



Full wwPDB NMR Structure Validation Report ⓘ

Mar 26, 2026 – 11:55 AM UTC

PDB ID : 2KH2 / pdb_00002kh2
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

<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

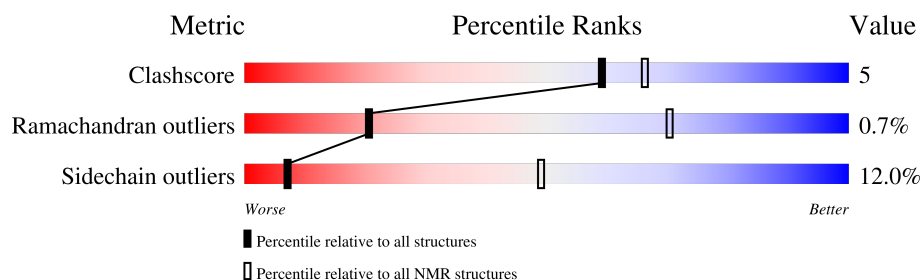
1 Overall quality at a glance

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	153	 88% 12%
2	B	254	 75% 18% 7%

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)	0.97	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	

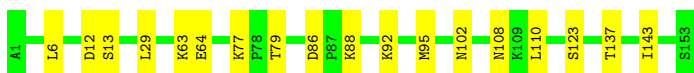
4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, 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.

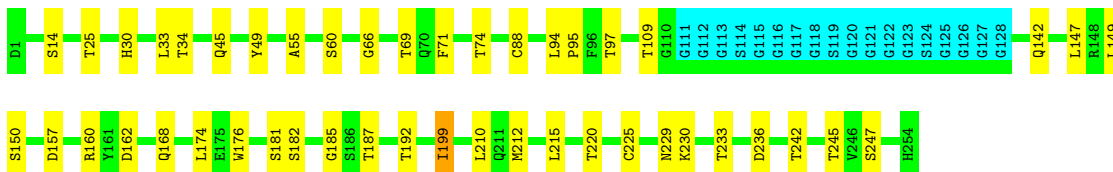
- Molecule 1: Interleukin-1 beta

Chain A:  88% 12%



- Molecule 2: scFv

Chain B:  75% 18% 7%



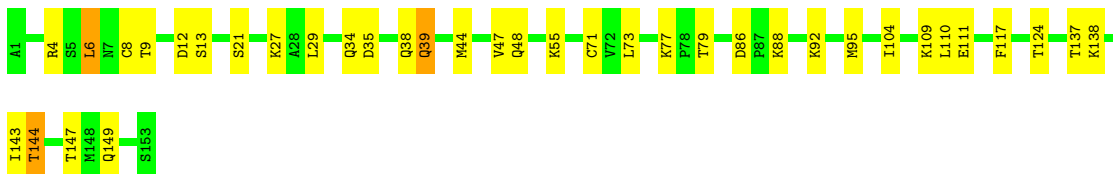
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

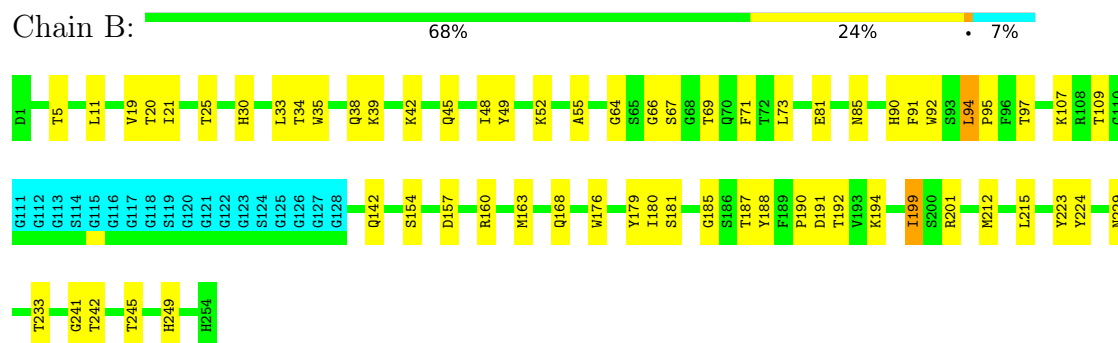
4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Interleukin-1 beta

Chain A:  76% 22% .

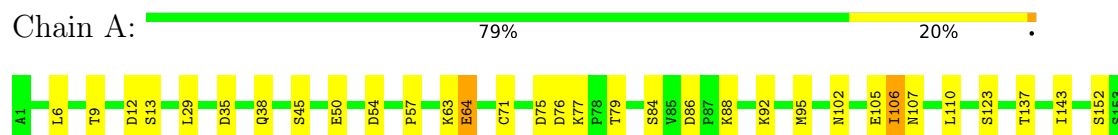


- Molecule 2: scFv

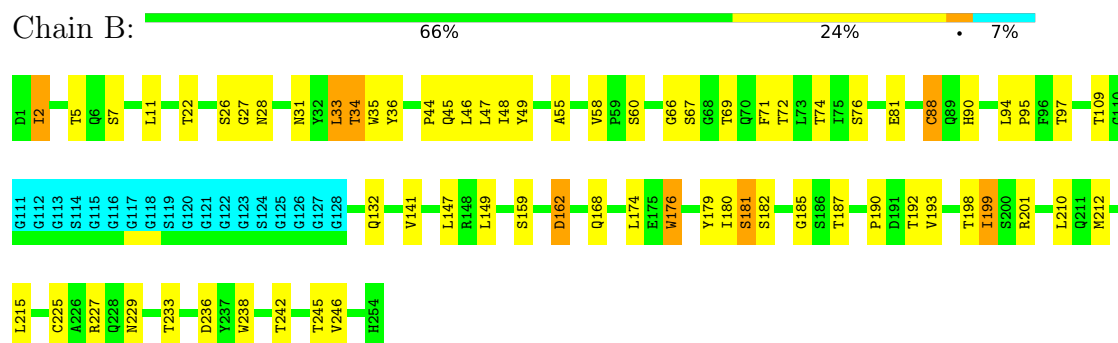


4.2.2 Score per residue for model 2

- Molecule 1: Interleukin-1 beta

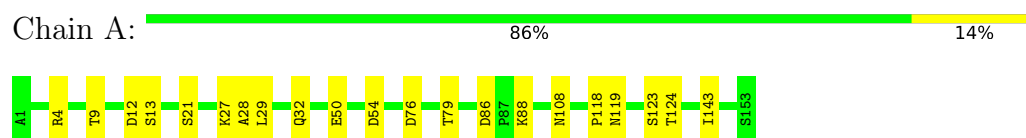


- Molecule 2: scFv

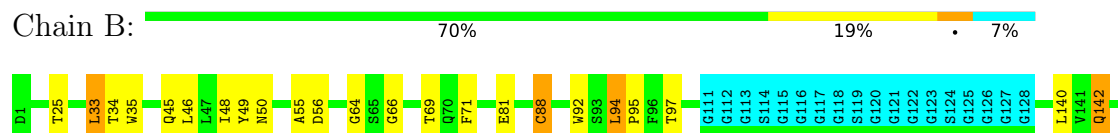


4.2.3 Score per residue for model 3

- Molecule 1: Interleukin-1 beta



- Molecule 2: scFv





4.2.4 Score per residue for model 4

- Molecule 1: Interleukin-1 beta

Chain A: 86% 14%



- Molecule 2: scFv

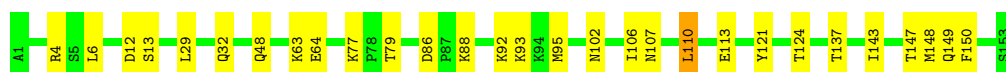
Chain B: 72% 19% 7%



4.2.5 Score per residue for model 5

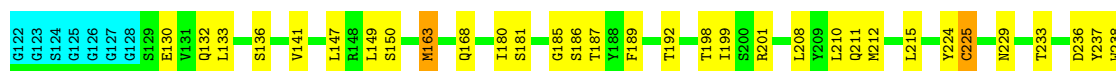
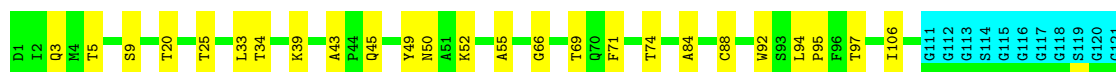
- Molecule 1: Interleukin-1 beta

Chain A: 81% 18%



- Molecule 2: scFv

Chain B: 70% 22% 7%



4.2.6 Score per residue for model 6

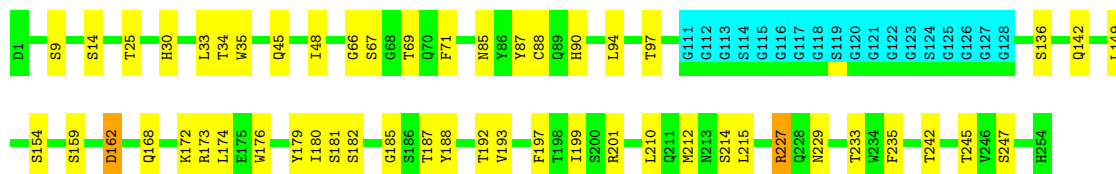
- Molecule 1: Interleukin-1 beta

Chain A:  84% 16%



• Molecule 2: scFv

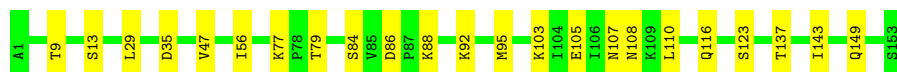
Chain B:  72% 20% 7%



4.2.7 Score per residue for model 7

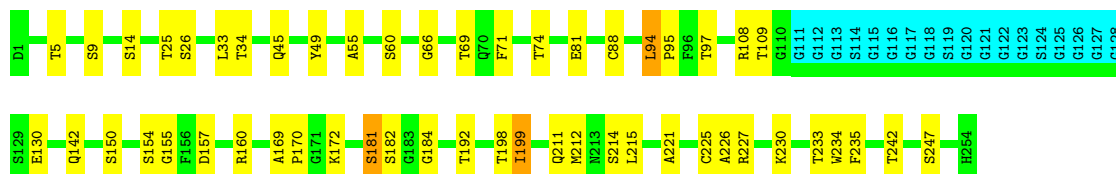
• Molecule 1: Interleukin-1 beta

Chain A:  85% 15%



• Molecule 2: scFv

Chain B:  72% 19% 7%



4.2.8 Score per residue for model 8

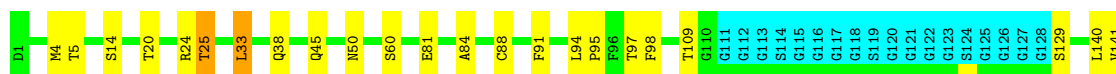
• Molecule 1: Interleukin-1 beta

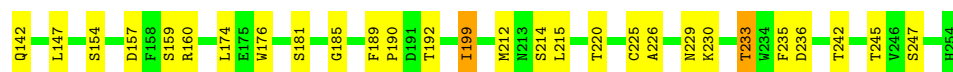
Chain A:  84% 16%



• Molecule 2: scFv

Chain B:  73% 19% 7%

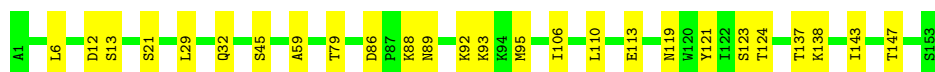




4.2.9 Score per residue for model 9

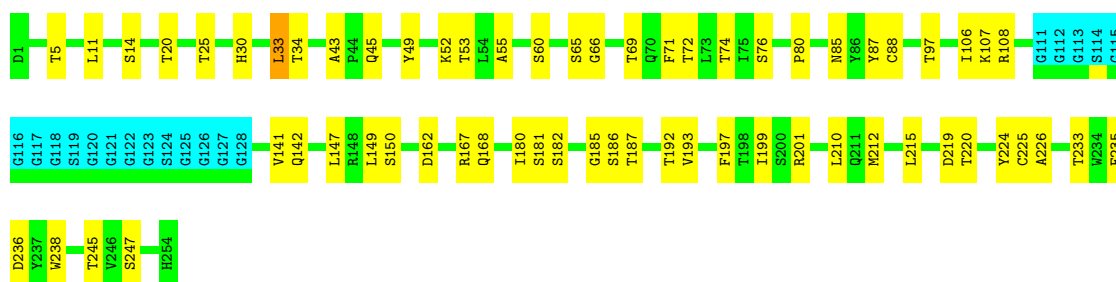
- Molecule 1: Interleukin-1 beta

Chain A: 83% 17%



- Molecule 2: scFv

Chain B: 68% 24% 7%



4.2.10 Score per residue for model 10

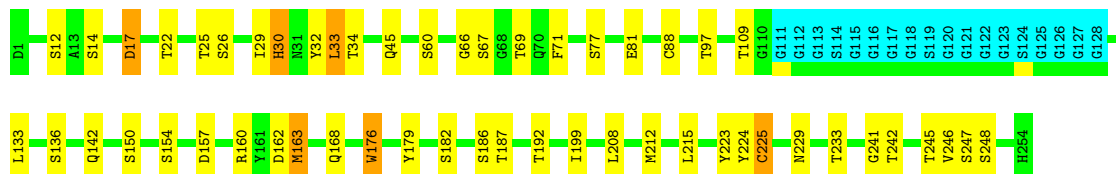
- Molecule 1: Interleukin-1 beta

Chain A: 85% 14%



- Molecule 2: scFv

Chain B: 72% 19% 7%



4.2.11 Score per residue for model 11

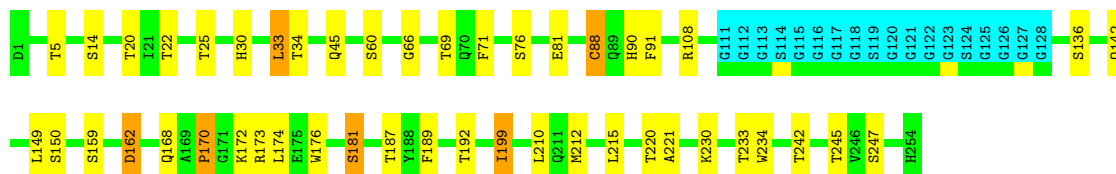
- Molecule 1: Interleukin-1 beta

Chain A:  85% 14% .



• Molecule 2: scFv

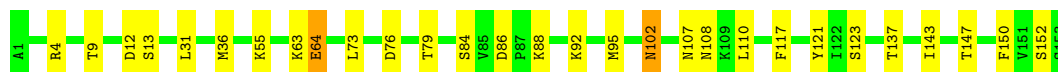
Chain B:  74% 16% 7% .



4.2.12 Score per residue for model 12

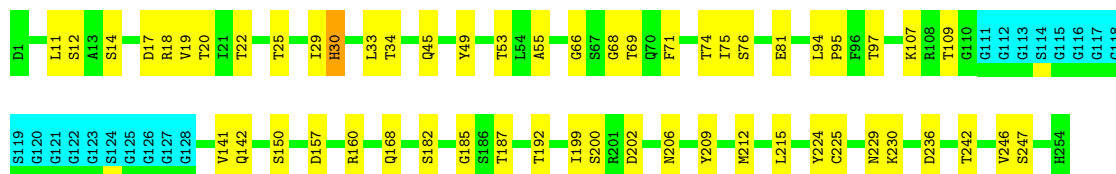
• Molecule 1: Interleukin-1 beta

Chain A:  81% 18% .



• Molecule 2: scFv

Chain B:  71% 21% 7% .



4.2.13 Score per residue for model 13

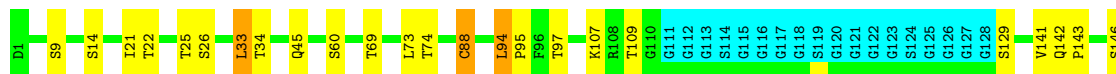
• Molecule 1: Interleukin-1 beta

Chain A:  85% 15% .



• Molecule 2: scFv

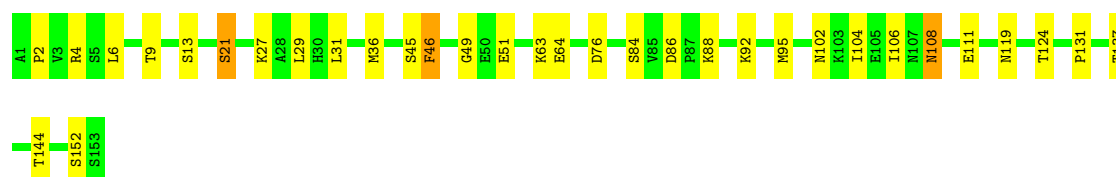
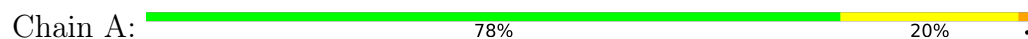
Chain B:  74% 17% 7% .



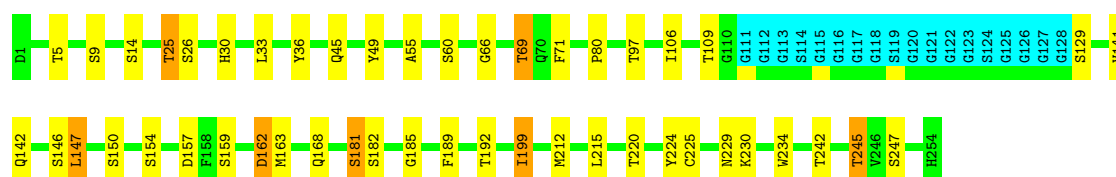


4.2.14 Score per residue for model 14

- Molecule 1: Interleukin-1 beta

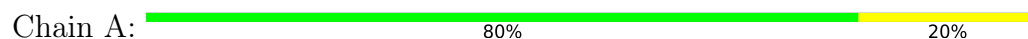


- Molecule 2: scFv

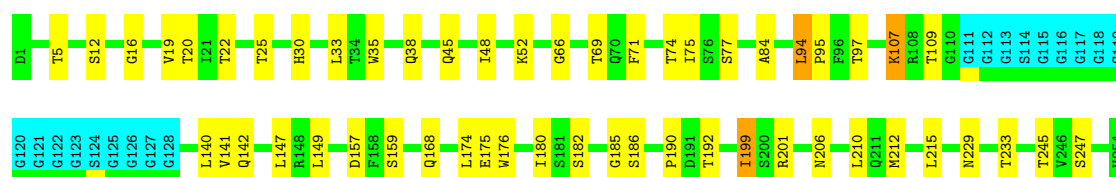


4.2.15 Score per residue for model 15

- Molecule 1: Interleukin-1 beta



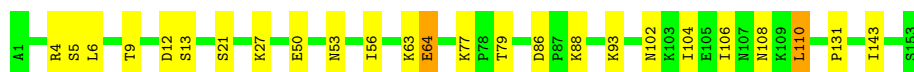
- Molecule 2: scFv



4.2.16 Score per residue for model 16

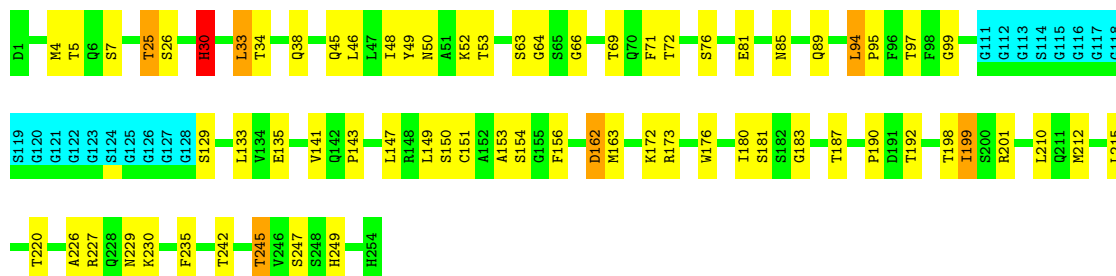
- Molecule 1: Interleukin-1 beta

Chain A:  84% 15% .



• Molecule 2: scFv

Chain B:  66% 24% 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% 21% 7% .



4.2.18 Score per residue for model 18

• Molecule 1: Interleukin-1 beta

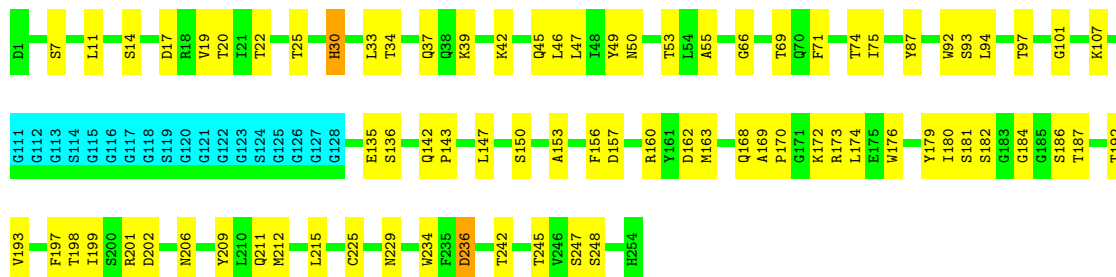
Chain A:  75% 24% .





• Molecule 2: scFv

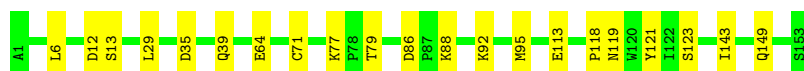
Chain B: 62% 30% 7%



4.2.19 Score per residue for model 19

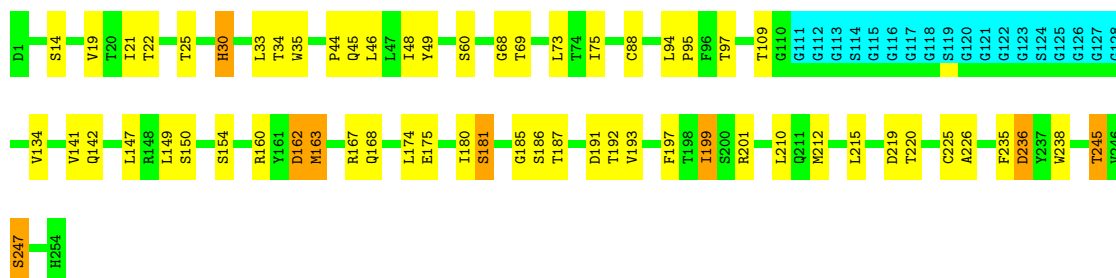
• Molecule 1: Interleukin-1 beta

Chain A: 86% 14%



• Molecule 2: scFv

Chain B: 69% 21% 7%



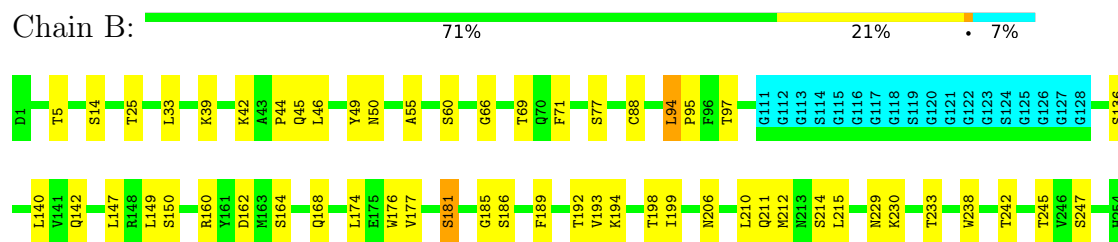
4.2.20 Score per residue for model 20

• Molecule 1: Interleukin-1 beta

Chain A: 82% 17%

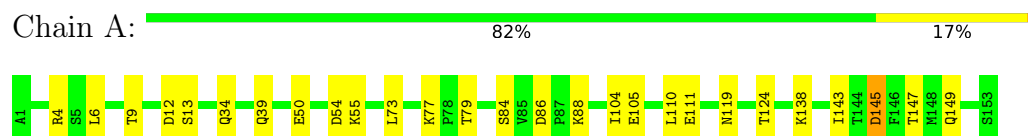


• Molecule 2: scFv

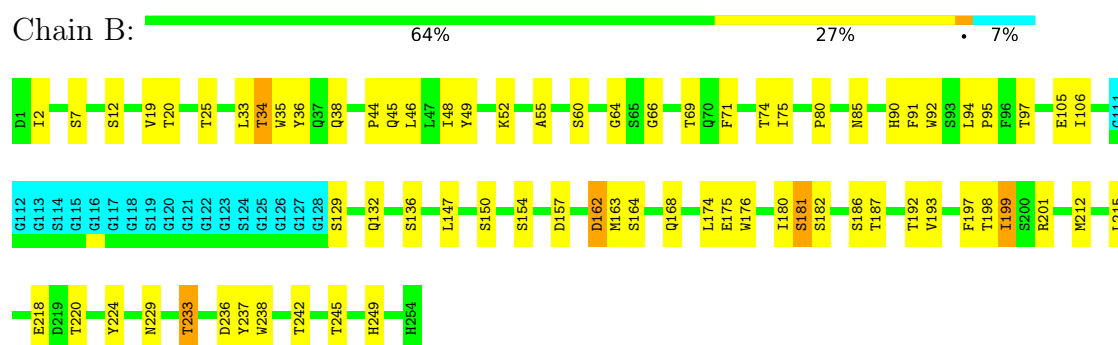


4.2.21 Score per residue for model 21

- Molecule 1: Interleukin-1 beta

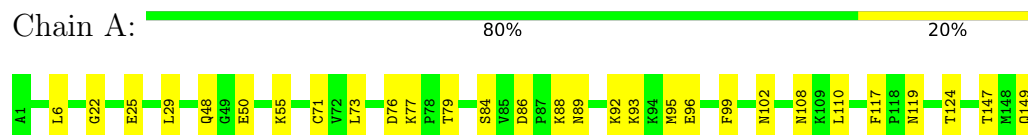


- Molecule 2: scFv

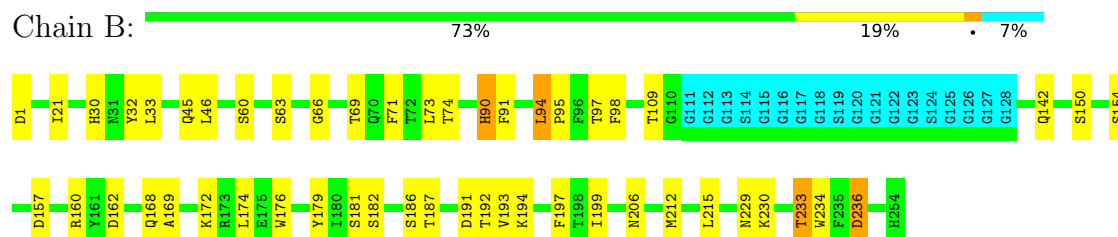


4.2.22 Score per residue for model 22

- Molecule 1: Interleukin-1 beta



- Molecule 2: scFv



4.2.23 Score per residue for model 23

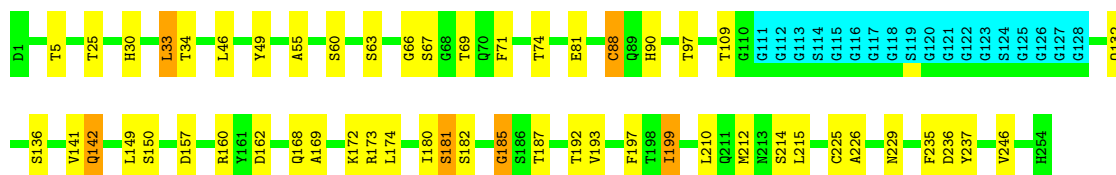
- Molecule 1: Interleukin-1 beta

Chain A:  87% 12%



- Molecule 2: scFv

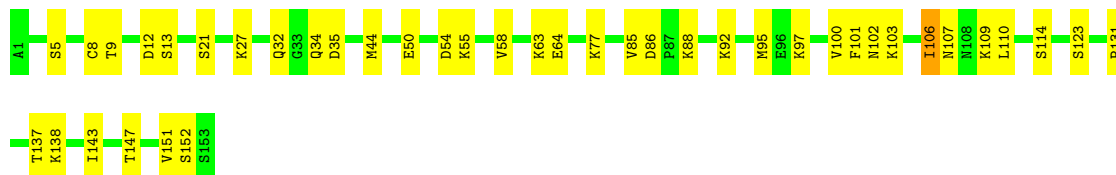
Chain B:  72% 19% 7%



4.2.24 Score per residue for model 24

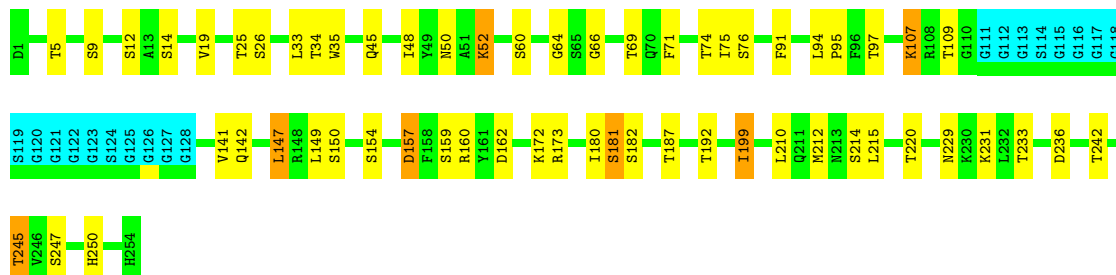
- Molecule 1: Interleukin-1 beta

Chain A:  73% 26%



- Molecule 2: scFv

Chain B:  70% 20% 7%



4.2.25 Score per residue for model 25

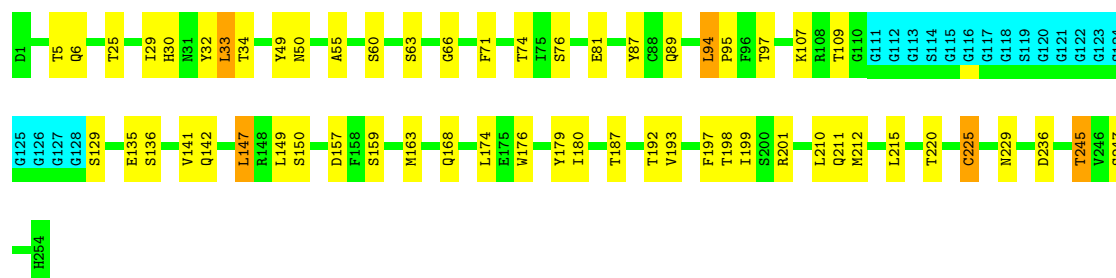
- Molecule 1: Interleukin-1 beta

Chain A:  79% 20%



- Molecule 2: scFv

Chain B: 70% 21% 7%



4.2.26 Score per residue for model 26

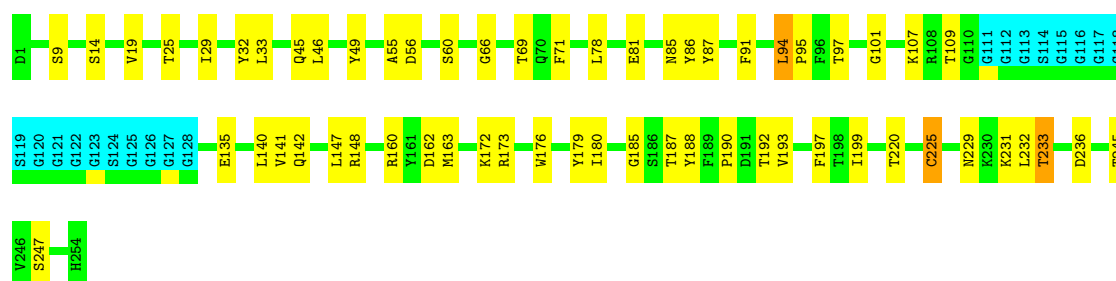
- Molecule 1: Interleukin-1 beta

Chain A: 84% 15%



- Molecule 2: scFv

Chain B: 70% 22% 7%



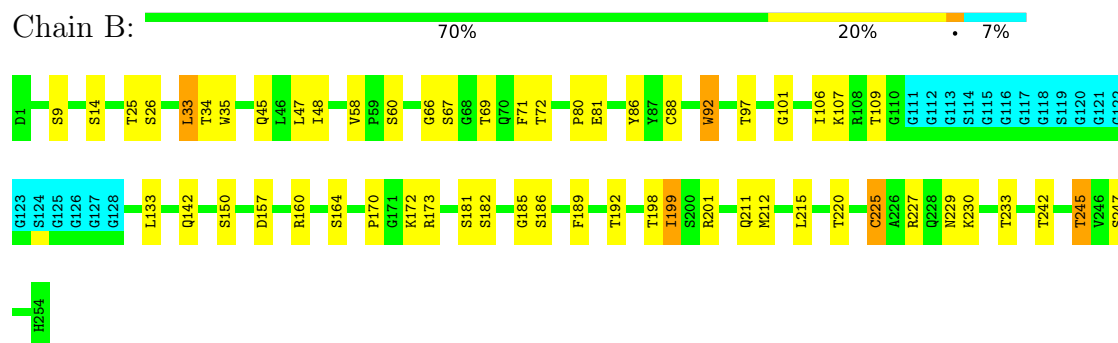
4.2.27 Score per residue for model 27

- Molecule 1: Interleukin-1 beta

Chain A: 86% 13%

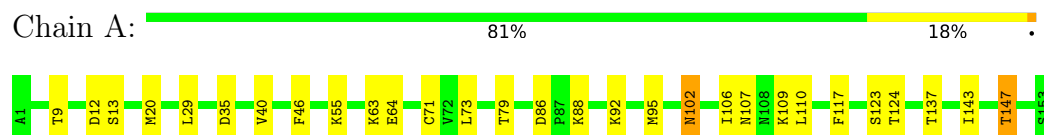


- Molecule 2: scFv

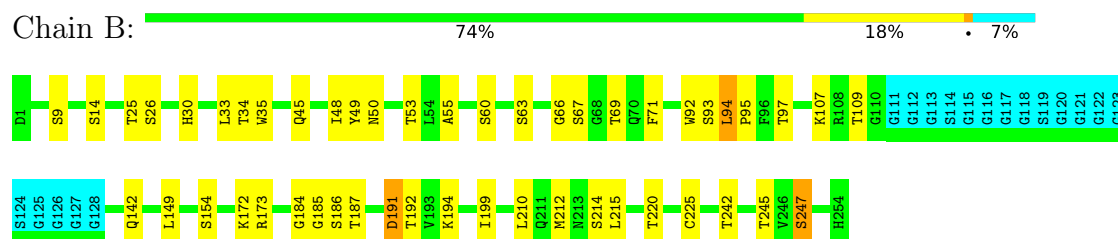


4.2.28 Score per residue for model 28

- Molecule 1: Interleukin-1 beta

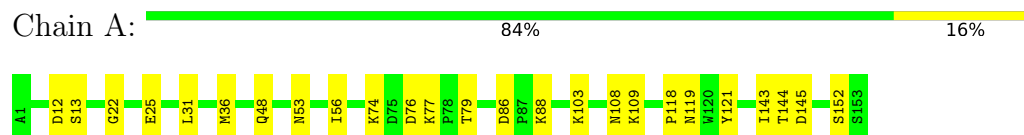


- Molecule 2: scFv

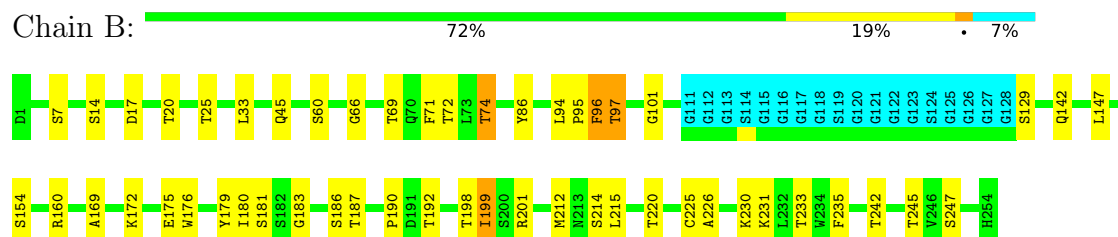


4.2.29 Score per residue for model 29

- Molecule 1: Interleukin-1 beta



- Molecule 2: scFv



4.2.30 Score per residue for model 30

- Molecule 1: Interleukin-1 beta

Chain A:  84% 15% .



- Molecule 2: scFv

Chain B:  69% 22% 7% .



4.2.31 Score per residue for model 31

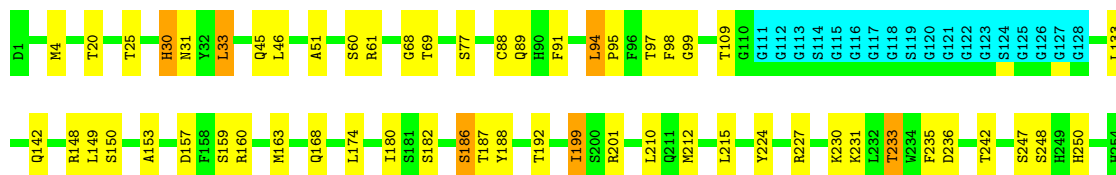
- Molecule 1: Interleukin-1 beta

Chain A:  78% 22%



- Molecule 2: scFv

Chain B:  70% 20% 7% .



4.2.32 Score per residue for model 32

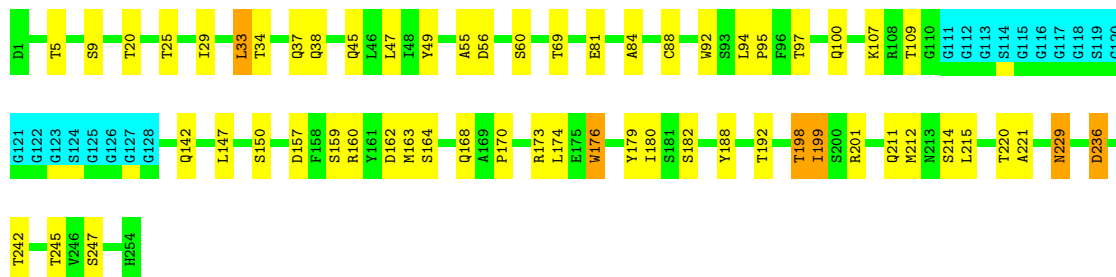
- Molecule 1: Interleukin-1 beta

Chain A:  86% 14%



- Molecule 2: scFv

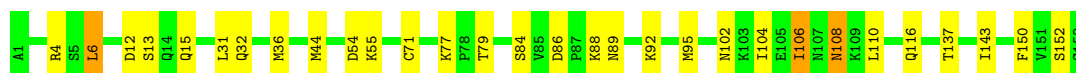
Chain B: 70% 21% 7%



4.2.33 Score per residue for model 33

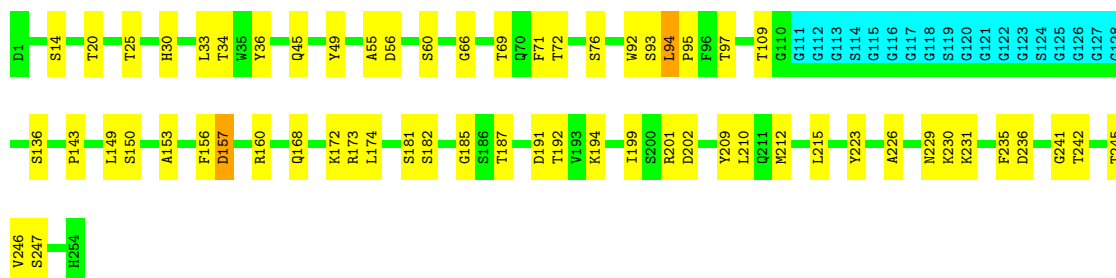
- Molecule 1: Interleukin-1 beta

Chain A: 80% 18% 2%



- Molecule 2: scFv

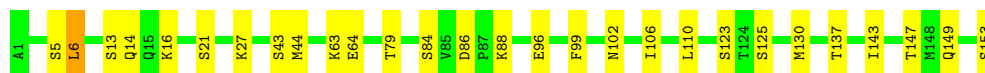
Chain B: 69% 23% 7%



4.2.34 Score per residue for model 34

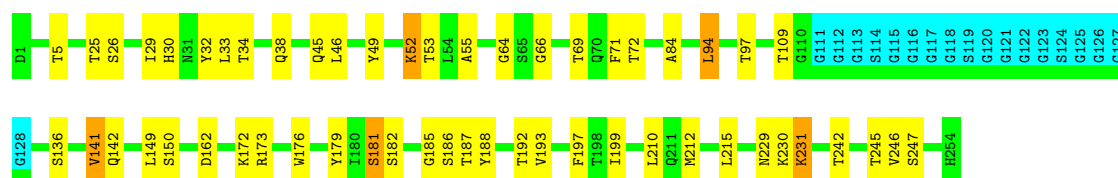
- Molecule 1: Interleukin-1 beta

Chain A: 82% 18% 0%



- Molecule 2: scFv

Chain B:  72% 19% 7%



4.2.35 Score per residue for model 35

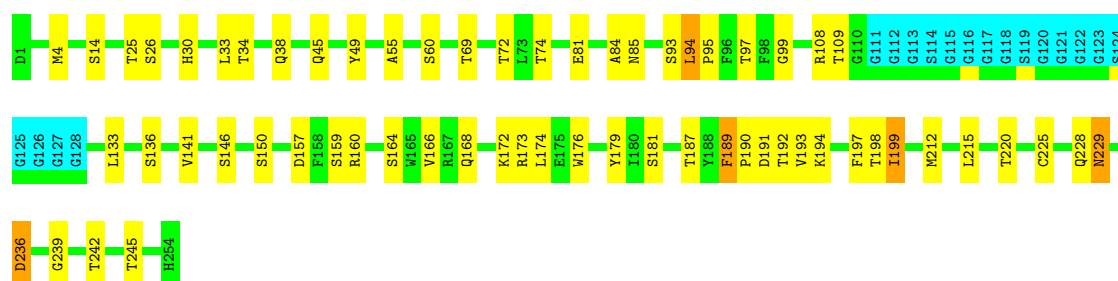
- Molecule 1: Interleukin-1 beta

Chain A:  82% 16%



- Molecule 2: scFv

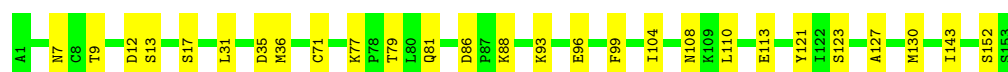
Chain B:  69% 22% 7%



4.2.36 Score per residue for model 36

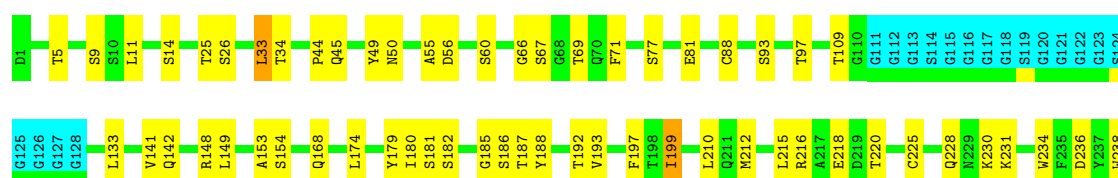
- Molecule 1: Interleukin-1 beta

Chain A:  82% 18%



- Molecule 2: scFv

Chain B:  69% 24% 7%

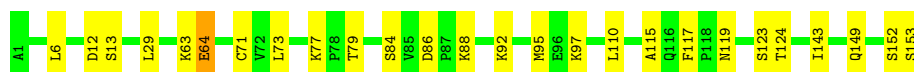




4.2.37 Score per residue for model 37

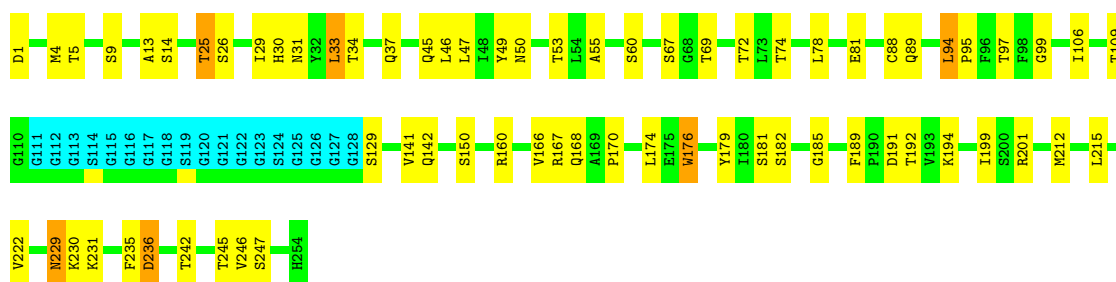
- Molecule 1: Interleukin-1 beta

Chain A: 83% 16%



- Molecule 2: scFv

Chain B: 66% 25% 7%



4.2.38 Score per residue for model 38

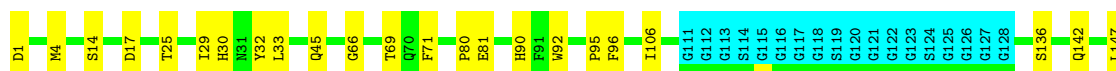
- Molecule 1: Interleukin-1 beta

Chain A: 85% 15%



- Molecule 2: scFv

Chain B: 72% 20% 7%



4.2.39 Score per residue for model 39

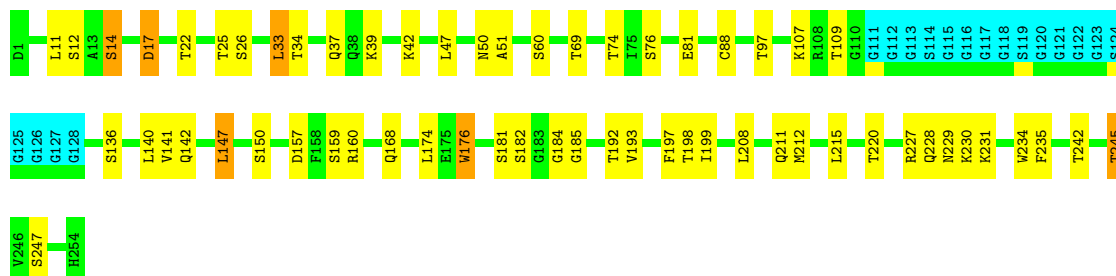
- Molecule 1: Interleukin-1 beta

Chain A:  86% 12% .



• Molecule 2: scFv

Chain B:  69% 21% 7% .



4.2.40 Score per residue for model 40

• Molecule 1: Interleukin-1 beta

Chain A:  84% 14% .



• Molecule 2: scFv

Chain B:  65% 25% 7% .



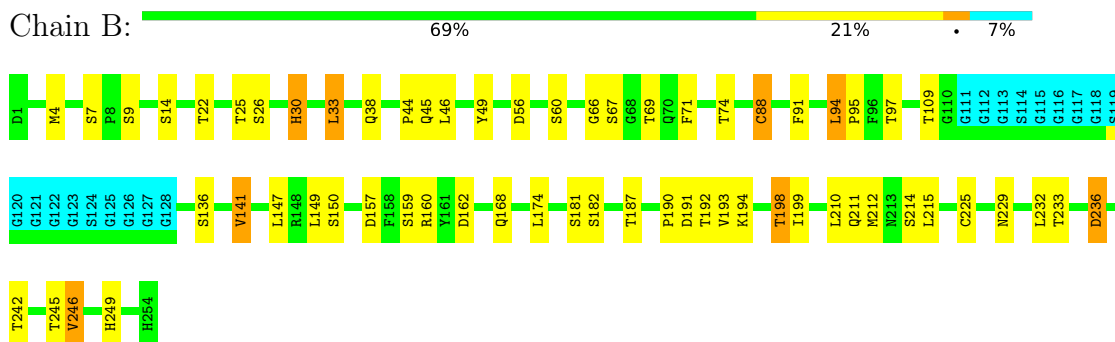
4.2.41 Score per residue for model 41

• Molecule 1: Interleukin-1 beta

Chain A:  80% 18% .

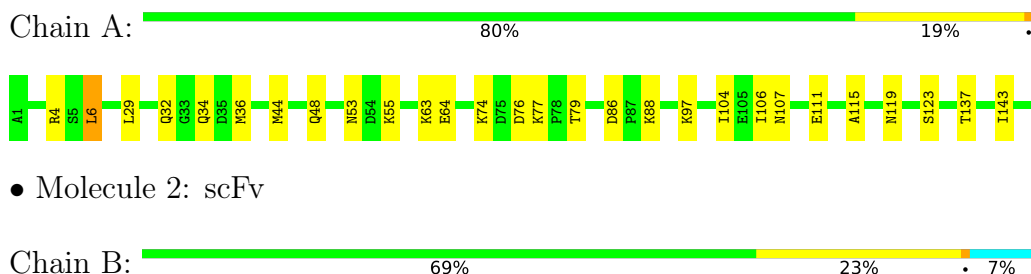


- Molecule 2: scFv

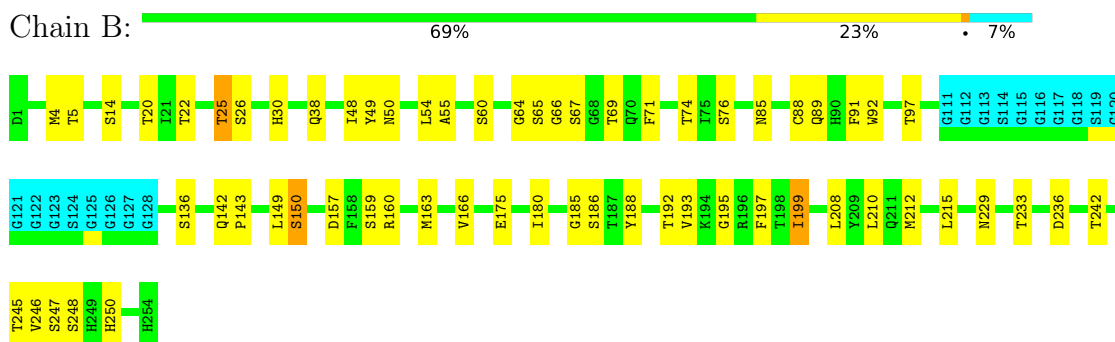


4.2.42 Score per residue for model 42

- Molecule 1: Interleukin-1 beta

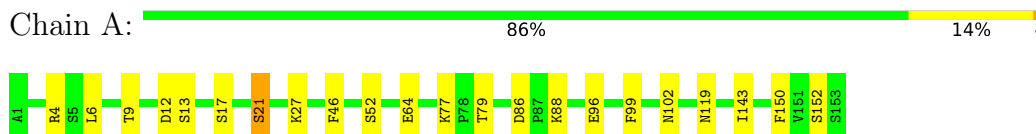


- Molecule 2: scFv



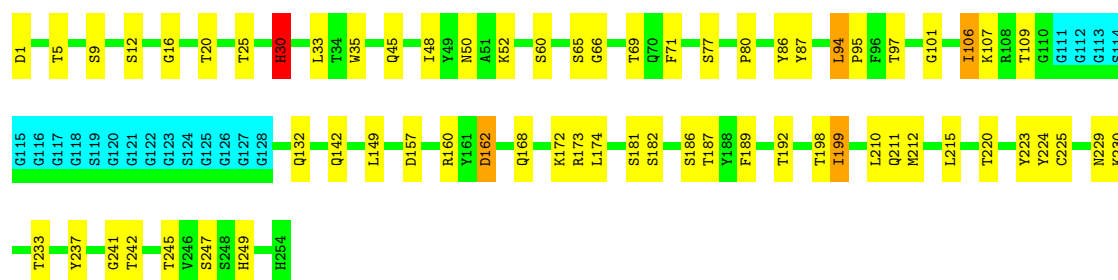
4.2.43 Score per residue for model 43

- Molecule 1: Interleukin-1 beta



- Molecule 2: scFv





4.2.44 Score per residue for model 44

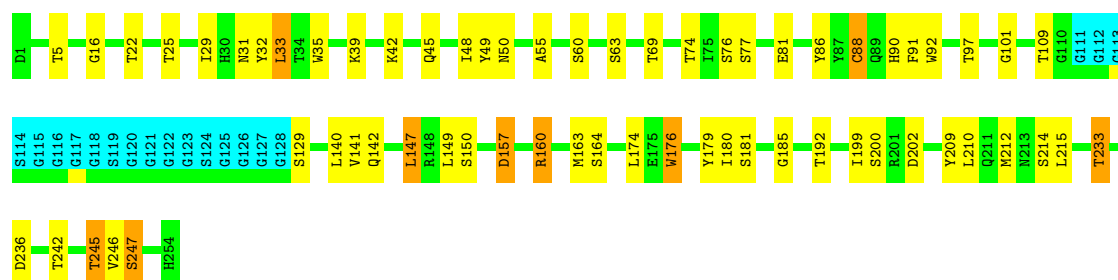
- Molecule 1: Interleukin-1 beta

Chain A: 86% 14%



- Molecule 2: scFv

Chain B: 68% 21% 7%



4.2.45 Score per residue for model 45

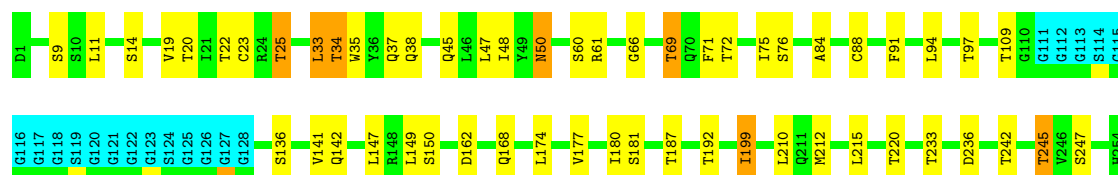
- Molecule 1: Interleukin-1 beta

Chain A: 80% 19%



- Molecule 2: scFv

Chain B: 71% 19% 7%



4.2.46 Score per residue for model 46

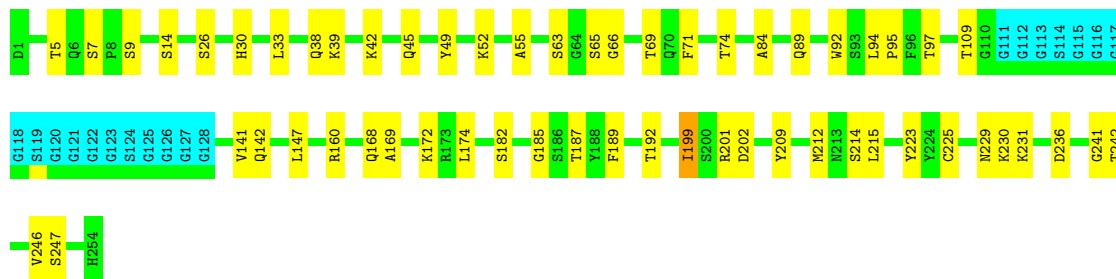
- Molecule 1: Interleukin-1 beta

Chain A: 



- Molecule 2: scFv

Chain B: 



4.2.47 Score per residue for model 47

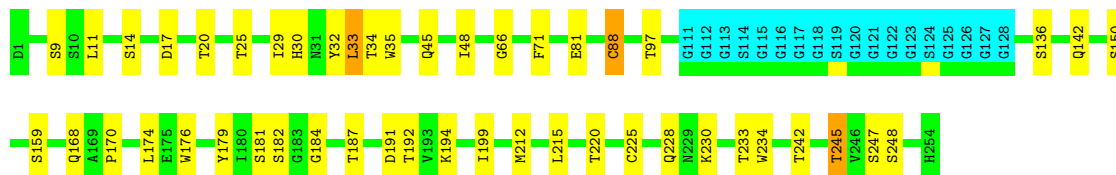
- Molecule 1: Interleukin-1 beta

Chain A: 



- Molecule 2: scFv

Chain B: 



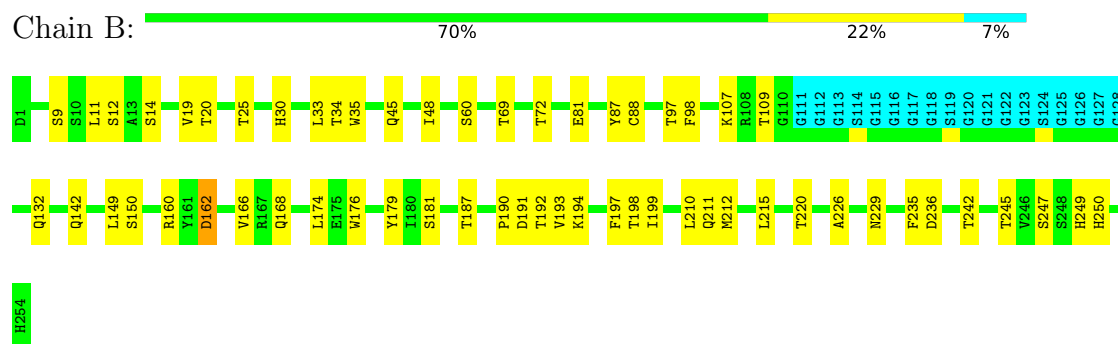
4.2.48 Score per residue for model 48

- Molecule 1: Interleukin-1 beta

Chain A: 

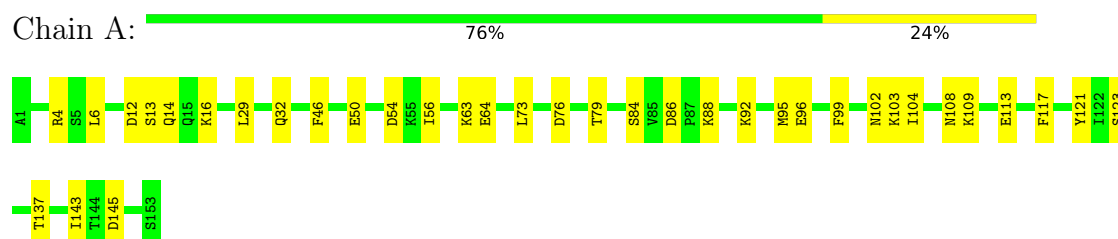


- Molecule 2: scFv

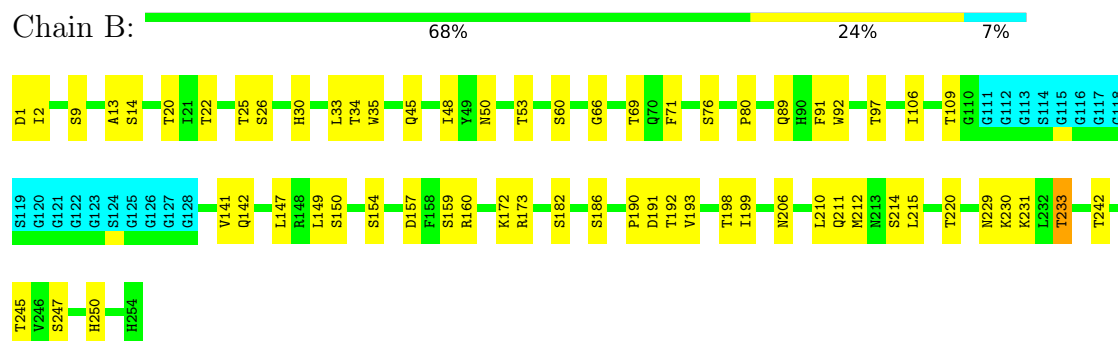


4.2.49 Score per residue for model 49

- Molecule 1: Interleukin-1 beta

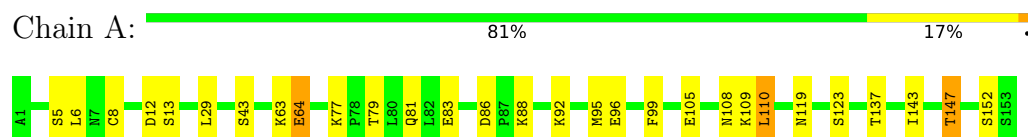


- Molecule 2: scFv

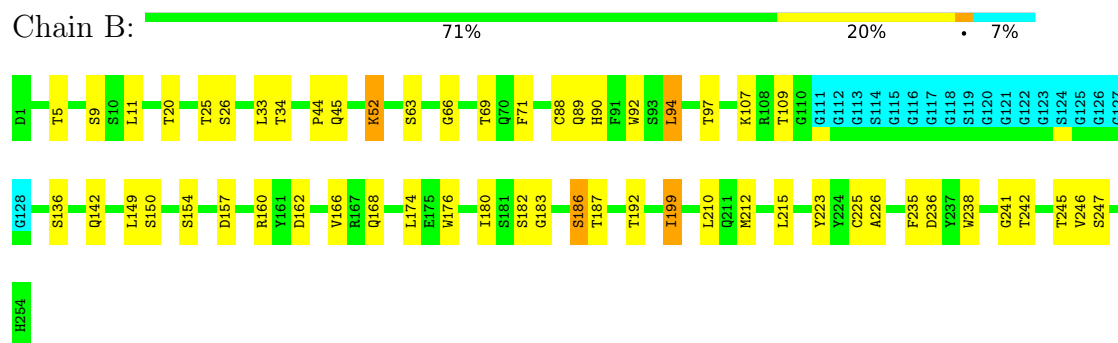


4.2.50 Score per residue for model 50

- Molecule 1: Interleukin-1 beta

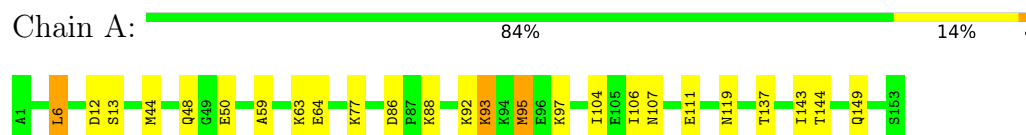


- Molecule 2: scFv

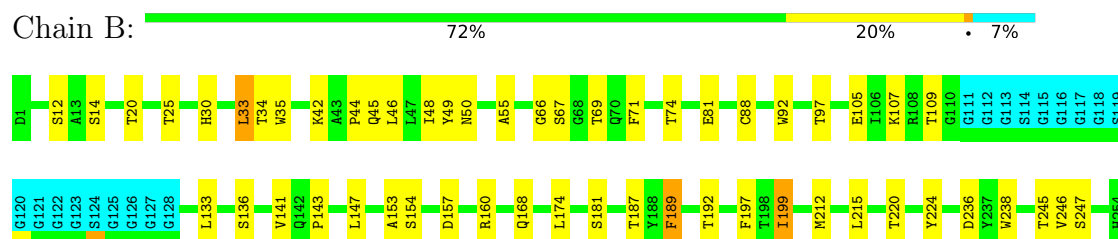


4.2.51 Score per residue for model 51

- Molecule 1: Interleukin-1 beta

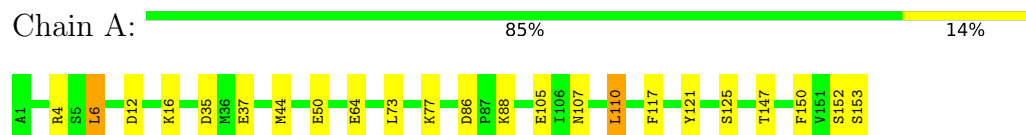


- Molecule 2: scFv

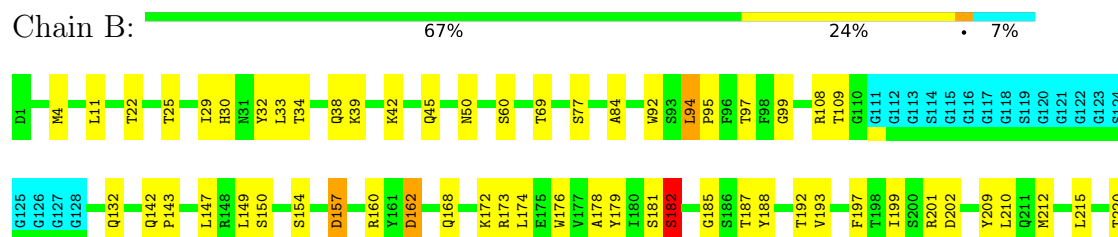


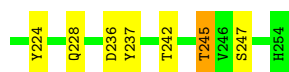
4.2.52 Score per residue for model 52

- Molecule 1: Interleukin-1 beta



- Molecule 2: scFv

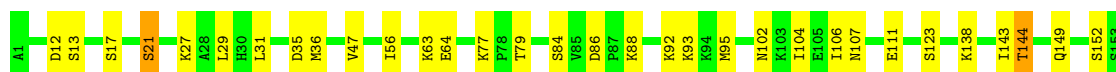




4.2.53 Score per residue for model 53

- Molecule 1: Interleukin-1 beta

Chain A: 79% 20% .



- Molecule 2: scFv

Chain B: 75% 17% 7% .



4.2.54 Score per residue for model 54

- Molecule 1: Interleukin-1 beta

Chain A: 81% 18% .



- Molecule 2: scFv

Chain B: 72% 20% 7% .



4.2.55 Score per residue for model 55

- Molecule 1: Interleukin-1 beta

Chain A: 78% 21% .



- Molecule 2: scFv

Chain B: 67% 24% 7%



4.2.56 Score per residue for model 56

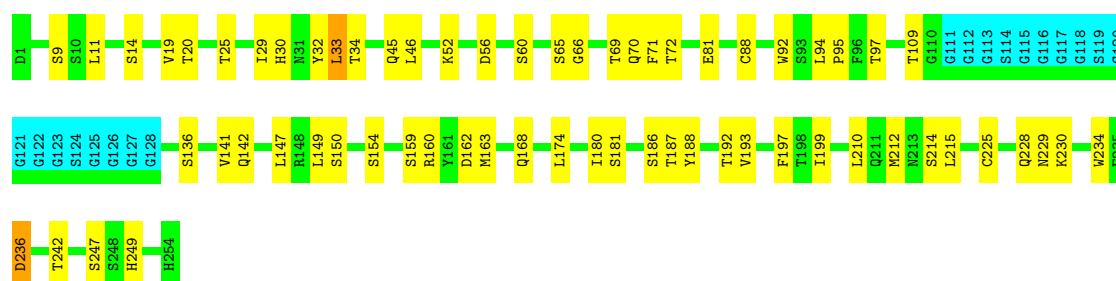
- Molecule 1: Interleukin-1 beta

Chain A: 83% 16% 1%



- Molecule 2: scFv

Chain B: 68% 24% 7%



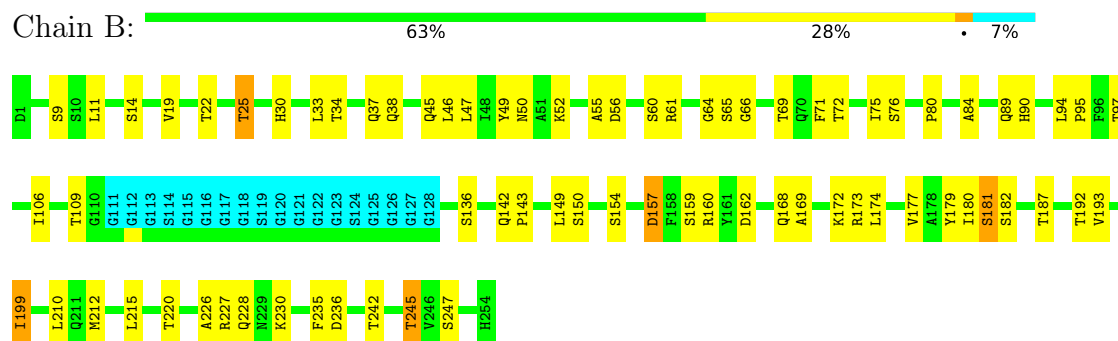
4.2.57 Score per residue for model 57

- Molecule 1: Interleukin-1 beta

Chain A: 86% 12% 2%

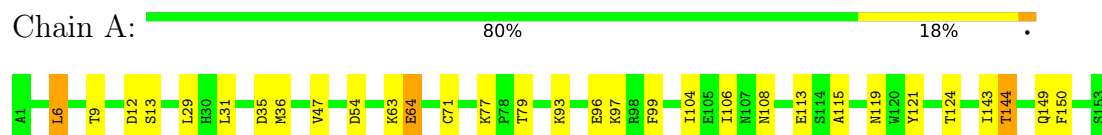


- Molecule 2: scFv

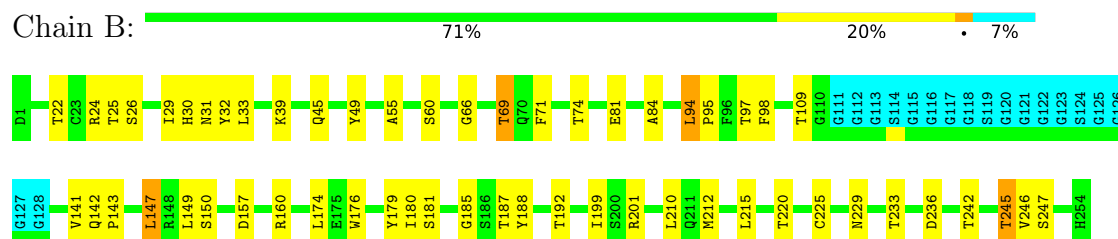


4.2.58 Score per residue for model 58

- Molecule 1: Interleukin-1 beta

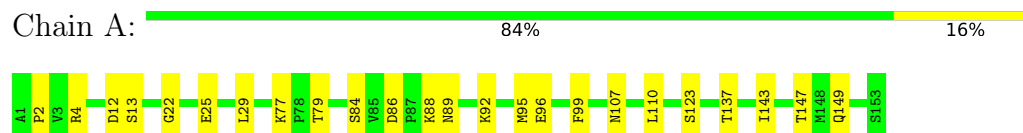


- Molecule 2: scFv

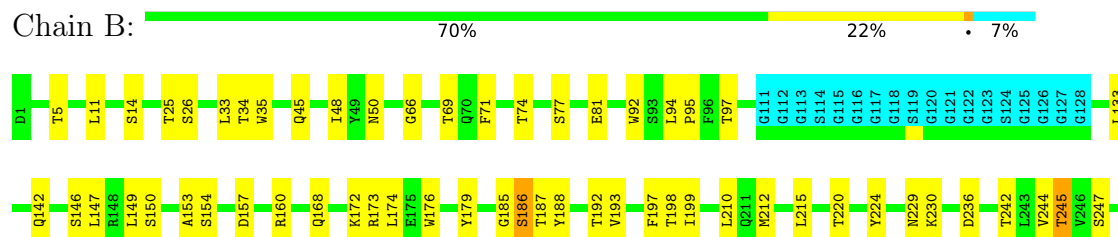


4.2.59 Score per residue for model 59

- Molecule 1: Interleukin-1 beta



- Molecule 2: scFv



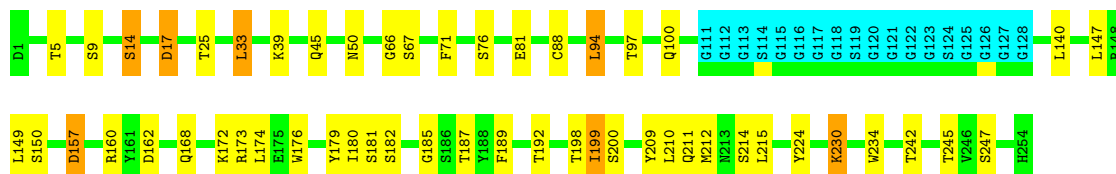
H254

4.2.60 Score per residue for model 60

- Molecule 1: Interleukin-1 beta

Chain A:  82% 17%

- Molecule 2: scFv

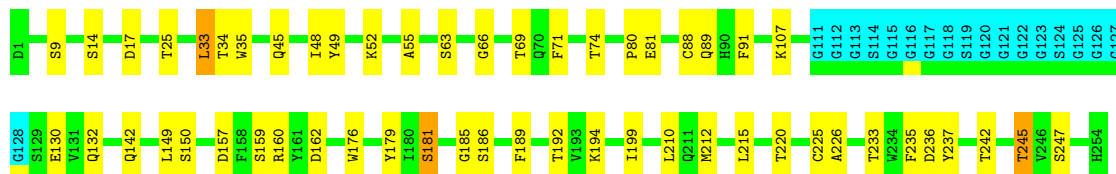
Chain B:  72% 18% 7%

4.2.61 Score per residue for model 61

- Molecule 1: Interleukin-1 beta

Chain A:  88% 12%

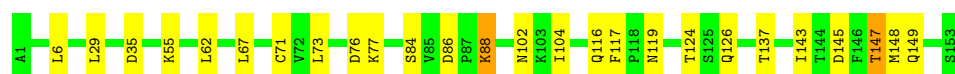
- Molecule 2: scFv

Chain B:  72% 20% 7%

4.2.62 Score per residue for model 62

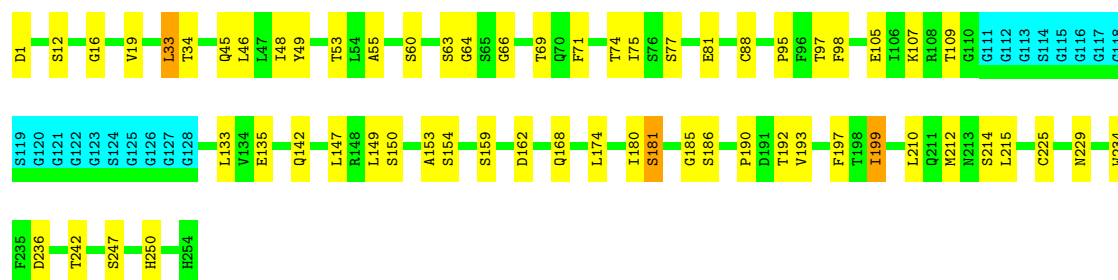
- Molecule 1: Interleukin-1 beta

Chain A:  83% 16%



• Molecule 2: scFv

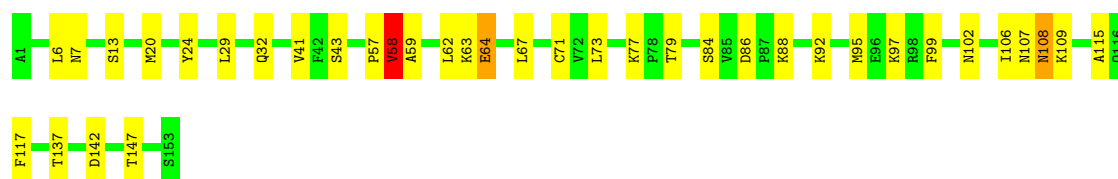
Chain B: 69% 23% 7%



4.2.63 Score per residue for model 63

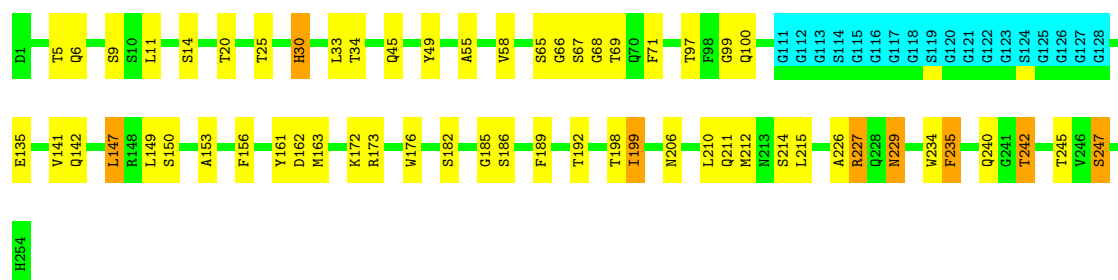
• Molecule 1: Interleukin-1 beta

Chain A: 76% 22% 2%



• Molecule 2: scFv

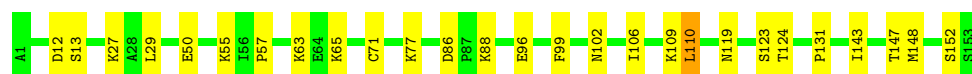
Chain B: 70% 20% 7%



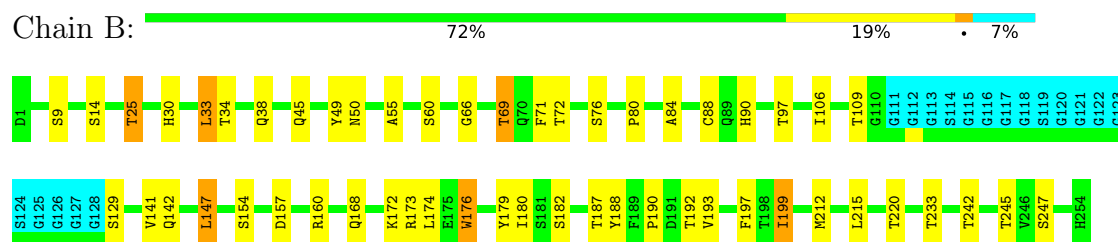
4.2.64 Score per residue for model 64

• Molecule 1: Interleukin-1 beta

Chain A: 82% 17% 1%

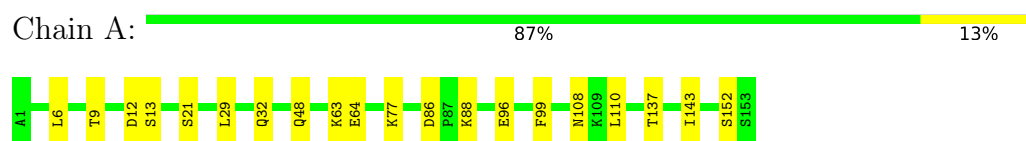


- Molecule 2: scFv

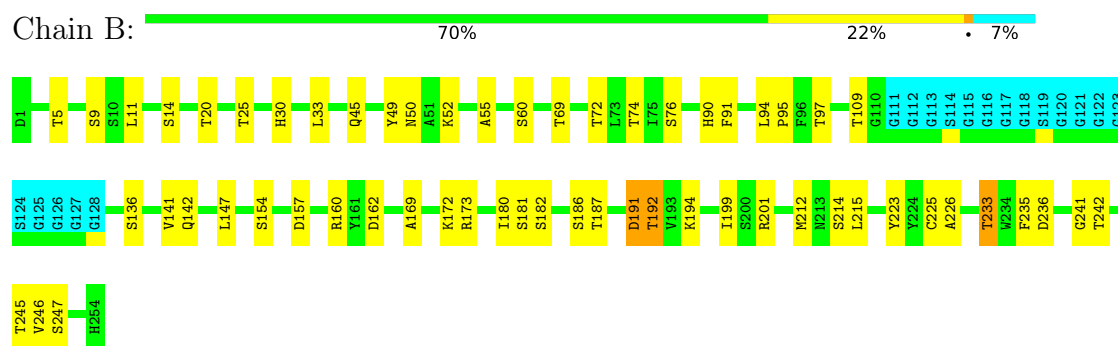


4.2.65 Score per residue for model 65

- Molecule 1: Interleukin-1 beta

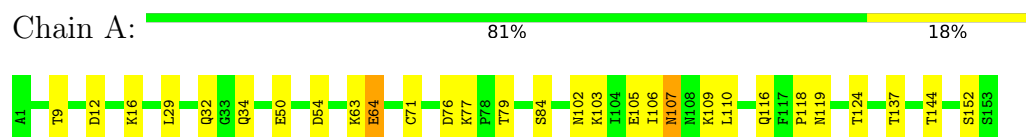


- Molecule 2: scFv

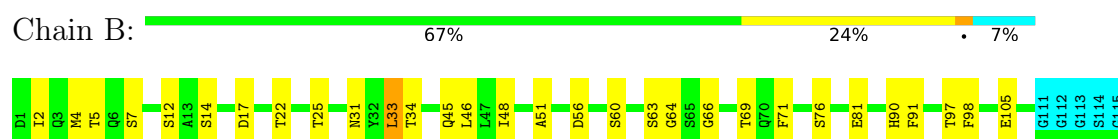


4.2.66 Score per residue for model 66

- Molecule 1: Interleukin-1 beta



- Molecule 2: scFv





4.2.67 Score per residue for model 67

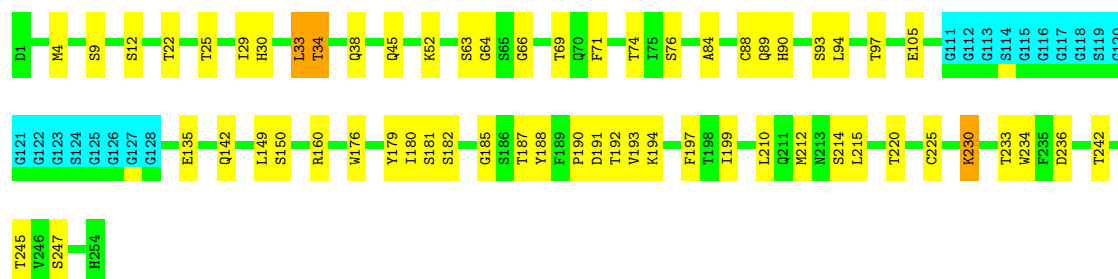
- Molecule 1: Interleukin-1 beta

Chain A: 84% 14% .



- Molecule 2: scFv

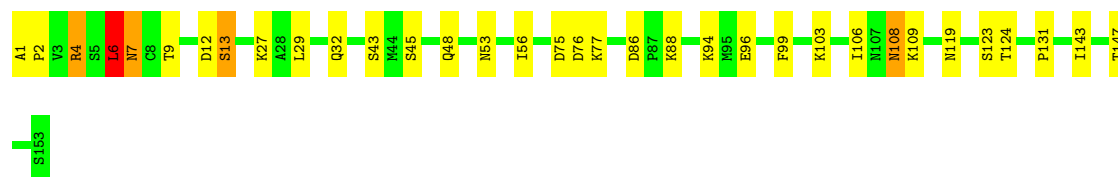
Chain B: 69% 22% 7% .



4.2.68 Score per residue for model 68

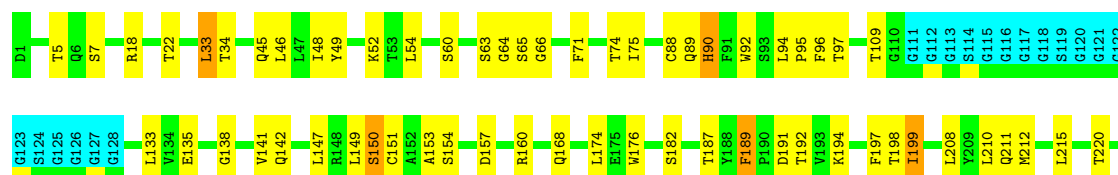
- Molecule 1: Interleukin-1 beta

Chain A: 78% 19% . .



- Molecule 2: scFv

Chain B: 67% 24% 7% .





4.2.69 Score per residue for model 69

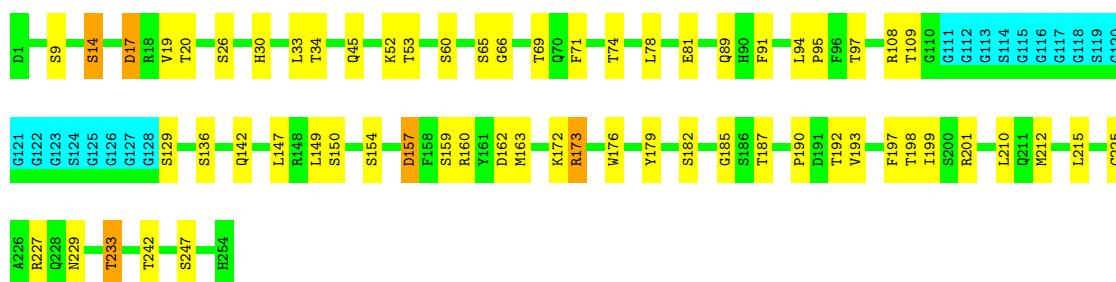
- Molecule 1: Interleukin-1 beta

Chain A: 82% 18% .



- Molecule 2: scFv

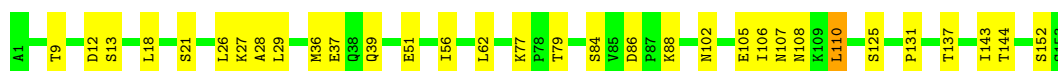
Chain B: 69% 22% 7% .



4.2.70 Score per residue for model 70

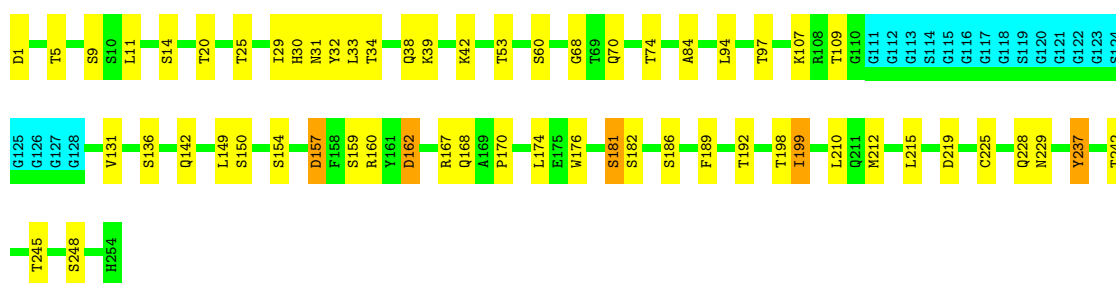
- Molecule 1: Interleukin-1 beta

Chain A: 79% 20% .



- Molecule 2: scFv

Chain B: 70% 21% 7% .



4.2.71 Score per residue for model 71

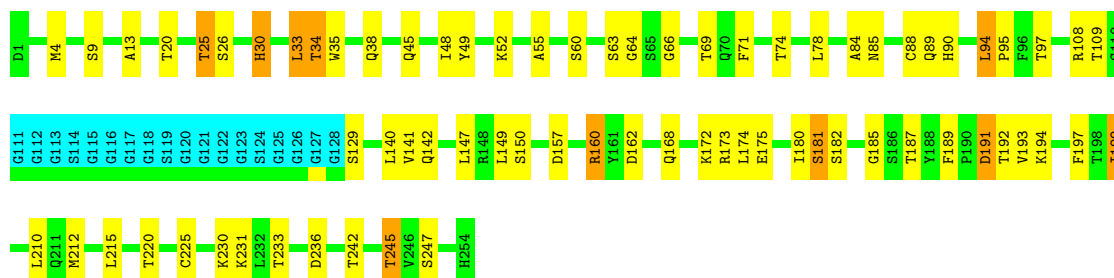
- Molecule 1: Interleukin-1 beta

Chain A: 



- Molecule 2: scFv

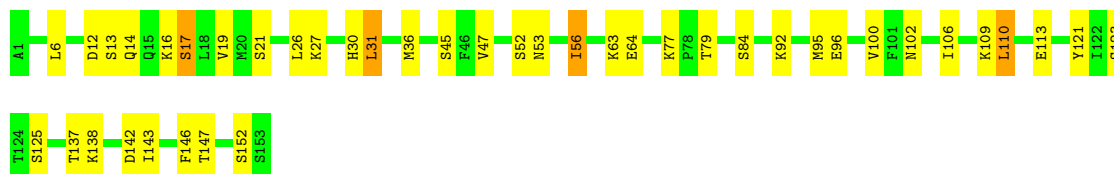
Chain B: 



4.2.72 Score per residue for model 72

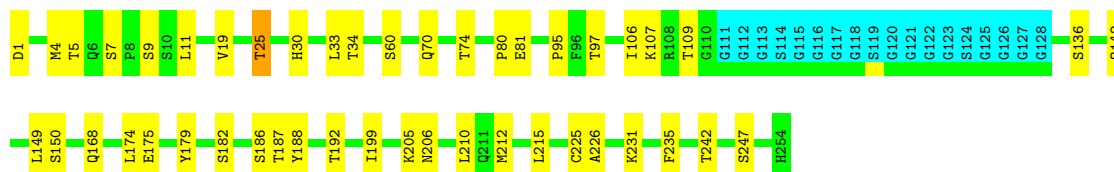
- Molecule 1: Interleukin-1 beta

Chain A: 



- Molecule 2: scFv

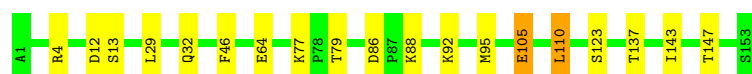
Chain B: 



4.2.73 Score per residue for model 73

- Molecule 1: Interleukin-1 beta

Chain A: 



- Molecule 2: scFv

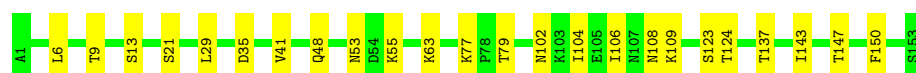
Chain B: 67% 24% 7%



4.2.74 Score per residue for model 74

- Molecule 1: Interleukin-1 beta

Chain A: 84% 16%



- Molecule 2: scFv

Chain B: 66% 23% 7%



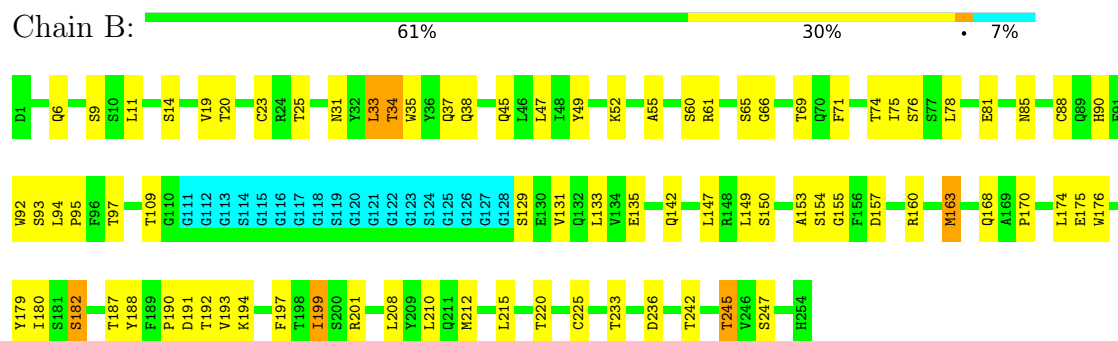
4.2.75 Score per residue for model 75

- Molecule 1: Interleukin-1 beta

Chain A: 82% 18%

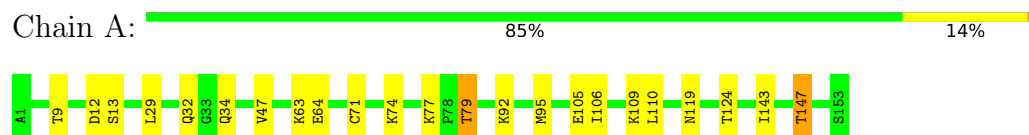


- Molecule 2: scFv

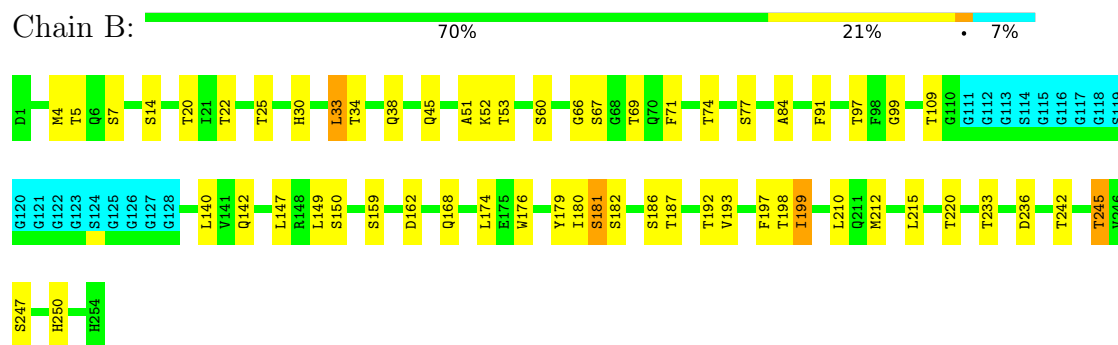


4.2.76 Score per residue for model 76

- Molecule 1: Interleukin-1 beta

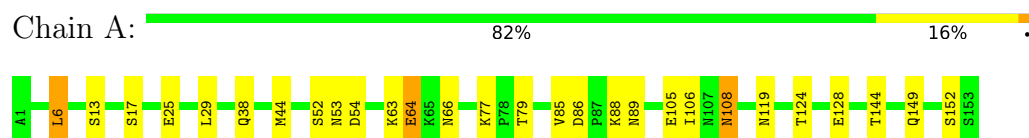


- Molecule 2: scFv

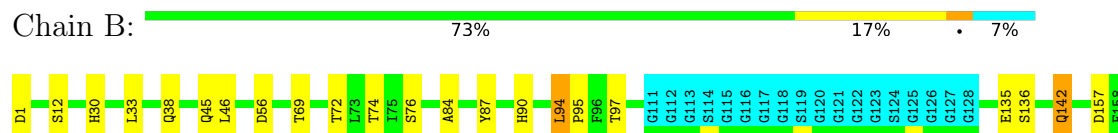


4.2.77 Score per residue for model 77

- Molecule 1: Interleukin-1 beta



- Molecule 2: scFv



S159	D162	Q168	R173	L174	E175	W176	V177	A178	Y179	I180	S181	S182	G185	S186	T187	Y189	D191	T192	V193	F197	T198	I199	W212	L215	T220	K230	W234	F235	D236	T242	T245	V246	S247	H254
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

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.

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

Continued on next page...

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Mol	Chain	Non-H	H(model)	H(added)	Clashes
All	All	236621	234003	230307	2133

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 5.

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:52:LYS:HG2	2:B:65:SER:HA	0.69	1.64	46	5
2:B:202:ASP:HB2	2:B:209:TYR:HE2	0.69	1.48	18	6
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:HH11	2:B:227:ARG:HB3	0.68	1.48	63	1
2:B:230:LYS:HG3	2:B:231:LYS:H	0.68	1.46	33	8
1:A:102:ASN:HB2	1:A:113:GLU:HB3	0.68	1.63	72	4
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:157:ASP:HB3	2:B:160:ARG:HB3	0.64	1.70	54	10
2:B:180:ILE:HD11	2:B:201:ARG:HB3	0.64	1.70	1	15
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:44:PRO:HD2	2:B:238:TRP:HB2	0.60	1.73	19	6
2:B:142:GLN:HA	2:B:247:SER:O	0.60	1.97	49	60
1:A:21:SER:HB2	1:A:27:LYS:HG3	0.60	1.71	39	21
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
2:B:95:PRO:O	2:B:96:PHE:HB2	0.59	1.96	29	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: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:105:GLU:HB3	1:A:110:LEU:HB3	0.58	1.76	73	2
1:A:4:ARG:HB3	2:B:92:TRP:CH2	0.57	2.34	18	1
1:A:4:ARG:HB3	2:B:92:TRP:CZ2	0.57	2.34	75	13
1:A:92:LYS:HE3	1:A:95:MET:HA	0.57	1.76	5	40
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
1:A:108:ASN:HB3	2:B:185:GLY:CA	0.56	2.30	17	1
2:B:135:GLU:HG2	2:B:225:CYS:HB3	0.56	1.76	68	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:11:LEU:HD11	2:B:19:VAL:HG13	0.55	1.78	45	8
2:B:38:GLN:O	2:B:84:ALA:HB1	0.55	2.02	8	19
1:A:74:LYS:HD2	1:A:79:THR:HB	0.55	1.79	13	4
2:B:193:VAL:HB	2:B:197:PHE:HD2	0.55	1.62	52	8
1:A:8:CYS:HB3	1:A:150:PHE:HD1	0.54	1.62	45	1
2:B:212:MET:HE2	2:B:215:LEU:HD21	0.54	1.78	49	5
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:46:LEU:HB2	2:B:236:ASP:HA	0.54	1.78	19	4
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
1:A:36:MET:HE1	2:B:195:GLY:N	0.53	2.17	42	1
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
2:B:179:TYR:HB3	2:B:188:TYR:HB2	0.52	1.80	77	10
1:A:28:ALA:HB3	1:A:124:THR:HG21	0.52	1.80	3	2
2:B:141:VAL:O	2:B:246:VAL:HA	0.52	2.04	41	15
2:B:94:LEU:HG	2:B:95:PRO:CA	0.52	2.31	19	4
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
2:B:193:VAL:HB	2:B:197:PHE:CD1	0.51	2.40	77	15
1:A:125:SER:HB2	1:A:130:MET:HG3	0.51	1.82	34	4
1:A:56:ILE:HD11	2:B:231:LYS:NZ	0.51	2.20	72	3
1:A:138:LYS:HG3	1:A:144:THR:HB	0.51	1.82	1	1
1:A:123:SER:HA	1:A:143:ILE:O	0.51	2.05	37	36
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
2:B:43:ALA:HB1	2:B:238:TRP:HB2	0.51	1.82	5	2
2:B:4:MET:HE1	2:B:25:THR:HB	0.51	1.82	37	8
1:A:48:GLN:HB3	1:A:94:LYS:HD3	0.51	1.82	17	1
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
1:A:106:ILE:HG13	1:A:107:ASN:H	0.51	1.66	24	7
2:B:176:TRP:CH2	2:B:179:TYR:HB2	0.51	2.40	10	8
1:A:45:SER:HB2	1:A:59:ALA:HB3	0.51	1.83	9	1
1:A:150:PHE:CE2	2:B:93:SER:HA	0.51	2.40	33	1
1:A:14:GLN:HB3	1:A:16:LYS:HG3	0.51	1.82	49	2
1:A:147:THR:HB	1:A:149:GLN:OE1	0.51	2.06	56	2
1:A:108:ASN:OD1	2:B:183:GLY:HA3	0.50	2.06	50	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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
1:A:138:LYS:HA	1:A:144:THR:HG21	0.50	1.82	18	3
2:B:80:PRO:HA	2:B:106:ILE:HG12	0.50	1.83	43	2
2:B:169:ALA:HB3	2:B:172:LYS:HE3	0.50	1.84	73	2
1:A:9:THR:HG21	1:A:39:GLN:HG3	0.50	1.84	1	1
2:B:14:SER:O	2:B:17:ASP:HB2	0.50	2.06	10	4
1:A:41:VAL:HB	1:A:63:LYS:HD3	0.50	1.82	63	3
1:A:73:LEU:HG	1:A:117:PHE:CZ	0.50	2.41	37	15
2:B:100:GLN:HA	2:B:173:ARG:HD3	0.50	1.84	32	1
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
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:H	2:B:199:ILE:HD13	0.49	1.67	8	17
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
2:B:47:LEU:HA	2:B:58:VAL:HG21	0.49	1.84	2	4
1:A:108:ASN:OD1	2:B:181:SER:HB2	0.49	2.08	7	1
1:A:47:VAL:HA	1:A:93:LYS:O	0.49	2.07	35	5
1:A:55:LYS:HE2	1:A:104:ILE:HG12	0.49	1.83	62	2
2:B:191:ASP:HA	2:B:194:LYS:HE3	0.49	1.84	1	1
2:B:94:LEU:CB	2:B:95:PRO:HA	0.49	2.38	13	4
2:B:193:VAL:HB	2:B:197:PHE:CD2	0.49	2.42	26	7
2:B:89:GLN:HG2	2:B:90:HIS:H	0.49	1.68	68	2
2:B:167:ARG:HH12	2:B:219:ASP:HA	0.49	1.68	9	3
1:A:22:GLY:H	1:A:25:GLU:HB3	0.49	1.67	22	7
2:B:33:LEU:CD1	2:B:88:CYS:HB2	0.49	2.37	45	1
1:A:70:SER:HB2	1:A:99:PHE:CE1	0.49	2.42	55	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
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:189:PHE:HE1	2:B:199:ILE:HD12	0.49	1.68	46	3
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:176:TRP:HE3	2:B:190:PRO:HG3	0.48	1.67	64	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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
1:A:20:MET:HG2	1:A:40:VAL:HG21	0.48	1.85	28	6
1:A:150:PHE:HB3	2:B:94:LEU:HD13	0.48	1.83	33	1
2:B:189:PHE:HE2	2:B:199:ILE:HD12	0.48	1.68	43	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:107:ASN:O	1:A:108:ASN:HB2	0.48	2.08	63	1
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:1:ASP:HB2	2:B:95:PRO:HD3	0.47	1.85	40	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
1:A:63:LYS:C	1:A:64:GLU:HG2	0.47	2.34	77	10
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
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:36:MET:HG2	1:A:39:GLN:NE2	0.47	2.24	70	1
1:A:109:LYS:HE3	1:A:147:THR:CG2	0.47	2.40	25	6
2:B:177:VAL:O	2:B:193:VAL:HG21	0.47	2.08	20	3
1:A:104:ILE:HD12	1:A:121:TYR:CE2	0.47	2.44	35	1
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:6:LEU:HD12	1:A:44:MET:HB2	0.47	1.86	25	3
1:A:104:ILE:HD12	1:A:121:TYR:HE2	0.47	1.70	35	3
2:B:157:ASP:CB	2:B:160:ARG:HB2	0.47	2.40	4	2
2:B:29:ILE:HG22	2:B:92:TRP:HB2	0.47	1.87	40	1
1:A:55:LYS:HD3	1:A:102:ASN:HB3	0.47	1.87	46	1
1:A:152:SER:HA	2:B:94:LEU:HD13	0.47	1.86	60	3
2:B:24:ARG:HG2	2:B:69:THR:O	0.47	2.10	58	1
2:B:176:TRP:CE3	2:B:190:PRO:HG3	0.46	2.45	35	5
2:B:141:VAL:HG12	2:B:142:GLN:H	0.46	1.69	23	1
1:A:149:GLN:HG3	2:B:188:TYR:CE1	0.46	2.45	56	1
2:B:5:THR:HA	2:B:100:GLN:OE1	0.46	2.10	63	2
2:B:133:LEU:HD23	2:B:153:ALA:HA	0.46	1.87	75	10
2:B:50:ASN:HB3	2:B:53:THR:HG22	0.46	1.88	16	5
1:A:6:LEU:HD11	1:A:44:MET:HE2	0.46	1.88	33	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
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
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:NE1	0.46	2.26	30	1
1:A:4:ARG:HB3	2:B:92:TRP:HZ2	0.46	1.71	59	3
2:B:193:VAL:HB	2:B:197:PHE:HD1	0.46	1.71	18	4
2:B:227:ARG:O	2:B:235:PHE:HA	0.46	2.10	39	4
2:B:228:GLN:HG3	2:B:234:TRP:O	0.46	2.11	36	3
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:35:ASP:HB3	1:A:38:GLN:HE21	0.46	1.71	1	1
1:A:54:ASP:O	1:A:104:ILE:HA	0.46	2.11	49	2
2:B:149:LEU:HB2	2:B:210:LEU:HB3	0.45	1.87	3	4
2:B:32:TYR:O	2:B:90:HIS:HA	0.45	2.11	22	3
2:B:132:GLN:HA	2:B:237:TYR:CE2	0.45	2.47	23	1
1:A:8:CYS:SG	1:A:44:MET:HE3	0.45	2.51	24	2
1:A:108:ASN:HB2	2:B:181:SER:HB3	0.45	1.87	36	1
2:B:48:ILE:HD13	2:B:54:LEU:HG	0.45	1.87	68	2
1:A:6:LEU:HD13	1:A:150:PHE:HE1	0.45	1.71	58	3
1:A:20:MET:SD	1:A:26:LEU:HG	0.45	2.50	55	1
2:B:153:ALA:HB1	2:B:156:PHE:CE1	0.45	2.46	73	2
1:A:6:LEU:HD23	2:B:93:SER:OG	0.45	2.11	75	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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
2:B:230:LYS:CG	2:B:231:LYS:H	0.45	2.22	33	1
1:A:109:LYS:HG3	1:A:145:ASP:HB2	0.45	1.88	40	1
1:A:107:ASN:CG	1:A:108:ASN:H	0.45	2.20	12	2
2:B:36:TYR:OH	2:B:234:TRP:HB2	0.45	2.11	14	1
1:A:55:LYS:HE3	1:A:104:ILE:HG12	0.45	1.88	31	2
1:A:96:GLU:HB2	1:A:99:PHE:CD2	0.45	2.46	43	4
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:169:ALA:HB3	2:B:172:LYS:HD2	0.44	1.87	23	2
2:B:172:LYS:HG3	2:B:173:ARG:N	0.44	2.26	71	1
2:B:133:LEU:HD13	2:B:225:CYS:HB3	0.44	1.90	10	4
2:B:143:PRO:HD3	2:B:247:SER:O	0.44	2.13	30	7
1:A:8:CYS:SG	1:A:44:MET:HE2	0.44	2.52	18	1
2:B:230:LYS:HE3	2:B:234:TRP:HZ2	0.44	1.72	40	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:46:LEU:CB	2:B:236:ASP:HA	0.44	2.42	21	1
2:B:29:ILE:HD11	2:B:33:LEU:HD23	0.44	1.89	37	2
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:131:VAL:HB	2:B:237:TYR:CZ	0.44	2.47	70	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
1:A:150:PHE:HE2	2:B:93:SER:HA	0.44	1.73	33	1
2:B:23:CYS:HB2	2:B:35:TRP:CH2	0.44	2.48	75	2
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: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
2:B:85:ASN:HB2	2:B:87:TYR:CE1	0.43	2.46	26	1
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
1:A:93:LYS:HA	1:A:93:LYS:HE2	0.43	1.89	51	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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
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:162:ASP:HB3	2:B:228:GLN:NE2	0.43	2.28	52	1
2:B:180:ILE:HB	2:B:199:ILE:CG1	0.43	2.41	64	1
1:A:26:LEU:HD11	1:A:62:LEU:HD11	0.43	1.90	70	1
1:A:93:LYS:HA	1:A:93:LYS:HE3	0.43	1.90	71	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:O	1:A:65:LYS:HG2	0.43	2.14	64	1
2:B:157:ASP:OD1	2:B:160:ARG:HD3	0.43	2.14	57	3
2:B:4:MET:HE2	2:B:33:LEU:HD21	0.43	1.90	41	3
2:B:189:PHE:CZ	2:B:197:PHE:HB2	0.43	2.48	51	2
1:A:1:ALA:HB3	2:B:28:ASN:HB2	0.43	1.90	55	1
2:B:200:SER:HB2	2:B:209:TYR:HB2	0.43	1.90	55	3
2:B:61:ARG:HD2	2:B:77:SER:O	0.43	2.14	31	1
2:B:150:SER:HA	2:B:208:LEU:O	0.43	2.14	40	3
2:B:157:ASP:HB2	2:B:160:ARG:HB2	0.43	1.90	42	1
2:B:80:PRO:HA	2:B:106:ILE:CD1	0.43	2.43	49	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:91:PHE:CE2	2:B:232:LEU:HD13	0.42	2.49	41	1
1:A:95:MET:HE3	1:A:99:PHE:HB3	0.42	1.91	63	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
1:A:62:LEU:HD22	1:A:67:LEU:HD12	0.42	1.91	62	2
2:B:37:GLN:HB2	2:B:47:LEU:CD1	0.42	2.42	75	1
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:66:GLY:HA3	2:B:71:PHE:CD1	0.42	2.50	54	1
1:A:13:SER:HB3	1:A:109:LYS:NZ	0.42	2.30	68	1
2:B:87:TYR:OH	2:B:173:ARG:HA	0.42	2.14	77	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:20:THR:HG23	2:B:74:THR:HG23	0.42	1.91	29	1
2:B:157:ASP:HB3	2:B:160:ARG:CB	0.42	2.42	54	1
2:B:18:ARG:NH1	2:B:76:SER:HA	0.42	2.29	12	1
2:B:235:PHE:HB2	2:B:238:TRP:HE1	0.42	1.74	66	1
2:B:135:GLU:HA	2:B:151:CYS:HA	0.42	1.90	16	1
2:B:91:PHE:HE2	2:B:232:LEU:HD13	0.42	1.74	41	2
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
2:B:147:LEU:HD13	2:B:244:VAL:HG13	0.42	1.92	59	1
1:A:126:GLN:NE2	1:A:143:ILE:HG13	0.42	2.29	62	1
1:A:8:CYS:HB3	1:A:150:PHE:CD1	0.42	2.49	75	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
2:B:230:LYS:HD3	2:B:234:TRP:HZ3	0.42	1.74	60	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
1:A:151:VAL:C	2:B:94:LEU:HD12	0.41	2.40	45	1
2:B:13:ALA:O	2:B:106:ILE:HA	0.41	2.15	49	1
1:A:63:LYS:HG2	1:A:64:GLU:CD	0.41	2.39	57	1
1:A:7:ASN:HB3	1:A:41:VAL:HG11	0.41	1.91	63	1
2:B:52:LYS:HE2	2:B:65:SER:HA	0.41	1.92	74	3
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:CE2	1:A:138:LYS:HB2	0.41	2.50	60	2
2:B:6:GLN:OE1	2:B:87:TYR:HA	0.41	2.15	25	1
2:B:167:ARG:HA	2:B:222:VAL:O	0.41	2.16	37	1
2:B:143:PRO:HA	2:B:246:VAL:HG12	0.41	1.92	42	1
1:A:121:TYR:HB2	1:A:144:THR:HG22	0.41	1.93	58	1
1:A:109:LYS:HE3	2:B:185:GLY:HA3	0.41	1.92	63	1
2:B:18:ARG:HA	2:B:75:ILE:O	0.41	2.15	68	1
2:B:135:GLU:HA	2:B:150:SER:O	0.41	2.15	68	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:15:GLN:OE1	1:A:15:GLN:HA	0.41	2.15	25	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:37:GLN:CD	2:B:39:LYS:HE3	0.41	2.39	30	1
2:B:52:LYS:HB3	2:B:64:GLY:O	0.41	2.14	34	1
1:A:4:ARG:NH2	2:B:30:HIS:HB2	0.41	2.30	43	1
2:B:25:THR:CG2	2:B:69:THR:HA	0.41	2.45	30	2
2:B:87:TYR:CE1	2:B:101:GLY:HA3	0.41	2.51	43	1
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:94:LEU:H	2:B:94:LEU:HD12	0.41	1.75	6	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
1:A:149:GLN:HA	2:B:188:TYR:CE1	0.41	2.50	32	1
2:B:2:ILE:HG22	2:B:26:SER:HB2	0.41	1.93	2	1
2:B:227:ARG:HH21	2:B:236:ASP:CG	0.41	2.24	55	2
2:B:230:LYS:HB3	2:B:231:LYS:H	0.41	1.55	29	1
2:B:143:PRO:HA	2:B:246:VAL:CG1	0.41	2.46	42	1
2:B:199:ILE:HD13	2:B:199:ILE:H	0.41	1.76	57	3
1:A:21:SER:HB2	1:A:27:LYS:HG2	0.41	1.90	70	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:172:LYS:HG2	2:B:173:ARG:N	0.41	2.30	18	2
2:B:78:LEU:HD21	2:B:106:ILE:HG13	0.41	1.92	37	1
1:A:81:GLN:NE2	1:A:83:GLU:HG3	0.41	2.31	50	1
2:B:138:GLY:H	2:B:242:THR:HG21	0.41	1.76	68	1
2:B:38:GLN:HB3	2:B:85:ASN:ND2	0.41	2.31	75	2
1:A:4:ARG:NH1	2:B:30:HIS:HB3	0.40	2.31	1	1
2:B:34:THR:HB	2:B:36:TYR:HE1	0.40	1.75	2	1
1:A:37:GLU:OE2	1:A:37:GLU:HA	0.40	2.15	26	1
2:B:228:GLN:HA	2:B:234:TRP:O	0.40	2.16	39	1
1:A:141:GLN:H	1:A:141:GLN:CD	0.40	2.24	56	1
2:B:55:ALA:HB3	2:B:58:VAL:CG2	0.40	2.46	63	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
2:B:189:PHE:CE1	2:B:199:ILE:HD12	0.40	2.51	11	1
1:A:21:SER:CB	1:A:27:LYS:HE2	0.40	2.46	16	2
1:A:54:ASP:HA	2:B:231:LYS:HZ1	0.40	1.76	31	1
2:B:166:VAL:HG12	2:B:176:TRP:HA	0.40	1.93	35	1
2:B:228:GLN:HG2	2:B:234:TRP:O	0.40	2.16	47	1
2:B:87:TYR:CD1	2:B:101:GLY:HA3	0.40	2.51	18	1
1:A:108:ASN:HB3	2:B:181:SER:HB2	0.40	1.92	22	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:106:ILE:HG13	1:A:107:ASN:N	0.40	2.32	66	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	151/153 (99%)	142±2 (94±2%)	9±2 (6±2%)	1±1 (1±1%)	26	74
2	B	234/254 (92%)	217±3 (93±1%)	15±3 (6±1%)	2±1 (1±0%)	18	68
All	All	29645/31339 (95%)	27623 (93%)	1820 (6%)	202 (1%)	20	70

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
1	A	107	ASN	8
2	B	170	PRO	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
2	B	27	GLY	1
2	B	28	ASN	1
1	A	49	GLY	1
1	A	85	VAL	1
1	A	101	PHE	1

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Mol	Chain	Res	Type	Models (Total)
1	A	114	SER	1
2	B	96	PHE	1
2	B	97	THR	1
2	B	177	VAL	1
2	B	31	ASN	1
2	B	230	LYS	1
1	A	58	VAL	1
2	B	192	THR	1
1	A	4	ARG	1
1	A	6	LEU	1
1	A	32	GLN	1
2	B	241	GLY	1
1	A	46	PHE	1
2	B	52	LYS	1
1	A	52	SER	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%)	127±3 (91±2%)	13±3 (9±2%)	11	56
2	B	200/203 (99%)	172±4 (86±2%)	28±4 (14±2%)	5	45
All	All	26180/26411 (99%)	23033 (88%)	3147 (12%)	7	49

All 193 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	33	LEU	76
2	B	192	THR	76
2	B	97	THR	74
2	B	199	ILE	74
2	B	45	GLN	70
1	A	13	SER	67
2	B	25	THR	67
2	B	69	THR	67
1	A	77	LYS	62

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Mol	Chain	Res	Type	Models (Total)
2	B	242	THR	62
2	B	187	THR	57
1	A	29	LEU	56
2	B	60	SER	56
2	B	150	SER	56
2	B	109	THR	55
2	B	34	THR	54
1	A	79	THR	52
2	B	14	SER	48
1	A	137	THR	45
1	A	110	LEU	44
2	B	236	ASP	44
2	B	181	SER	43
2	B	245	THR	42
1	A	6	LEU	40
2	B	147	LEU	40
2	B	225	CYS	39
2	B	74	THR	38
2	B	182	SER	36
2	B	154	SER	35
2	B	9	SER	35
2	B	81	GLU	34
1	A	84	SER	34
1	A	102	ASN	34
2	B	5	THR	33
1	A	71	CYS	32
1	A	119	ASN	32
2	B	136	SER	32
1	A	124	THR	31
2	B	20	THR	31
1	A	64	GLU	31
2	B	233	THR	31
1	A	149	GLN	29
2	B	94	LEU	28
2	B	159	SER	28
2	B	162	ASP	28
1	A	152	SER	27
2	B	26	SER	27
1	A	76	ASP	26
2	B	22	THR	24
2	B	176	TRP	24
2	B	50	ASN	24

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Mol	Chain	Res	Type	Models (Total)
2	B	186	SER	24
1	A	9	THR	23
2	B	76	SER	23
1	A	108	ASN	22
2	B	230	LYS	22
2	B	214	SER	20
1	A	35	ASP	19
2	B	88	CYS	19
2	B	30	HIS	19
1	A	144	THR	18
2	B	11	LEU	18
1	A	32	GLN	18
2	B	67	SER	17
2	B	107	LYS	17
2	B	129	SER	17
1	A	147	THR	17
2	B	90	HIS	16
2	B	163	MET	16
2	B	72	THR	16
1	A	53	ASN	16
2	B	157	ASP	16
1	A	106	ILE	15
1	A	48	GLN	14
2	B	198	THR	14
1	A	93	LYS	14
2	B	63	SER	14
1	A	50	GLU	12
2	B	17	ASP	12
2	B	7	SER	11
2	B	56	ASP	11
2	B	189	PHE	11
1	A	45	SER	10
2	B	250	HIS	10
2	B	246	VAL	10
2	B	175	GLU	10
2	B	141	VAL	10
2	B	31	ASN	9
2	B	52	LYS	9
2	B	53	THR	9
1	A	121	TYR	9
2	B	206	ASN	9
1	A	34	GLN	8

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Mol	Chain	Res	Type	Models (Total)
2	B	249	HIS	8
2	B	164	SER	8
2	B	191	ASP	8
2	B	108	ARG	8
2	B	227	ARG	7
1	A	5	SER	7
1	A	138	LYS	7
2	B	77	SER	7
2	B	142	GLN	6
1	A	56	ILE	6
1	A	116	GLN	6
1	A	105	GLU	6
1	A	37	GLU	6
1	A	43	SER	6
2	B	234	TRP	6
1	A	125	SER	6
1	A	39	GLN	5
2	B	228	GLN	5
2	B	231	LYS	5
1	A	109	LYS	5
2	B	146	SER	5
2	B	93	SER	5
2	B	247	SER	5
1	A	17	SER	5
2	B	166	VAL	5
1	A	54	ASP	4
1	A	75	ASP	4
1	A	123	SER	4
1	A	52	SER	4
1	A	51	GLU	4
1	A	145	ASP	4
2	B	148	ARG	4
2	B	92	TRP	4
2	B	89	GLN	4
2	B	160	ARG	4
1	A	8	CYS	3
2	B	132	GLN	3
1	A	128	GLU	3
2	B	248	SER	3
1	A	73	LEU	3
2	B	65	SER	3
2	B	1	ASP	3

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Mol	Chain	Res	Type	Models (Total)
1	A	142	ASP	3
2	B	70	GLN	3
1	A	38	GLN	2
2	B	2	ILE	2
2	B	106	ILE	2
2	B	130	GLU	2
2	B	12	SER	2
1	A	89	ASN	2
2	B	216	ARG	2
2	B	200	SER	2
2	B	218	GLU	2
1	A	55	LYS	2
1	A	151	VAL	2
1	A	7	ASN	2
1	A	153	SER	2
2	B	235	PHE	2
1	A	97	LYS	2
1	A	150	PHE	2
1	A	26	LEU	2
2	B	3	GLN	1
2	B	24	ARG	1
1	A	66	ASN	1
1	A	4	ARG	1
2	B	29	ILE	1
1	A	46	PHE	1
1	A	132	VAL	1
2	B	134	VAL	1
1	A	21	SER	1
1	A	104	ILE	1
1	A	41	VAL	1
2	B	85	ASN	1
1	A	81	GLN	1
2	B	203	ASN	1
1	A	86	ASP	1
2	B	54	LEU	1
1	A	92	LYS	1
2	B	174	LEU	1
1	A	141	GLN	1
1	A	95	MET	1
2	B	42	LYS	1
1	A	11	ARG	1
2	B	179	TYR	1

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Mol	Chain	Res	Type	Models (Total)
1	A	88	LYS	1
1	A	148	MET	1
1	A	20	MET	1
1	A	58	VAL	1
2	B	240	GLN	1
1	A	36	MET	1
1	A	83	GLU	1
1	A	94	LYS	1
2	B	173	ARG	1
2	B	237	TYR	1
1	A	19	VAL	1
1	A	30	HIS	1
1	A	31	LEU	1
2	B	205	LYS	1
1	A	25	GLU	1
2	B	135	GLU	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 ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided