



Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 11:13 pm GMT

PDB ID : 2KH2
Title : Solution structure of a scFv-IL-1B complex
Authors : Wilkinson, I.C.; Hall, C.J.; Veverka, V.; Muskett, F.W.; Stephens, P.E.; Taylor, R.J.; Henry, A.J.; Carr, M.D.
Deposited on : 2009-03-23

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
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : trunk28760
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

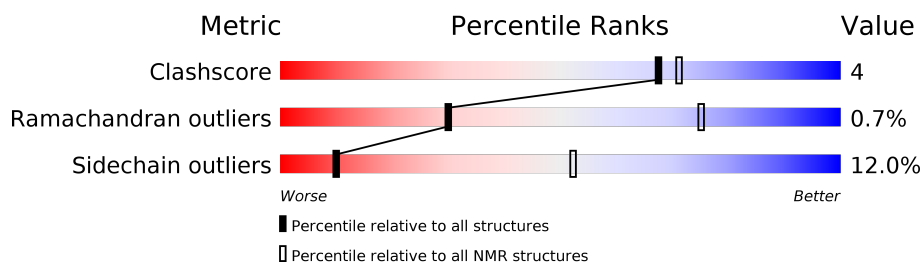
1 Overall quality at a glance

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	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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	153	
2	B	254	

2 Ensemble composition and analysis

This entry contains 77 models. Model 1 is the overall representative, medoid model (most similar to other models).

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:1-A:153, B:1-B:110, B:129-B:254 (389)	0.56	1

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

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

The models can be grouped into 11 clusters and 9 single-model clusters were found.

Cluster number	Models
1	1, 3, 7, 8, 15, 16, 17, 19, 20, 21, 24, 25, 29, 33, 42, 55, 58, 60
2	23, 31, 35, 37, 39, 40, 48, 56, 62, 66
3	45, 57, 64, 67, 68, 71, 74, 75, 77
4	5, 12, 30, 34, 43, 46, 59, 70, 72
5	6, 11, 22, 38, 54, 69
6	10, 14, 49, 53
7	36, 50, 61
8	2, 4, 41
9	47, 65
10	9, 27
11	44, 63
Single-model clusters	13; 18; 26; 28; 32; 51; 52; 73; 76

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 6250 atoms, of which 3099 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Interleukin-1 beta.

Mol	Chain	Residues	Atoms						Trace
1	A	153	Total	C	H	N	O	S	0
			2457	773	1238	201	237	8	

- Molecule 2 is a protein called scFv.

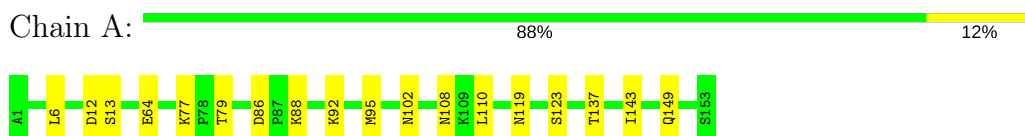
Mol	Chain	Residues	Atoms						Trace
2	B	254	Total	C	H	N	O	S	0
			3793	1208	1861	345	372	7	

4 Residue-property plots [i](#)

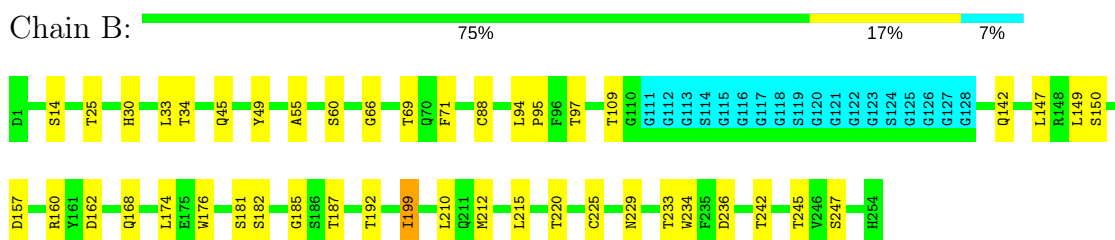
4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Interleukin-1 beta



- Molecule 2: scFv

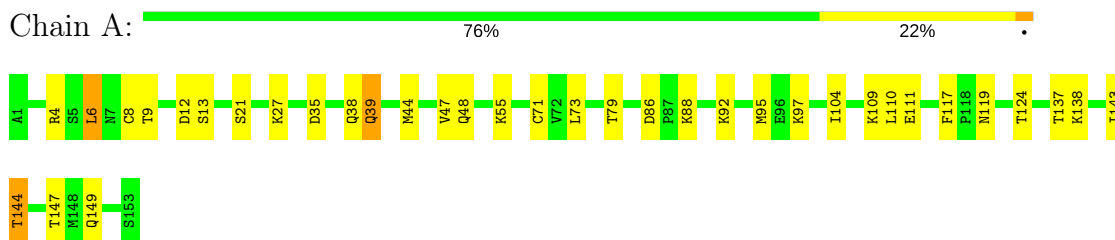


4.2 Scores per residue for each member of the ensemble

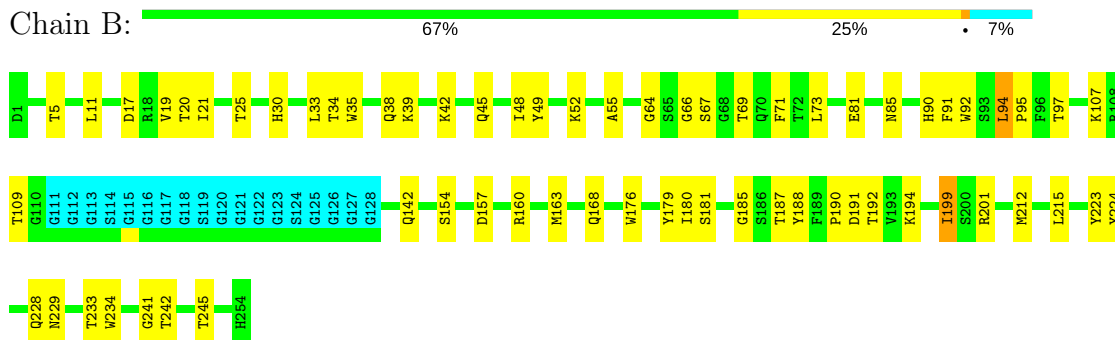
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Interleukin-1 beta

