A:245:LYS:HB2	0.51	2.06	36	2
1:A:191:LEU:O	1:A:193:LEU:HG	0.51	2.06	61	1
1:A:264:PHE:O	1:A:268:ALA:HB2	0.51	2.06	65	2
1:A:220:SER:HA	1:A:223:LEU:HG	0.51	1.81	66	2
1:A:175:TYR:HE2	1:A:222:LEU:HD22	0.51	1.66	66	1
2:B:335:LEU:HD13	2:B:366:GLU:HG2	0.51	1.82	33	2
1:A:299:THR:HA	1:A:302:LEU:HD12	0.51	1.83	32	2
1:A:202:VAL:HA	1:A:205:VAL:HG22	0.51	1.83	42	1
2:B:335:LEU:HD21	2:B:363:LEU:HG	0.50	1.83	37	3
2:B:381:LYS:HG3	2:B:382:MET:N	0.50	2.20	72	2
1:A:304:MET:HE2	2:B:336:LYS:HB2	0.50	1.81	22	3
2:B:367:ALA:HA	2:B:370:MET:HE2	0.50	1.82	19	2
1:A:244:LEU:O	1:A:247:LEU:HB2	0.50	2.06	73	3
2:B:338:TYR:CZ	2:B:386:LEU:HB2	0.50	2.41	3	1
1:A:183:GLU:HA	1:A:186:GLU:HG3	0.50	1.82	56	1
1:A:277:THR:HA	1:A:280:ASP:HB2	0.50	1.82	29	1
1:A:169:THR:HG22	1:A:207:LEU:HD21	0.50	1.83	56	1
2:B:434:PHE:HZ	2:B:441:LYS:HG2	0.50	1.66	49	3
1:A:256:ARG:HD2	2:B:349:HIS:HB2	0.50	1.82	36	1
1:A:200:VAL:N	1:A:201:PRO:HD2	0.50	2.21	61	3
2:B:368:ILE:HG23	2:B:429:PHE:CE2	0.50	2.41	54	2
2:B:430:VAL:HG11	2:B:447:CYS:SG	0.50	2.46	10	1
2:B:428:ARG:O	2:B:432:GLU:HB2	0.50	2.07	17	3
1:A:248:PRO:HB3	1:A:290:GLN:HG3	0.50	1.84	38	4
1:A: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:199:GLY:O	1:A:203:LEU:HB2	0.50	2.06	42	1
1:A:226:LEU:O	1:A:231:MET:HB3	0.50	2.07	57	1
1:A:222:LEU:O	1:A:226:LEU:HG	0.49	2.06	49	10
1:A:300:VAL:HG13	2:B:340:LEU:HB3	0.49	1.83	15	1
1:A:247:LEU:N	1:A:248:PRO:CD	0.49	2.74	17	3
1:A:220:SER:HA	1:A:223:LEU:HD12	0.49	1.83	45	1
1:A:225:ASP:C	1:A:227:CYS:H	0.49	2.14	68	1
1:A:299:THR:HA	1:A:302:LEU:HB3	0.49	1.83	24	1
1:A:176:PHE:HB3	1:A:215:HIS:CD2	0.49	2.42	56	2
1:A:173:GLN:O	1:A:177:GLU:HG2	0.49	2.07	65	2
1:A:185:ALA:O	1:A:189:ARG:HG3	0.49	2.08	41	2
1:A:178:HIS:CG	1:A:179:GLY:H	0.49	2.26	52	1
2:B:365:TYR:HB2	2:B:408:ILE:HD11	0.49	1.85	54	1
2:B:348:GLU:HG2	2:B:390:LEU:HD22	0.49	1.85	11	1
1:A:221:LYS:O	1:A:225:ASP:HB2	0.49	2.07	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:171:ILE:HG23	1:A:187:MET:SD	0.49	2.47	69	2
2:B:360:HIS:HB2	2:B:400:GLN:CG	0.49	2.36	65	2
1:A:300:VAL:HA	2:B:340:LEU:HD22	0.49	1.83	21	1
1:A:269:VAL:HB	1:A:302:LEU:HD11	0.49	1.85	30	1
2:B:384:LEU:HG	2:B:388:LYS:HE2	0.49	1.84	39	1
1:A:266:ALA:HB2	1:A:298:ALA:HB1	0.49	1.84	51	1
1:A:304:MET:HE2	2:B:333:MET:HA	0.49	1.83	27	1
2:B:343:ASP:HB2	2:B:346:GLU:HG2	0.49	1.82	55	1
2:B:346:GLU:HA	2:B:346:GLU:OE1	0.49	2.07	55	3
2:B:377:GLU:HA	2:B:380:PHE:HB2	0.49	1.84	6	2
2:B:423:TYR:HA	2:B:426:LEU:HB3	0.49	1.84	21	1
1:A:178:HIS:CE1	1:A:180:ASP:HB2	0.49	2.43	32	1
2:B:344:ILE:HA	2:B:347:ALA:HB3	0.49	1.84	34	1
1:A:266:ALA:HB2	1:A:298:ALA:HA	0.49	1.83	45	1
2:B:361:HIS:CD2	2:B:403:ARG:HB3	0.49	2.43	61	1
2:B:368:ILE:HG21	2:B:408:ILE:HG13	0.49	1.84	66	4
1:A:172:ILE:HD12	1:A:207:LEU:HD12	0.49	1.85	25	1
1:A:253:ASP:O	1:A:255:PRO:HD3	0.49	2.08	66	1
1:A:184:VAL:O	1:A:188:LEU:HG	0.48	2.08	27	8
1:A:237:GLU:HG2	1:A:274:LEU:HD12	0.48	1.84	27	2
2:B:346:GLU:O	2:B:350:CYS:SG	0.48	2.71	44	1
2:B:360:HIS:HB2	2:B:400:GLN:HG2	0.48	1.85	59	1
1:A:175:TYR:OH	1:A:222:LEU:HB2	0.48	2.08	14	2
1:A:184:VAL:O	1:A:188:LEU:HB2	0.48	2.07	41	1
1:A:240:PHE:O	1:A:244:LEU:HG	0.48	2.08	4	2
1:A:214:SER:O	1:A:218:MET:HG2	0.48	2.09	8	1
1:A:240:PHE:HE2	1:A:265:ILE:HA	0.48	1.68	18	1
1:A:240:PHE:HE2	1:A:265:ILE:HG12	0.48	1.68	54	1
