



Full wwPDB NMR Structure Validation Report ⓘ

Mar 4, 2026 – 11:32 PM UTC

PDB ID : 1Y4E / pdb_00001y4e
Title : NMR structure of transmembrane segment IV of the NHE1 isoform of the Na⁺/H⁺ exchanger
Authors : Slepko, E.R.; Rainey, J.K.; Li, X.; Liu, Y.; Lindhout, D.A.; Sykes, B.D.; Fliegel, L.
Deposited on : 2004-11-30

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
Mogul	:	2022.3.0, CSD as543be (2022)
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

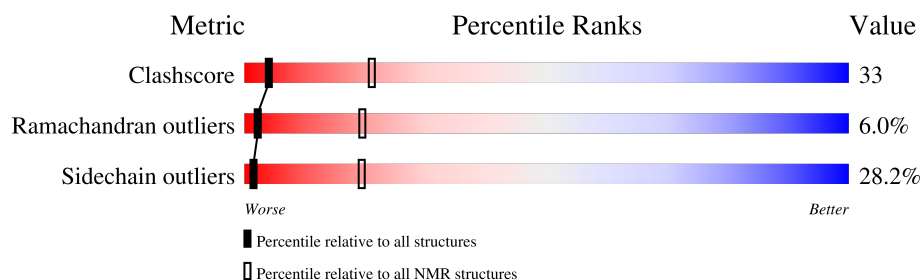
1 Overall quality at a glance

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	27	11% 15% . 70%

2 Ensemble composition and analysis

This entry contains 100 models. Model 9 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:169-A:176 (8)	0.35	9

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 15 clusters and 3 single-model clusters were found.

Cluster number	Models
1	9, 13, 14, 18, 24, 25, 28, 29, 30, 31, 32, 37, 38, 40, 43, 47, 50, 52, 57, 61, 65, 66, 68, 73, 74, 77, 81, 90, 92, 95
2	1, 7, 10, 26, 27, 39, 44, 46, 51, 56, 71, 76, 89, 94, 97
3	3, 8, 16, 21, 22, 36, 55, 75, 86, 87, 96, 99, 100
4	35, 41, 42, 70, 80, 84, 88, 93
5	2, 11, 23, 49, 69, 79, 98
6	12, 54, 64
7	17, 19, 58
8	33, 60, 72
9	4, 59, 91
10	15, 48
11	67, 83
12	6, 45
13	63, 85
14	20, 34
15	5, 53
Single-model clusters	62; 78; 82

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 458 atoms, of which 233 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Sodium/hydrogen exchanger 1.

Mol	Chain	Residues	Atoms					Trace
1	A	27	Total	C	H	N	O	0
			458	159	233	31	35	

There is a discrepancy between the modelled and reference sequences:

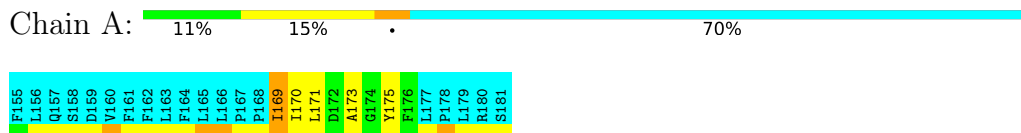
Chain	Residue	Modelled	Actual	Comment	Reference
A	181	HSL	-	insertion	UNP P19634

4 Residue-property plots

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: Sodium/hydrogen exchanger 1

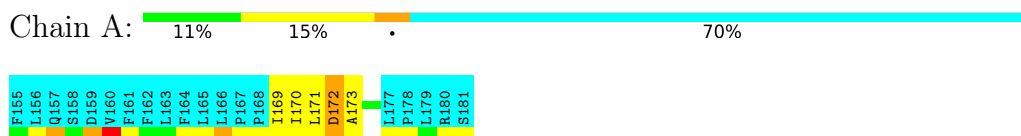


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Sodium/hydrogen exchanger 1



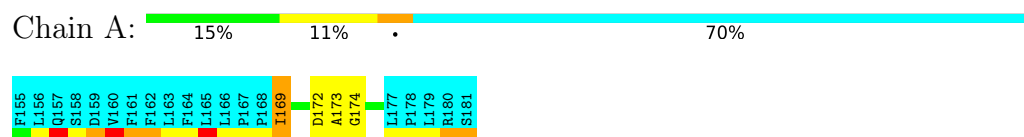
4.2.2 Score per residue for model 2

- Molecule 1: Sodium/hydrogen exchanger 1



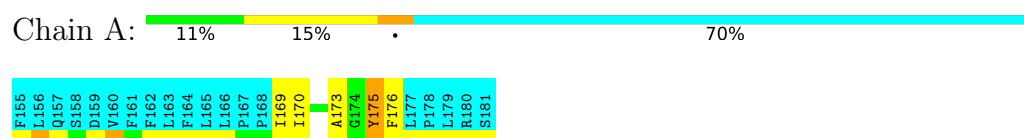
4.2.3 Score per residue for model 3

- Molecule 1: Sodium/hydrogen exchanger 1



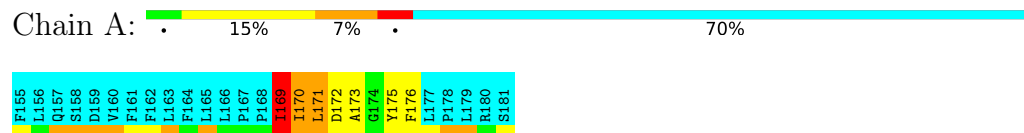
4.2.4 Score per residue for model 4

- Molecule 1: Sodium/hydrogen exchanger 1



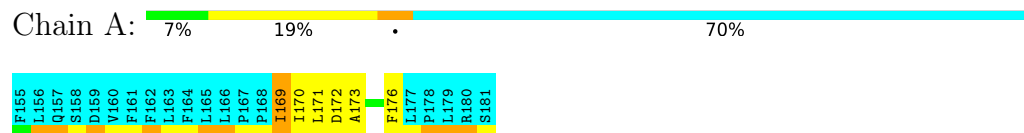
4.2.5 Score per residue for model 5

- Molecule 1: Sodium/hydrogen exchanger 1



4.2.6 Score per residue for model 6

- Molecule 1: Sodium/hydrogen exchanger 1



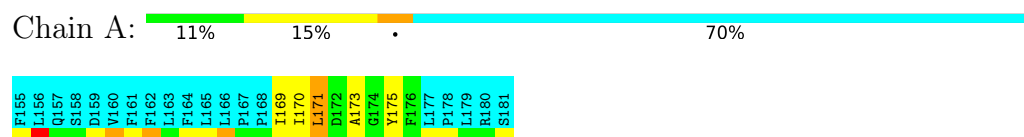
4.2.7 Score per residue for model 7

- Molecule 1: Sodium/hydrogen exchanger 1



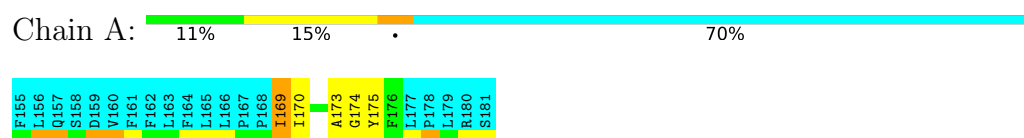
4.2.8 Score per residue for model 8

- Molecule 1: Sodium/hydrogen exchanger 1



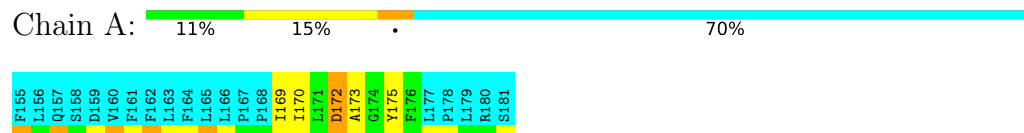
4.2.9 Score per residue for model 9 (medoid)