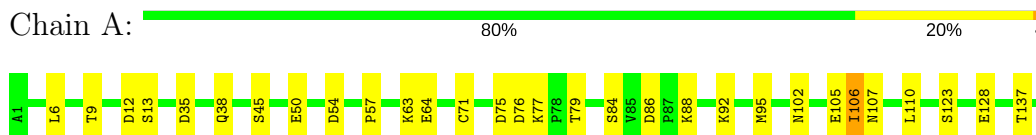


- Molecule 2: scFv

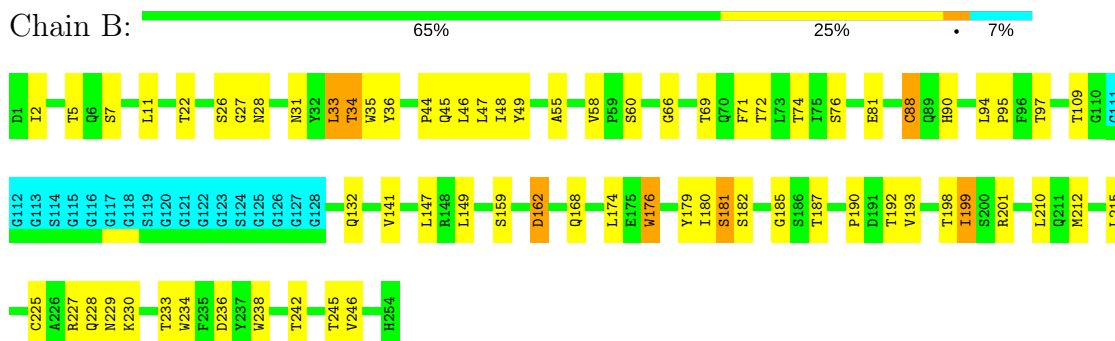


4.2.2 Score per residue for model 2

- Molecule 1: Interleukin-1 beta

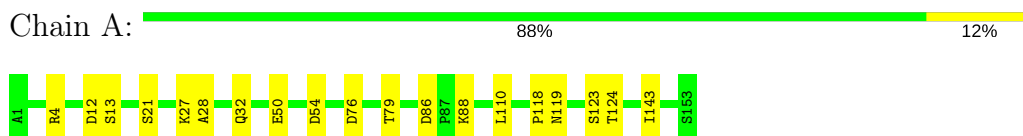


- Molecule 2: scFv

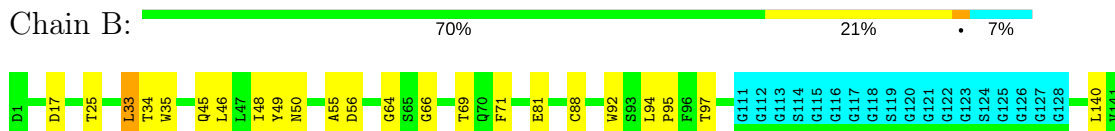


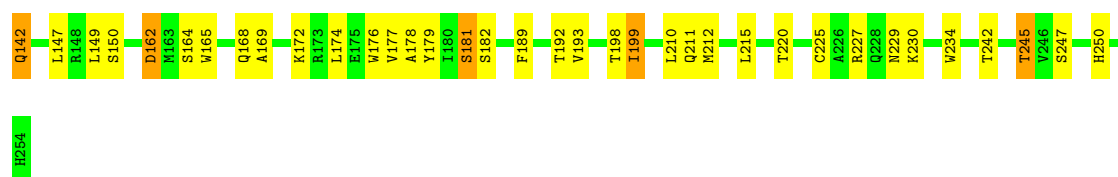
4.2.3 Score per residue for model 3

- Molecule 1: Interleukin-1 beta



- Molecule 2: scFv





4.2.4 Score per residue for model 4

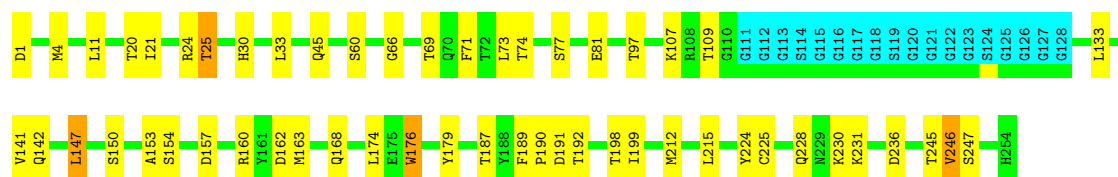
- Molecule 1: Interleukin-1 beta

Chain A: 88% 11%



- Molecule 2: scFv

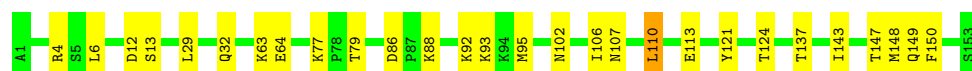
Chain B: 72% 20% 7%



4.2.5 Score per residue for model 5

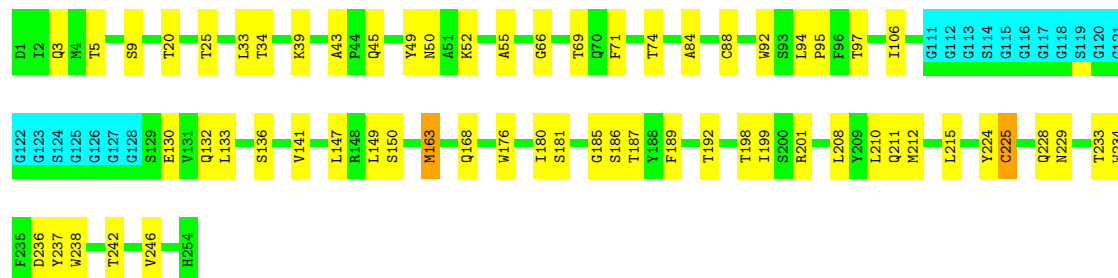
- Molecule 1: Interleukin-1 beta

Chain A: 82% 18%



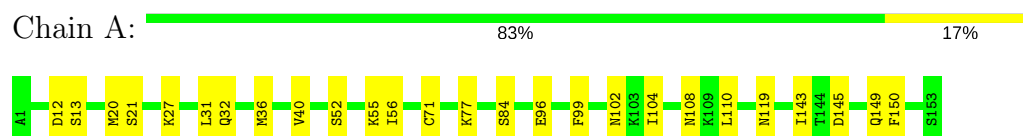
- Molecule 2: scFv

Chain B: 69% 24% 7%

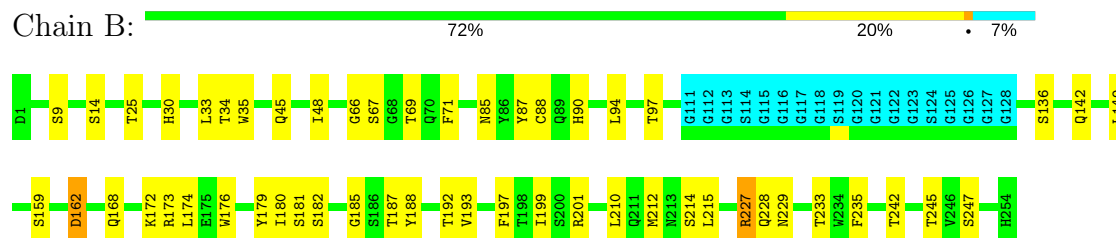


4.2.6 Score per residue for model 6

- Molecule 1: Interleukin-1 beta

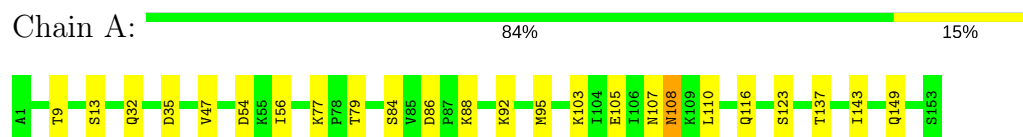


- Molecule 2: scFv

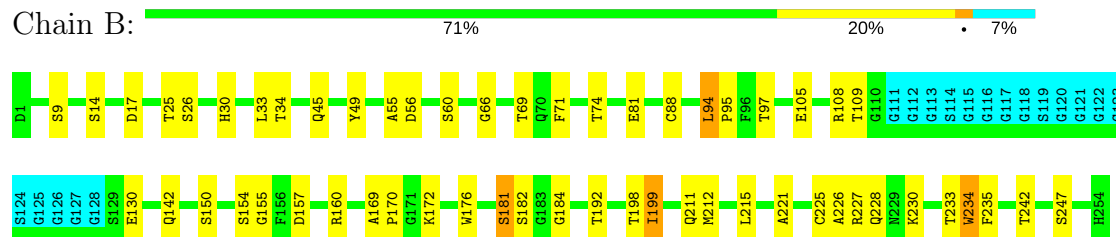


4.2.7 Score per residue for model 7

- Molecule 1: Interleukin-1 beta

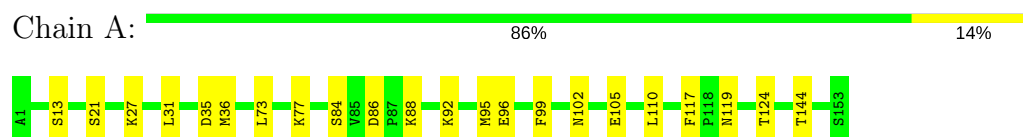


- Molecule 2: scFv

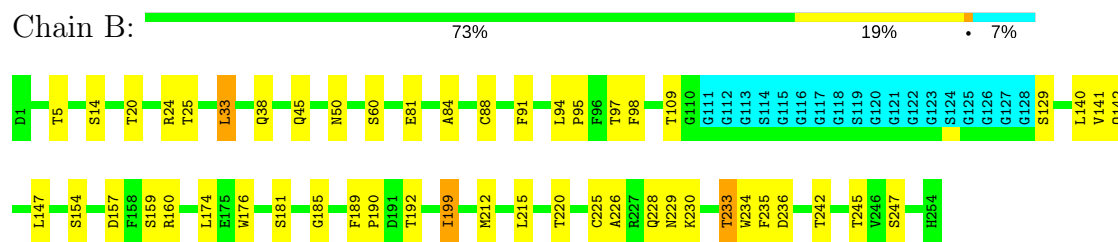


4.2.8 Score per residue for model 8

- Molecule 1: Interleukin-1 beta

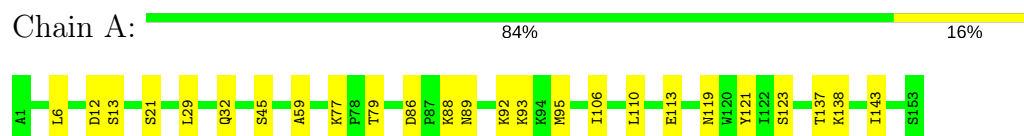


- Molecule 2: scFv

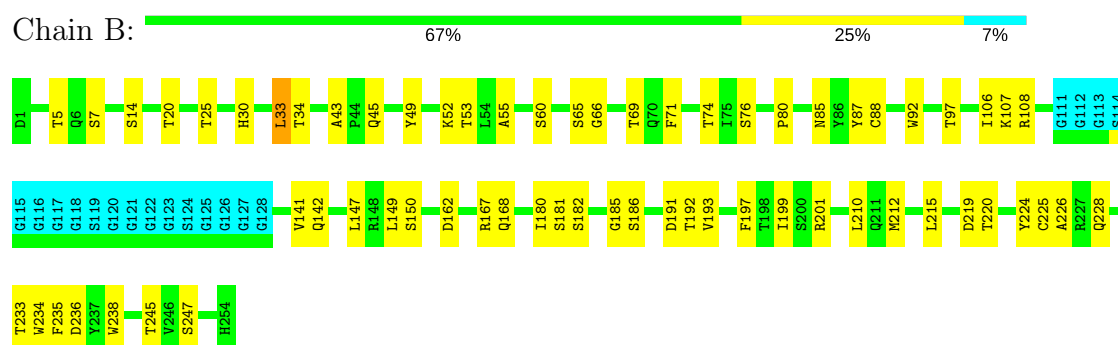


4.2.9 Score per residue for model 9

- Molecule 1: Interleukin-1 beta

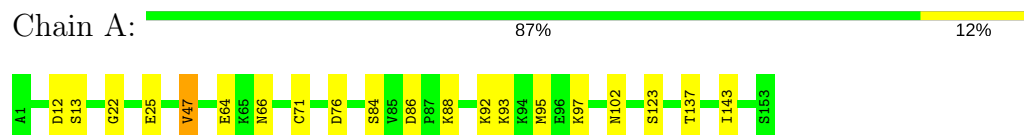


- Molecule 2: scFv

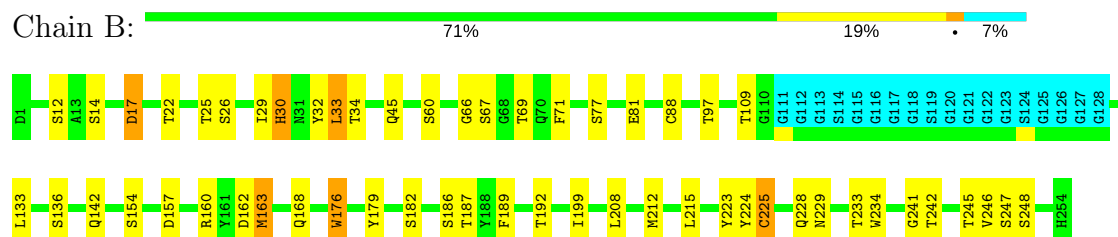


4.2.10 Score per residue for model 10

- Molecule 1: Interleukin-1 beta




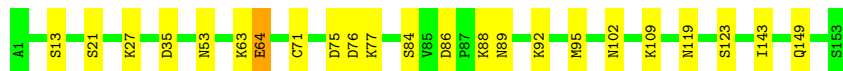
- Molecule 2: scFv



4.2.11 Score per residue for model 11

- Molecule 1: Interleukin-1 beta

Chain A:  85% 14%




- Molecule 2: scFv

Chain B:  73% 17% 7%



4.2.12 Score per residue for model 12

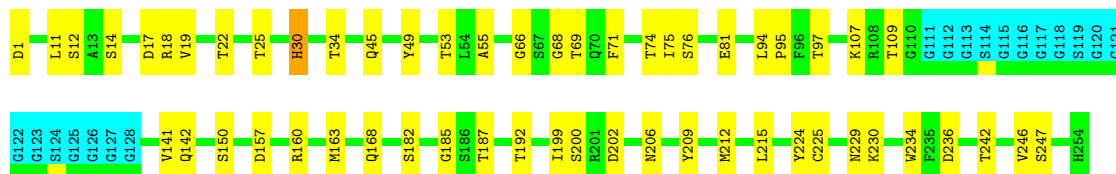
- Molecule 1: Interleukin-1 beta

Chain A:  82% 18%



- Molecule 2: scFv

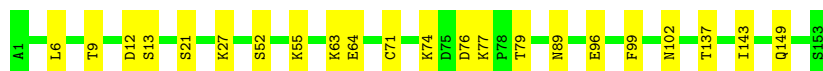
Chain B:  71% 21% 7%



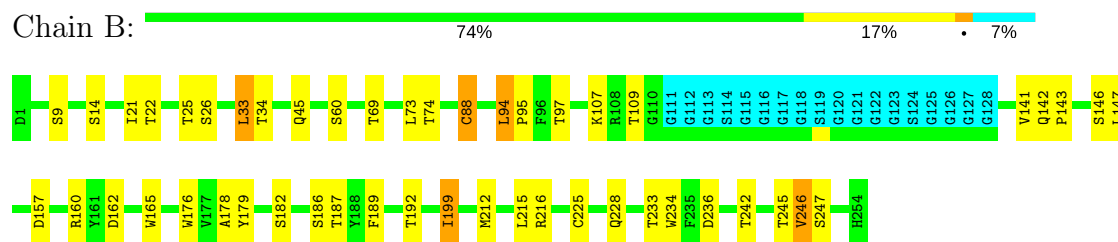
4.2.13 Score per residue for model 13

- Molecule 1: Interleukin-1 beta

Chain A:  86% 14%

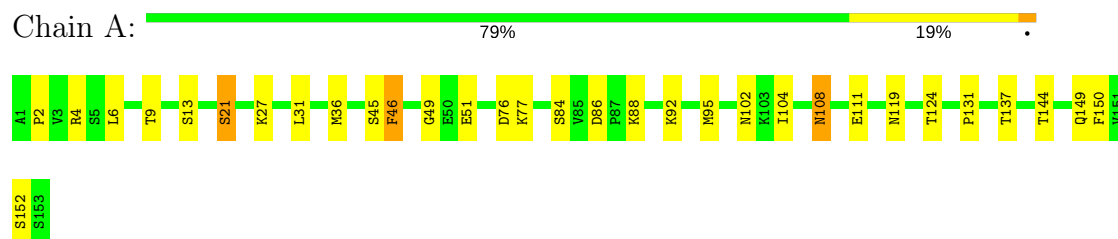


- Molecule 2: scFv

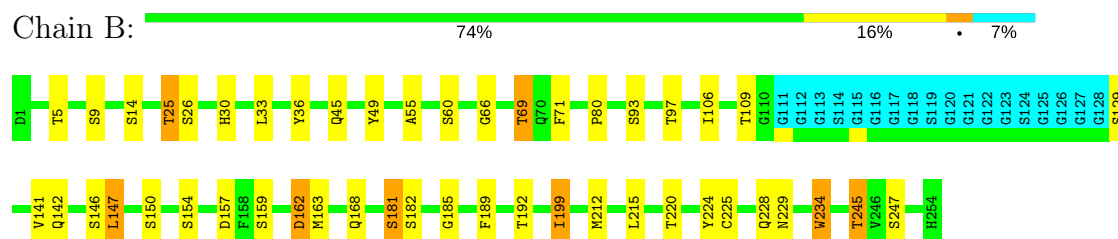


4.2.14 Score per residue for model 14

- Molecule 1: Interleukin-1 beta

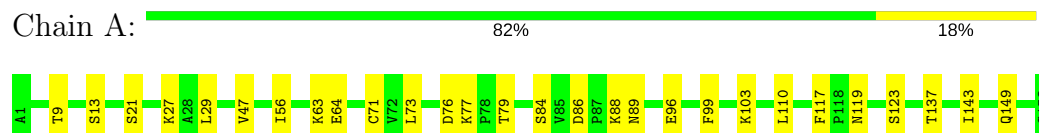


- Molecule 2: scFv

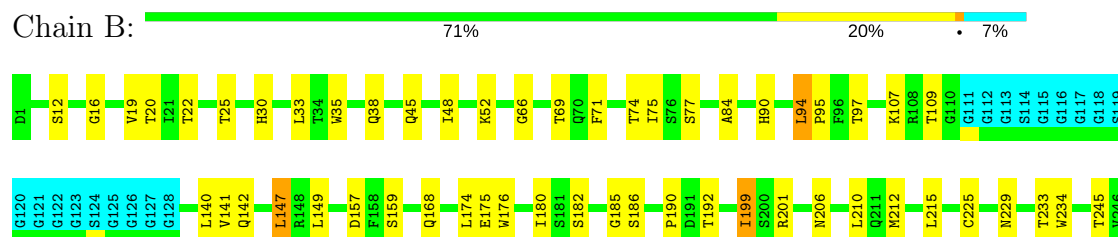


4.2.15 Score per residue for model 15

- Molecule 1: Interleukin-1 beta



- Molecule 2: scFv

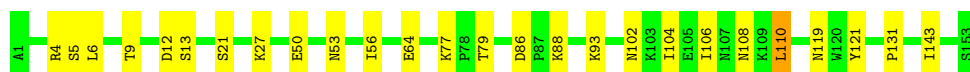




4.2.16 Score per residue for model 16

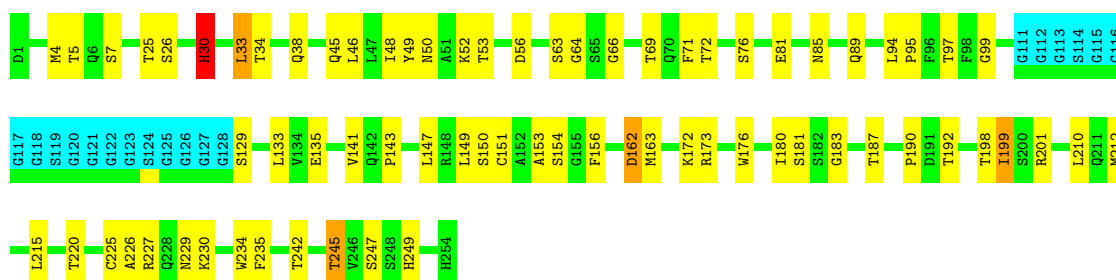
- Molecule 1: Interleukin-1 beta

Chain A: 83% 16% .



- Molecule 2: scFv

Chain B: 65% 26% 7% .



4.2.17 Score per residue for model 17

- Molecule 1: Interleukin-1 beta

Chain A: 84% 15% .



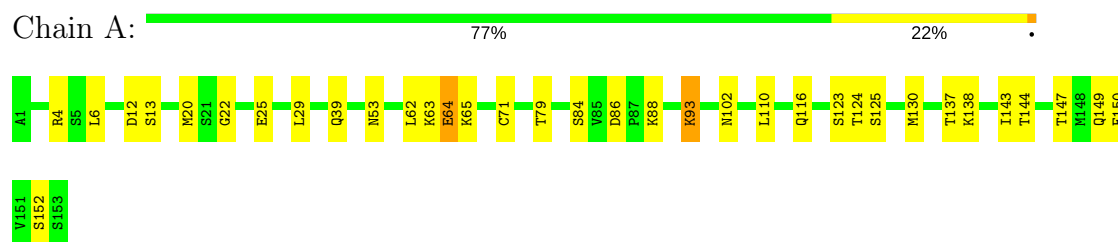
- Molecule 2: scFv

Chain B: 69% 22% 7% .

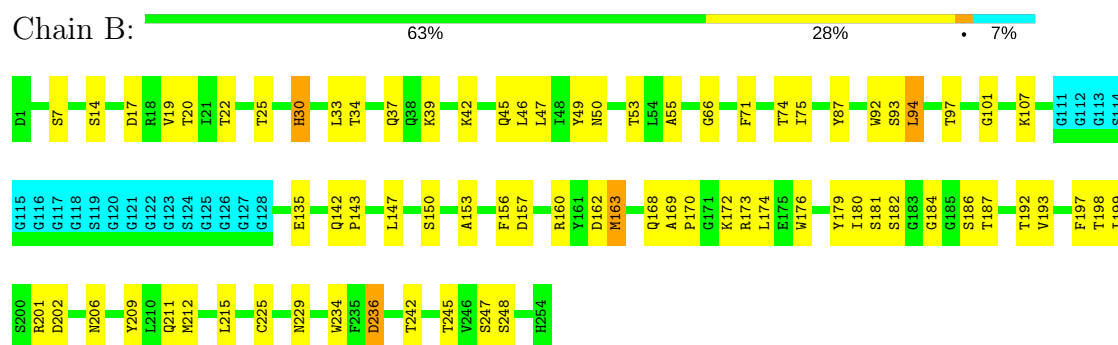


4.2.18 Score per residue for model 18

- Molecule 1: Interleukin-1 beta

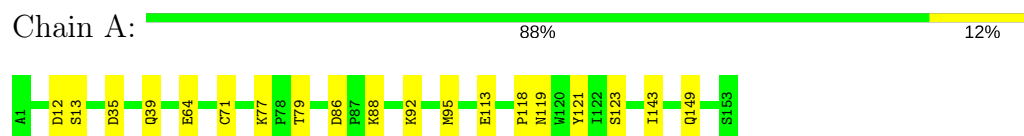


- Molecule 2: scFv

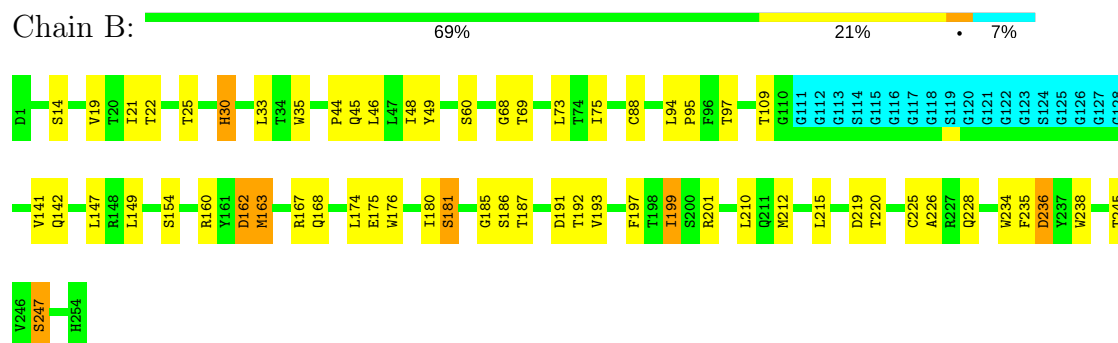


4.2.19 Score per residue for model 19

- Molecule 1: Interleukin-1 beta

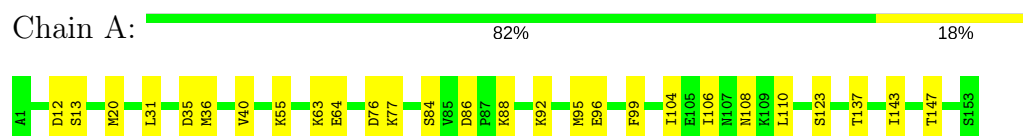


- Molecule 2: scFv

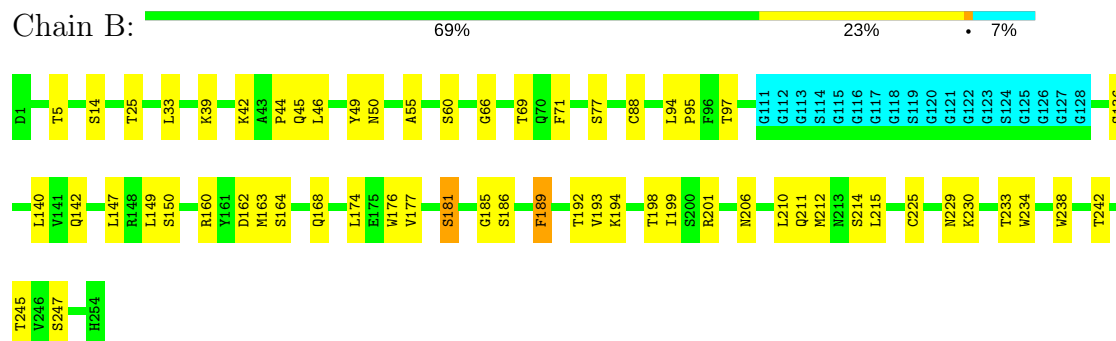


4.2.20 Score per residue for model 20

- Molecule 1: Interleukin-1 beta

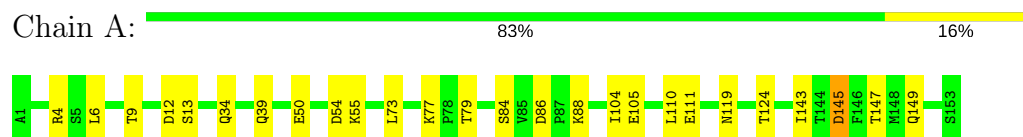


- Molecule 2: scFv

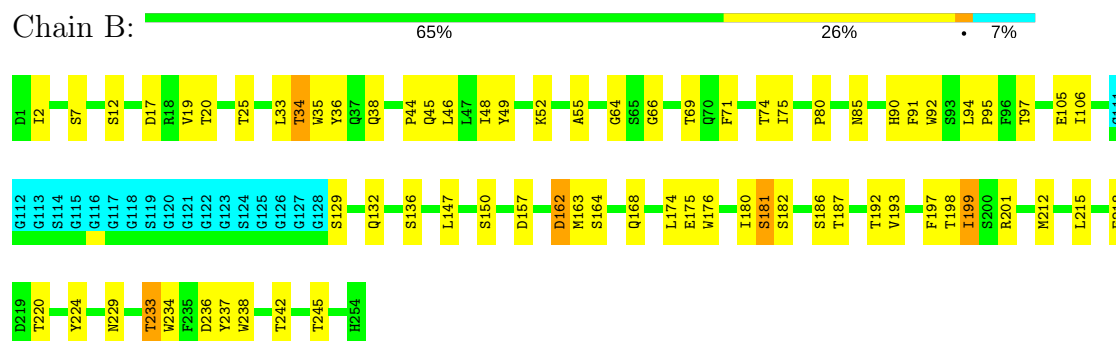


4.2.21 Score per residue for model 21

- Molecule 1: Interleukin-1 beta

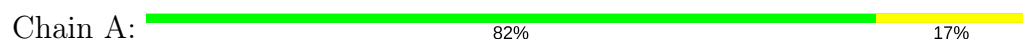


- Molecule 2: scFv



4.2.22 Score per residue for model 22

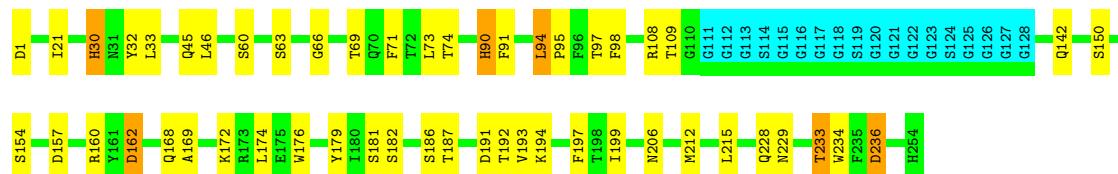
- Molecule 1: Interleukin-1 beta





• Molecule 2: scFv

Chain B: 72% 18% 7%



4.2.23 Score per residue for model 23

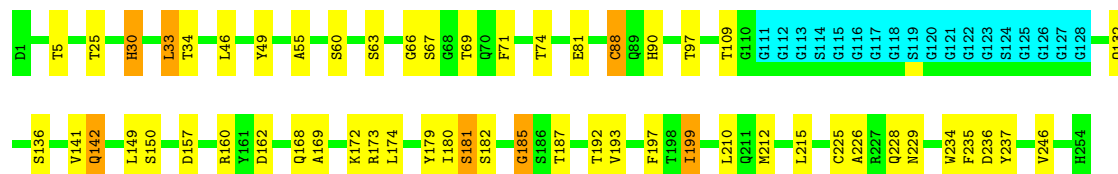
• Molecule 1: Interleukin-1 beta

Chain A: 88% 12%



• Molecule 2: scFv

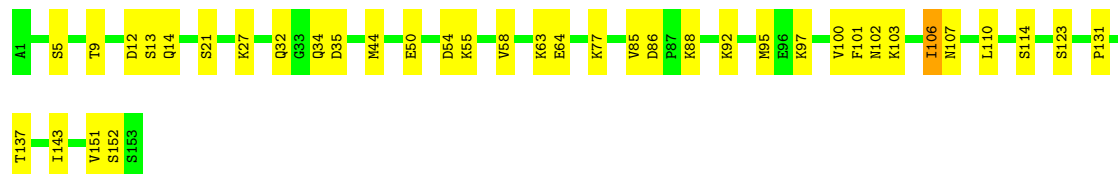
Chain B: 71% 19% 7%



4.2.24 Score per residue for model 24

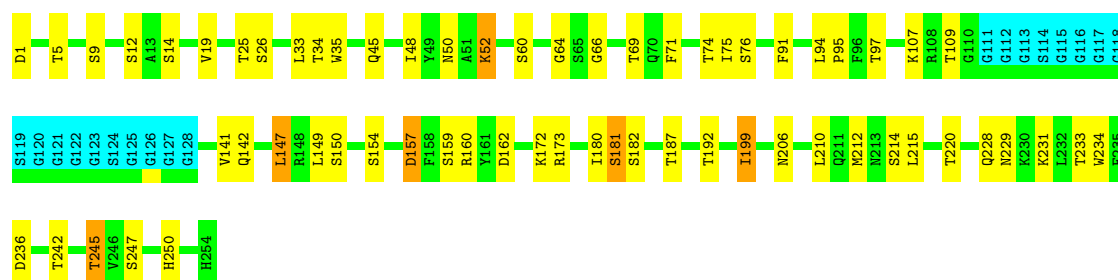
• Molecule 1: Interleukin-1 beta

Chain A: 75% 24%



• Molecule 2: scFv

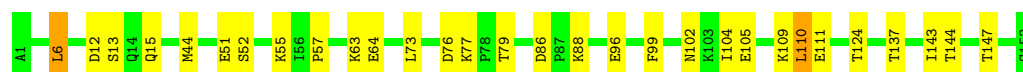
Chain B: 68% 22% 7%



4.2.25 Score per residue for model 25

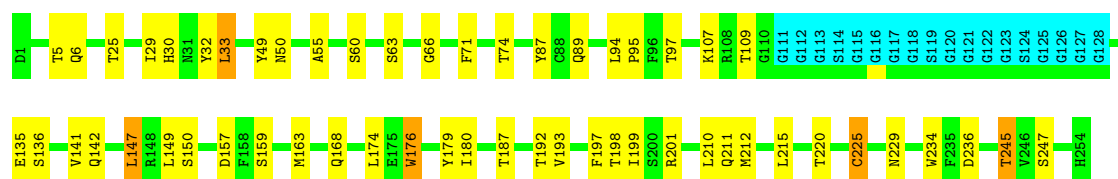
- Molecule 1: Interleukin-1 beta

Chain A: 80% 18% •



- Molecule 2: scFv

Chain B: 71% 20% 7% •



4.2.26 Score per residue for model 26

- Molecule 1: Interleukin-1 beta

Chain A: 82% 16% •



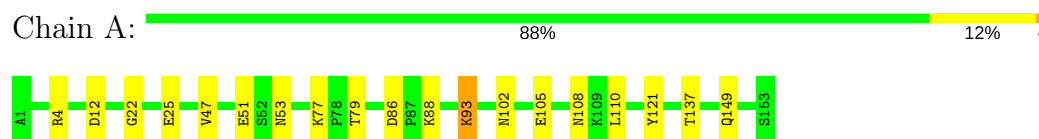
- Molecule 2: scFv

Chain B: 69% 22% 7% •

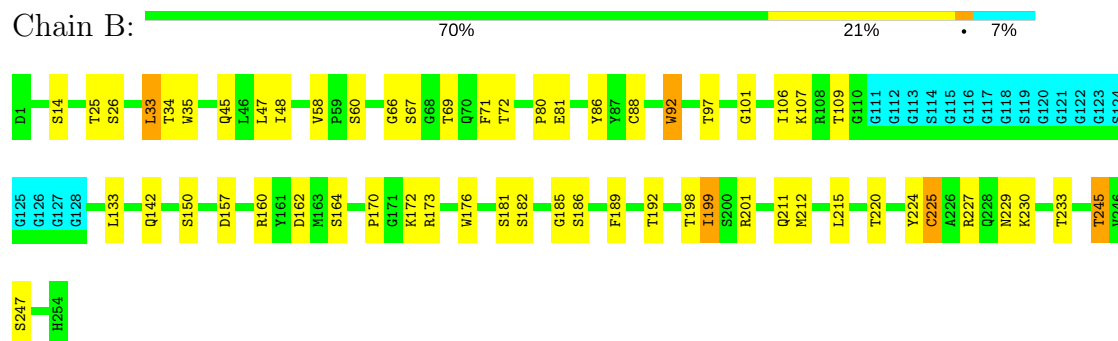


4.2.27 Score per residue for model 27

- Molecule 1: Interleukin-1 beta

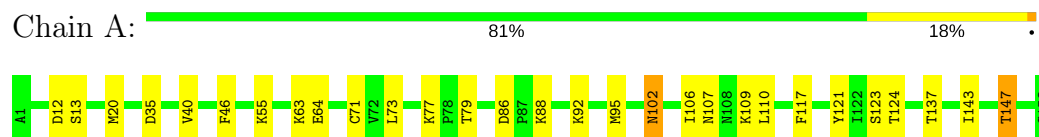


- Molecule 2: scFv

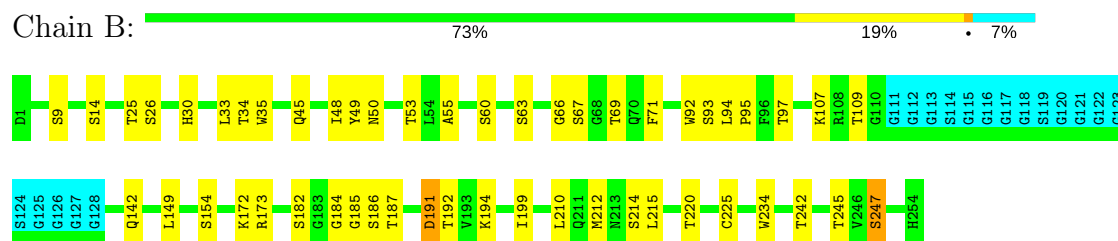


4.2.28 Score per residue for model 28

- Molecule 1: Interleukin-1 beta

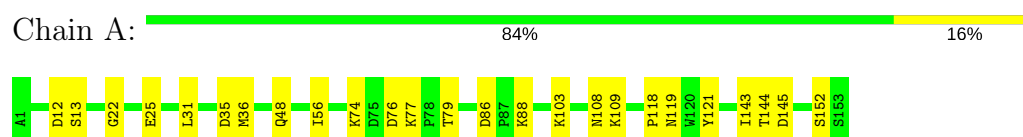


- Molecule 2: scFv

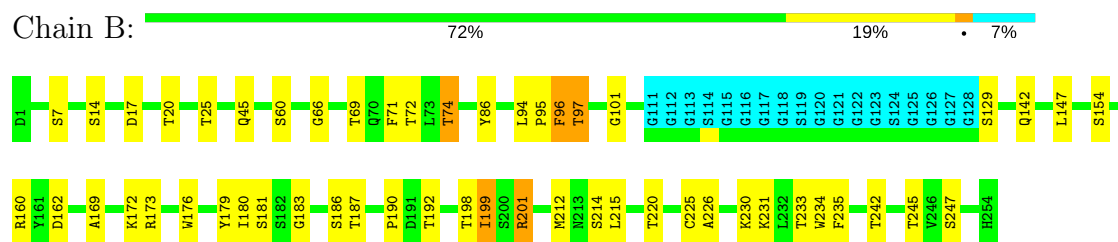


4.2.29 Score per residue for model 29

- Molecule 1: Interleukin-1 beta

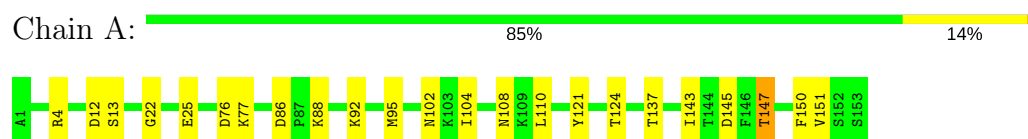


- Molecule 2: scFv

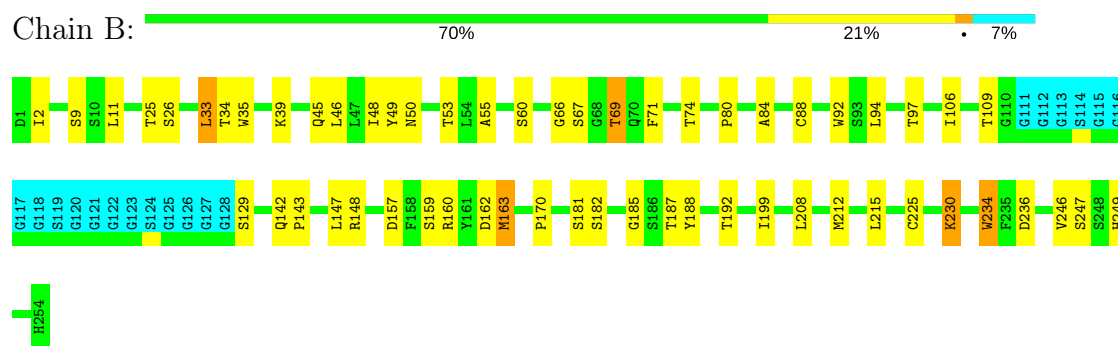


4.2.30 Score per residue for model 30

- Molecule 1: Interleukin-1 beta

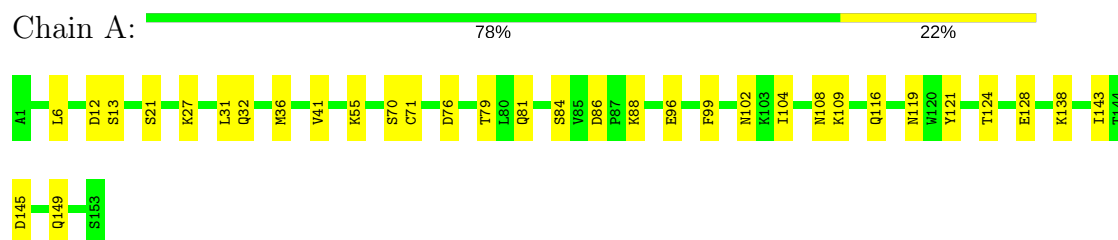


- Molecule 2: scFv



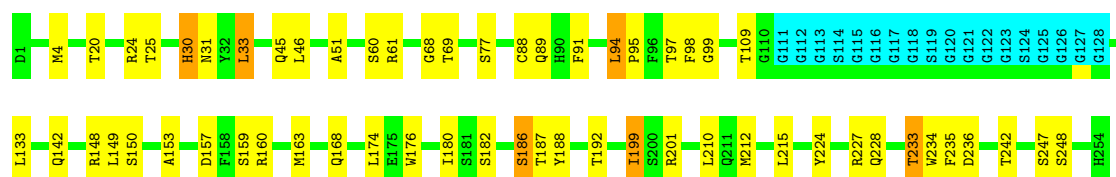
4.2.31 Score per residue for model 31

- Molecule 1: Interleukin-1 beta



- Molecule 2: scFv





4.2.32 Score per residue for model 32

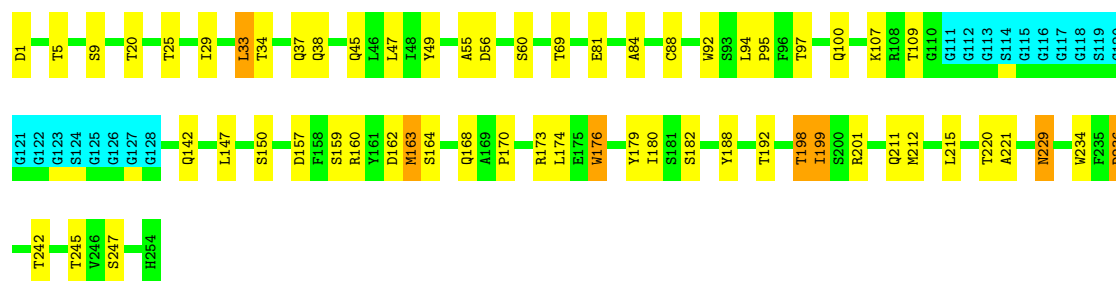
- Molecule 1: Interleukin-1 beta

Chain A: 89% 10%



- Molecule 2: scFv

Chain B: 69% 21% 7%



4.2.33 Score per residue for model 33

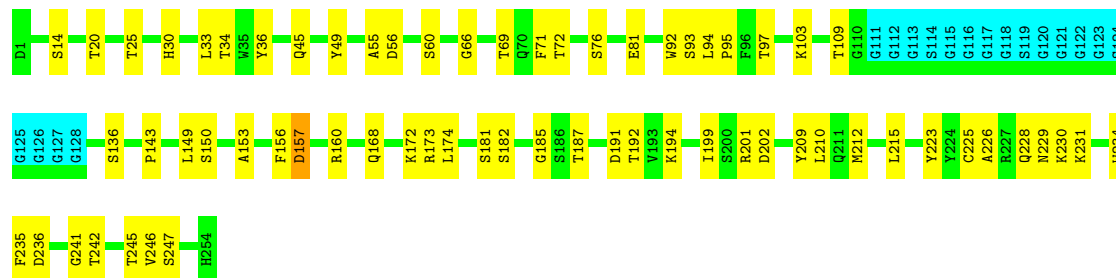
- Molecule 1: Interleukin-1 beta

Chain A: 81% 17%



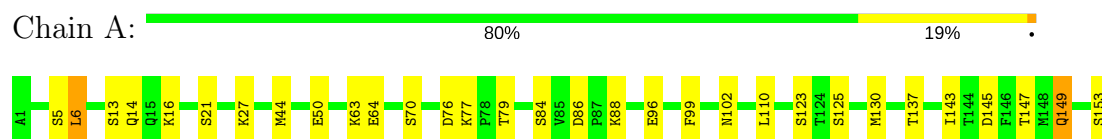
- Molecule 2: scFv

Chain B: 67% 26% 7%

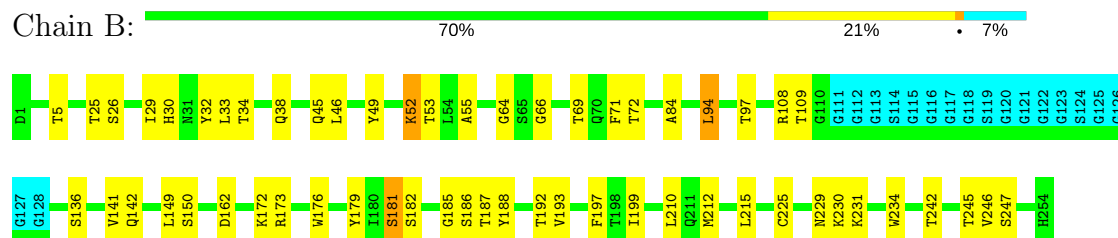


4.2.34 Score per residue for model 34

- Molecule 1: Interleukin-1 beta

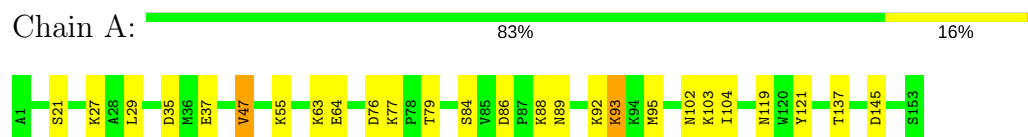


- Molecule 2: scFv

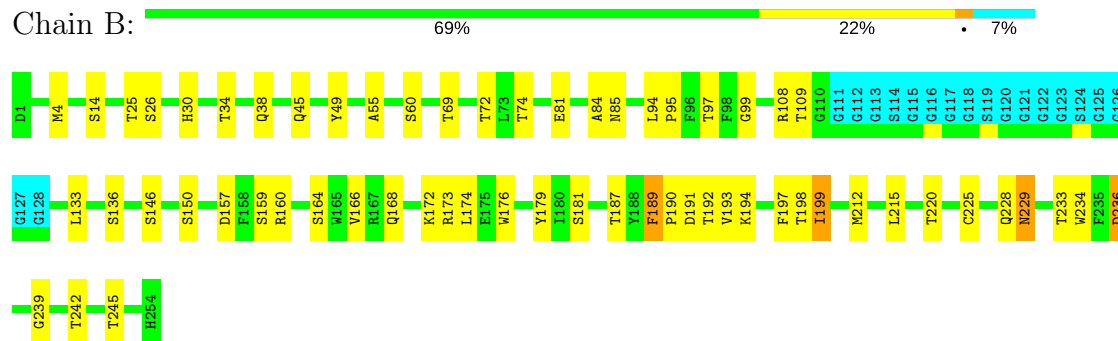


4.2.35 Score per residue for model 35

- Molecule 1: Interleukin-1 beta

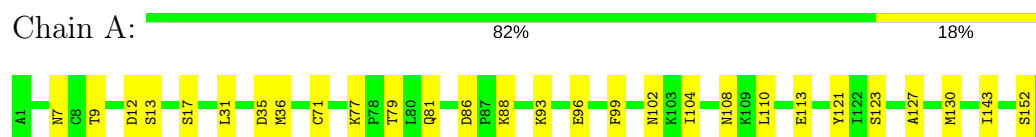


- Molecule 2: scFv

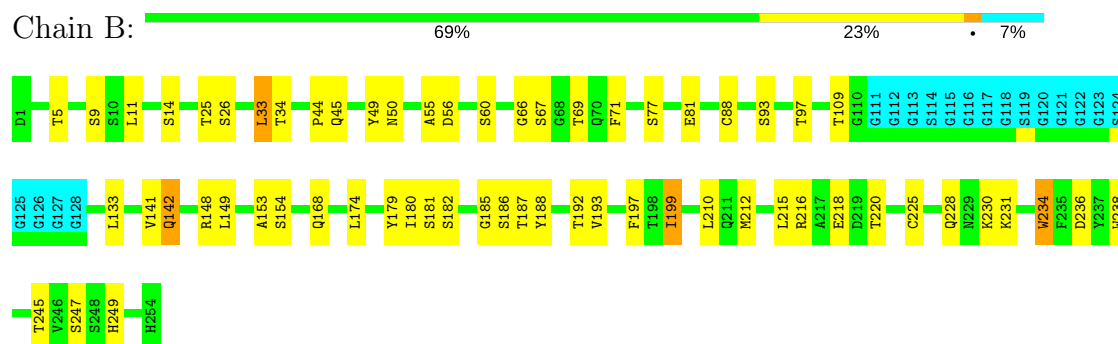


4.2.36 Score per residue for model 36

- Molecule 1: Interleukin-1 beta

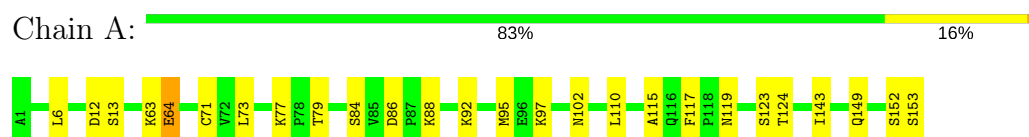


- Molecule 2: scFv

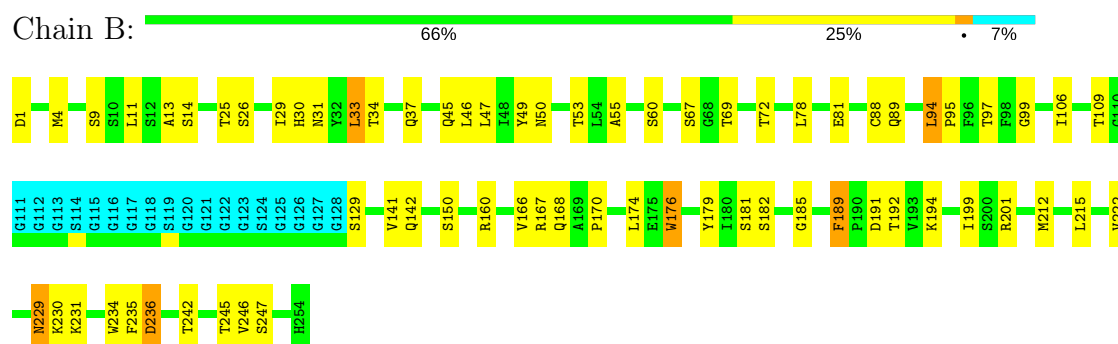


4.2.37 Score per residue for model 37

- Molecule 1: Interleukin-1 beta

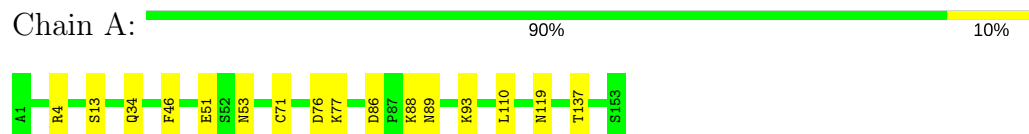


- Molecule 2: scFv



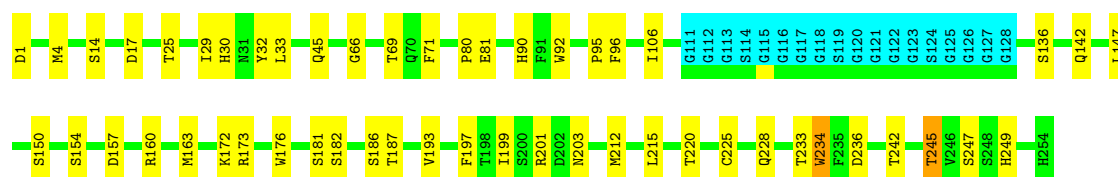
4.2.38 Score per residue for model 38

- Molecule 1: Interleukin-1 beta



- Molecule 2: scFv

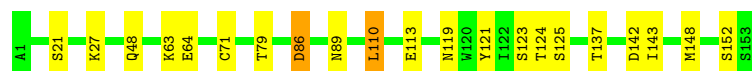




4.2.39 Score per residue for model 39

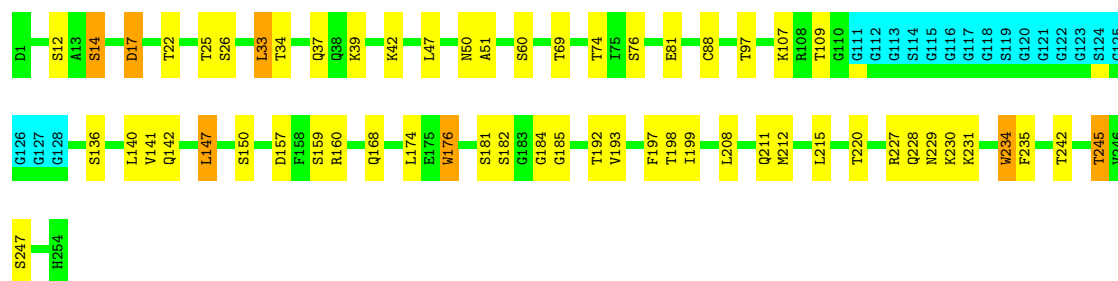
- Molecule 1: Interleukin-1 beta

Chain A: 86% 12% •



- Molecule 2: scFv

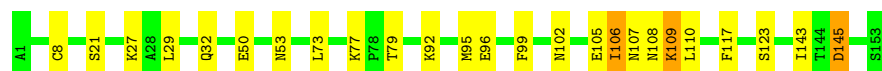
Chain B: 70% 20% 7% •



4.2.40 Score per residue for model 40

- Molecule 1: Interleukin-1 beta

Chain A: 84% 14% •




- Molecule 2: scFv

Chain B: 66% 24% 7% •



4.2.41 Score per residue for model 41

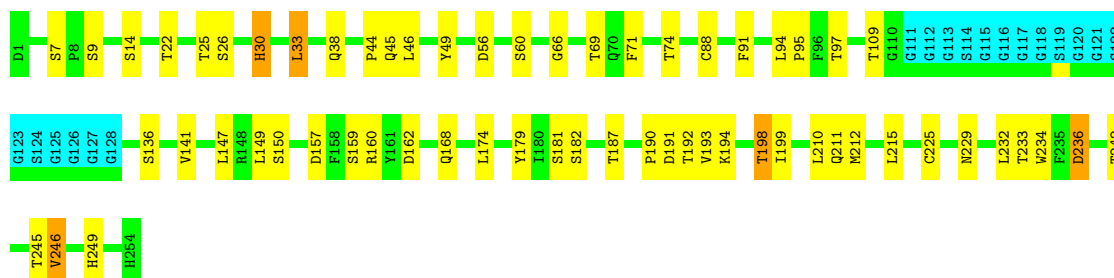
- Molecule 1: Interleukin-1 beta

Chain A: 




- Molecule 2: scFv

Chain B: 



4.2.42 Score per residue for model 42

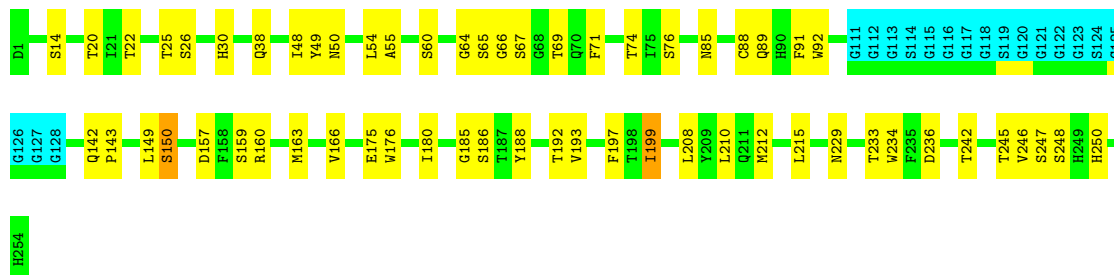
- Molecule 1: Interleukin-1 beta

Chain A: 



- Molecule 2: scFv

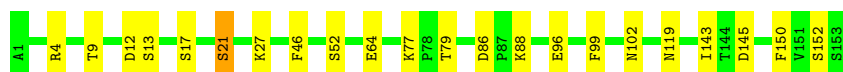
Chain B: 



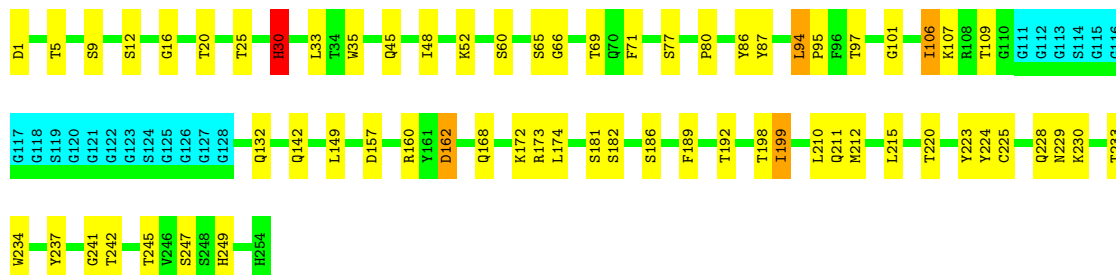
4.2.43 Score per residue for model 43

- Molecule 1: Interleukin-1 beta

Chain A: 

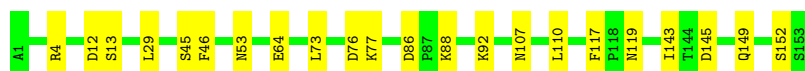


- Molecule 2: scFv

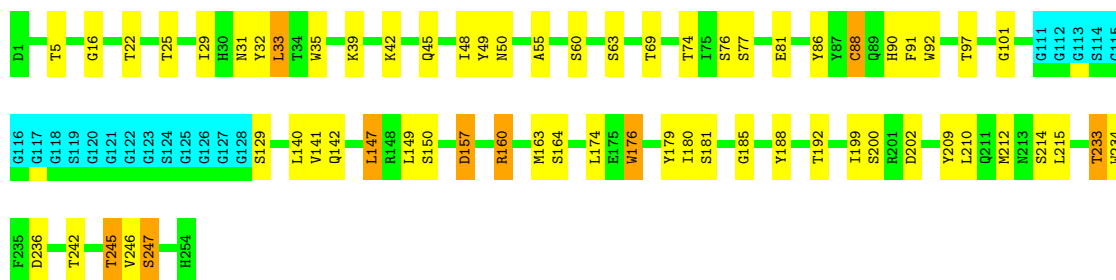


4.2.44 Score per residue for model 44

- Molecule 1: Interleukin-1 beta

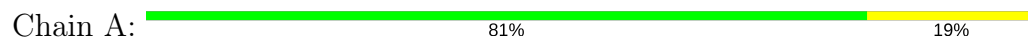


- Molecule 2: scFv

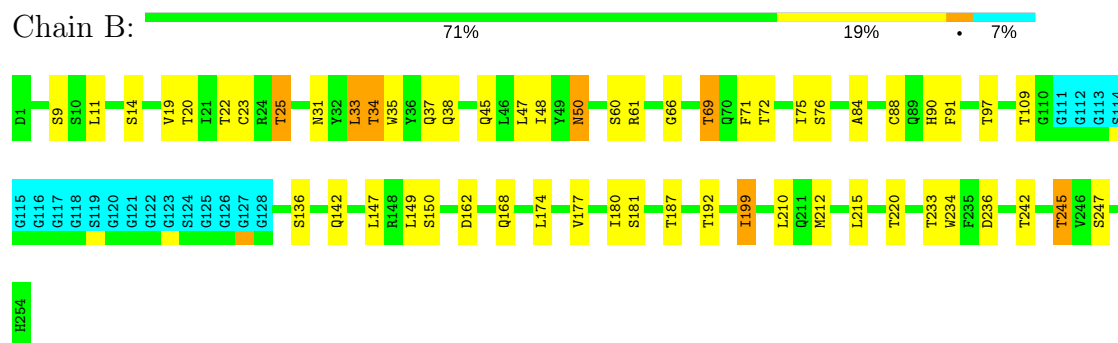


4.2.45 Score per residue for model 45

- Molecule 1: Interleukin-1 beta

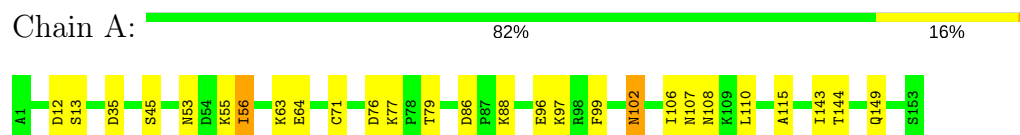


- Molecule 2: scFv

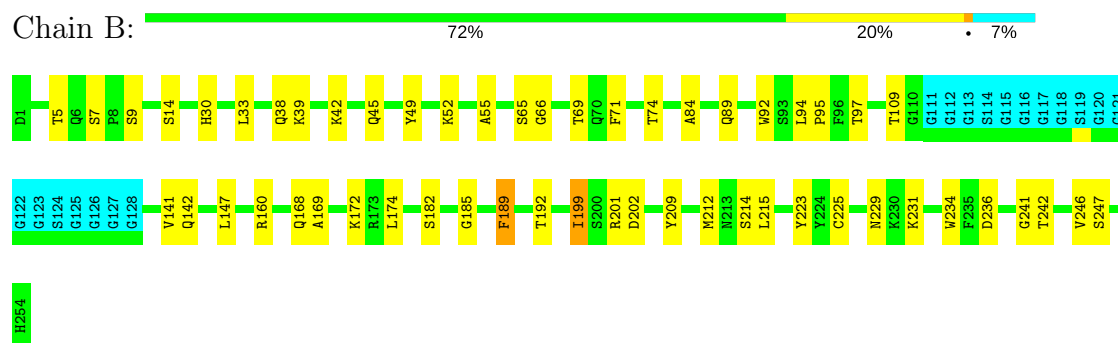


4.2.46 Score per residue for model 46

- Molecule 1: Interleukin-1 beta

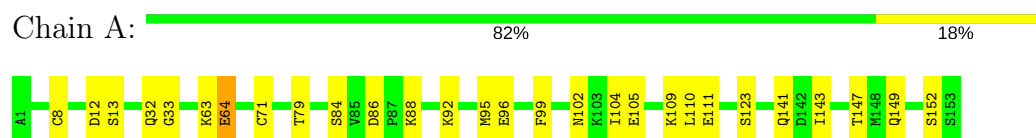


- Molecule 2: scFv

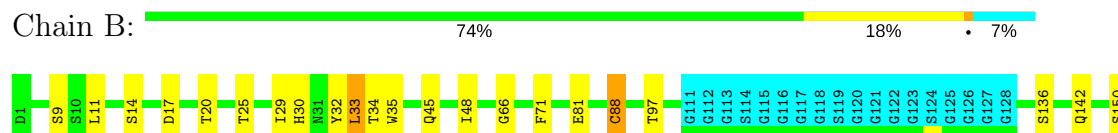


4.2.47 Score per residue for model 47

- Molecule 1: Interleukin-1 beta



- Molecule 2: scFv

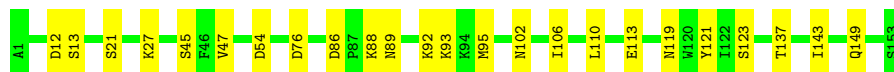




4.2.48 Score per residue for model 48

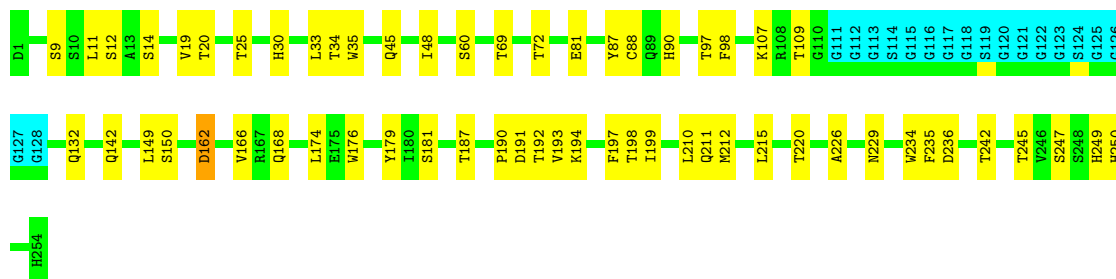
- Molecule 1: Interleukin-1 beta

Chain A: 84% 16%



- Molecule 2: scFv

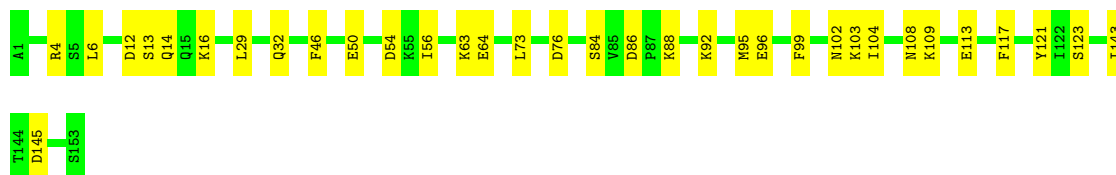
Chain B: 70% 23% 7%



4.2.49 Score per residue for model 49

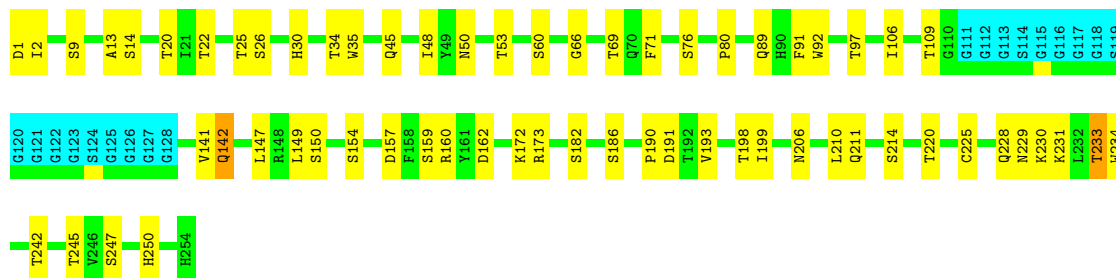
- Molecule 1: Interleukin-1 beta

Chain A: 78% 22%




- Molecule 2: scFv

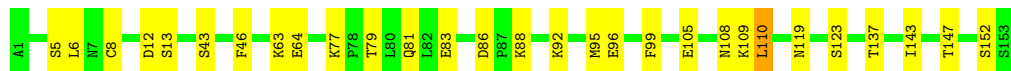
Chain B: 68% 24% 7%



4.2.50 Score per residue for model 50

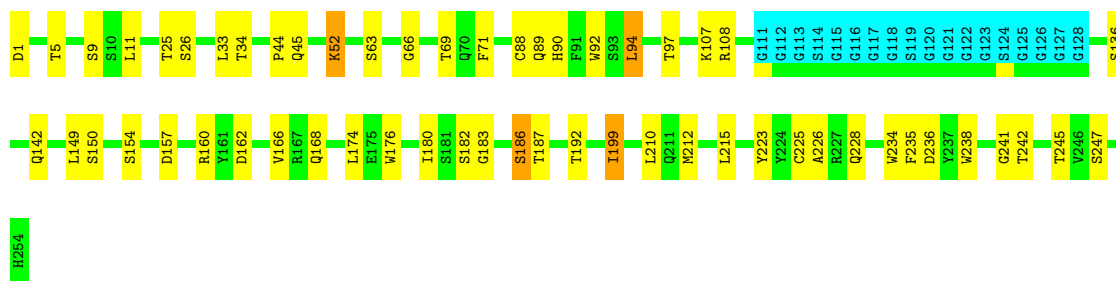
- Molecule 1: Interleukin-1 beta

Chain A:  81% 18%




- Molecule 2: scFv

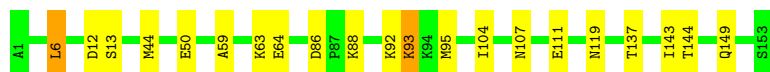
Chain B:  70% 21% 7%



4.2.51 Score per residue for model 51

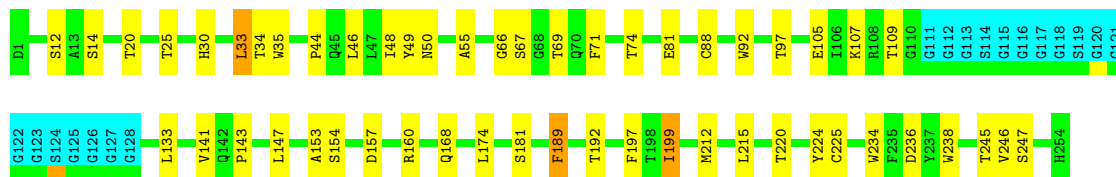
- Molecule 1: Interleukin-1 beta

Chain A:  86% 12%




- Molecule 2: scFv

Chain B:  72% 19% 7%



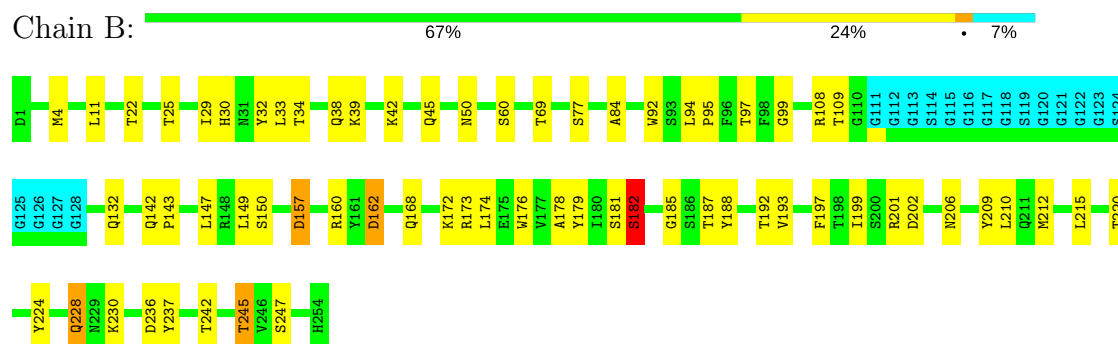
4.2.52 Score per residue for model 52

- Molecule 1: Interleukin-1 beta

Chain A:  84% 15%

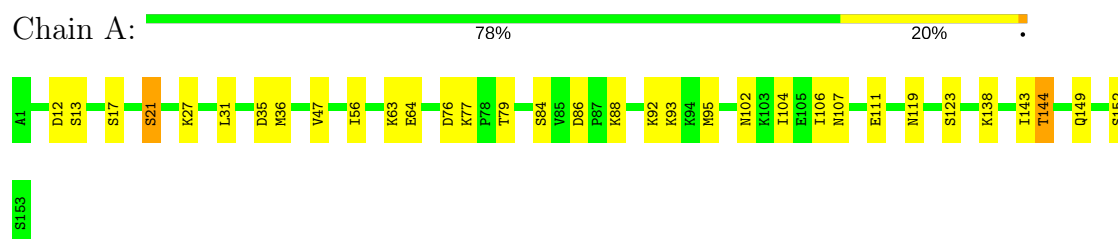


- Molecule 2: scFv

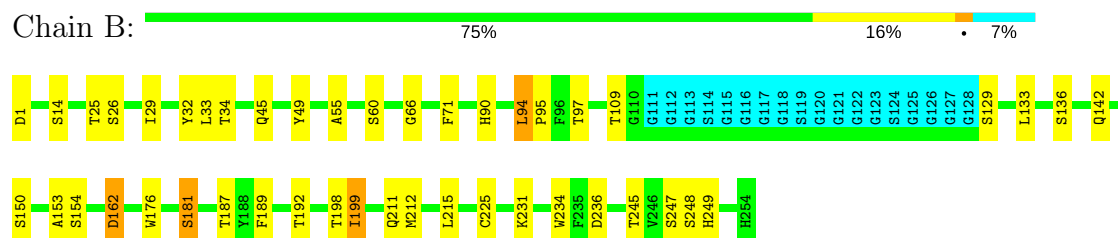


4.2.53 Score per residue for model 53

- Molecule 1: Interleukin-1 beta

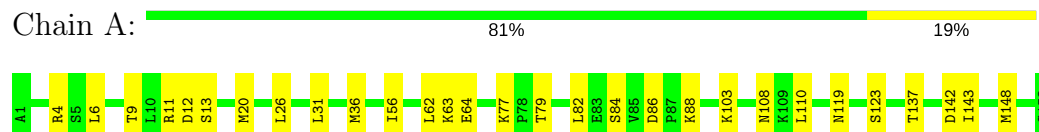


- Molecule 2: scFv



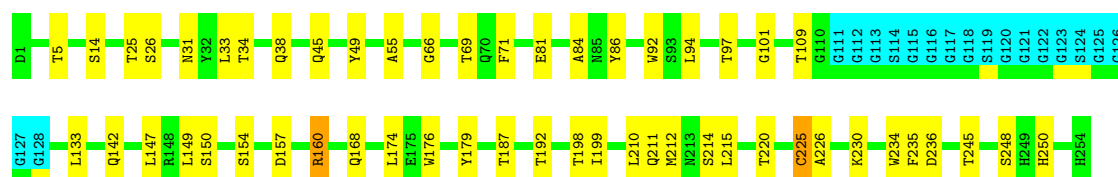
4.2.54 Score per residue for model 54

- Molecule 1: Interleukin-1 beta



- Molecule 2: scFv

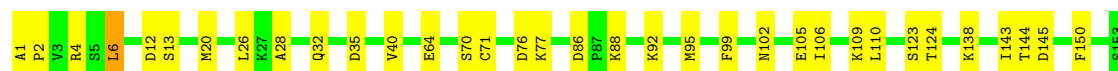




4.2.55 Score per residue for model 55

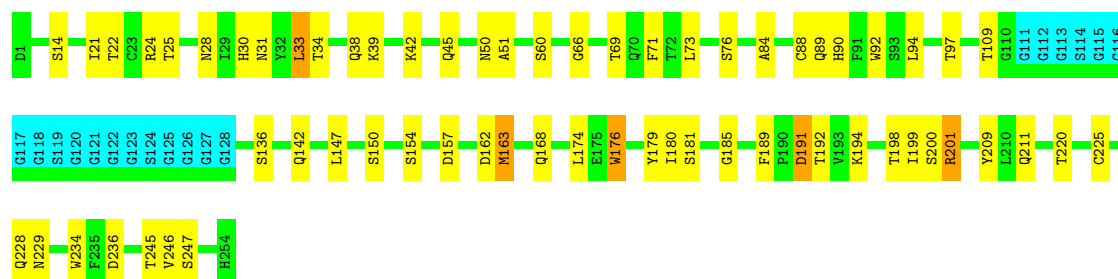
- Molecule 1: Interleukin-1 beta

Chain A: 78% 22%



- Molecule 2: scFv

Chain B: 68% 23% 7%



4.2.56 Score per residue for model 56

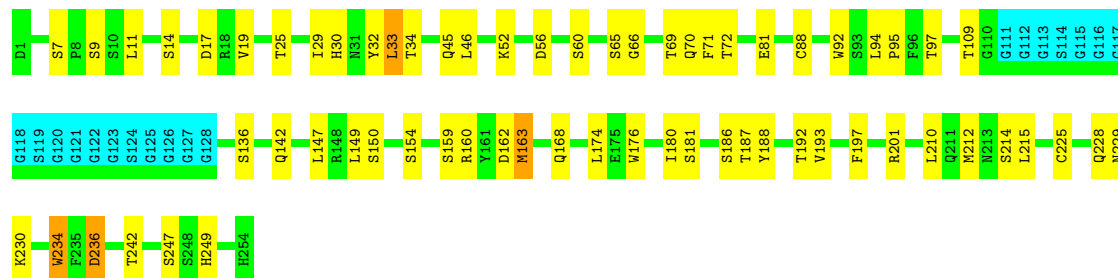
- Molecule 1: Interleukin-1 beta

Chain A: 86% 12%



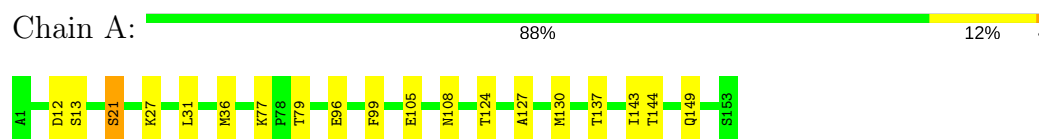
- Molecule 2: scFv

Chain B: 67% 24% 7%

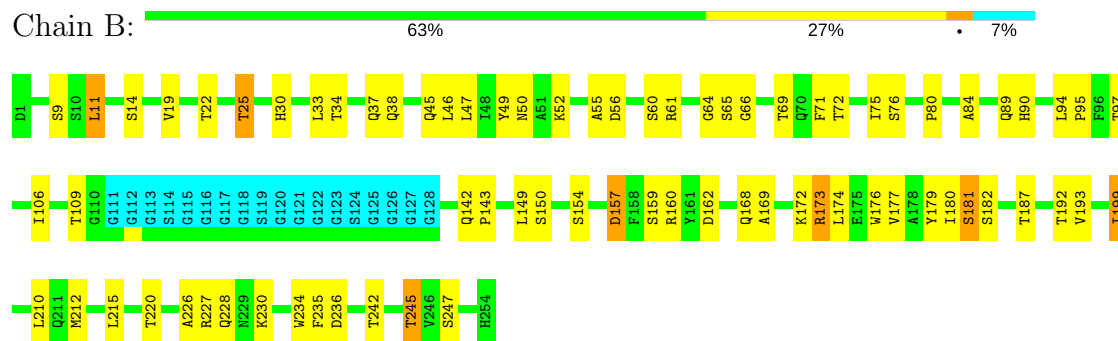


4.2.57 Score per residue for model 57

- Molecule 1: Interleukin-1 beta

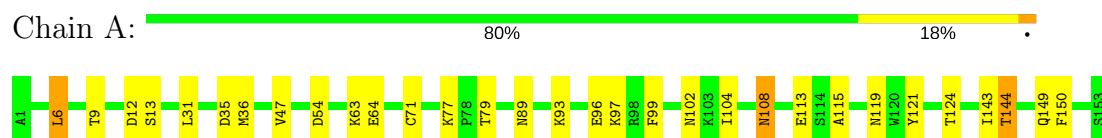


- Molecule 2: scFv

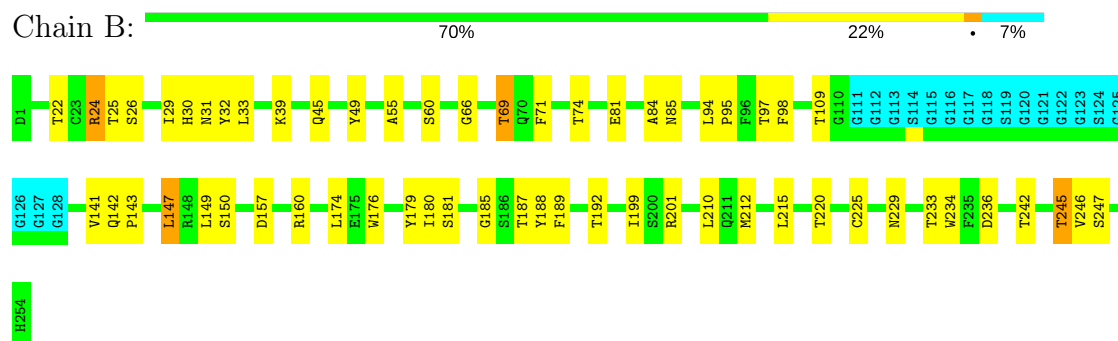


4.2.58 Score per residue for model 58

- Molecule 1: Interleukin-1 beta

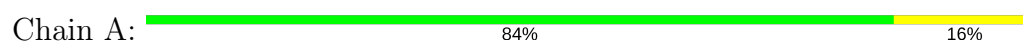


- Molecule 2: scFv



4.2.59 Score per residue for model 59

- Molecule 1: Interleukin-1 beta



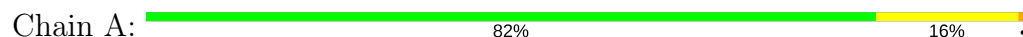


- Molecule 2: scFv

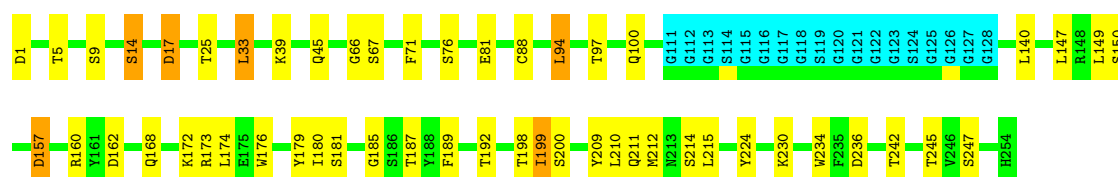


4.2.60 Score per residue for model 60

- Molecule 1: Interleukin-1 beta

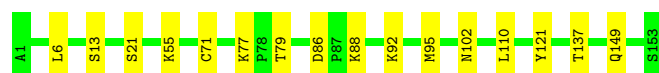


- Molecule 2: scFv



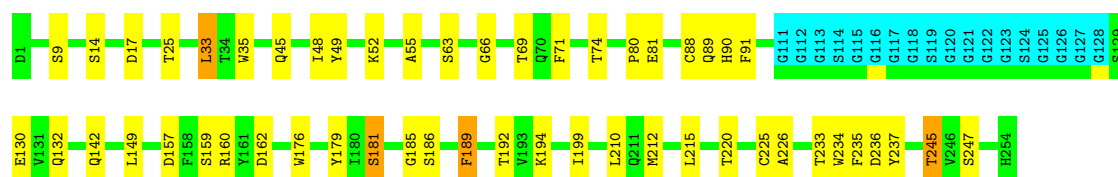
4.2.61 Score per residue for model 61

- Molecule 1: Interleukin-1 beta



- Molecule 2: scFv

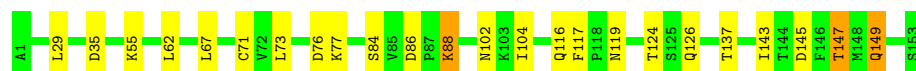




4.2.62 Score per residue for model 62

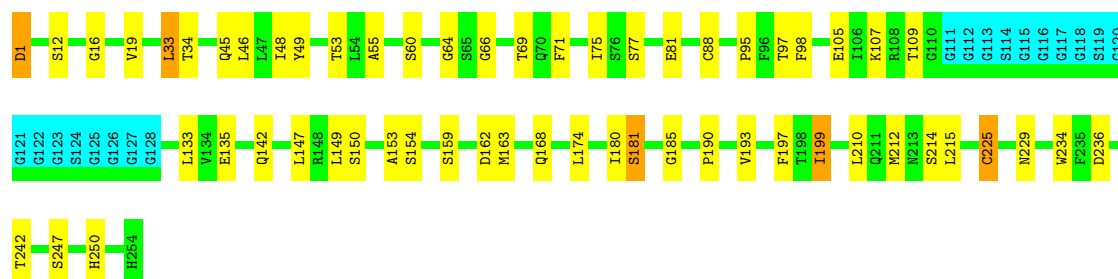
- Molecule 1: Interleukin-1 beta

Chain A: 84% 14% .



- Molecule 2: scFv

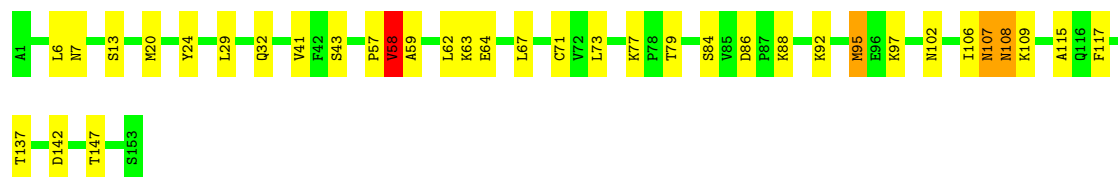
Chain B: 70% 21% 7% .



4.2.63 Score per residue for model 63

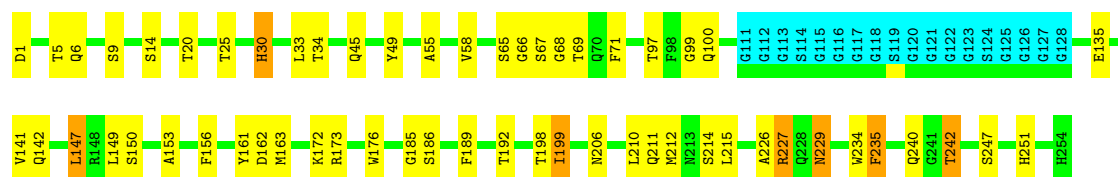
- Molecule 1: Interleukin-1 beta

Chain A: 76% 21% .




- Molecule 2: scFv

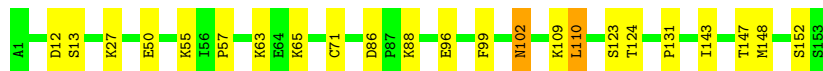
Chain B: 70% 20% 7% .



4.2.64 Score per residue for model 64

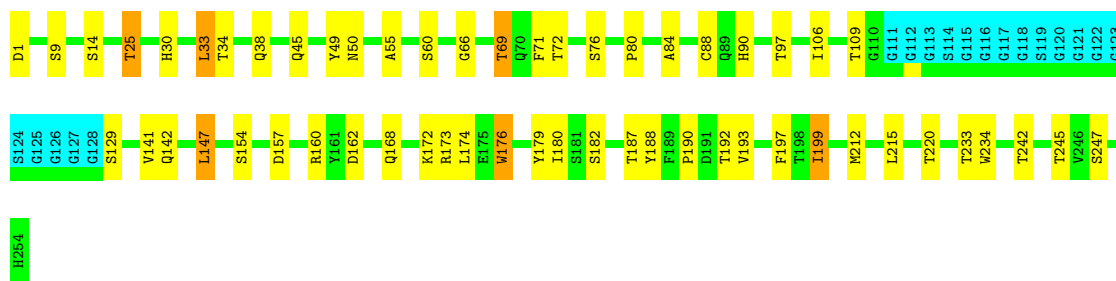
- Molecule 1: Interleukin-1 beta

Chain A:  85% 14%




- Molecule 2: scFv

Chain B:  71% 20% 7%



4.2.65 Score per residue for model 65

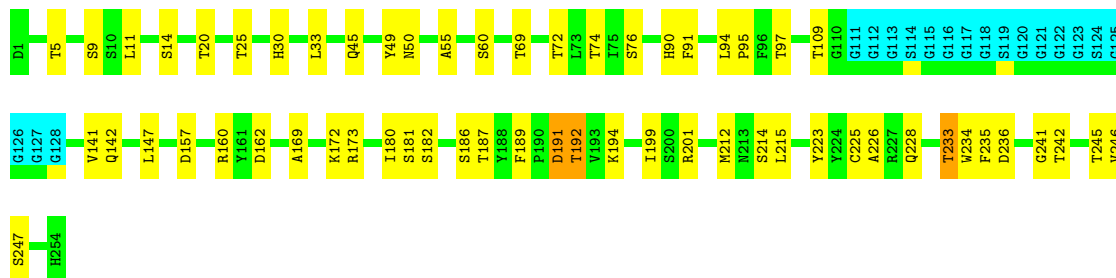
- Molecule 1: Interleukin-1 beta

Chain A:  86% 14%




- Molecule 2: scFv

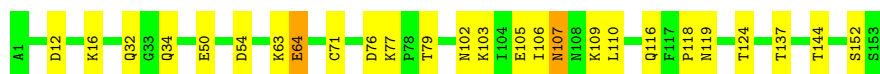
Chain B:  70% 22% 7%



4.2.66 Score per residue for model 66

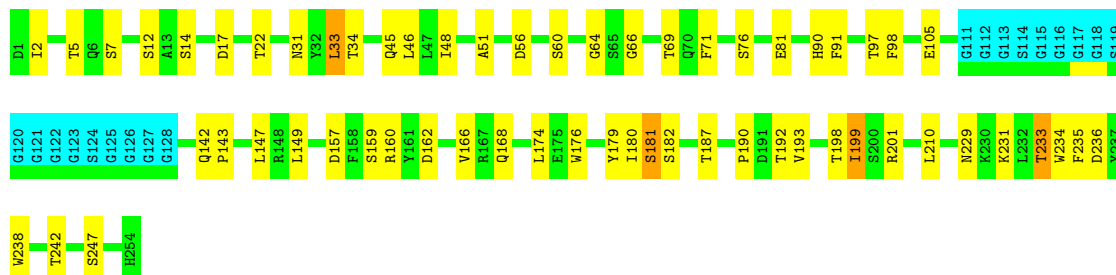
- Molecule 1: Interleukin-1 beta

Chain A:  83% 16%



- Molecule 2: scFv

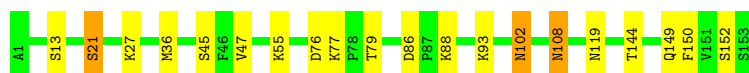
Chain B: 69% 22% 7%



4.2.67 Score per residue for model 67

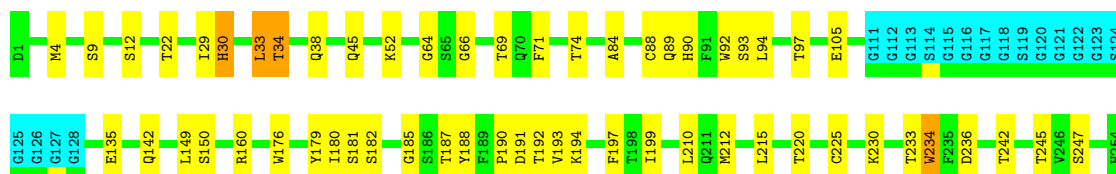
- Molecule 1: Interleukin-1 beta

Chain A: 87% 11% 2%



- Molecule 2: scFv

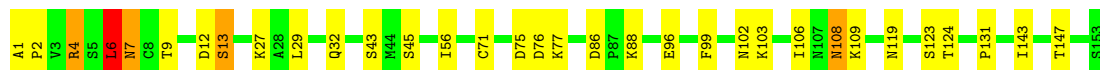
Chain B: 70% 21% 7%



4.2.68 Score per residue for model 68

- Molecule 1: Interleukin-1 beta

Chain A: 78% 18% 4%



- Molecule 2: scFv

Chain B: 66% 24% 7%



4.2.69 Score per residue for model 69

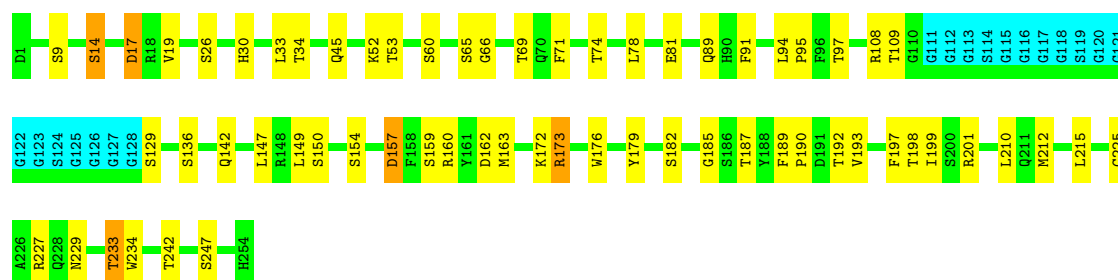
- Molecule 1: Interleukin-1 beta

Chain A: 83% 16%



- Molecule 2: scFv

Chain B: 68% 23% 7%



4.2.70 Score per residue for model 70

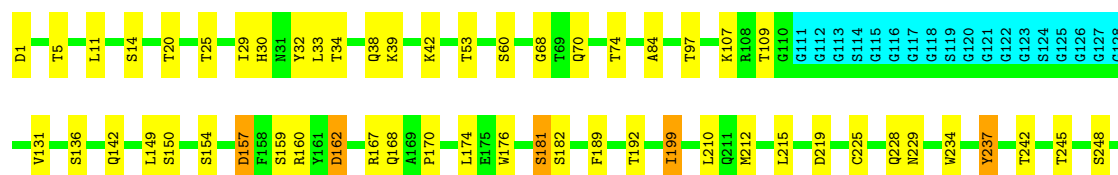
- Molecule 1: Interleukin-1 beta

Chain A: 80% 19%



- Molecule 2: scFv

Chain B: 71% 20% 7%



H254

4.2.71 Score per residue for model 71

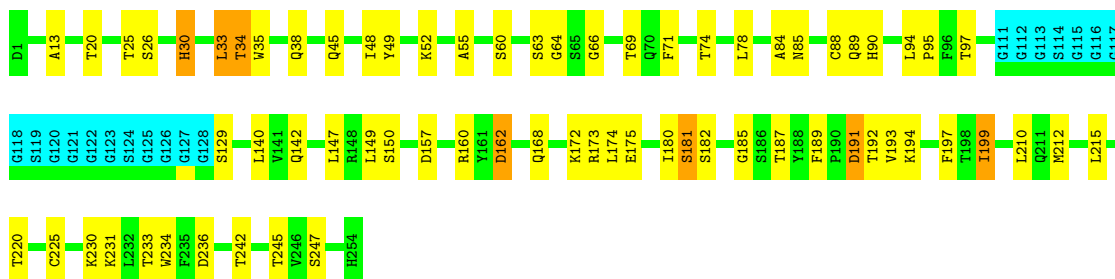
- Molecule 1: Interleukin-1 beta

Chain A: 79% 19%



- Molecule 2: scFv

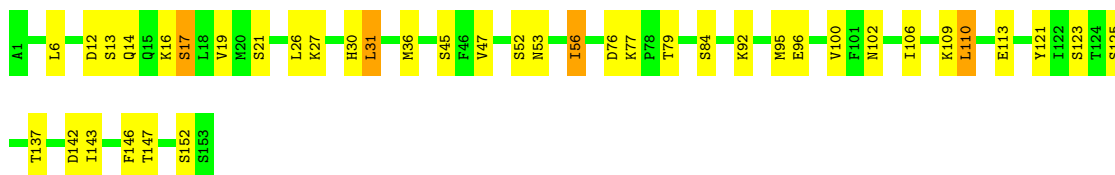
Chain B: 66% 24% 3% 7%



4.2.72 Score per residue for model 72

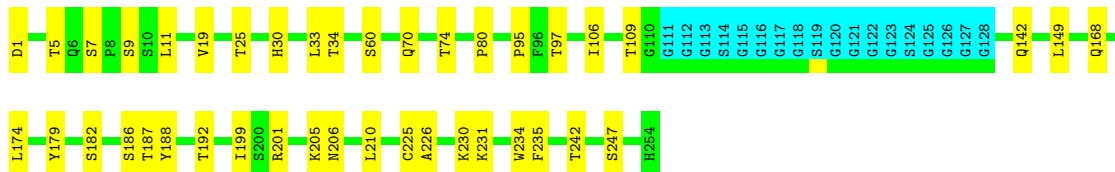
- Molecule 1: Interleukin-1 beta

Chain A: 74% 24%




- Molecule 2: scFv

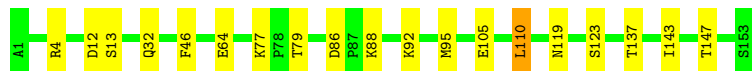
Chain B: 77% 16% 7%



4.2.73 Score per residue for model 73

- Molecule 1: Interleukin-1 beta

Chain A:  88% 12%




- Molecule 2: scFv

Chain B:  69% 22% 7%



4.2.74 Score per residue for model 74

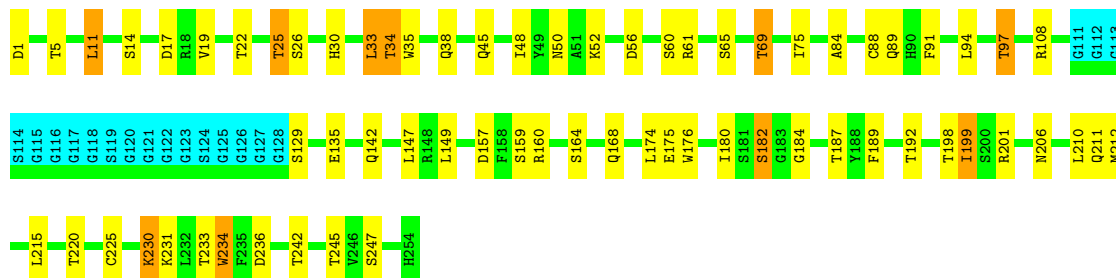
- Molecule 1: Interleukin-1 beta

Chain A:  86% 14%




- Molecule 2: scFv

Chain B:  66% 23% 7%



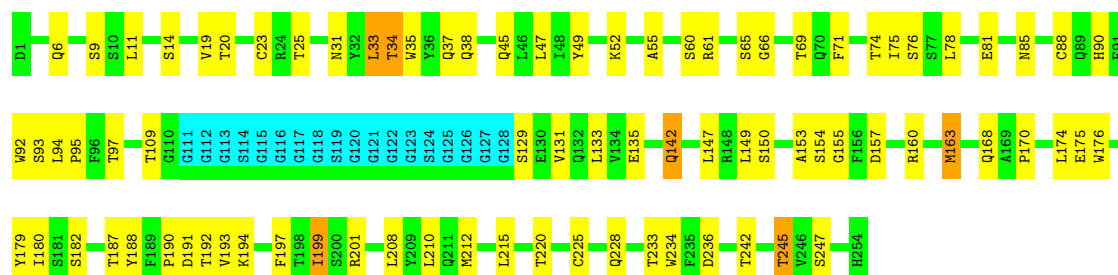
4.2.75 Score per residue for model 75

- Molecule 1: Interleukin-1 beta

Chain A:  81% 18%

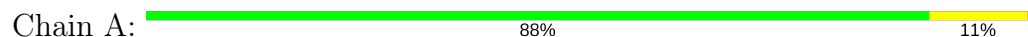


- Molecule 2: scFv

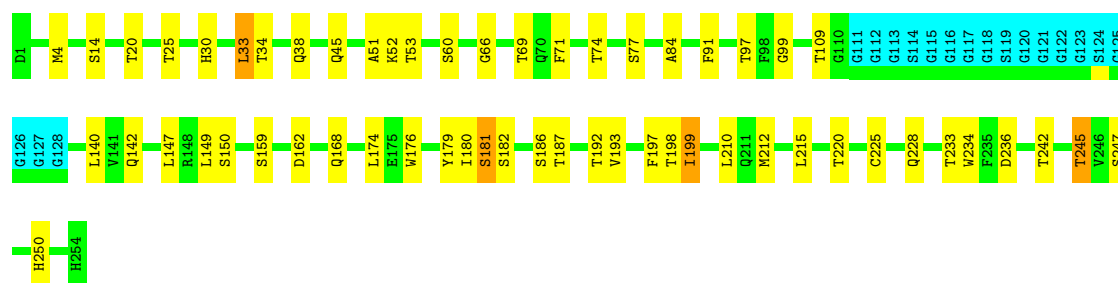


4.2.76 Score per residue for model 76

- Molecule 1: Interleukin-1 beta

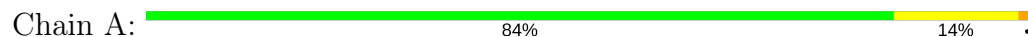


- Molecule 2: scFv

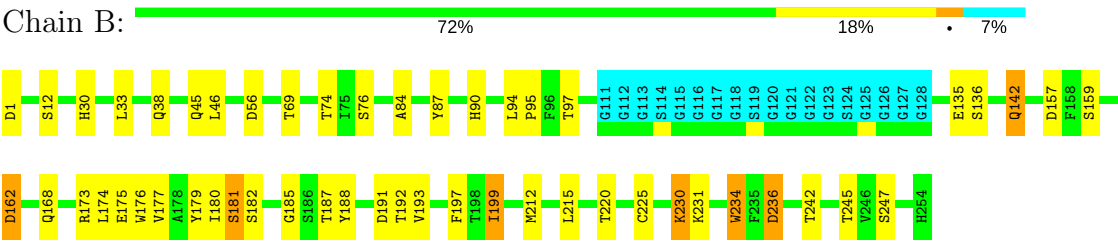


4.2.77 Score per residue for model 77

- Molecule 1: Interleukin-1 beta



- Molecule 2: scFv



5 Refinement protocol and experimental data overview

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

Of the 77 calculated structures, 77 were deposited, based on the following criterion: *all calculated structures submitted*.

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

Software name	Classification	Version
Haddock	structure solution	2.0
Haddock	refinement	2.0

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 [i](#)

6.1 Standard geometry [i](#)

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

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
1	A	0.1±0.5	0.0±0.0
2	B	0.0±0.2	0.0±0.0
All	All	8	0

There are no bond-length outliers.

There are no bond-angle outliers.

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

Mol	Chain	Res	Type	Atoms	Models (Total)
2	B	76	SER	CA	1
1	A	58	VAL	CA	1
1	A	59	ALA	CA	1
1	A	1	ALA	CA	1
1	A	4	ARG	CA	1
1	A	6	LEU	CA	1
1	A	7	ASN	CA	1
2	B	205	LYS	CA	1

There are no planarity outliers.

6.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1219	1238	1218	9±3
2	B	1854	1801	1773	20±5

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Mol	Chain	Non-H	H(model)	H(added)	Clashes
All	All	236621	234003	230307	2095

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 4.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:94:LEU:HG	2:B:95:PRO:HA	0.94	1.36	58	32
1:A:12:ASP:HB2	1:A:143:ILE:HG21	0.84	1.48	55	51
1:A:108:ASN:HB3	2:B:185:GLY:HA3	0.83	1.49	23	10
2:B:142:GLN:HG2	2:B:248:SER:HA	0.81	1.49	54	5
2:B:168:GLN:HB2	2:B:174:LEU:HG	0.80	1.54	31	9
2:B:180:ILE:HB	2:B:199:ILE:HG13	0.77	1.55	50	24
2:B:212:MET:HB3	2:B:215:LEU:HD21	0.76	1.56	51	72
1:A:104:ILE:HB	1:A:111:GLU:HG3	0.71	1.61	42	4
2:B:49:TYR:HE1	2:B:55:ALA:HA	0.71	1.44	63	31
2:B:180:ILE:HB	2:B:199:ILE:HD12	0.71	1.61	67	2
1:A:63:LYS:HG2	1:A:64:GLU:HG2	0.71	1.62	45	2
1:A:109:LYS:HE3	1:A:147:THR:HG23	0.69	1.62	64	7
2:B:202:ASP:HB2	2:B:209:TYR:HE2	0.69	1.48	18	6
2:B:52:LYS:HG2	2:B:65:SER:HA	0.69	1.64	46	5
2:B:157:ASP:HB2	2:B:160:ARG:HB3	0.69	1.64	70	23
2:B:4:MET:HB2	2:B:99:GLY:HA2	0.69	1.65	37	6
2:B:227:ARG:HB3	2:B:227:ARG:HH11	0.68	1.48	63	1
1:A:102:ASN:HB2	1:A:113:GLU:HB3	0.68	1.63	72	4
2:B:230:LYS:HG3	2:B:231:LYS:H	0.68	1.46	33	8
1:A:4:ARG:HB2	1:A:46:PHE:HD2	0.67	1.48	43	5
2:B:189:PHE:HZ	2:B:197:PHE:HB2	0.67	1.47	17	2
2:B:46:LEU:HD22	2:B:236:ASP:HA	0.67	1.66	62	9
2:B:30:HIS:HA	2:B:68:GLY:HA2	0.67	1.64	70	5
2:B:91:PHE:HB2	2:B:233:THR:HG23	0.67	1.65	76	18
1:A:44:MET:HB2	1:A:58:VAL:HB	0.66	1.65	24	1
1:A:109:LYS:HB3	1:A:145:ASP:HB2	0.66	1.67	29	4
2:B:48:ILE:HG21	2:B:64:GLY:HA3	0.66	1.67	68	7
2:B:34:THR:O	2:B:88:CYS:HA	0.66	1.91	45	5
2:B:165:TRP:HB2	2:B:178:ALA:HB3	0.65	1.68	13	2
1:A:31:LEU:HG	1:A:36:MET:HA	0.65	1.68	57	17
2:B:33:LEU:HD11	2:B:88:CYS:HB2	0.65	1.67	75	11
2:B:39:LYS:HB2	2:B:42:LYS:HB2	0.65	1.68	20	9
1:A:150:PHE:HB3	2:B:94:LEU:HD11	0.65	1.67	6	6
2:B:66:GLY:HA3	2:B:71:PHE:HA	0.65	1.68	68	59

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:180:ILE:HD11	2:B:201:ARG:HB3	0.64	1.70	1	15
2:B:157:ASP:HB3	2:B:160:ARG:HB3	0.64	1.70	54	10
1:A:150:PHE:HB3	2:B:94:LEU:HD21	0.64	1.69	18	1
1:A:105:GLU:HA	1:A:110:LEU:HA	0.64	1.69	73	1
2:B:29:ILE:HB	2:B:32:TYR:HB2	0.64	1.68	56	13
2:B:168:GLN:HB2	2:B:174:LEU:HD23	0.64	1.68	17	40
2:B:33:LEU:HD11	2:B:88:CYS:HB3	0.63	1.69	27	18
1:A:4:ARG:HB2	2:B:92:TRP:HZ3	0.63	1.53	27	1
1:A:86:ASP:OD2	1:A:88:LYS:HG2	0.63	1.93	61	61
2:B:229:ASN:HD22	2:B:236:ASP:HB3	0.63	1.51	35	3
2:B:163:MET:HG2	2:B:180:ILE:HG23	0.63	1.69	18	6
1:A:54:ASP:HA	2:B:231:LYS:NZ	0.63	2.07	24	1
1:A:18:LEU:HD23	1:A:28:ALA:HB2	0.62	1.71	70	1
2:B:141:VAL:HG21	2:B:147:LEU:HG	0.62	1.69	16	17
2:B:49:TYR:HE2	2:B:55:ALA:HA	0.62	1.54	57	8
2:B:149:LEU:HD12	2:B:210:LEU:HD23	0.62	1.72	23	48
1:A:149:GLN:HG3	2:B:188:TYR:HD1	0.61	1.55	34	2
2:B:19:VAL:HB	2:B:75:ILE:HB	0.61	1.71	19	8
2:B:220:THR:HG23	2:B:245:THR:HA	0.61	1.71	71	41
2:B:176:TRP:HZ2	2:B:179:TYR:HB2	0.61	1.54	75	19
2:B:12:SER:HB3	2:B:107:LYS:HD3	0.61	1.71	12	3
2:B:142:GLN:HA	2:B:247:SER:O	0.60	1.97	49	60
2:B:44:PRO:HD2	2:B:238:TRP:HB2	0.60	1.73	19	6
1:A:21:SER:HB2	1:A:27:LYS:HG3	0.60	1.71	39	21
2:B:95:PRO:O	2:B:96:PHE:HB2	0.60	1.96	29	1
2:B:94:LEU:CG	2:B:95:PRO:HA	0.60	2.21	41	20
2:B:198:THR:HB	2:B:211:GLN:HB3	0.60	1.73	39	22
2:B:33:LEU:HB3	2:B:51:ALA:HB2	0.59	1.73	66	6
1:A:54:ASP:HB2	1:A:105:GLU:HB2	0.59	1.74	66	1
1:A:97:LYS:HE3	1:A:115:ALA:HB1	0.59	1.73	46	2
2:B:35:TRP:HB2	2:B:48:ILE:HB	0.59	1.73	6	21
2:B:191:ASP:HA	2:B:194:LYS:HD2	0.59	1.72	71	15
2:B:162:ASP:OD1	2:B:181:SER:HA	0.59	1.98	48	26
2:B:37:GLN:HB2	2:B:47:LEU:HD11	0.59	1.74	45	7
1:A:4:ARG:HB2	2:B:92:TRP:CZ2	0.59	2.33	55	2
2:B:170:PRO:HD3	2:B:221:ALA:HA	0.58	1.76	32	3
2:B:157:ASP:HB3	2:B:160:ARG:HB2	0.58	1.75	71	7
2:B:230:LYS:HB2	2:B:234:TRP:HE1	0.58	1.59	11	2
2:B:230:LYS:HD3	2:B:234:TRP:HZ2	0.58	1.58	77	6
1:A:105:GLU:HG2	1:A:110:LEU:HD22	0.58	1.74	69	6
2:B:178:ALA:HB3	2:B:199:ILE:HD11	0.58	1.73	52	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:110:LEU:HD21	1:A:148:MET:HB2	0.58	1.74	5	4
2:B:39:LYS:HG2	2:B:84:ALA:HB2	0.58	1.74	58	3
1:A:105:GLU:HB3	1:A:110:LEU:HB3	0.58	1.76	73	2
1:A:56:ILE:HB	1:A:103:LYS:HE3	0.58	1.76	15	8
2:B:18:ARG:HH11	2:B:76:SER:HA	0.58	1.59	12	1
2:B:46:LEU:HD21	2:B:49:TYR:HB3	0.58	1.75	16	3
1:A:4:ARG:HB3	2:B:92:TRP:CH2	0.57	2.34	18	1
1:A:92:LYS:HE3	1:A:95:MET:HA	0.57	1.76	5	40
1:A:4:ARG:HB3	2:B:92:TRP:CZ2	0.57	2.34	75	13
2:B:80:PRO:HA	2:B:106:ILE:HD13	0.57	1.76	57	8
2:B:190:PRO:HG2	2:B:193:VAL:HG22	0.57	1.76	48	6
1:A:149:GLN:HG3	2:B:188:TYR:CD1	0.57	2.34	34	3
1:A:97:LYS:HA	1:A:100:VAL:HG23	0.57	1.76	24	1
2:B:34:THR:HB	2:B:89:GLN:HB3	0.57	1.76	69	3
2:B:87:TYR:HB3	2:B:98:PHE:HD2	0.57	1.58	48	1
1:A:96:GLU:HB2	1:A:99:PHE:HD2	0.57	1.60	40	26
1:A:86:ASP:OD1	1:A:88:LYS:HG2	0.56	2.00	27	3
2:B:176:TRP:CZ2	2:B:179:TYR:HB2	0.56	2.35	75	14
2:B:135:GLU:HG2	2:B:225:CYS:HB3	0.56	1.76	68	1
1:A:108:ASN:HB3	2:B:185:GLY:CA	0.56	2.30	17	1
2:B:163:MET:HG3	2:B:208:LEU:HD11	0.56	1.76	10	4
1:A:147:THR:HB	2:B:186:SER:HA	0.56	1.77	22	4
1:A:55:LYS:HE2	1:A:102:ASN:HB3	0.56	1.76	67	7
1:A:21:SER:HB2	1:A:27:LYS:HE2	0.56	1.78	35	3
2:B:172:LYS:HG2	2:B:173:ARG:H	0.55	1.61	38	22
1:A:55:LYS:HG2	1:A:104:ILE:HG12	0.55	1.79	25	6
2:B:46:LEU:HD11	2:B:49:TYR:HB3	0.55	1.79	19	10
2:B:140:LEU:HD12	2:B:245:THR:HB	0.55	1.78	71	2
2:B:85:ASN:HB2	2:B:87:TYR:HE1	0.55	1.62	26	3
2:B:202:ASP:HB2	2:B:209:TYR:CE2	0.55	2.35	33	3
2:B:38:GLN:O	2:B:84:ALA:HB1	0.55	2.02	8	19
2:B:193:VAL:HB	2:B:197:PHE:HD2	0.55	1.62	52	8
1:A:74:LYS:HD2	1:A:79:THR:HB	0.55	1.79	13	4
2:B:11:LEU:HD11	2:B:19:VAL:HG13	0.55	1.78	45	8
1:A:8:CYS:HB3	1:A:150:PHE:HD1	0.54	1.62	45	1
2:B:98:PHE:HB2	2:B:174:LEU:HB2	0.54	1.78	8	3
1:A:86:ASP:HB3	1:A:89:ASN:HB2	0.54	1.78	39	13
2:B:169:ALA:HB3	2:B:172:LYS:HB3	0.54	1.78	7	6
1:A:6:LEU:HB3	1:A:150:PHE:HE1	0.54	1.63	74	1
2:B:94:LEU:HB3	2:B:95:PRO:HA	0.54	1.79	59	5
2:B:46:LEU:HB2	2:B:236:ASP:HA	0.54	1.78	19	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:157:ASP:CB	2:B:160:ARG:HB3	0.54	2.33	43	11
1:A:126:GLN:HE22	1:A:143:ILE:HG13	0.54	1.63	62	1
1:A:63:LYS:O	1:A:64:GLU:HG2	0.53	2.03	5	25
2:B:1:ASP:HB3	2:B:95:PRO:HD3	0.53	1.81	77	8
2:B:153:ALA:HB1	2:B:156:PHE:CZ	0.53	2.39	33	3
1:A:6:LEU:HD12	1:A:44:MET:HB3	0.53	1.80	77	2
1:A:4:ARG:HB2	2:B:92:TRP:HZ2	0.53	1.63	68	1
2:B:142:GLN:HG2	2:B:143:PRO:HD2	0.53	1.78	18	2
2:B:162:ASP:OD2	2:B:181:SER:HA	0.53	2.04	24	3
1:A:28:ALA:HB3	1:A:124:THR:HG21	0.52	1.80	3	2
2:B:179:TYR:HB3	2:B:188:TYR:HB2	0.52	1.80	77	10
2:B:94:LEU:HG	2:B:95:PRO:CA	0.52	2.31	19	4
2:B:141:VAL:O	2:B:246:VAL:HA	0.52	2.04	41	15
1:A:97:LYS:HE2	1:A:115:ALA:HB1	0.52	1.80	26	4
2:B:52:LYS:HG3	2:B:64:GLY:O	0.52	2.04	67	3
1:A:46:PHE:HE2	2:B:92:TRP:HE1	0.52	1.47	28	4
2:B:226:ALA:HB1	2:B:235:PHE:CD1	0.52	2.40	72	17
2:B:229:ASN:ND2	2:B:236:ASP:HB3	0.52	2.19	37	2
2:B:168:GLN:HB3	2:B:224:TYR:HE1	0.51	1.65	12	14
1:A:125:SER:HB2	1:A:130:MET:HG3	0.51	1.82	34	4
2:B:193:VAL:HB	2:B:197:PHE:CD1	0.51	2.40	77	15
1:A:56:ILE:HD11	2:B:231:LYS:NZ	0.51	2.20	72	3
1:A:123:SER:HA	1:A:143:ILE:O	0.51	2.05	37	36
1:A:138:LYS:HG3	1:A:144:THR:HB	0.51	1.82	1	1
1:A:105:GLU:HG2	1:A:110:LEU:HB3	0.51	1.82	52	3
2:B:89:GLN:HG2	2:B:90:HIS:N	0.51	2.20	68	4
1:A:48:GLN:HB3	1:A:94:LYS:HD3	0.51	1.82	17	1
2:B:43:ALA:HB1	2:B:238:TRP:HB2	0.51	1.82	5	2
2:B:182:SER:HA	2:B:201:ARG:CZ	0.51	2.35	74	15
2:B:142:GLN:HG3	2:B:248:SER:HA	0.51	1.81	10	1
1:A:105:GLU:HG3	1:A:110:LEU:HB3	0.51	1.83	25	1
2:B:176:TRP:CH2	2:B:179:TYR:HB2	0.51	2.40	10	8
1:A:106:ILE:HG13	1:A:107:ASN:H	0.51	1.66	24	7
1:A:147:THR:HB	1:A:149:GLN:OE1	0.51	2.06	56	2
1:A:14:GLN:HB3	1:A:16:LYS:HG3	0.51	1.82	49	2
1:A:150:PHE:CE2	2:B:93:SER:HA	0.51	2.40	33	1
1:A:45:SER:HB2	1:A:59:ALA:HB3	0.51	1.83	9	1
1:A:108:ASN:OD1	2:B:183:GLY:HA3	0.50	2.06	50	1
1:A:4:ARG:NH1	2:B:30:HIS:HB2	0.50	2.21	71	3
1:A:109:LYS:HE3	1:A:147:THR:HG22	0.50	1.84	75	2
2:B:38:GLN:HB2	2:B:44:PRO:HB3	0.50	1.83	41	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:138:LYS:HA	1:A:144:THR:HG21	0.50	1.82	18	3
2:B:169:ALA:HB3	2:B:172:LYS:HE3	0.50	1.84	73	2
2:B:80:PRO:HA	2:B:106:ILE:HG12	0.50	1.83	43	2
1:A:9:THR:HG21	1:A:39:GLN:HG3	0.50	1.84	1	1
1:A:41:VAL:HB	1:A:63:LYS:HD3	0.50	1.82	63	3
2:B:14:SER:O	2:B:17:ASP:HB2	0.50	2.06	10	4
1:A:73:LEU:HG	1:A:117:PHE:CZ	0.50	2.41	37	15
1:A:44:MET:HA	1:A:59:ALA:O	0.50	2.07	51	1
2:B:151:CYS:HB3	2:B:208:LEU:HB2	0.50	1.84	68	1
2:B:100:GLN:HA	2:B:173:ARG:HD3	0.50	1.84	32	1
1:A:1:ALA:N	1:A:2:PRO:HD3	0.49	2.21	68	1
1:A:14:GLN:HB2	1:A:16:LYS:HD3	0.49	1.81	72	1
2:B:199:ILE:HD13	2:B:199:ILE:H	0.49	1.67	8	15
2:B:133:LEU:HB2	2:B:239:GLY:HA2	0.49	1.84	35	1
2:B:25:THR:HG23	2:B:69:THR:HA	0.49	1.83	45	4
1:A:107:ASN:O	1:A:108:ASN:HB2	0.49	2.08	63	1
2:B:47:LEU:HA	2:B:58:VAL:HG21	0.49	1.84	2	4
1:A:47:VAL:HA	1:A:93:LYS:O	0.49	2.07	35	5
1:A:108:ASN:OD1	2:B:181:SER:HB2	0.49	2.08	7	1
1:A:55:LYS:HE2	1:A:104:ILE:HG12	0.49	1.83	62	2
2:B:193:VAL:HB	2:B:197:PHE:CD2	0.49	2.42	26	7
2:B:94:LEU:CB	2:B:95:PRO:HA	0.49	2.38	13	4
2:B:89:GLN:HG2	2:B:90:HIS:H	0.49	1.68	68	2
2:B:191:ASP:HA	2:B:194:LYS:HE3	0.49	1.84	1	1
1:A:22:GLY:H	1:A:25:GLU:HB3	0.49	1.67	22	7
2:B:167:ARG:HH12	2:B:219:ASP:HA	0.49	1.68	9	3
1:A:70:SER:HB2	1:A:99:PHE:CE1	0.49	2.42	55	1
2:B:33:LEU:CD1	2:B:88:CYS:HB2	0.49	2.37	45	1
1:A:27:LYS:HA	1:A:131:PRO:HA	0.49	1.85	70	8
1:A:103:LYS:HD2	1:A:110:LEU:HD13	0.49	1.84	54	2
2:B:189:PHE:HE1	2:B:199:ILE:HD12	0.49	1.68	46	3
1:A:113:GLU:HB2	1:A:121:TYR:CE2	0.49	2.43	36	9
2:B:132:GLN:HA	2:B:237:TYR:OH	0.49	2.08	61	4
2:B:227:ARG:HB3	2:B:227:ARG:NH1	0.49	2.21	63	1
2:B:52:LYS:HG2	2:B:64:GLY:O	0.48	2.08	1	2
1:A:111:GLU:HG2	1:A:145:ASP:HA	0.48	1.83	17	2
1:A:46:PHE:HA	1:A:58:VAL:HG12	0.48	1.85	71	1
1:A:17:SER:HB2	1:A:31:LEU:HD22	0.48	1.85	72	1
2:B:94:LEU:HD21	2:B:190:PRO:HA	0.48	1.85	15	2
2:B:12:SER:HA	2:B:105:GLU:O	0.48	2.08	62	5
2:B:189:PHE:O	2:B:194:LYS:HE3	0.48	2.09	73	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:176:TRP:HE3	2:B:190:PRO:HG3	0.48	1.67	64	3
1:A:20:MET:HG2	1:A:40:VAL:HG21	0.48	1.85	28	6
2:B:189:PHE:HE2	2:B:199:ILE:HD12	0.48	1.68	43	1
1:A:150:PHE:HB3	2:B:94:LEU:HD13	0.48	1.83	33	1
2:B:6:GLN:OE1	2:B:99:GLY:HA3	0.48	2.08	63	1
2:B:140:LEU:HD11	2:B:247:SER:HB2	0.48	1.86	60	8
2:B:156:PHE:CE2	2:B:227:ARG:HD2	0.48	2.43	16	1
2:B:50:ASN:HA	2:B:91:PHE:HZ	0.48	1.69	74	2
1:A:21:SER:OG	1:A:27:LYS:HE2	0.48	2.08	72	1
1:A:104:ILE:HB	1:A:111:GLU:HB2	0.48	1.84	53	4
1:A:54:ASP:HA	1:A:105:GLU:HB2	0.48	1.84	77	1
2:B:223:TYR:O	2:B:241:GLY:HA2	0.48	2.09	65	7
2:B:13:ALA:HB3	2:B:78:LEU:HD22	0.48	1.85	71	2
1:A:6:LEU:O	1:A:7:ASN:HB3	0.48	2.08	68	1
1:A:110:LEU:HD12	1:A:148:MET:HB2	0.48	1.85	54	1
2:B:135:GLU:CG	2:B:225:CYS:HB2	0.48	2.38	18	9
1:A:6:LEU:HG	1:A:44:MET:HB2	0.48	1.85	52	2
2:B:29:ILE:HG22	2:B:92:TRP:HB3	0.47	1.86	32	1
1:A:123:SER:HB3	1:A:142:ASP:HB3	0.47	1.85	39	1
2:B:16:GLY:HA2	2:B:77:SER:HB3	0.47	1.85	44	2
2:B:39:LYS:HE2	2:B:81:GLU:O	0.47	2.08	60	1
2:B:1:ASP:HB2	2:B:95:PRO:HD3	0.47	1.85	40	1
1:A:4:ARG:HB2	1:A:46:PHE:HB2	0.47	1.86	14	1
2:B:96:PHE:CE1	2:B:233:THR:HG21	0.47	2.44	68	2
2:B:61:ARG:O	2:B:75:ILE:HA	0.47	2.09	74	4
2:B:12:SER:HB3	2:B:107:LYS:HD2	0.47	1.86	73	5
1:A:147:THR:HB	2:B:188:TYR:CE1	0.47	2.44	52	1
2:B:142:GLN:HG3	2:B:249:HIS:HD2	0.47	1.70	30	3
2:B:38:GLN:HB3	2:B:85:ASN:OD1	0.47	2.09	16	4
1:A:36:MET:HG2	1:A:39:GLN:NE2	0.47	2.24	70	1
2:B:46:LEU:HB2	2:B:235:PHE:O	0.47	2.10	16	1
1:A:153:SER:H	2:B:94:LEU:HD13	0.47	1.69	34	1
1:A:109:LYS:HE3	1:A:147:THR:CG2	0.47	2.40	25	6
1:A:104:ILE:HD12	1:A:121:TYR:CE2	0.47	2.44	35	1
2:B:177:VAL:O	2:B:193:VAL:HG21	0.47	2.08	20	3
1:A:4:ARG:HB2	1:A:46:PHE:CD2	0.47	2.45	44	3
1:A:96:GLU:O	1:A:100:VAL:HG23	0.47	2.10	72	1
1:A:6:LEU:HD12	1:A:44:MET:HB2	0.47	1.86	25	3
2:B:157:ASP:CB	2:B:160:ARG:HB2	0.47	2.40	4	2
1:A:104:ILE:HD12	1:A:121:TYR:HE2	0.47	1.70	35	3
2:B:24:ARG:HG2	2:B:69:THR:O	0.47	2.10	58	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:152:SER:HA	2:B:94:LEU:HD13	0.47	1.86	60	3
1:A:55:LYS:HD3	1:A:102:ASN:HB3	0.47	1.87	46	1
2:B:29:ILE:HG22	2:B:92:TRP:HB2	0.47	1.87	40	1
2:B:5:THR:HA	2:B:100:GLN:OE1	0.46	2.10	63	2
2:B:176:TRP:CE3	2:B:190:PRO:HG3	0.46	2.45	35	5
1:A:149:GLN:HG3	2:B:188:TYR:CE1	0.46	2.45	56	1
2:B:141:VAL:HG12	2:B:142:GLN:H	0.46	1.69	23	1
2:B:50:ASN:HB3	2:B:53:THR:HG22	0.46	1.88	16	5
2:B:133:LEU:HD23	2:B:153:ALA:HA	0.46	1.87	75	10
1:A:105:GLU:HG3	1:A:110:LEU:HD22	0.46	1.87	21	1
2:B:86:TYR:O	2:B:101:GLY:HA2	0.46	2.11	44	6
1:A:106:ILE:HD12	1:A:109:LYS:HG2	0.46	1.87	40	1
1:A:106:ILE:HG22	1:A:107:ASN:H	0.46	1.71	40	1
1:A:55:LYS:HB2	1:A:104:ILE:HG12	0.46	1.86	1	1
1:A:20:MET:HG2	1:A:40:VAL:HG22	0.46	1.88	6	1
2:B:45:GLN:HE22	2:B:237:TYR:HD1	0.46	1.53	21	1
2:B:163:MET:HB2	2:B:180:ILE:HG23	0.46	1.87	44	3
1:A:4:ARG:HB3	2:B:92:TRP:HZ2	0.46	1.71	59	3
1:A:4:ARG:HB3	2:B:92:TRP:NE1	0.46	2.26	30	1
2:B:193:VAL:HB	2:B:197:PHE:HD1	0.46	1.71	18	4
2:B:228:GLN:HG3	2:B:234:TRP:O	0.46	2.11	36	3
2:B:227:ARG:O	2:B:235:PHE:HA	0.46	2.10	39	4
2:B:49:TYR:CE1	2:B:55:ALA:HA	0.46	2.43	75	4
1:A:62:LEU:HB3	1:A:65:LYS:HD2	0.46	1.87	18	1
1:A:54:ASP:O	1:A:104:ILE:HA	0.46	2.11	49	2
1:A:35:ASP:HB3	1:A:38:GLN:HE21	0.46	1.71	1	1
2:B:153:ALA:HB1	2:B:156:PHE:CE1	0.45	2.46	73	2
2:B:32:TYR:O	2:B:90:HIS:HA	0.45	2.11	22	3
2:B:149:LEU:HB2	2:B:210:LEU:HB3	0.45	1.87	3	4
1:A:6:LEU:HD13	1:A:150:PHE:HE1	0.45	1.71	58	3
1:A:108:ASN:HB2	2:B:181:SER:HB3	0.45	1.87	36	1
1:A:6:LEU:HD23	2:B:93:SER:OG	0.45	2.11	75	1
2:B:48:ILE:HD13	2:B:54:LEU:HG	0.45	1.87	68	2
1:A:20:MET:SD	1:A:26:LEU:HG	0.45	2.50	55	1
2:B:132:GLN:HA	2:B:237:TYR:CE2	0.45	2.47	23	1
1:A:24:TYR:HE1	1:A:67:LEU:HD22	0.45	1.71	63	1
1:A:50:GLU:O	1:A:57:PRO:HD3	0.45	2.11	64	2
1:A:118:PRO:O	1:A:119:ASN:HB2	0.45	2.11	3	4
1:A:109:LYS:HG3	1:A:145:ASP:HB2	0.45	1.88	40	1
2:B:230:LYS:CG	2:B:231:LYS:H	0.45	2.22	33	1
1:A:55:LYS:HE3	1:A:104:ILE:HG12	0.45	1.88	31	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:36:TYR:OH	2:B:234:TRP:HB2	0.45	2.11	14	1
1:A:96:GLU:HB2	1:A:99:PHE:CD2	0.45	2.46	43	4
2:B:199:ILE:H	2:B:199:ILE:HD13	0.45	1.71	3	5
2:B:182:SER:HA	2:B:201:ARG:NH2	0.45	2.26	66	2
1:A:52:SER:HB2	1:A:55:LYS:HB2	0.44	1.90	13	1
2:B:35:TRP:CD1	2:B:48:ILE:HB	0.44	2.47	28	2
1:A:7:ASN:HB3	1:A:41:VAL:CG1	0.44	2.43	63	1
2:B:230:LYS:HD3	2:B:234:TRP:CZ2	0.44	2.47	7	1
2:B:172:LYS:HG3	2:B:173:ARG:N	0.44	2.26	71	1
2:B:169:ALA:HB3	2:B:172:LYS:HD2	0.44	1.87	23	2
2:B:143:PRO:HD3	2:B:247:SER:O	0.44	2.13	30	7
2:B:133:LEU:HD13	2:B:225:CYS:HB3	0.44	1.90	10	4
2:B:230:LYS:HE3	2:B:234:TRP:HZ2	0.44	1.72	40	1
2:B:46:LEU:CB	2:B:236:ASP:HA	0.44	2.42	21	1
2:B:21:ILE:HD12	2:B:73:LEU:HD23	0.44	1.89	55	7
2:B:177:VAL:HG12	2:B:193:VAL:HG11	0.44	1.89	3	1
2:B:29:ILE:HD11	2:B:33:LEU:HD23	0.44	1.89	37	2
2:B:131:VAL:HB	2:B:237:TYR:CZ	0.44	2.47	70	1
2:B:44:PRO:HD2	2:B:238:TRP:CD1	0.44	2.48	51	1
1:A:26:LEU:HD12	1:A:82:LEU:HD21	0.44	1.90	54	1
2:B:34:THR:HB	2:B:36:TYR:CE1	0.44	2.48	2	2
2:B:190:PRO:HD2	2:B:193:VAL:HG22	0.44	1.88	2	2
1:A:55:LYS:HA	1:A:103:LYS:O	0.44	2.13	35	2
2:B:23:CYS:HB2	2:B:35:TRP:CH2	0.44	2.48	75	2
1:A:150:PHE:HE2	2:B:93:SER:HA	0.44	1.73	33	1
1:A:58:VAL:HG23	1:A:59:ALA:N	0.44	2.28	63	1
1:A:47:VAL:HG21	1:A:100:VAL:HG13	0.44	1.90	72	1
2:B:85:ASN:HB2	2:B:87:TYR:CE1	0.43	2.46	26	1
2:B:35:TRP:HD1	2:B:48:ILE:HB	0.43	1.73	15	1
2:B:131:VAL:HG13	2:B:156:PHE:CD2	0.43	2.48	17	1
2:B:189:PHE:CD1	2:B:194:LYS:HG2	0.43	2.48	20	2
1:A:93:LYS:HE2	1:A:93:LYS:HA	0.43	1.89	51	3
1:A:104:ILE:O	1:A:110:LEU:HA	0.43	2.13	16	1
1:A:108:ASN:ND2	2:B:183:GLY:HA3	0.43	2.28	16	1
2:B:176:TRP:HE1	2:B:235:PHE:HZ	0.43	1.55	39	1
1:A:127:ALA:HB3	1:A:130:MET:HG3	0.43	1.89	57	2
1:A:26:LEU:HD11	1:A:62:LEU:HD11	0.43	1.90	70	1
2:B:19:VAL:HG21	2:B:78:LEU:HD13	0.43	1.90	75	3
1:A:12:ASP:OD2	1:A:16:LYS:HB2	0.43	2.12	52	2
2:B:180:ILE:HB	2:B:199:ILE:CG1	0.43	2.41	64	1
1:A:93:LYS:HA	1:A:93:LYS:HE3	0.43	1.90	71	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:162:ASP:HB3	2:B:228:GLN:NE2	0.43	2.28	52	1
1:A:108:ASN:HD21	2:B:183:GLY:HA3	0.43	1.73	29	1
2:B:190:PRO:HD2	2:B:193:VAL:CG2	0.43	2.43	2	2
2:B:135:GLU:HG2	2:B:225:CYS:HB2	0.43	1.90	18	2
2:B:98:PHE:CD1	2:B:174:LEU:HB2	0.43	2.49	62	3
2:B:6:GLN:HG2	2:B:88:CYS:SG	0.43	2.53	75	1
1:A:147:THR:HG22	2:B:188:TYR:CE1	0.43	2.47	26	2
2:B:187:THR:HB	2:B:189:PHE:CE2	0.43	2.49	60	1
1:A:63:LYS:C	1:A:64:GLU:HG2	0.43	2.34	77	2
1:A:63:LYS:O	1:A:65:LYS:HG2	0.43	2.14	64	1
2:B:189:PHE:CZ	2:B:197:PHE:HB2	0.43	2.48	51	2
2:B:157:ASP:OD1	2:B:160:ARG:HD3	0.43	2.14	57	3
1:A:1:ALA:HB3	2:B:28:ASN:HB2	0.43	1.90	55	1
2:B:157:ASP:HB2	2:B:160:ARG:HB2	0.43	1.90	42	1
2:B:150:SER:HA	2:B:208:LEU:O	0.43	2.14	40	3
2:B:200:SER:HB2	2:B:209:TYR:HB2	0.43	1.90	55	3
2:B:80:PRO:HA	2:B:106:ILE:CD1	0.43	2.43	49	1
2:B:61:ARG:HD2	2:B:77:SER:O	0.43	2.14	31	1
2:B:91:PHE:CE2	2:B:232:LEU:HD13	0.42	2.49	41	1
2:B:189:PHE:HZ	2:B:199:ILE:HD12	0.42	1.73	13	1
1:A:51:GLU:HA	1:A:57:PRO:HD3	0.42	1.90	25	2
2:B:36:TYR:HE2	2:B:235:PHE:O	0.42	1.97	33	1
2:B:163:MET:SD	2:B:227:ARG:HG3	0.42	2.54	69	1
2:B:16:GLY:HA2	2:B:77:SER:OG	0.42	2.14	62	2
2:B:161:TYR:CD1	2:B:229:ASN:HA	0.42	2.49	63	1
1:A:108:ASN:O	2:B:185:GLY:HA3	0.42	2.14	14	1
2:B:142:GLN:HG3	2:B:143:PRO:HD2	0.42	1.91	66	2
1:A:110:LEU:HG	1:A:146:PHE:O	0.42	2.15	72	1
2:B:216:ARG:HB2	2:B:218:GLU:HG2	0.42	1.90	36	1
2:B:37:GLN:HB2	2:B:47:LEU:CD1	0.42	2.42	75	1
1:A:62:LEU:HD22	1:A:67:LEU:HD12	0.42	1.91	62	2
2:B:189:PHE:CZ	2:B:199:ILE:HD12	0.42	2.50	13	1
1:A:150:PHE:H	2:B:188:TYR:HD1	0.42	1.57	42	1
2:B:87:TYR:OH	2:B:173:ARG:HA	0.42	2.14	77	1
1:A:13:SER:HB3	1:A:109:LYS:NZ	0.42	2.30	68	1
2:B:66:GLY:HA3	2:B:71:PHE:CD1	0.42	2.50	54	1
1:A:105:GLU:HG3	1:A:110:LEU:HG	0.42	1.91	7	1
2:B:12:SER:CB	2:B:107:LYS:HD2	0.42	2.45	24	1
2:B:157:ASP:HB3	2:B:160:ARG:CB	0.42	2.42	54	1
2:B:20:THR:HG23	2:B:74:THR:HG23	0.42	1.91	29	1
2:B:18:ARG:NH1	2:B:76:SER:HA	0.42	2.29	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:235:PHE:HB2	2:B:238:TRP:HE1	0.42	1.74	66	1
2:B:91:PHE:HE2	2:B:232:LEU:HD13	0.42	1.74	41	2
2:B:135:GLU:HA	2:B:151:CYS:HA	0.42	1.90	16	1
1:A:57:PRO:O	1:A:58:VAL:CB	0.42	2.68	63	1
2:B:4:MET:SD	2:B:90:HIS:HD2	0.42	2.38	67	2
1:A:8:CYS:HB3	1:A:150:PHE:CD1	0.42	2.49	75	1
1:A:126:GLN:NE2	1:A:143:ILE:HG13	0.42	2.29	62	1
2:B:147:LEU:HD13	2:B:244:VAL:HG13	0.42	1.92	59	1
2:B:230:LYS:HD3	2:B:234:TRP:HZ3	0.42	1.74	60	1
2:B:94:LEU:HD21	2:B:190:PRO:HB3	0.42	1.90	1	1
2:B:49:TYR:CE2	2:B:55:ALA:HA	0.42	2.43	57	1
1:A:20:MET:SD	1:A:62:LEU:HD21	0.41	2.55	54	2
2:B:33:LEU:HD22	2:B:89:GLN:O	0.41	2.15	16	4
2:B:52:LYS:HE2	2:B:65:SER:HA	0.41	1.92	74	3
2:B:13:ALA:O	2:B:106:ILE:HA	0.41	2.15	49	1
1:A:7:ASN:HB3	1:A:41:VAL:HG11	0.41	1.91	63	1
1:A:121:TYR:CE2	1:A:138:LYS:HB2	0.41	2.50	60	2
2:B:140:LEU:HA	2:B:245:THR:O	0.41	2.15	15	1
1:A:70:SER:HB3	1:A:81:GLN:HG3	0.41	1.92	31	1
1:A:121:TYR:HB2	1:A:144:THR:HG22	0.41	1.93	58	1
2:B:143:PRO:HA	2:B:246:VAL:HG12	0.41	1.92	42	1
2:B:167:ARG:HA	2:B:222:VAL:O	0.41	2.16	37	1
2:B:135:GLU:HA	2:B:150:SER:O	0.41	2.15	68	1
2:B:18:ARG:HA	2:B:75:ILE:O	0.41	2.15	68	1
1:A:109:LYS:HE3	2:B:185:GLY:HA3	0.41	1.92	63	1
2:B:6:GLN:OE1	2:B:87:TYR:HA	0.41	2.15	25	1
2:B:52:LYS:HE2	2:B:66:GLY:O	0.41	2.15	50	2
1:A:32:GLN:HG2	1:A:33:GLY:H	0.41	1.76	47	1
1:A:57:PRO:O	1:A:58:VAL:HB	0.41	2.16	63	1
2:B:2:ILE:HB	2:B:90:HIS:CE1	0.41	2.50	66	2
1:A:4:ARG:NH2	2:B:30:HIS:HB2	0.41	2.30	43	1
2:B:52:LYS:HB3	2:B:64:GLY:O	0.41	2.14	34	1
1:A:15:GLN:OE1	1:A:15:GLN:HA	0.41	2.15	25	1
2:B:87:TYR:CE1	2:B:101:GLY:HA3	0.41	2.51	43	1
2:B:25:THR:CG2	2:B:69:THR:HA	0.41	2.45	30	2
2:B:2:ILE:HD11	2:B:92:TRP:HE3	0.41	1.75	49	1
2:B:66:GLY:CA	2:B:71:PHE:HA	0.41	2.46	63	1
2:B:130:GLU:O	2:B:155:GLY:HA3	0.41	2.15	7	1
1:A:92:LYS:HG2	1:A:95:MET:SD	0.41	2.56	11	1
2:B:94:LEU:HD12	2:B:94:LEU:H	0.41	1.75	6	1
1:A:149:GLN:HA	2:B:188:TYR:CE1	0.41	2.50	32	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:2:ILE:HG22	2:B:26:SER:HB2	0.41	1.93	2	1
1:A:21:SER:HB2	1:A:27:LYS:HG2	0.41	1.90	70	1
2:B:143:PRO:HA	2:B:246:VAL:CG1	0.41	2.46	42	1
2:B:131:VAL:HA	2:B:155:GLY:HA3	0.41	1.93	75	1
1:A:66:ASN:HB2	1:A:85:VAL:O	0.41	2.15	77	1
2:B:230:LYS:HB3	2:B:231:LYS:H	0.41	1.55	29	1
2:B:172:LYS:HG2	2:B:173:ARG:N	0.41	2.30	18	2
1:A:81:GLN:NE2	1:A:83:GLU:HG3	0.41	2.31	50	1
2:B:78:LEU:HD21	2:B:106:ILE:HG13	0.41	1.92	37	1
2:B:38:GLN:HB3	2:B:85:ASN:ND2	0.41	2.31	75	2
2:B:138:GLY:H	2:B:242:THR:HG21	0.41	1.76	68	1
2:B:34:THR:HB	2:B:36:TYR:HE1	0.40	1.75	2	1
1:A:37:GLU:HA	1:A:37:GLU:OE2	0.40	2.15	26	1
1:A:4:ARG:NH1	2:B:30:HIS:HB3	0.40	2.31	1	1
2:B:55:ALA:HB3	2:B:58:VAL:CG2	0.40	2.46	63	1
2:B:228:GLN:HA	2:B:234:TRP:O	0.40	2.16	39	1
2:B:54:LEU:HD21	2:B:62:PHE:O	0.40	2.15	40	1
2:B:135:GLU:HB2	2:B:242:THR:OG1	0.40	2.16	63	1
2:B:89:GLN:HB2	2:B:97:THR:O	0.40	2.17	74	1
2:B:4:MET:SD	2:B:25:THR:HB	0.40	2.56	4	1
1:A:21:SER:CB	1:A:27:LYS:HE2	0.40	2.46	16	2
2:B:189:PHE:CE1	2:B:199:ILE:HD12	0.40	2.51	11	1
2:B:228:GLN:HG2	2:B:234:TRP:O	0.40	2.16	47	1
2:B:166:VAL:HG12	2:B:176:TRP:HA	0.40	1.93	35	1
1:A:107:ASN:CG	1:A:108:ASN:H	0.40	2.20	12	1
1:A:15:GLN:HA	1:A:15:GLN:OE1	0.40	2.17	33	1
2:B:87:TYR:CD1	2:B:101:GLY:HA3	0.40	2.51	18	1
1:A:106:ILE:HG13	1:A:107:ASN:N	0.40	2.32	66	1
1:A:108:ASN:HB3	2:B:181:SER:HB2	0.40	1.92	22	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	151/153 (99%)	142±2 (94±2%)	9±2 (6±2%)	1±1 (1±1%)	37	78

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	234/254 (92%)	217±3 (93±1%)	15±3 (6±1%)	2±1 (1±0%)	27	73
All	All	29645/31339 (95%)	27623 (93%)	1820 (6%)	202 (1%)	30	75

All 35 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	229	ASN	42
2	B	30	HIS	29
2	B	185	GLY	27
1	A	106	ILE	15
1	A	21	SER	11
1	A	47	VAL	10
2	B	160	ARG	9
2	B	170	PRO	8
1	A	107	ASN	8
2	B	184	GLY	6
2	B	186	SER	6
1	A	2	PRO	4
1	A	108	ASN	3
1	A	53	ASN	2
2	B	182	SER	2
1	A	46	PHE	1
2	B	96	PHE	1
2	B	192	THR	1
2	B	31	ASN	1
2	B	28	ASN	1
1	A	85	VAL	1
1	A	114	SER	1
1	A	58	VAL	1
2	B	241	GLY	1
1	A	49	GLY	1
2	B	27	GLY	1
2	B	177	VAL	1
2	B	97	THR	1
1	A	32	GLN	1
1	A	101	PHE	1
1	A	52	SER	1
2	B	230	LYS	1
1	A	6	LEU	1
2	B	52	LYS	1
1	A	4	ARG	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	140/140 (100%)	128±3 (91±2%)	12±3 (9±2%)	17	62
2	B	200/203 (99%)	171±4 (86±2%)	29±4 (14±2%)	7	47
All	All	26180/26411 (99%)	23050 (88%)	3130 (12%)	10	52

All 197 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)
2	B	199	ILE	73
2	B	192	THR	73
2	B	97	THR	73
2	B	33	LEU	72
2	B	234	TRP	70
2	B	45	GLN	69
1	A	13	SER	67
2	B	25	THR	67
2	B	69	THR	65
1	A	77	LYS	61
2	B	242	THR	58
2	B	60	SER	55
1	A	102	ASN	54
2	B	187	THR	53
2	B	109	THR	52
2	B	150	SER	52
2	B	225	CYS	50
2	B	34	THR	50
1	A	79	THR	50
2	B	14	SER	48
2	B	236	ASP	47
1	A	110	LEU	44
1	A	137	THR	44
2	B	181	SER	43
2	B	147	LEU	42
1	A	119	ASN	38
2	B	245	THR	37
2	B	162	ASP	37

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Mol	Chain	Res	Type	Models (Total)
2	B	74	THR	36
1	A	149	GLN	34
2	B	182	SER	33
1	A	76	ASP	33
2	B	176	TRP	33
2	B	233	THR	32
1	A	6	LEU	32
2	B	81	GLU	32
2	B	9	SER	32
2	B	228	GLN	32
1	A	71	CYS	30
2	B	154	SER	30
1	A	84	SER	30
2	B	5	THR	28
2	B	159	SER	27
2	B	26	SER	26
2	B	20	THR	26
1	A	124	THR	25
2	B	136	SER	25
1	A	152	SER	24
2	B	163	MET	23
2	B	30	HIS	23
2	B	189	PHE	22
1	A	108	ASN	22
2	B	22	THR	22
2	B	186	SER	22
2	B	50	ASN	22
2	B	76	SER	21
1	A	32	GLN	21
1	A	35	ASP	20
1	A	64	GLU	20
2	B	90	HIS	20
1	A	9	THR	19
2	B	17	ASP	19
2	B	230	LYS	18
1	A	144	THR	17
2	B	11	LEU	17
1	A	29	LEU	17
2	B	157	ASP	17
2	B	94	LEU	16
2	B	88	CYS	16
1	A	145	ASP	15

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Mol	Chain	Res	Type	Models (Total)
2	B	129	SER	15
2	B	67	SER	14
2	B	72	THR	14
2	B	56	ASP	14
2	B	214	SER	14
1	A	53	ASN	14
2	B	1	ASP	14
1	A	93	LYS	13
2	B	107	LYS	12
1	A	147	THR	12
2	B	198	THR	12
2	B	7	SER	12
1	A	50	GLU	11
2	B	206	ASN	11
1	A	121	TYR	11
2	B	191	ASP	10
2	B	108	ARG	10
2	B	31	ASN	9
2	B	53	THR	9
2	B	246	VAL	9
1	A	45	SER	9
2	B	63	SER	9
2	B	175	GLU	8
2	B	164	SER	8
2	B	52	LYS	8
2	B	142	GLN	8
2	B	250	HIS	8
2	B	77	SER	7
2	B	227	ARG	7
1	A	5	SER	7
1	A	116	GLN	6
2	B	249	HIS	6
1	A	56	ILE	6
2	B	201	ARG	6
1	A	54	ASP	6
2	B	92	TRP	6
1	A	48	GLN	5
1	A	17	SER	5
1	A	34	GLN	5
2	B	93	SER	5
1	A	150	PHE	5
2	B	24	ARG	5

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Mol	Chain	Res	Type	Models (Total)
2	B	146	SER	5
1	A	39	GLN	5
2	B	166	VAL	5
1	A	125	SER	5
1	A	8	CYS	4
1	A	43	SER	4
2	B	89	GLN	4
2	B	148	ARG	4
1	A	51	GLU	4
1	A	109	LYS	4
1	A	75	ASP	4
1	A	52	SER	4
2	B	247	SER	4
1	A	128	GLU	3
2	B	179	TYR	3
2	B	65	SER	3
1	A	37	GLU	3
1	A	73	LEU	3
2	B	132	GLN	3
1	A	105	GLU	3
1	A	89	ASN	3
2	B	248	SER	3
2	B	231	LYS	3
2	B	70	GLN	3
2	B	173	ARG	3
1	A	142	ASP	3
1	A	123	SER	3
1	A	138	LYS	2
1	A	46	PHE	2
2	B	200	SER	2
2	B	235	PHE	2
1	A	153	SER	2
1	A	106	ILE	2
1	A	55	LYS	2
2	B	85	ASN	2
2	B	130	GLU	2
2	B	12	SER	2
1	A	97	LYS	2
2	B	106	ILE	2
1	A	151	VAL	2
2	B	160	ARG	2
1	A	7	ASN	2

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Mol	Chain	Res	Type	Models (Total)
2	B	141	VAL	2
1	A	19	VAL	1
2	B	103	LYS	1
1	A	25	GLU	1
2	B	240	GLN	1
2	B	2	ILE	1
1	A	41	VAL	1
2	B	140	LEU	1
1	A	30	HIS	1
1	A	26	LEU	1
2	B	203	ASN	1
1	A	81	GLN	1
1	A	66	ASN	1
2	B	174	LEU	1
1	A	92	LYS	1
1	A	58	VAL	1
2	B	135	GLU	1
1	A	36	MET	1
2	B	3	GLN	1
2	B	105	GLU	1
2	B	237	TYR	1
2	B	216	ARG	1
2	B	205	LYS	1
1	A	14	GLN	1
1	A	88	LYS	1
1	A	95	MET	1
1	A	141	GLN	1
2	B	224	TYR	1
1	A	11	ARG	1
1	A	104	ILE	1
1	A	12	ASP	1
2	B	251	HIS	1
1	A	86	ASP	1
2	B	218	GLU	1
1	A	38	GLN	1
1	A	70	SER	1
1	A	31	LEU	1
1	A	4	ARG	1
1	A	20	MET	1
2	B	188	TYR	1
1	A	107	ASN	1
2	B	54	LEU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	21	SER	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