2:B:366:GLU:HA	2:B:369:VAL:CG2	0.48	2.38	35	1
1:A:223:LEU:HB3	1:A:273:ILE:HD13	0.48	1.83	48	1
1:A:286:VAL:HB	1:A:292:ARG:NH1	0.48	2.22	73	1
1:A:201:PRO:O	1:A:205:VAL:HB	0.48	2.08	4	2
2:B:338:TYR:HE1	2:B:344:ILE:HG12	0.48	1.68	12	3
1:A:168:LEU:HD11	1:A:200:VAL:HG13	0.48	1.86	25	2
2:B:334:LEU:HD11	2:B:350:CYS:HB3	0.48	1.84	72	1
1:A:297:LYS:HZ3	2:B:346:GLU:CD	0.48	2.17	8	2
2:B:419:VAL:HG12	2:B:421:HIS:CD2	0.48	2.44	17	1
2:B:424:SER:O	2:B:428:ARG:HB2	0.48	2.09	57	4
2:B:377:GLU:O	2:B:381:LYS:HG2	0.48	2.09	8	3
1:A:257:ALA:N	1:A:258:PRO:HD2	0.48	2.23	4	14
2:B:380:PHE:O	2:B:384:LEU:HB2	0.48	2.09	47	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:244:LEU:O	1:A:248:PRO:HD3	0.48	2.09	17	1
2:B:419:VAL:HG12	2:B:421:HIS:HD2	0.48	1.67	17	1
1:A:304:MET:HG3	2:B:332:ASP:OD2	0.48	2.09	34	1
1:A:220:SER:O	1:A:223:LEU:HB2	0.48	2.09	66	2
1:A:286:VAL:HB	1:A:292:ARG:HG3	0.48	1.86	8	1
1:A:303:SER:HB3	2:B:336:LYS:HD2	0.48	1.86	27	1
1:A:304:MET:CE	2:B:333:MET:HA	0.48	2.39	31	1
2:B:367:ALA:O	2:B:371:VAL:HG23	0.48	2.07	24	10
2:B:368:ILE:HG23	2:B:429:PHE:HE2	0.48	1.69	54	2
1:A:300:VAL:HG13	2:B:340:LEU:CB	0.48	2.39	59	2
2:B:434:PHE:CE1	2:B:441:LYS:HA	0.48	2.43	7	8
1:A:168:LEU:HD12	1:A:171:ILE:HD12	0.48	1.86	17	1
1:A:206:SER:HA	1:A:209:LEU:HD12	0.48	1.86	24	1
2:B:381:LYS:O	2:B:385:ASP:HB2	0.48	2.09	43	3
2:B:442:GLN:O	2:B:446:LEU:HG	0.48	2.08	63	3
2:B:387:LEU:HD11	2:B:433:CYS:SG	0.48	2.49	67	1
1:A:172:ILE:CD1	1:A:207:LEU:HD12	0.47	2.39	25	1
1:A:268:ALA:HB1	1:A:273:ILE:HG13	0.47	1.86	29	1
2:B:343:ASP:HB3	2:B:346:GLU:HG3	0.47	1.84	36	2
2:B:351:LEU:HD23	2:B:390:LEU:HD22	0.47	1.85	35	1
1:A:268:ALA:HB1	1:A:274:LEU:HB2	0.47	1.85	59	2
1:A:181:THR:CG2	1:A:222:LEU:HA	0.47	2.39	60	3
2:B:428:ARG:O	2:B:432:GLU:N	0.47	2.47	27	3
1:A:206:SER:HA	1:A:209:LEU:HG	0.47	1.86	45	1
2:B:350:CYS:HA	2:B:353:GLU:HG3	0.47	1.85	70	1
1:A:205:VAL:O	1:A:219:THR:HB	0.47	2.09	72	1
2:B:412:ILE:HG23	2:B:416:ASN:ND2	0.47	2.24	66	2
2:B:393:SER:O	2:B:394:SER:CB	0.47	2.62	21	2
2:B:383:ILE:O	2:B:386:LEU:HB3	0.47	2.09	28	2
1:A:300:VAL:HG21	2:B:341:SER:OG	0.47	2.09	57	3
1:A:248:PRO:HG3	1:A:288:CYS:SG	0.47	2.49	3	1
2:B:419:VAL:N	2:B:420:PRO:HD3	0.47	2.25	26	2
1:A:304:MET:HG3	2:B:336:LYS:HE2	0.47	1.86	56	1
1:A:256:ARG:NH1	2:B:349:HIS:HB3	0.47	2.24	61	1
1:A:181:THR:HG21	1:A:225:ASP:CB	0.47	2.39	46	2
2:B:391:TRP:HH2	2:B:398:ILE:HA	0.47	1.70	42	1
1:A:266:ALA:HB3	1:A:301:LEU:HD23	0.47	1.85	6	1
1:A:205:VAL:O	1:A:209:LEU:HB2	0.47	2.09	30	1
2:B:434:PHE:HA	2:B:439:ILE:CD1	0.47	2.33	70	3
1:A:176:PHE:HZ	1:A:219:THR:HG23	0.47	1.70	32	1
2:B:430:VAL:HG21	2:B:447:CYS:SG	0.47	2.50	66	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:300:VAL:HG21	2:B:341:SER:HA	0.47	1.86	51	1
1:A:158:PRO:HB2	1:A:161:GLU:HG2	0.47	1.86	54	1
2:B:379:ALA:O	2:B:383:ILE:HG13	0.47	2.10	58	1
1:A:277:THR:O	1:A:280:ASP:N	0.47	2.45	68	3
1:A:232:SER:O	1:A:235:ASP:HB2	0.47	2.10	2	1
1:A:259:GLN:HA	1:A:297:LYS:CD	0.47	2.40	9	1
1:A:179:GLY:HA3	1:A:218:MET:HE1	0.47	1.87	25	1
1:A:184:VAL:HG11	1:A:222:LEU:HD11	0.47	1.85	67	2
2:B:409:TYR:HA	2:B:412:ILE:CG1	0.47	2.40	57	1
1:A:304:MET:HG2	2:B:336:LYS:HB3	0.47	1.87	58	1
1:A:200:VAL:H	1:A:201:PRO:HD2	0.47	1.70	37	2
2:B:406:GLU:HG2	2:B:446:LEU:HD22	0.47	1.86	62	1
1:A:172:ILE:HD12	1:A:203:LEU:HD23	0.47	1.87	63	1
1:A:164:PHE:CE1	1:A:200:VAL:HG22	0.47	2.45	72	1
1:A:263:GLN:HG3	1:A:301:LEU:HG	0.47	1.84	72	1
1:A:304:MET:HG2	2:B:332:ASP:OD2	0.47	2.10	5	3
2:B:405:TYR:HE1	2:B:430:VAL:HG22	0.47	1.69	28	2
2:B:366:GLU:O	2:B:369:VAL:HB	0.46	2.10	72	1
2:B:402:LYS:HD2	2:B:443:LEU:HD13	0.46	1.88	20	1
1:A:185:ALA:CB	1:A:226:LEU:HD22	0.46	2.40	56	1
2:B:367:ALA:O	2:B:383:ILE:HG21	0.46	2.10	66	1
1:A:263:GLN:HA	1:A:301:LEU:HD22	0.46	1.87	4	1
1:A:269:VAL:HA	1:A:274:LEU:O	0.46	2.10	72	3
1:A:249:GLU:O	1:A:252:LEU:HB2	0.46	2.11	73	2
1:A:247:LEU:HD11	1:A:261:VAL:HG11	0.46	1.87	20	2
2:B:433:CYS:HB3	2:B:438:ILE:HD11	0.46	1.87	73	4
1:A:217:GLU:HG3	1:A:267:ARG:HH22	0.46	1.71	35	2
2:B:402:LYS:HG2	2:B:406:GLU:OE2	0.46	2.10	45	1
2:B:435:GLN:C	2:B:437:GLY:H	0.46	2.18	36	5
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
1:A:208:ALA:C	1:A:210:GLU:H	0.46	2.19	64	2
2:B:345:SER:O	2:B:349:HIS:HB2	0.46	2.10	42	2
1:A:256:ARG:HA	1:A:259:GLN:NE2	0.46	2.25	46	1
1:A:201:PRO:O	1:A:205:VAL:HG23	0.46	2.10	12	7
1:A:161:GLU:O	1:A:165:GLU:HG3	0.46	2.10	14	4
1:A:162:ARG:N	1:A:162:ARG:HD2	0.46	2.25	34	1
1:A:300:VAL:HG22	1:A:304:MET:HE2	0.46	1.86	37	1
1:A:257:ALA:HB3	1:A:258:PRO:HD3	0.46	1.88	54	2
2:B:444:ARG:O	2:B:447:CYS:HB2	0.46	2.11	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:168:LEU:HA	1:A:171:ILE:HD12	0.46	1.88	28	1
1:A:240:PHE:CE1	1:A:265:ILE:HG12	0.46	2.44	31	1
2:B:380:PHE:CE1	2:B:429:PHE:HB3	0.46	2.45	31	1
1:A:222:LEU:O	1:A:226:LEU:HB2	0.46	2.10	34	1
1:A:179:GLY:HA2	1:A:218:MET:HE1	0.46	1.88	43	1
1:A:240:PHE:HE2	1:A:265:ILE:HG23	0.46	1.71	61	1
1:A:203:LEU:O	1:A:207:LEU:N	0.46	2.49	72	2
1:A:236:VAL:HG11	1:A:273:ILE:O	0.46	2.11	13	2
2:B:402:LYS:O	2:B:406:GLU:HG3	0.46	2.10	22	1
2:B:389:SER:HA	2:B:392:LYS:CD	0.46	2.40	8	1
2:B:335:LEU:CD1	2:B:366:GLU:HB3	0.46	2.41	31	2
1:A:263:GLN:HE21	1:A:301:LEU:HD22	0.46	1.70	36	1
2:B:338:TYR:CZ	2:B:344:ILE:HG23	0.46	2.46	54	1
1:A:268:ALA:HA	1:A:271:ASP:OD1	0.46	2.11	29	1
2:B:368:ILE:O	2:B:371:VAL:HG12	0.46	2.11	48	3
1:A:172:ILE:HG13	1:A:173:GLN:N	0.46	2.26	64	1
1:A:240:PHE:O	1:A:243:LEU:HB2	0.45	2.10	13	1
1:A:300:VAL:CG2	2:B:340:LEU:HB3	0.45	2.41	46	2
2:B:398:ILE:O	2:B:402:LYS:HG3	0.45	2.10	33	1
1:A:276:ASN:C	1:A:278:TYR:H	0.45	2.19	73	2
1:A:193:LEU:HD22	1:A:196:MET:HB3	0.45	1.88	58	1
1:A:304:MET:HE1	2:B:333:MET:HG3	0.45	1.87	29	2
2:B:351:LEU:HD21	2:B:363:LEU:HD13	0.45	1.87	20	1
1:A:209:LEU:HD21	1:A:264:PHE:HE2	0.45	1.72	53	1
2:B:384:LEU:HB2	2:B:429:PHE:CE1	0.45	2.45	66	1
1:A:265:ILE:HD13	1:A:295:LEU:HD23	0.45	1.87	8	1
1:A:304:MET:SD	2:B:333:MET:HG3	0.45	2.51	41	2
1:A:249:GLU:HA	1:A:252:LEU:HG	0.45	1.88	65	1
1:A:225:ASP:C	1:A:227:CYS:N	0.45	2.74	68	1
1:A:282:TYR:HA	1:A:285:THR:OG1	0.45	2.10	57	4
2:B:333:MET:O	2:B:337:GLU:HG3	0.45	2.11	29	1
2:B:424:SER:O	2:B:428:ARG:HG2	0.45	2.12	36	1
1:A:300:VAL:HG11	2:B:337:GLU:CA	0.45	2.38	48	1
2:B:348:GLU:O	2:B:352:LYS:HD2	0.45	2.12	8	1
1:A:300:VAL:CG1	2:B:340:LEU:HB2	0.45	2.42	23	4
2:B:371:VAL:HG11	2:B:380:PHE:HD1	0.45	1.70	29	1
2:B:434:PHE:HD1	2:B:439:ILE:HD11	0.45	1.71	30	1
2:B:429:PHE:O	2:B:432:GLU:HB3	0.45	2.11	57	1
1:A:249:GLU:O	1:A:251:ALA:N	0.45	2.50	72	1
2:B:334:LEU:HD21	2:B:351:LEU:HB2	0.45	1.88	2	1
2:B:338:TYR:CD2	2:B:386:LEU:HD13	0.45	2.47	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:201:PRO:HG3	1:A:231:MET:SD	0.45	2.52	32	2
1:A:266:ALA:HA	1:A:269:VAL:HG23	0.45	1.87	8	1
1:A:268:ALA:CB	1:A:273:ILE:HB	0.45	2.42	13	1
1:A:169:THR:N	1:A:170:PRO:HD2	0.45	2.27	63	4
2:B:338:TYR:O	2:B:342:GLY:HA2	0.45	2.11	69	2
2:B:382:MET:O	2:B:386:LEU:HB2	0.45	2.11	68	1
1:A:187:MET:O	1:A:191:LEU:HG	0.45	2.12	8	2
2:B:338:TYR:O	2:B:382:MET:HE3	0.45	2.11	18	1
1:A:171:ILE:HG12	1:A:187:MET:SD	0.45	2.52	25	1
1:A:240:PHE:HB3	1:A:278:TYR:OH	0.45	2.12	35	1
2:B:368:ILE:CD1	2:B:408:ILE:HG13	0.45	2.40	61	2
1:A:258:PRO:HB2	1:A:293:ALA:HB1	0.45	1.87	66	1
1:A:176:PHE:CZ	1:A:208:ALA:HB2	0.45	2.46	17	2
1:A:296:ASP:O	1:A:300:VAL:HG23	0.45	2.10	70	3
1:A:304:MET:HG2	2:B:336:LYS:HG3	0.45	1.89	22	1
1:A:304:MET:HE1	2:B:333:MET:HA	0.45	1.89	28	1
1:A:217:GLU:HA	1:A:267:ARG:NH2	0.45	2.26	49	1
2:B:384:LEU:HB2	2:B:429:PHE:HE1	0.45	1.71	66	1
2:B:334:LEU:CD2	2:B:347:ALA:HA	0.45	2.42	11	2
2:B:405:TYR:CE1	2:B:430:VAL:HG22	0.45	2.47	40	2
1:A:208:ALA:HA	1:A:215:HIS:ND1	0.45	2.27	39	1
1:A:198:SER:C	1:A:200:VAL:H	0.45	2.19	64	1
2:B:442:GLN:HB3	2:B:446:LEU:HD12	0.45	1.88	64	1
1:A:244:LEU:HA	1:A:247:LEU:HD13	0.45	1.89	59	4
1:A:300:VAL:HB	2:B:340:LEU:CB	0.45	2.41	21	1
2:B:331:ILE:O	2:B:335:LEU:HG	0.45	2.12	29	1
2:B:354:LEU:O	2:B:355:GLU:HB2	0.45	2.11	49	1
2:B:334:LEU:HD21	2:B:350:CYS:CB	0.44	2.42	50	1
1:A:289:VAL:HA	1:A:292:ARG:HB2	0.44	1.89	21	2
2:B:367:ALA:HB1	2:B:383:ILE:HD12	0.44	1.87	36	1
2:B:348:GLU:O	2:B:352:LYS:HG2	0.44	2.12	61	1
2:B:398:ILE:O	2:B:402:LYS:HB2	0.44	2.11	71	1
2:B:330:GLU:HG3	2:B:331:ILE:N	0.44	2.27	18	1
2:B:352:LYS:C	2:B:354:LEU:H	0.44	2.19	72	2
1:A:205:VAL:HG22	1:A:219:THR:CG2	0.44	2.42	54	1
2:B:338:TYR:CE2	2:B:344:ILE:HA	0.44	2.47	30	1
1:A:267:ARG:O	1:A:271:ASP:HB2	0.44	2.12	73	2
1:A:181:THR:HG22	1:A:222:LEU:HD12	0.44	1.89	71	3
1:A:193:LEU:O	1:A:197:LYS:HB2	0.44	2.12	21	1
1:A:240:PHE:HA	1:A:243:LEU:HB3	0.44	1.88	52	1
2:B:402:LYS:HE3	2:B:442:GLN:OE1	0.44	2.12	53	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:361:HIS:HB2	2:B:400:GLN:HA	0.44	1.88	73	1
2:B:338:TYR:CD1	2:B:382:MET:HB3	0.44	2.47	45	1
1:A:274:LEU:HG	1:A:275:CYS:N	0.44	2.28	62	2
1:A:169:THR:H	1:A:170:PRO:HD2	0.44	1.73	66	1
2:B:361:HIS:HB3	2:B:400:GLN:CB	0.44	2.41	72	1
1:A:202:VAL:HG23	1:A:239:SER:HB3	0.44	1.90	8	3
1:A:257:ALA:HA	1:A:260:LEU:HD12	0.44	1.90	44	2
2:B:406:GLU:HA	2:B:409:TYR:CE2	0.44	2.48	59	4
2:B:424:SER:O	2:B:428:ARG:HB3	0.44	2.13	9	2
1:A:174:GLU:C	1:A:176:PHE:H	0.44	2.21	49	1
2:B:402:LYS:HG2	2:B:443:LEU:HD22	0.44	1.88	66	1
1:A:304:MET:HB3	2:B:333:MET:HE3	0.44	1.87	72	1
1:A:300:VAL:HG13	1:A:304:MET:HE2	0.44	1.90	2	1
2:B:331:ILE:HD13	2:B:362:GLU:HB3	0.44	1.89	14	1
1:A:227:CYS:SG	1:A:273:ILE:HG22	0.44	2.53	27	2
2:B:379:ALA:O	2:B:383:ILE:HG12	0.44	2.13	33	3
2:B:352:LYS:HD2	2:B:352:LYS:N	0.44	2.27	29	1
2:B:371:VAL:HB	2:B:383:ILE:HG21	0.44	1.89	69	2
2:B:347:ALA:O	2:B:351:LEU:HB2	0.44	2.13	56	1
2:B:384:LEU:O	2:B:388:LYS:HE3	0.44	2.13	59	1
1:A:168:LEU:HD21	1:A:200:VAL:HG13	0.44	1.88	63	1
2:B:399:ASP:HA	2:B:402:LYS:HG3	0.44	1.90	73	1
1:A:244:LEU:HD11	1:A:295:LEU:HD21	0.43	1.89	41	2
1:A:259:GLN:HB3	2:B:346:GLU:OE1	0.43	2.13	50	1
1:A:247:LEU:HD23	1:A:290:GLN:HB3	0.43	1.88	53	1
1:A:300:VAL:HG22	2:B:340:LEU:HB2	0.43	1.90	1	1
1:A:304:MET:HA	2:B:336:LYS:NZ	0.43	2.28	2	1
2:B:373:GLU:HA	2:B:373:GLU:OE1	0.43	2.13	13	1
2:B:338:TYR:OH	2:B:385:ASP:HB3	0.43	2.14	30	1
1:A:203:LEU:O	1:A:207:LEU:HG	0.43	2.13	41	2
1:A:174:GLU:HA	1:A:177:GLU:HG2	0.43	1.89	45	1
1:A:269:VAL:HG11	1:A:276:ASN:HB3	0.43	1.90	61	1
1:A:216:ARG:NH1	1:A:260:LEU:HD13	0.43	2.28	73	1
2:B:348:GLU:O	2:B:352:LYS:HG3	0.43	2.13	28	1
1:A:256:ARG:HG2	1:A:260:LEU:HG	0.43	1.90	42	1
1:A:210:GLU:H	1:A:210:GLU:CD	0.43	2.21	46	1
2:B:391:TRP:CZ2	2:B:398:ILE:HB	0.43	2.42	60	1
1:A:280:ASP:O	1:A:283:LYS:HB2	0.43	2.14	9	2
2:B:391:TRP:HA	2:B:396:ILE:HB	0.43	1.89	21	1
1:A:172:ILE:HG22	1:A:176:PHE:CZ	0.43	2.49	46	2
1:A:224:SER:HA	1:A:273:ILE:HG21	0.43	1.89	22	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:402:LYS:O	2:B:406:GLU:HB2	0.43	2.12	27	2
1:A:240:PHE:CZ	1:A:274:LEU:HD22	0.43	2.48	47	1
1:A:263:GLN:HB2	1:A:301:LEU:HD13	0.43	1.90	51	1
2:B:334:LEU:HD22	2:B:350:CYS:SG	0.43	2.53	57	1
1:A:175:TYR:C	1:A:177:GLU:H	0.43	2.21	64	2
1:A:178:HIS:O	1:A:180:ASP:N	0.43	2.51	22	1
2:B:405:TYR:O	2:B:408:ILE:HB	0.43	2.12	22	1
2:B:352:LYS:HD2	2:B:352:LYS:H	0.43	1.73	29	1
1:A:158:PRO:HB3	1:A:196:MET:HG2	0.43	1.90	62	1
1:A:300:VAL:HG13	2:B:336:LYS:HB3	0.43	1.89	54	1
2:B:351:LEU:HD23	2:B:395:THR:HG21	0.43	1.91	61	1
1:A:232:SER:H	1:A:235:ASP:HB3	0.43	1.74	71	1
1:A:204:ALA:HA	1:A:207:LEU:HD12	0.43	1.89	4	1
2:B:358:HIS:HA	2:B:400:GLN:HE22	0.43	1.74	21	1
1:A:256:ARG:HH21	2:B:346:GLU:CD	0.43	2.22	24	1
2:B:364:VAL:HG23	2:B:365:TYR:H	0.43	1.74	50	1
2:B:412:ILE:N	2:B:413:PRO:HD2	0.43	2.28	72	1
1:A:181:THR:HG22	1:A:222:LEU:HA	0.43	1.89	7	3
1:A:300:VAL:HG11	2:B:337:GLU:HG3	0.43	1.91	4	1
2:B:343:ASP:HB3	2:B:346:GLU:CG	0.43	2.42	13	1
2:B:331:ILE:HD13	2:B:362:GLU:HB2	0.43	1.90	26	1
1:A:200:VAL:HB	1:A:201:PRO:CD	0.43	2.44	34	8
1:A:292:ARG:HD2	1:A:292:ARG:HA	0.43	1.63	20	1
1:A:247:LEU:HA	1:A:250:LEU:HB2	0.43	1.89	21	1
2:B:342:GLY:HA2	2:B:382:MET:HE2	0.43	1.89	29	1
2:B:431:GLU:HG3	2:B:432:GLU:N	0.43	2.29	55	3
2:B:440:SER:OG	2:B:443:LEU:HB2	0.43	2.14	42	1
2:B:355:GLU:O	2:B:356:VAL:C	0.43	2.61	50	1
2:B:331:ILE:CG2	2:B:363:LEU:HA	0.43	2.44	58	1
1:A:277:THR:O	1:A:280:ASP:HB2	0.43	2.14	59	1
2:B:380:PHE:O	2:B:384:LEU:HB3	0.43	2.13	61	1
2:B:360:HIS:CB	2:B:400:GLN:HG3	0.43	2.38	65	1
1:A:197:LYS:O	1:A:200:VAL:HG23	0.43	2.13	38	1
2:B:401:MET:HE3	2:B:405:TYR:HE2	0.43	1.74	44	1
1:A:258:PRO:HG2	1:A:259:GLN:OE1	0.43	2.13	46	1
2:B:371:VAL:O	2:B:374:SER:HB2	0.43	2.14	60	1
2:B:361:HIS:HB2	2:B:400:GLN:O	0.42	2.14	23	1
2:B:336:LYS:HD3	2:B:370:MET:HE2	0.42	1.91	33	1
1:A:226:LEU:O	1:A:227:CYS:C	0.42	2.62	56	1
2:B:351:LEU:HD11	2:B:363:LEU:HD11	0.42	1.90	56	1
1:A:195:GLU:HA	1:A:238:LYS:NZ	0.42	2.29	70	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:297:LYS:HZ1	2:B:346:GLU:CD	0.42	2.23	9	1
1:A:251:ALA:CB	1:A:258:PRO:HG3	0.42	2.44	70	2
2:B:364:VAL:O	2:B:368:ILE:HG13	0.42	2.14	63	2
2:B:336:LYS:O	2:B:339:LEU:HB3	0.42	2.14	36	1
1:A:286:VAL:CG1	1:A:291:ALA:HB3	0.42	2.43	38	1
1:A:292:ARG:O	1:A:296:ASP:HB2	0.42	2.15	66	2
1:A:300:VAL:HG21	2:B:341:SER:CA	0.42	2.44	51	1
2:B:348:GLU:HG2	2:B:390:LEU:HD23	0.42	1.90	54	1
2:B:368:ILE:O	2:B:371:VAL:HB	0.42	2.13	4	1
1:A:216:ARG:HB3	1:A:264:PHE:CE1	0.42	2.49	15	1
1:A:181:THR:HG21	1:A:225:ASP:HB3	0.42	1.90	28	1
2:B:380:PHE:HE1	2:B:429:PHE:HB3	0.42	1.74	31	1
2:B:335:LEU:HD11	2:B:366:GLU:HB3	0.42	1.90	65	1
1:A:158:PRO:HA	1:A:196:MET:SD	0.42	2.53	66	1
1:A:283:LYS:O	1:A:283:LYS:HG2	0.42	2.13	7	1
2:B:390:LEU:HD12	2:B:396:ILE:HD11	0.42	1.90	14	1
2:B:416:ASN:HB3	2:B:420:PRO:HB3	0.42	1.91	35	1
1:A:226:LEU:HB3	1:A:231:MET:HE2	0.42	1.91	57	1
1:A:244:LEU:HB3	1:A:291:ALA:CB	0.42	2.45	13	1
1:A:301:LEU:HD22	2:B:333:MET:HE1	0.42	1.92	23	1
2:B:443:LEU:HD12	2:B:446:LEU:HD12	0.42	1.91	26	1
1:A:279:ILE:HG23	1:A:295:LEU:HD22	0.42	1.90	29	1
1:A:300:VAL:HG23	2:B:340:LEU:HD12	0.42	1.89	2	1
2:B:397:THR:OG1	2:B:400:GLN:HG2	0.42	2.14	10	1
2:B:346:GLU:OE1	2:B:346:GLU:HA	0.42	2.15	14	1
1:A:216:ARG:HB3	1:A:264:PHE:CZ	0.42	2.44	18	1
2:B:344:ILE:O	2:B:348:GLU:HB2	0.42	2.15	22	2
1:A:236:VAL:HG21	1:A:273:ILE:HG21	0.42	1.90	66	1
2:B:424:SER:O	2:B:428:ARG:HD3	0.42	2.15	70	1
1:A:277:THR:O	1:A:278:TYR:C	0.42	2.63	71	1
2:B:348:GLU:O	2:B:352:LYS:HD3	0.42	2.14	23	1
2:B:351:LEU:HD22	2:B:390:LEU:HD13	0.42	1.91	27	1
2:B:354:LEU:HB3	2:B:355:GLU:H	0.42	1.57	64	2
1:A:172:ILE:HD13	1:A:204:ALA:HB2	0.42	1.92	30	1
2:B:345:SER:HA	2:B:348:GLU:CD	0.42	2.40	59	1
1:A:251:ALA:O	1:A:253:ASP:N	0.42	2.53	42	1
1:A:300:VAL:HA	2:B:340:LEU:HD13	0.42	1.92	64	2
2:B:348:GLU:HB3	2:B:352:LYS:HE2	0.42	1.90	54	1
1:A:297:LYS:HE3	2:B:346:GLU:OE2	0.42	2.15	55	1
2:B:360:HIS:O	2:B:363:LEU:HB3	0.42	2.15	61	1
1:A:189:ARG:C	1:A:191:LEU:H	0.42	2.23	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:206:SER:O	1:A:209:LEU:HB2	0.42	2.15	15	1
2:B:409:TYR:CZ	2:B:447:CYS:HB3	0.42	2.49	52	1
2:B:338:TYR:CD1	2:B:386:LEU:HD13	0.42	2.50	8	1
1:A:178:HIS:H	1:A:178:HIS:CD2	0.41	2.32	52	1
1:A:212:LYS:O	1:A:216:ARG:HG3	0.41	2.15	70	1
1:A:188:LEU:HA	1:A:191:LEU:HD12	0.41	1.91	71	1
2:B:412:ILE:HD13	2:B:412:ILE:HA	0.41	1.81	21	1
2:B:339:LEU:HB2	2:B:383:ILE:HD11	0.41	1.91	56	1
1:A:180:ASP:HB3	1:A:183:GLU:HB2	0.41	1.91	3	1
1:A:206:SER:HA	1:A:209:LEU:HB2	0.41	1.91	38	1
2:B:388:LYS:HG3	2:B:438:ILE:HD13	0.41	1.91	48	1
1:A:216:ARG:HD3	1:A:260:LEU:HD22	0.41	1.92	56	1
1:A:259:GLN:NE2	2:B:346:GLU:HB3	0.41	2.30	73	1
1:A:164:PHE:CD2	1:A:196:MET:HE3	0.41	2.50	25	1
2:B:412:ILE:O	2:B:416:ASN:HB2	0.41	2.16	25	1
2:B:431:GLU:HA	2:B:434:PHE:HB3	0.41	1.93	52	1
1:A:267:ARG:NH2	2:B:333:MET:HE1	0.41	2.29	56	1
1:A:213:ALA:HA	1:A:216:ARG:CZ	0.41	2.46	64	1
1:A:170:PRO:O	1:A:174:GLU:HG2	0.41	2.14	70	1
2:B:338:TYR:O	2:B:341:SER:O	0.41	2.37	73	1
1:A:254:THR:HG22	1:A:256:ARG:H	0.41	1.76	8	1
1:A:247:LEU:HD21	1:A:258:PRO:CA	0.41	2.42	13	1
2:B:438:ILE:HG13	2:B:439:ILE:N	0.41	2.30	41	1
2:B:351:LEU:HD13	2:B:363:LEU:HD13	0.41	1.93	55	1
1:A:247:LEU:HA	1:A:250:LEU:HD12	0.41	1.91	59	1
2:B:356:VAL:HB	2:B:359:PHE:HB3	0.41	1.90	61	1
1:A:215:HIS:HD2	1:A:218:MET:SD	0.41	2.38	13	1
2:B:351:LEU:HD22	2:B:390:LEU:HD22	0.41	1.93	31	2
1:A:258:PRO:O	1:A:261:VAL:HB	0.41	2.16	23	1
1:A:181:THR:HG21	1:A:222:LEU:HA	0.41	1.93	31	1
1:A:259:GLN:HG2	2:B:346:GLU:CG	0.41	2.44	40	1
2:B:438:ILE:HG13	2:B:439:ILE:HG12	0.41	1.92	50	1
1:A:176:PHE:CE1	1:A:219:THR:HA	0.41	2.50	66	1
2:B:365:TYR:CE1	2:B:407:ARG:HG2	0.41	2.50	17	1
1:A:239:SER:O	1:A:243:LEU:HB2	0.41	2.15	70	2
2:B:367:ALA:HA	2:B:370:MET:HB2	0.41	1.92	44	1
1:A:219:THR:HB	1:A:264:PHE:HE1	0.41	1.74	56	2
1:A:213:ALA:HA	1:A:216:ARG:NH1	0.41	2.30	57	1
2:B:388:LYS:O	2:B:391:TRP:N	0.41	2.37	68	1
1:A:188:LEU:HD23	1:A:191:LEU:HD12	0.41	1.93	4	1
1:A:161:GLU:H	1:A:161:GLU:CD	0.41	2.24	30	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:297:LYS:NZ	2:B:337:GLU:OE1	0.41	2.52	57	1
2:B:409:TYR:CE1	2:B:447:CYS:HB3	0.41	2.51	57	1
1:A:168:LEU:HG	1:A:200:VAL:HG22	0.41	1.93	66	1
1:A:175:TYR:O	1:A:177:GLU:N	0.41	2.54	66	1
1:A:170:PRO:O	1:A:174:GLU:HB2	0.41	2.16	67	1
1:A:161:GLU:O	1:A:165:GLU:HB2	0.41	2.16	68	1
1:A:222:LEU:O	1:A:223:LEU:C	0.41	2.64	72	1
1:A:237:GLU:HG3	1:A:274:LEU:CD1	0.41	2.46	28	1
1:A:300:VAL:HG11	2:B:336:LYS:O	0.41	2.16	35	1
1:A:253:ASP:O	1:A:254:THR:CB	0.41	2.68	72	1
2:B:387:LEU:HD13	2:B:401:MET:HE1	0.40	1.92	3	1
1:A:304:MET:HE3	2:B:333:MET:HA	0.40	1.93	34	1
2:B:402:LYS:HE3	2:B:443:LEU:HD13	0.40	1.91	37	1
2:B:397:THR:O	2:B:400:GLN:HB2	0.40	2.16	42	1
1:A:248:PRO:O	1:A:252:LEU:HD12	0.40	2.16	53	1
2:B:344:ILE:H	2:B:344:ILE:HD12	0.40	1.76	10	1
2:B:434:PHE:CD1	2:B:439:ILE:HD11	0.40	2.51	30	1
1:A:246:ASP:C	1:A:248:PRO:HD2	0.40	2.41	42	1
1:A:297:LYS:HE3	1:A:301:LEU:HD21	0.40	1.93	44	1
1:A:178:HIS:O	1:A:179:GLY:C	0.40	2.64	71	1
2:B:334:LEU:HD11	2:B:350:CYS:HB2	0.40	1.91	17	1
2:B:354:LEU:HD22	2:B:354:LEU:HA	0.40	1.80	18	1
1:A:304:MET:HE1	2:B:337:GLU:HB2	0.40	1.93	19	1
1:A:169:THR:HB	1:A:170:PRO:CD	0.40	2.46	21	1
1:A:216:ARG:NH1	1:A:260:LEU:HD12	0.40	2.31	52	1
2:B:361:HIS:CE1	2:B:404:GLY:HA2	0.40	2.51	59	1
2:B:396:ILE:HG23	2:B:400:GLN:HB3	0.40	1.94	65	1
1:A:205:VAL:HG11	1:A:243:LEU:HD21	0.40	1.92	43	1
1:A:304:MET:HB3	2:B:333:MET:SD	0.40	2.56	21	1
1:A:167:THR:C	1:A:169:THR:H	0.40	2.25	25	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%)	12	60
2	B	119/131 (91%)	105±5 (88±4%)	13±4 (11±3%)	2±2 (1±1%)	12	60
All	All	19564/21462 (91%)	17506 (89%)	1805 (9%)	253 (1%)	12	60

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

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

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Mol	Chain	Res	Type	Models (Total)
1	A	201	PRO	2
1	A	305	SER	2
1	A	209	LEU	2
2	B	364	VAL	2
1	A	254	THR	2
1	A	227	CYS	2
1	A	247	LEU	2
1	A	255	PRO	2
1	A	199	GLY	2
1	A	216	ARG	2
1	A	190	ASP	1
2	B	360	HIS	1
2	B	362	GLU	1
1	A	241	ASP	1
1	A	175	TYR	1
1	A	181	THR	1
1	A	229	THR	1
2	B	357	PRO	1
2	B	380	PHE	1
2	B	420	PRO	1
1	A	219	THR	1
1	A	222	LEU	1
2	B	437	GLY	1
1	A	200	VAL	1
1	A	252	LEU	1
2	B	403	ARG	1
2	B	386	LEU	1
2	B	375	THR	1
1	A	233	THR	1
2	B	374	SER	1
1	A	180	ASP	1
1	A	256	ARG	1
1	A	161	GLU	1
1	A	244	LEU	1
2	B	344	ILE	1
1	A	174	GLU	1
1	A	288	CYS	1
1	A	258	PRO	1
1	A	176	PHE	1
1	A	223	LEU	1
1	A	292	ARG	1
1	A	212	LYS	1

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Mol	Chain	Res	Type	Models (Total)
1	A	226	LEU	1
2	B	389	SER	1
2	B	402	LYS	1
1	A	250	LEU	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%)	108±4 (85±3%)	19±4 (15±3%)	5	42
2	B	112/121 (93%)	95±4 (85±3%)	17±4 (15±3%)	5	42
All	All	17447/18761 (93%)	14823 (85%)	2624 (15%)	5	42

All 199 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	70
1	A	277	THR	66
1	A	214	SER	64
1	A	195	GLU	62
1	A	233	THR	60
2	B	378	SER	55
2	B	440	SER	49
1	A	283	LYS	48
2	B	424	SER	48
1	A	234	THR	44
1	A	292	ARG	42
2	B	405	TYR	42
1	A	225	ASP	41
2	B	375	THR	41
2	B	397	THR	40
1	A	181	THR	40
2	B	400	GLN	39
1	A	196	MET	38
1	A	224	SER	36
1	A	220	SER	36

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Mol	Chain	Res	Type	Models (Total)
2	B	421	HIS	36
2	B	345	SER	34
2	B	387	LEU	33
2	B	422	SER	33
1	A	299	THR	33
1	A	271	ASP	32
2	B	395	THR	28
2	B	407	ARG	28
1	A	221	LYS	27
1	A	246	ASP	27
2	B	354	LEU	27
1	A	256	ARG	25
2	B	356	VAL	25
2	B	449	SER	25
2	B	344	ILE	25
1	A	249	GLU	24
2	B	423	TYR	23
1	A	219	THR	23
1	A	210	GLU	23
1	A	232	SER	22
2	B	346	GLU	22
2	B	361	HIS	22
1	A	168	LEU	22
2	B	414	ASP	22
2	B	358	HIS	21
2	B	427	GLU	21
1	A	303	SER	21
2	B	393	SER	20
2	B	399	ASP	20
1	A	190	ASP	20
1	A	254	THR	20
2	B	353	GLU	19
1	A	280	ASP	18
2	B	444	ARG	17
1	A	241	ASP	16
2	B	341	SER	16
1	A	273	ILE	16
2	B	330	GLU	16
1	A	229	THR	16
1	A	160	ASP	15
1	A	253	ASP	15
2	B	337	GLU	15

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Mol	Chain	Res	Type	Models (Total)
1	A	296	ASP	15
1	A	237	GLU	15
2	B	348	GLU	15
1	A	305	SER	15
2	B	442	GLN	14
1	A	215	HIS	14
1	A	169	THR	13
2	B	359	PHE	13
2	B	391	TRP	13
1	A	174	GLU	13
1	A	206	SER	12
2	B	411	GLU	12
2	B	402	LYS	12
2	B	349	HIS	12
2	B	338	TYR	11
2	B	412	ILE	11
2	B	373	GLU	11
2	B	340	LEU	11
1	A	198	SER	10
1	A	263	GLN	10
1	A	178	HIS	10
1	A	239	SER	10
1	A	247	LEU	10
2	B	384	LEU	9
2	B	377	GLU	9
2	B	392	LYS	9
2	B	416	ASN	9
2	B	388	LYS	9
2	B	385	ASP	9
1	A	300	VAL	8
2	B	360	HIS	8
1	A	275	CYS	8
1	A	259	GLN	8
1	A	222	LEU	7
2	B	333	MET	7
2	B	435	GLN	7
1	A	197	LYS	7
2	B	418	ASP	7
1	A	167	THR	7
2	B	394	SER	7
2	B	431	GLU	7
2	B	371	VAL	7

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Mol	Chain	Res	Type	Models (Total)
1	A	207	LEU	7
2	B	336	LYS	6
1	A	217	GLU	6
2	B	351	LEU	6
1	A	161	GLU	6
1	A	238	LYS	6
1	A	193	LEU	6
2	B	363	LEU	6
2	B	433	CYS	6
1	A	304	MET	6
1	A	182	ASN	5
2	B	366	GLU	5
1	A	192	ASN	5
1	A	267	ARG	5
2	B	352	LYS	5
1	A	250	LEU	5
2	B	425	VAL	5
1	A	209	LEU	5
1	A	216	ARG	5
2	B	334	LEU	4
2	B	428	ARG	4
2	B	362	GLU	4
2	B	439	ILE	4
2	B	445	ASP	4
1	A	297	LYS	4
2	B	417	LEU	4
2	B	350	CYS	4
2	B	426	LEU	4
1	A	226	LEU	4
2	B	446	LEU	4
2	B	355	GLU	4
2	B	364	VAL	4
1	A	183	GLU	3
1	A	186	GLU	3
2	B	390	LEU	3
1	A	240	PHE	3
1	A	184	VAL	3
2	B	386	LEU	3
1	A	301	LEU	3
2	B	429	PHE	3
1	A	235	ASP	3
1	A	177	GLU	3

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Mol	Chain	Res	Type	Models (Total)
1	A	252	LEU	3
1	A	289	VAL	3
2	B	370	MET	3
1	A	281	SER	3
1	A	230	VAL	3
2	B	403	ARG	2
2	B	419	VAL	2
1	A	276	ASN	2
2	B	401	MET	2
2	B	332	ASP	2
1	A	172	ILE	2
1	A	162	ARG	2
2	B	372	LEU	2
2	B	381	LYS	2
1	A	261	VAL	2
1	A	202	VAL	2
1	A	188	LEU	2
2	B	430	VAL	2
2	B	398	ILE	2
2	B	365	TYR	2
1	A	165	GLU	2
1	A	203	LEU	2
1	A	159	LEU	2
2	B	383	ILE	1
1	A	212	LYS	1
2	B	432	GLU	1
1	A	245	LYS	1
1	A	243	LEU	1
2	B	382	MET	1
2	B	409	TYR	1
2	B	447	CYS	1
2	B	339	LEU	1
1	A	191	LEU	1
2	B	441	LYS	1
1	A	218	MET	1
2	B	331	ILE	1
2	B	380	PHE	1
1	A	173	GLN	1
1	A	236	VAL	1
1	A	287	ASP	1
2	B	343	ASP	1
1	A	175	TYR	1

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Mol	Chain	Res	Type	Models (Total)
1	A	223	LEU	1
1	A	264	PHE	1
1	A	274	LEU	1
2	B	369	VAL	1
1	A	260	LEU	1
2	B	408	ILE	1
1	A	180	ASP	1
1	A	290	GLN	1
2	B	335	LEU	1
2	B	389	SER	1
1	A	176	PHE	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides 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