- Molecule 1: Sodium/hydrogen exchanger 1



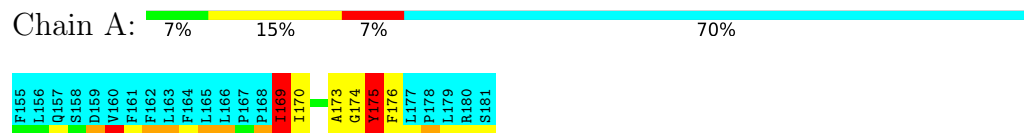
4.2.10 Score per residue for model 10

- Molecule 1: Sodium/hydrogen exchanger 1



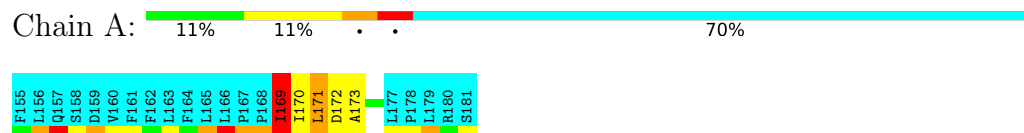
4.2.11 Score per residue for model 11

- Molecule 1: Sodium/hydrogen exchanger 1



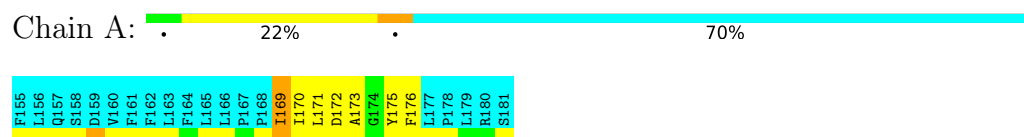
4.2.12 Score per residue for model 12

- Molecule 1: Sodium/hydrogen exchanger 1



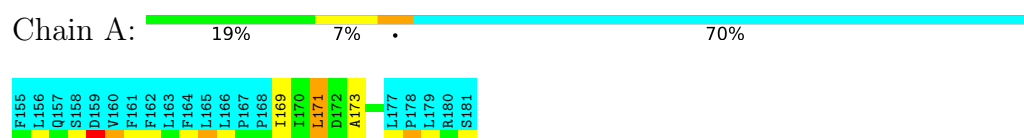
4.2.13 Score per residue for model 13

- Molecule 1: Sodium/hydrogen exchanger 1



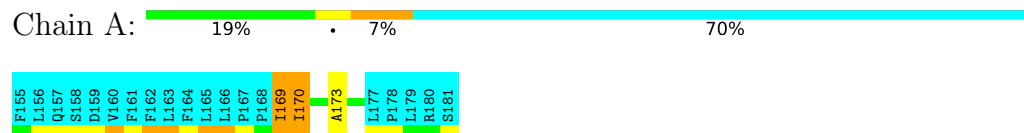
4.2.14 Score per residue for model 14

- Molecule 1: Sodium/hydrogen exchanger 1



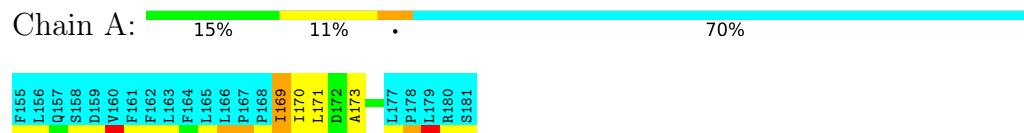
4.2.15 Score per residue for model 15

- Molecule 1: Sodium/hydrogen exchanger 1



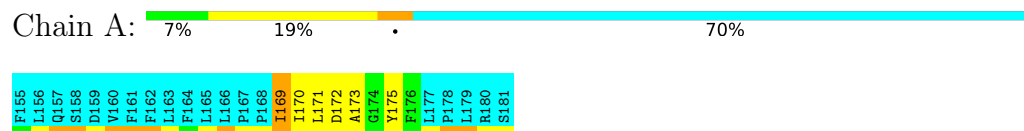
4.2.16 Score per residue for model 16

- Molecule 1: Sodium/hydrogen exchanger 1



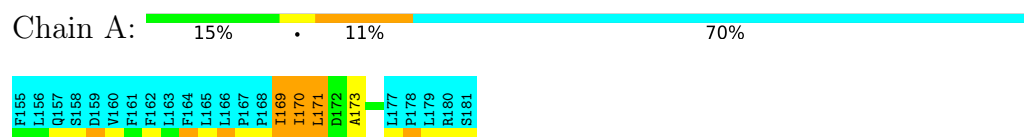
4.2.17 Score per residue for model 17

- Molecule 1: Sodium/hydrogen exchanger 1



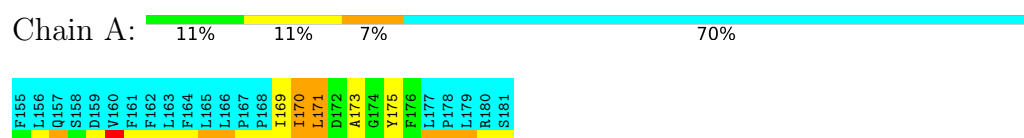
4.2.18 Score per residue for model 18

- Molecule 1: Sodium/hydrogen exchanger 1



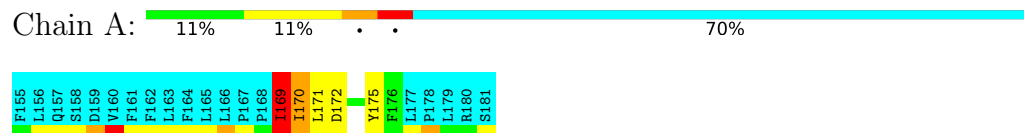
4.2.19 Score per residue for model 19

- Molecule 1: Sodium/hydrogen exchanger 1



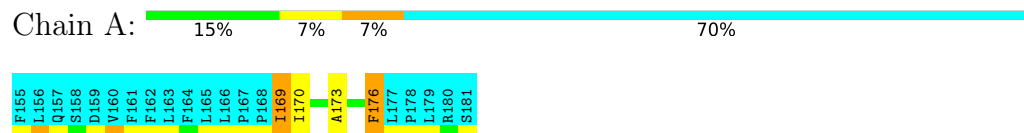
4.2.20 Score per residue for model 20

- Molecule 1: Sodium/hydrogen exchanger 1



4.2.21 Score per residue for model 21

- Molecule 1: Sodium/hydrogen exchanger 1



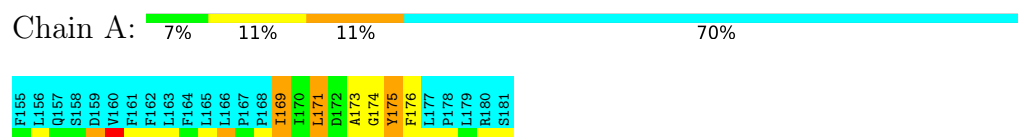
4.2.22 Score per residue for model 22

- Molecule 1: Sodium/hydrogen exchanger 1



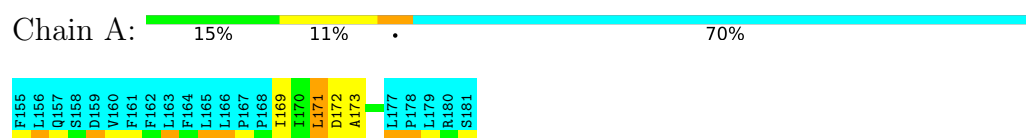
4.2.23 Score per residue for model 23

- Molecule 1: Sodium/hydrogen exchanger 1



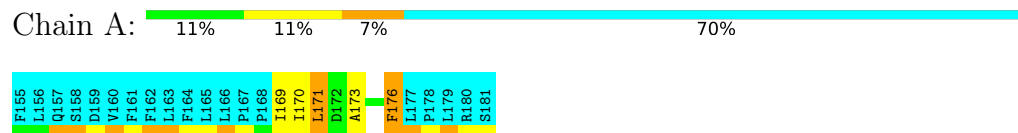
4.2.24 Score per residue for model 24

- Molecule 1: Sodium/hydrogen exchanger 1



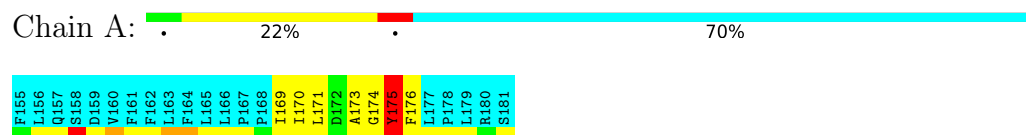
4.2.25 Score per residue for model 25

- Molecule 1: Sodium/hydrogen exchanger 1



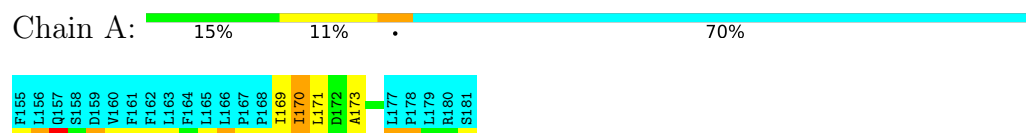
4.2.26 Score per residue for model 26

- Molecule 1: Sodium/hydrogen exchanger 1



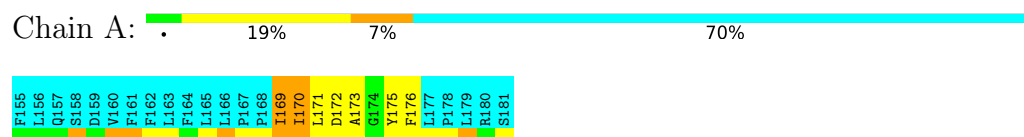
4.2.27 Score per residue for model 27

- Molecule 1: Sodium/hydrogen exchanger 1



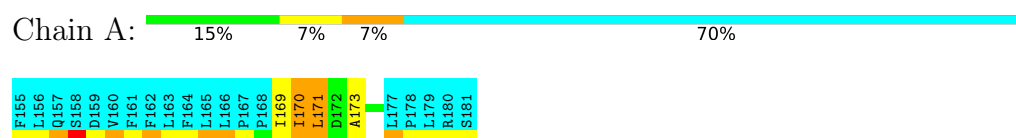
4.2.28 Score per residue for model 28

- Molecule 1: Sodium/hydrogen exchanger 1



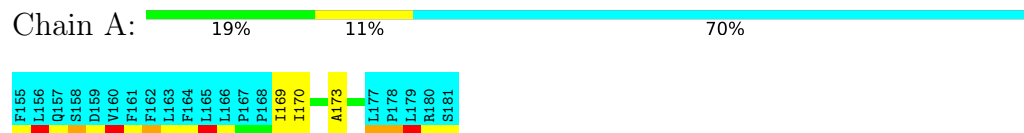
4.2.29 Score per residue for model 29

- Molecule 1: Sodium/hydrogen exchanger 1



4.2.30 Score per residue for model 30

- Molecule 1: Sodium/hydrogen exchanger 1



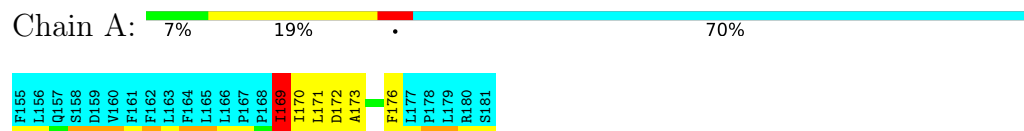
4.2.31 Score per residue for model 31

- Molecule 1: Sodium/hydrogen exchanger 1



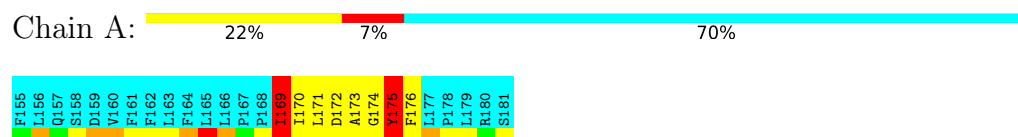
4.2.32 Score per residue for model 32

- Molecule 1: Sodium/hydrogen exchanger 1



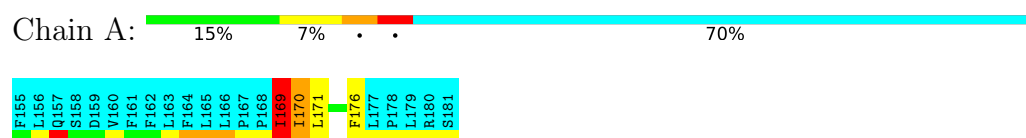
4.2.33 Score per residue for model 33

- Molecule 1: Sodium/hydrogen exchanger 1



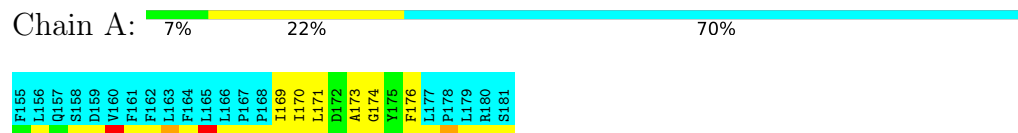
4.2.34 Score per residue for model 34

- Molecule 1: Sodium/hydrogen exchanger 1



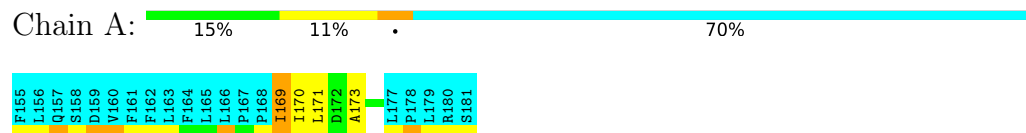
4.2.35 Score per residue for model 35

- Molecule 1: Sodium/hydrogen exchanger 1



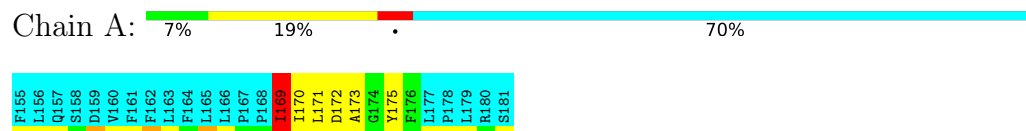
4.2.36 Score per residue for model 36

- Molecule 1: Sodium/hydrogen exchanger 1



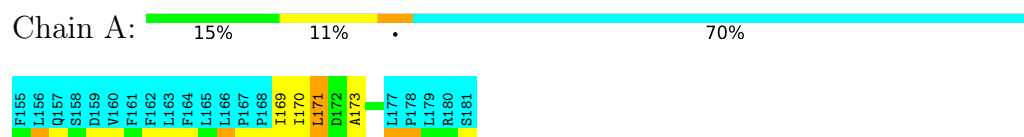
4.2.37 Score per residue for model 37

- Molecule 1: Sodium/hydrogen exchanger 1



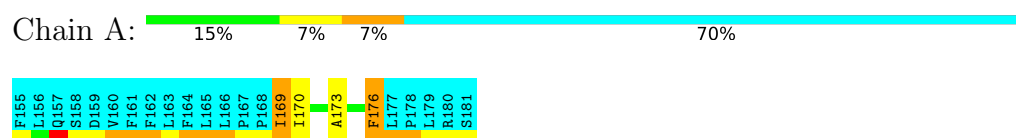
4.2.38 Score per residue for model 38

- Molecule 1: Sodium/hydrogen exchanger 1



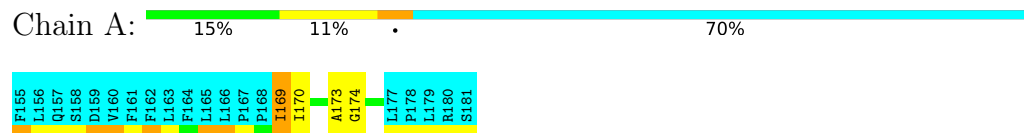
4.2.39 Score per residue for model 39

- Molecule 1: Sodium/hydrogen exchanger 1



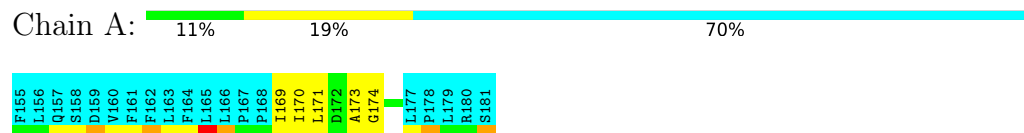
4.2.40 Score per residue for model 40

- Molecule 1: Sodium/hydrogen exchanger 1



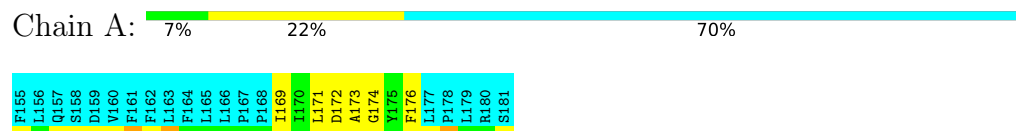
4.2.41 Score per residue for model 41

- Molecule 1: Sodium/hydrogen exchanger 1



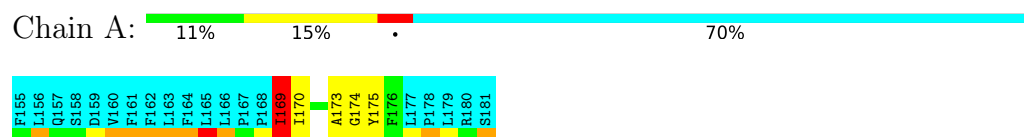
4.2.42 Score per residue for model 42

- Molecule 1: Sodium/hydrogen exchanger 1



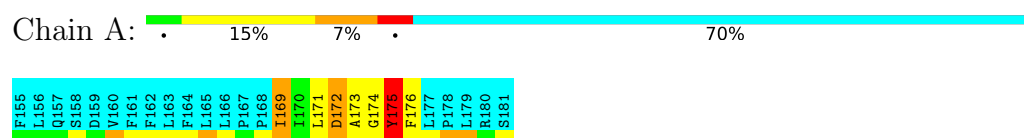
4.2.43 Score per residue for model 43

- Molecule 1: Sodium/hydrogen exchanger 1



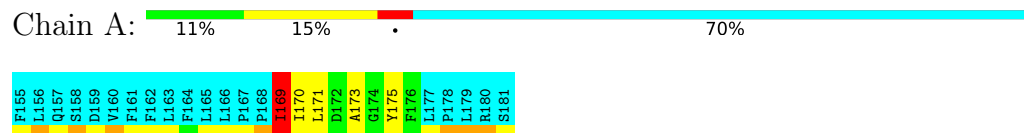
4.2.44 Score per residue for model 44

- Molecule 1: Sodium/hydrogen exchanger 1



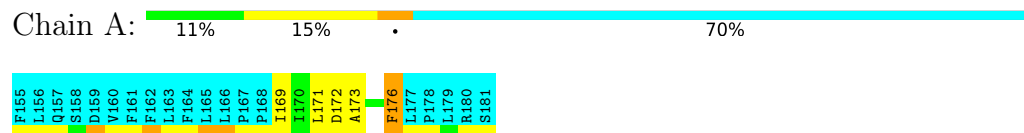
4.2.45 Score per residue for model 45

- Molecule 1: Sodium/hydrogen exchanger 1



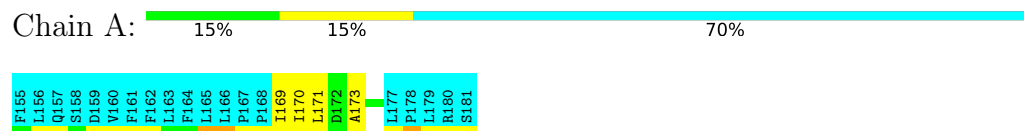
4.2.46 Score per residue for model 46

- Molecule 1: Sodium/hydrogen exchanger 1



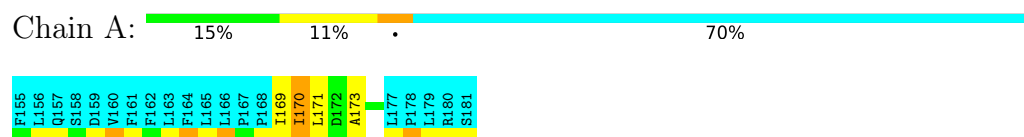
4.2.47 Score per residue for model 47

- Molecule 1: Sodium/hydrogen exchanger 1



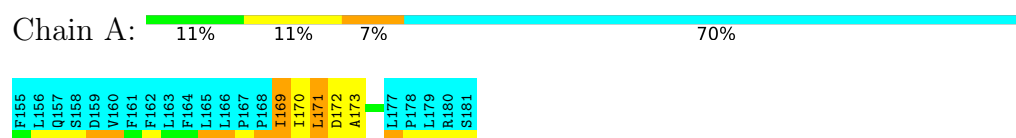
4.2.48 Score per residue for model 48

- Molecule 1: Sodium/hydrogen exchanger 1



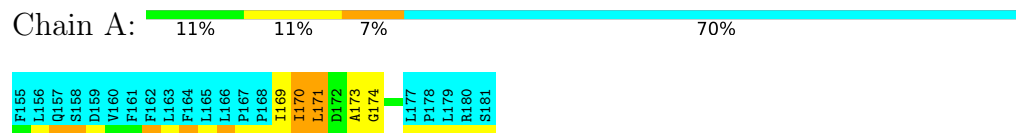
4.2.49 Score per residue for model 49

- Molecule 1: Sodium/hydrogen exchanger 1



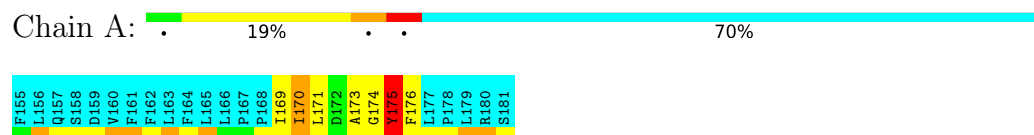
4.2.50 Score per residue for model 50

- Molecule 1: Sodium/hydrogen exchanger 1



4.2.51 Score per residue for model 51

- Molecule 1: Sodium/hydrogen exchanger 1



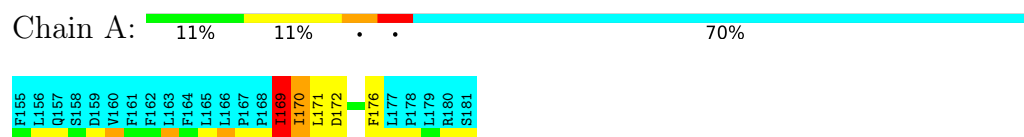
4.2.52 Score per residue for model 52

- Molecule 1: Sodium/hydrogen exchanger 1



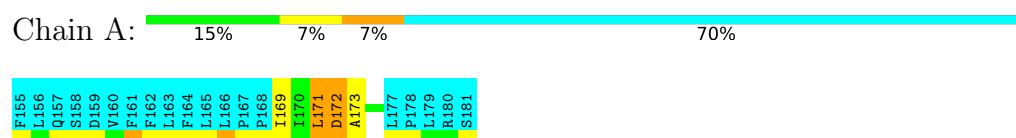
4.2.53 Score per residue for model 53

- Molecule 1: Sodium/hydrogen exchanger 1



4.2.54 Score per residue for model 54

- Molecule 1: Sodium/hydrogen exchanger 1



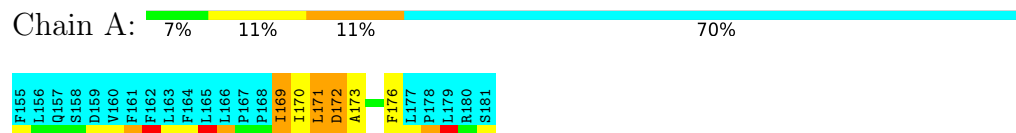
4.2.55 Score per residue for model 55

- Molecule 1: Sodium/hydrogen exchanger 1



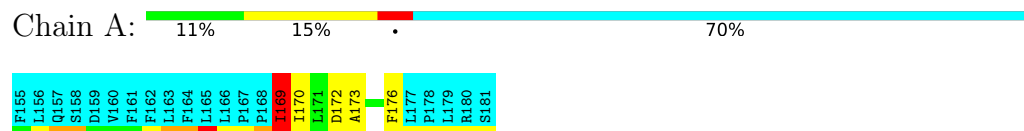
4.2.56 Score per residue for model 56

- Molecule 1: Sodium/hydrogen exchanger 1



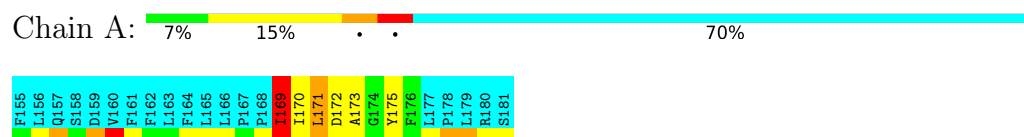
4.2.57 Score per residue for model 57

- Molecule 1: Sodium/hydrogen exchanger 1



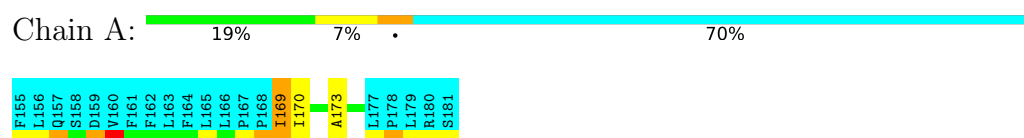
4.2.58 Score per residue for model 58

- Molecule 1: Sodium/hydrogen exchanger 1



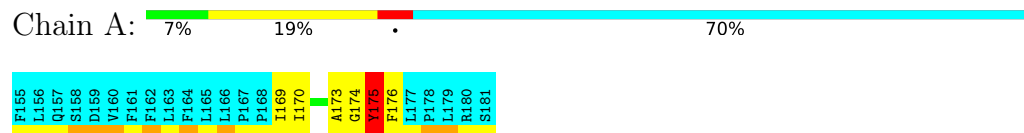
4.2.59 Score per residue for model 59

- Molecule 1: Sodium/hydrogen exchanger 1



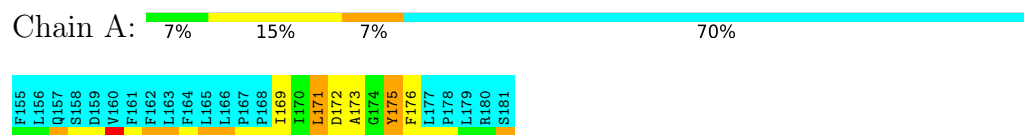
4.2.60 Score per residue for model 60

- Molecule 1: Sodium/hydrogen exchanger 1



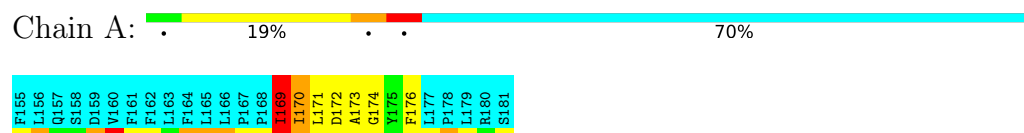
4.2.61 Score per residue for model 61

- Molecule 1: Sodium/hydrogen exchanger 1



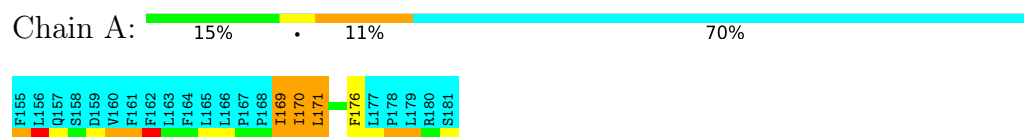
4.2.62 Score per residue for model 62

- Molecule 1: Sodium/hydrogen exchanger 1



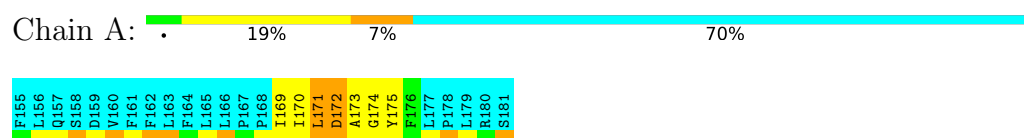
4.2.63 Score per residue for model 63

- Molecule 1: Sodium/hydrogen exchanger 1



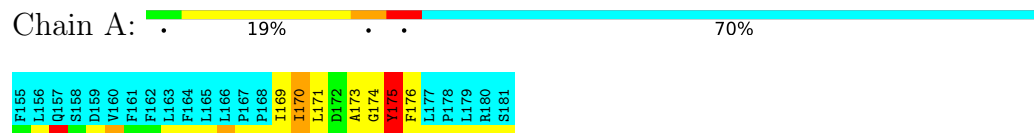
4.2.64 Score per residue for model 64

- Molecule 1: Sodium/hydrogen exchanger 1



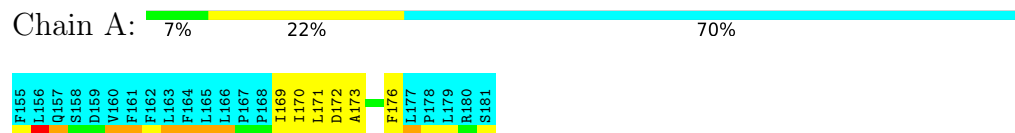
4.2.65 Score per residue for model 65

- Molecule 1: Sodium/hydrogen exchanger 1



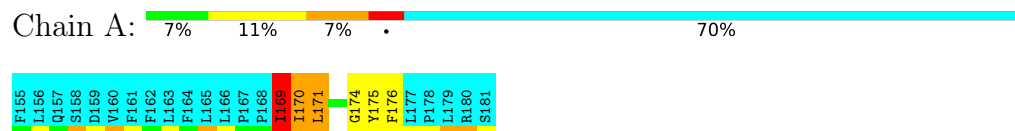
4.2.66 Score per residue for model 66

- Molecule 1: Sodium/hydrogen exchanger 1



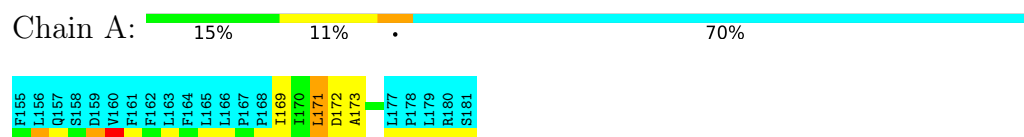
4.2.67 Score per residue for model 67

- Molecule 1: Sodium/hydrogen exchanger 1



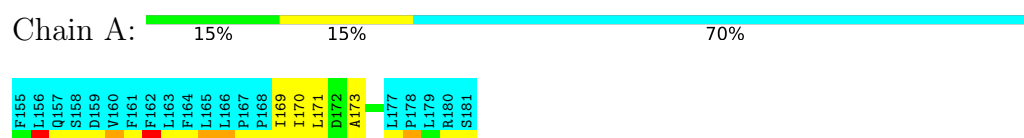
4.2.68 Score per residue for model 68

- Molecule 1: Sodium/hydrogen exchanger 1



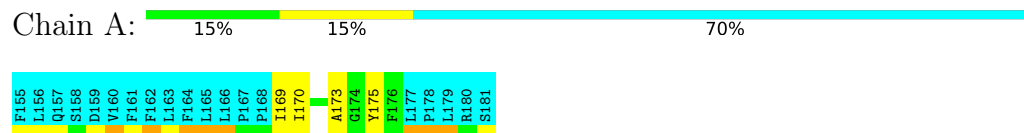
4.2.69 Score per residue for model 69

- Molecule 1: Sodium/hydrogen exchanger 1



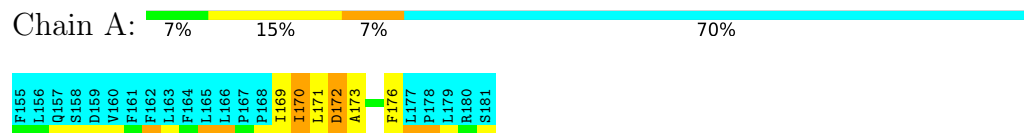
4.2.70 Score per residue for model 70

- Molecule 1: Sodium/hydrogen exchanger 1



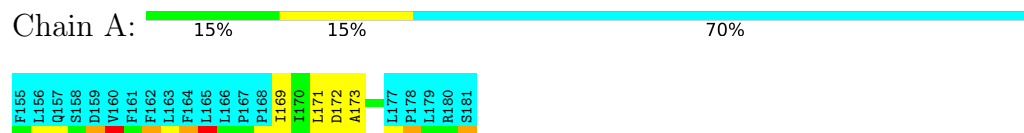
4.2.71 Score per residue for model 71

- Molecule 1: Sodium/hydrogen exchanger 1



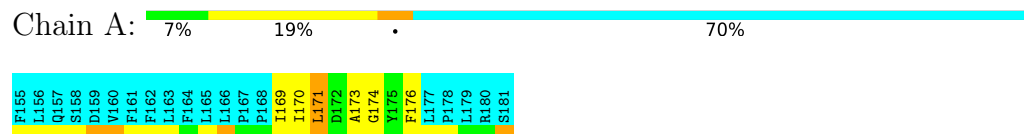
4.2.72 Score per residue for model 72

- Molecule 1: Sodium/hydrogen exchanger 1



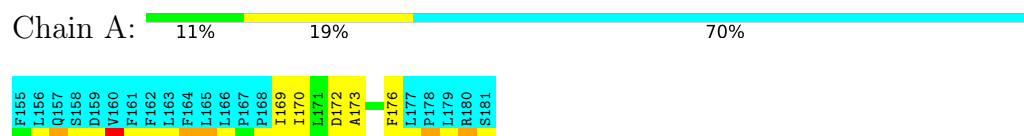
4.2.73 Score per residue for model 73

- Molecule 1: Sodium/hydrogen exchanger 1



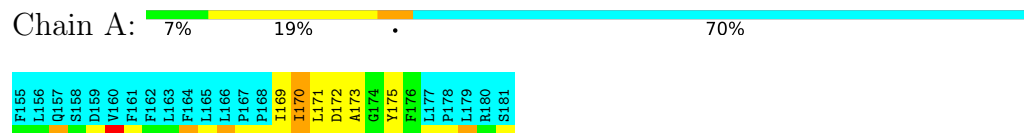
4.2.74 Score per residue for model 74

- Molecule 1: Sodium/hydrogen exchanger 1



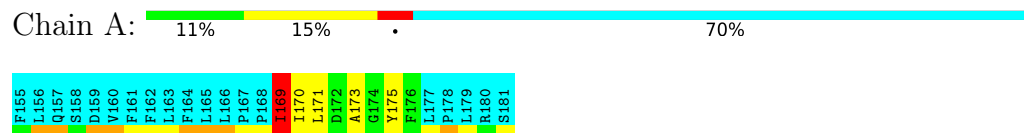
4.2.75 Score per residue for model 75

- Molecule 1: Sodium/hydrogen exchanger 1



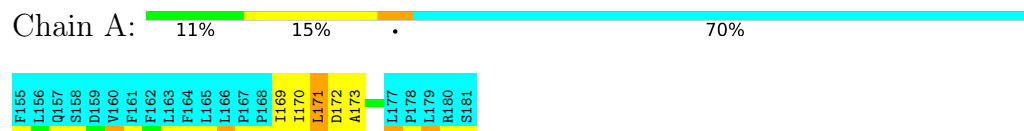
4.2.76 Score per residue for model 76

- Molecule 1: Sodium/hydrogen exchanger 1



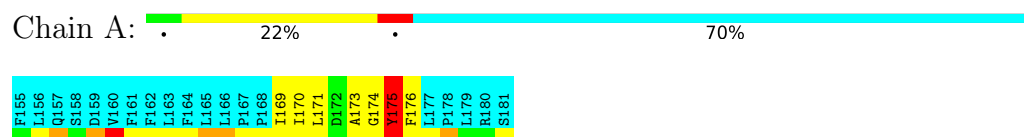
4.2.77 Score per residue for model 77

- Molecule 1: Sodium/hydrogen exchanger 1



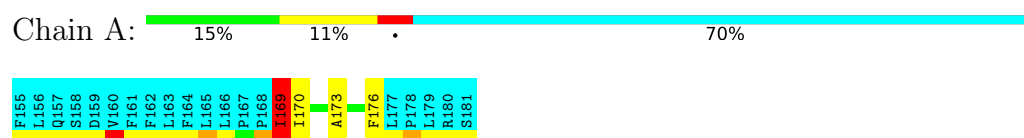
4.2.78 Score per residue for model 78

- Molecule 1: Sodium/hydrogen exchanger 1



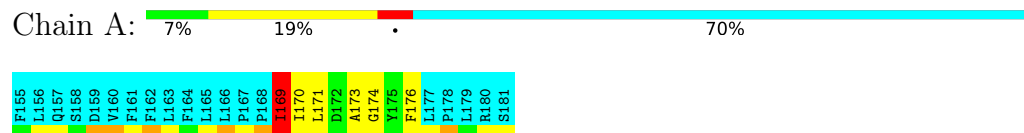
4.2.79 Score per residue for model 79

- Molecule 1: Sodium/hydrogen exchanger 1



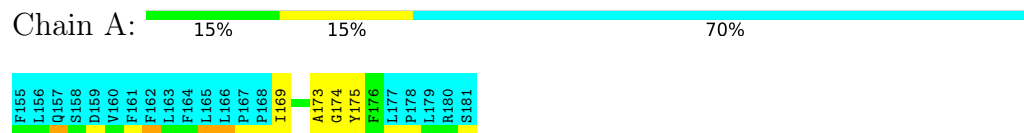
4.2.80 Score per residue for model 80

- Molecule 1: Sodium/hydrogen exchanger 1



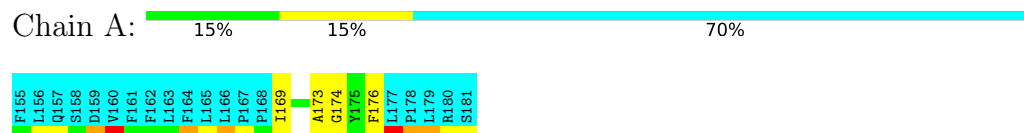
4.2.81 Score per residue for model 81

- Molecule 1: Sodium/hydrogen exchanger 1



4.2.82 Score per residue for model 82

- Molecule 1: Sodium/hydrogen exchanger 1



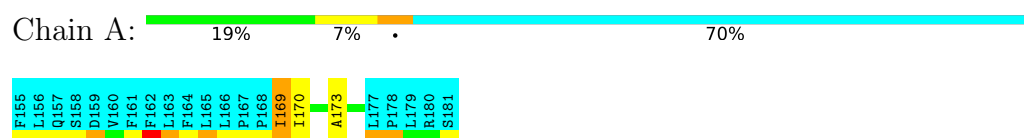
4.2.83 Score per residue for model 83

- Molecule 1: Sodium/hydrogen exchanger 1



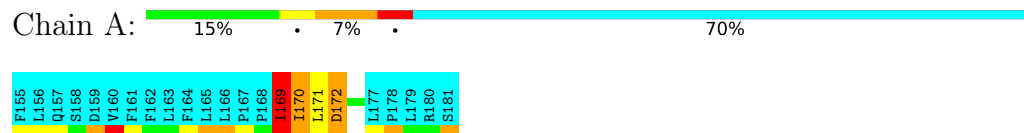
4.2.84 Score per residue for model 84

- Molecule 1: Sodium/hydrogen exchanger 1



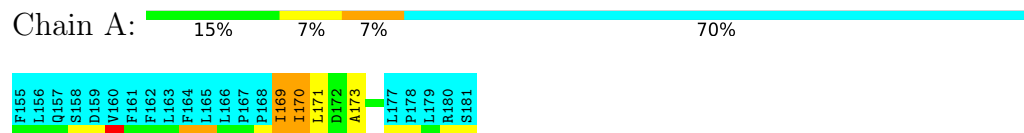
4.2.85 Score per residue for model 85

- Molecule 1: Sodium/hydrogen exchanger 1



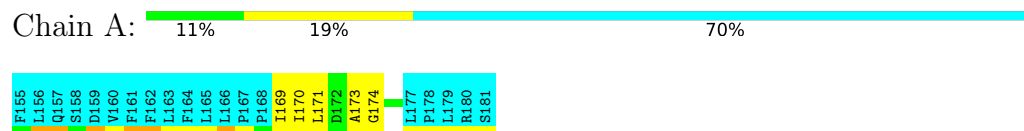
4.2.86 Score per residue for model 86

- Molecule 1: Sodium/hydrogen exchanger 1



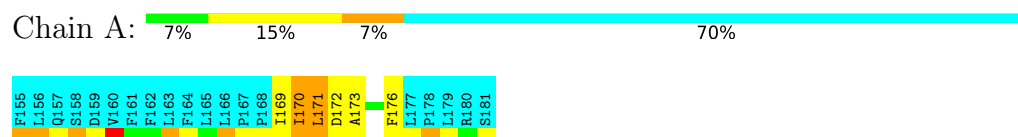
4.2.87 Score per residue for model 87

- Molecule 1: Sodium/hydrogen exchanger 1



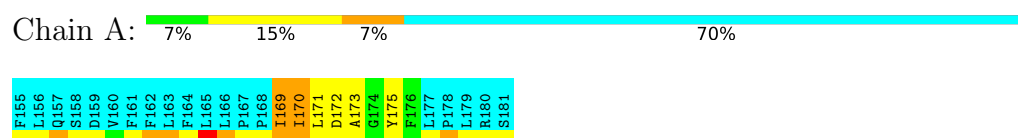
4.2.88 Score per residue for model 88

- Molecule 1: Sodium/hydrogen exchanger 1



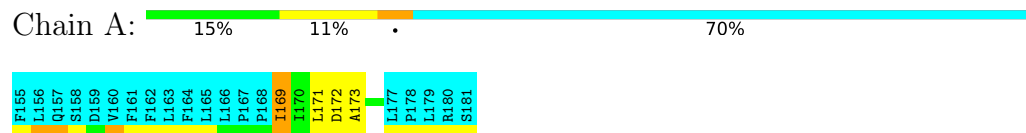
4.2.89 Score per residue for model 89

- Molecule 1: Sodium/hydrogen exchanger 1



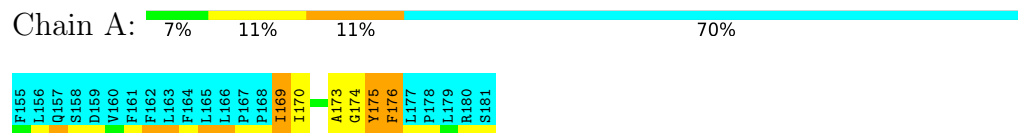
4.2.90 Score per residue for model 90

- Molecule 1: Sodium/hydrogen exchanger 1



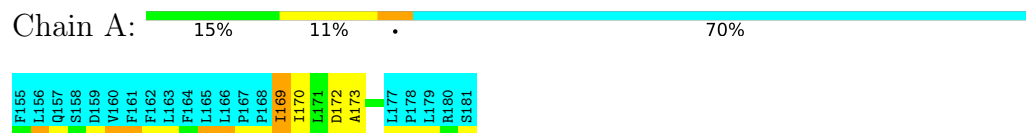
4.2.91 Score per residue for model 91

- Molecule 1: Sodium/hydrogen exchanger 1



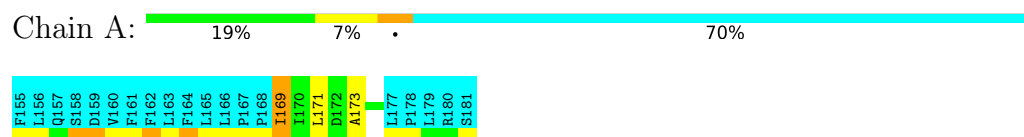
4.2.92 Score per residue for model 92

- Molecule 1: Sodium/hydrogen exchanger 1



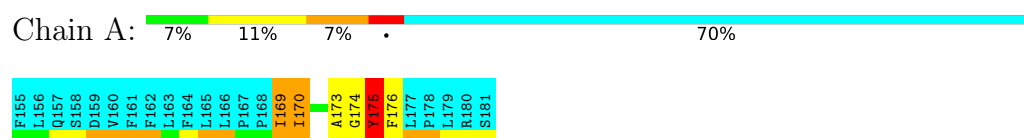
4.2.93 Score per residue for model 93

- Molecule 1: Sodium/hydrogen exchanger 1



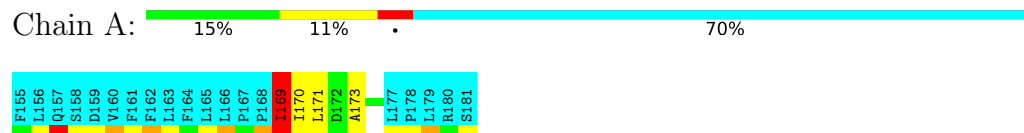
4.2.94 Score per residue for model 94

- Molecule 1: Sodium/hydrogen exchanger 1



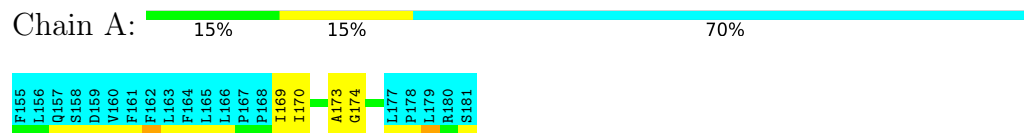
4.2.95 Score per residue for model 95

- Molecule 1: Sodium/hydrogen exchanger 1



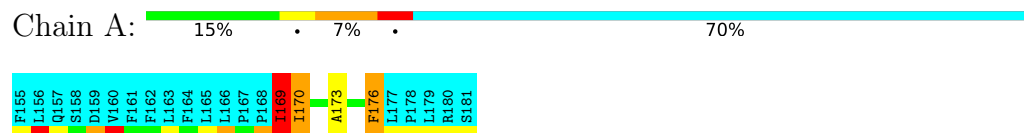
4.2.96 Score per residue for model 96

- Molecule 1: Sodium/hydrogen exchanger 1



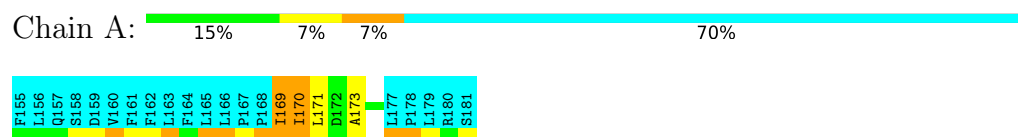
4.2.97 Score per residue for model 97

- Molecule 1: Sodium/hydrogen exchanger 1



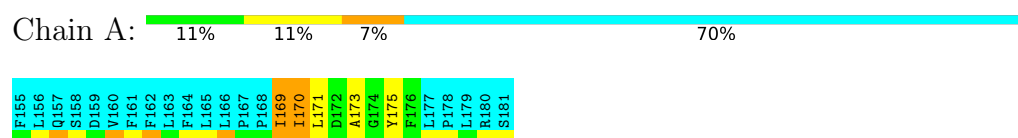
4.2.98 Score per residue for model 98

- Molecule 1: Sodium/hydrogen exchanger 1



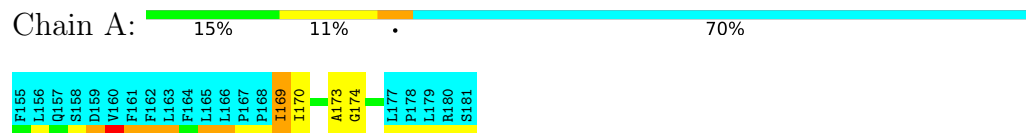
4.2.99 Score per residue for model 99

- Molecule 1: Sodium/hydrogen exchanger 1



4.2.100 Score per residue for model 100

- Molecule 1: Sodium/hydrogen exchanger 1



5 Refinement protocol and experimental data overview

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

Of the 1000 calculated structures, 100 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CNS	structure solution	1.1
CNS	refinement	1.1

No chemical shift data was provided.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HSL

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

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	64	63	63	4±3
All	All	6400	6300	6300	421

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 33.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:169:ILE:O	1:A:171:LEU:N	0.93	2.02	34	9
1:A:169:ILE:O	1:A:173:ALA:HB2	0.92	1.63	54	91
1:A:169:ILE:HG23	1:A:170:ILE:HD13	0.74	1.59	40	12
1:A:169:ILE:HG13	1:A:173:ALA:HB2	0.72	1.58	5	1
1:A:171:LEU:HD12	1:A:172:ASP:N	0.71	2.00	20	5
1:A:169:ILE:O	1:A:169:ILE:HD13	0.69	1.88	99	18
1:A:169:ILE:HD13	1:A:169:ILE:O	0.67	1.90	58	1
1:A:171:LEU:HD13	1:A:171:LEU:H	0.66	1.49	58	1
1:A:171:LEU:H	1:A:171:LEU:HD22	0.65	1.51	18	3
1:A:171:LEU:HD23	1:A:172:ASP:N	0.65	2.07	88	4
1:A:174:GLY:O	1:A:176:PHE:N	0.63	2.31	44	13
1:A:169:ILE:HG23	1:A:170:ILE:H	0.62	1.54	62	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:174:GLY:C	1:A:175:TYR:CG	0.59	2.80	11	10
1:A:174:GLY:O	1:A:175:TYR:CG	0.59	2.55	91	9
1:A:170:ILE:HD12	1:A:171:LEU:N	0.58	2.14	37	1
1:A:169:ILE:CG2	1:A:170:ILE:N	0.57	2.67	98	43
1:A:169:ILE:HG23	1:A:170:ILE:N	0.57	2.15	75	21
1:A:171:LEU:C	1:A:171:LEU:HD12	0.56	2.25	38	3
1:A:171:LEU:N	1:A:171:LEU:HD23	0.56	2.16	67	1
1:A:169:ILE:CG2	1:A:170:ILE:HD13	0.56	2.30	60	11
1:A:171:LEU:HD13	1:A:171:LEU:N	0.55	2.16	58	2
1:A:169:ILE:HG13	1:A:170:ILE:N	0.55	2.16	65	3
1:A:170:ILE:CD1	1:A:171:LEU:HD13	0.54	2.32	18	1
1:A:170:ILE:CG1	1:A:171:LEU:HD13	0.54	2.32	58	1
1:A:171:LEU:C	1:A:171:LEU:HD13	0.53	2.28	28	3
1:A:169:ILE:CG1	1:A:173:ALA:HB2	0.53	2.30	5	1
1:A:169:ILE:O	1:A:173:ALA:CB	0.52	2.52	60	25
1:A:169:ILE:HG13	1:A:170:ILE:HG23	0.52	1.79	19	1
1:A:171:LEU:HD23	1:A:172:ASP:H	0.52	1.63	64	2
1:A:169:ILE:HG22	1:A:170:ILE:HG23	0.52	1.81	15	2
1:A:169:ILE:O	1:A:173:ALA:N	0.52	2.43	4	5
1:A:171:LEU:HG	1:A:172:ASP:N	0.51	2.21	72	3
1:A:169:ILE:HG12	1:A:170:ILE:N	0.50	2.22	62	1
1:A:169:ILE:HG22	1:A:170:ILE:N	0.49	2.23	89	3
1:A:169:ILE:CG1	1:A:170:ILE:N	0.49	2.76	65	8
1:A:169:ILE:HD13	1:A:169:ILE:C	0.49	2.33	58	9
1:A:169:ILE:O	1:A:170:ILE:C	0.48	2.56	5	6
1:A:176:PHE:C	1:A:176:PHE:CD1	0.48	2.91	97	2
1:A:174:GLY:O	1:A:175:TYR:CD2	0.47	2.68	91	11
1:A:175:TYR:CD1	1:A:176:PHE:N	0.46	2.84	91	1
1:A:169:ILE:HG23	1:A:170:ILE:HG23	0.46	1.88	29	2
1:A:171:LEU:O	1:A:175:TYR:HA	0.45	2.11	58	8
1:A:169:ILE:HG23	1:A:170:ILE:CD1	0.45	2.41	52	2
1:A:169:ILE:O	1:A:172:ASP:N	0.45	2.50	5	1
1:A:169:ILE:CG2	1:A:170:ILE:CD1	0.44	2.95	22	5
1:A:174:GLY:O	1:A:176:PHE:CD2	0.44	2.71	23	1
1:A:175:TYR:CG	1:A:176:PHE:N	0.44	2.84	61	1
1:A:171:LEU:HD22	1:A:171:LEU:N	0.44	2.28	80	4
1:A:174:GLY:C	1:A:176:PHE:H	0.43	2.20	11	1
1:A:174:GLY:C	1:A:175:TYR:CD1	0.43	2.97	94	6
1:A:176:PHE:O	1:A:176:PHE:CG	0.43	2.71	67	9
1:A:176:PHE:O	1:A:176:PHE:CD2	0.43	2.72	80	4
1:A:170:ILE:HD12	1:A:170:ILE:H	0.42	1.74	59	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:174:GLY:O	1:A:175:TYR:HB3	0.42	2.14	9	4
1:A:171:LEU:N	1:A:171:LEU:HD22	0.42	2.29	53	1
1:A:172:ASP:OD1	1:A:175:TYR:CZ	0.42	2.73	10	1
1:A:169:ILE:HG22	1:A:170:ILE:HD12	0.42	1.90	31	2
1:A:171:LEU:N	1:A:171:LEU:CD2	0.42	2.82	45	3
1:A:171:LEU:CD2	1:A:171:LEU:N	0.42	2.82	95	1
1:A:171:LEU:O	1:A:175:TYR:N	0.42	2.52	67	1
1:A:175:TYR:CD1	1:A:175:TYR:C	0.41	2.98	4	1
1:A:170:ILE:HG13	1:A:171:LEU:HD13	0.41	1.90	58	1
1:A:170:ILE:HG12	1:A:171:LEU:HD13	0.41	1.93	58	1
1:A:175:TYR:CD1	1:A:175:TYR:N	0.41	2.89	65	2
1:A:171:LEU:HD13	1:A:172:ASP:N	0.41	2.31	28	1
1:A:176:PHE:O	1:A:176:PHE:CD1	0.40	2.74	11	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	8/27 (30%)	6±1 (71±12%)	2±1 (23±11%)	0±1 (6±9%)	2	19
All	All	800/2700 (30%)	566 (71%)	186 (23%)	48 (6%)	2	19

All 4 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	169	ILE	28
1	A	175	TYR	10
1	A	170	ILE	9
1	A	173	ALA	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	6/24 (25%)	4±1 (72±18%)	2±1 (28±18%)	1	19
All	All	600/2400 (25%)	431 (72%)	169 (28%)	1	19

All 6 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	169	ILE	48
1	A	171	LEU	40
1	A	172	ASP	24
1	A	175	TYR	21
1	A	170	ILE	19
1	A	176	PHE	17

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
1	HSL	A	181	1	6,7,7	0.93±0.01	1±0 (16±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is

considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
1	HSL	A	181	1	4,9,9	1.48±0.04	1±0 (27±7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HSL	A	181	1	-	-	0±0,1,1,1

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	181	HSL	OD-CG	2.16	1.40	1.46	4	100

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	181	HSL	OD-C-O	2.37	123.94	121.43	93	100
1	A	181	HSL	CG-OD-C	2.24	112.36	110.35	58	10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided