



Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 10:07 pm GMT

PDB ID : 2HTG
Title : Structural and functional characterization of TM VII of the NHE1 isoform of the Na⁺/H⁺ exchanger
Authors : Rainey, J.K.; Ding, J.; Xu, C.; Fliegel, L.; Sykes, B.D.
Deposited on : 2006-07-25

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : trunk28760
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

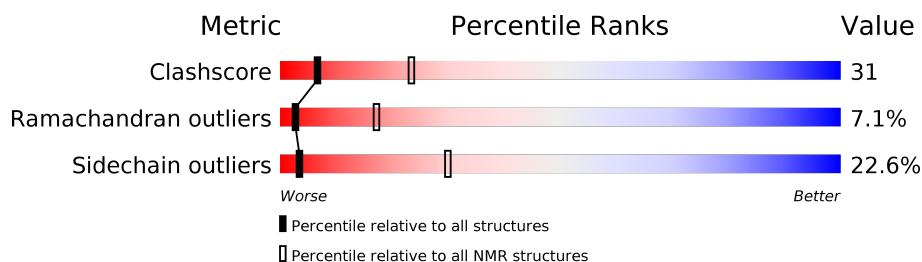
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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

Mol	Chain	Length	Quality of chain
1	A	28	<div> <div>43%</div> <div>57%</div> </div>

2 Ensemble composition and analysis

This entry contains 66 models. Model 35 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

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:264-A:275 (12)	0.60	35

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 10 clusters and 14 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 452 atoms, of which 234 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called NHE1 isoform of Na⁺/H⁺ exchanger 1.

Mol	Chain	Residues	Atoms					Trace
1	A	28	Total	C	H	N	O	1
			452	144	234	36	38	

There are 2 discrepancies between the modelled and reference sequences:

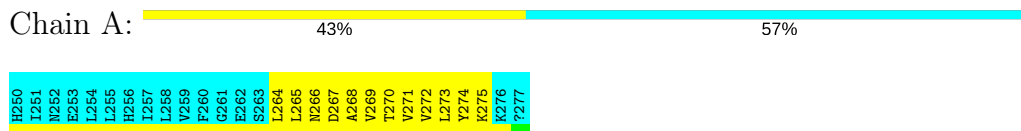
Chain	Residue	Modelled	Actual	Comment	Reference
A	275	LYS	-	CLONING ARTIFACT	UNP P19634
A	276	LYS	-	CLONING ARTIFACT	UNP P19634

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: NHE1 isoform of Na⁺/H⁺ exchanger 1

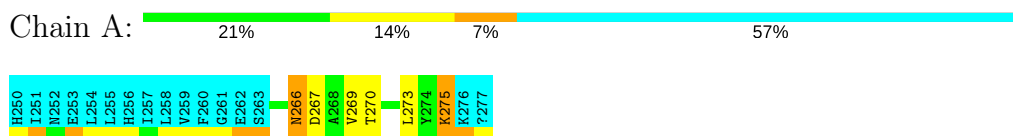


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

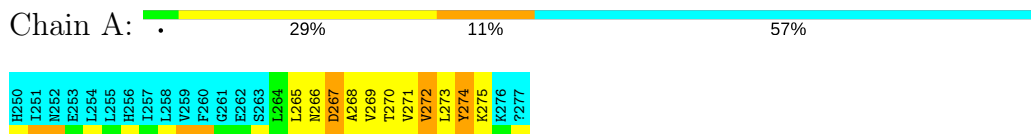
4.2.1 Score per residue for model 1

- Molecule 1: NHE1 isoform of Na⁺/H⁺ exchanger 1



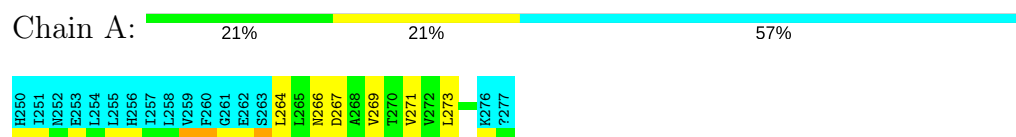
4.2.2 Score per residue for model 2

- Molecule 1: NHE1 isoform of Na⁺/H⁺ exchanger 1



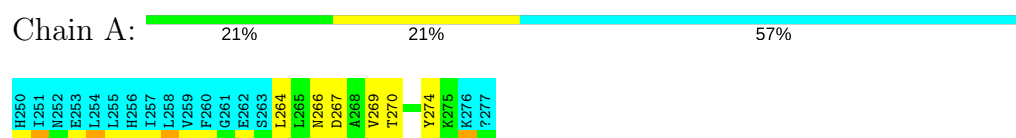
4.2.3 Score per residue for model 3

- Molecule 1: NHE1 isoform of Na⁺/H⁺ exchanger 1



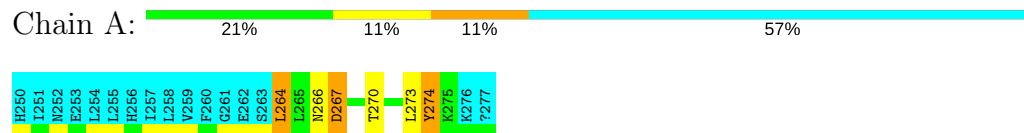
4.2.4 Score per residue for model 4

- Molecule 1: NHE1 isoform of Na⁺/H⁺ exchanger 1



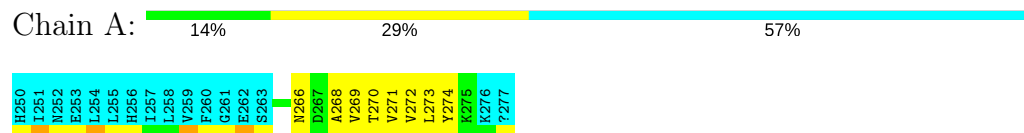
4.2.5 Score per residue for model 5

- Molecule 1: NHE1 isoform of Na⁺/H⁺ exchanger 1



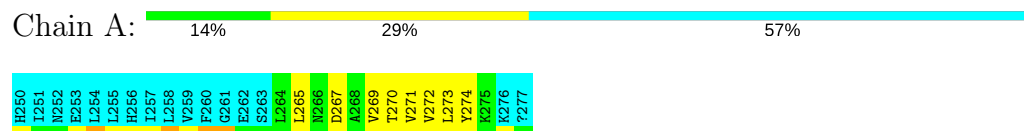
4.2.6 Score per residue for model 6

- Molecule 1: NHE1 isoform of Na⁺/H⁺ exchanger 1



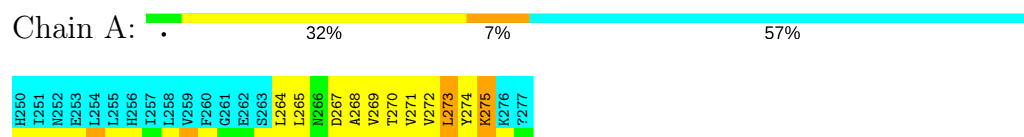
4.2.7 Score per residue for model 7

- Molecule 1: NHE1 isoform of Na⁺/H⁺ exchanger 1



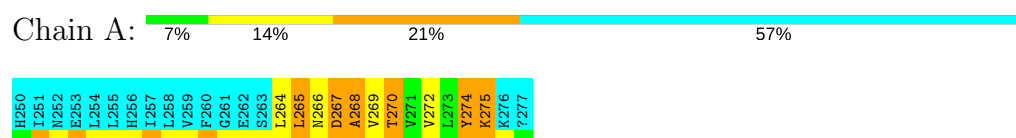
4.2.8 Score per residue for model 8

- Molecule 1: NHE1 isoform of Na⁺/H⁺ exchanger 1



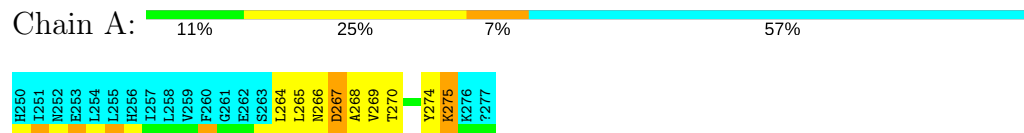
4.2.9 Score per residue for model 9

- Molecule 1: NHE1 isoform of Na⁺/H⁺ exchanger 1



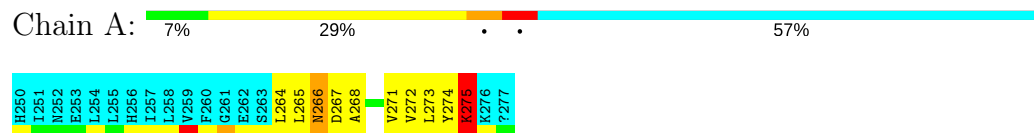
4.2.10 Score per residue for model 10

- Molecule 1: NHE1 isoform of Na⁺/H⁺ exchanger 1



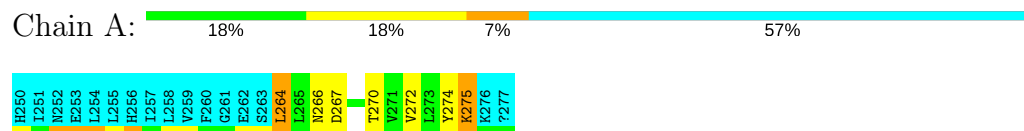
4.2.11 Score per residue for model 11

- Molecule 1: NHE1 isoform of Na⁺/H⁺ exchanger 1



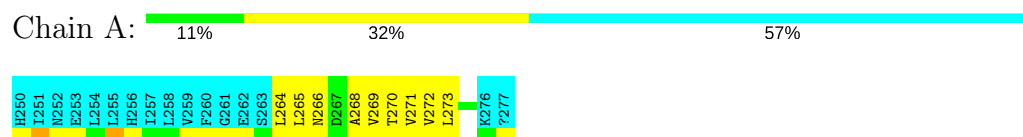
4.2.12 Score per residue for model 12

- Molecule 1: NHE1 isoform of Na⁺/H⁺ exchanger 1



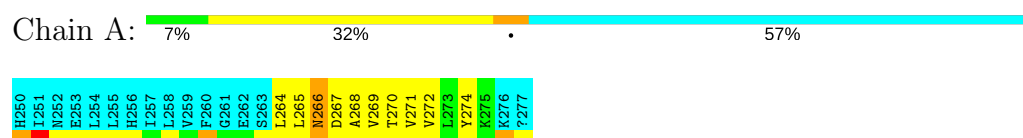
4.2.13 Score per residue for model 13

- Molecule 1: NHE1 isoform of Na⁺/H⁺ exchanger 1



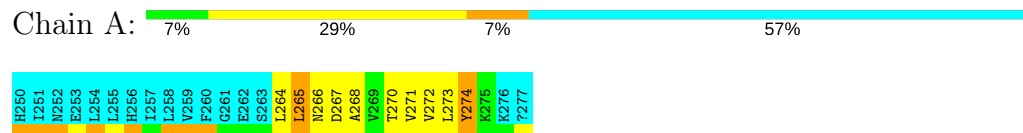
4.2.14 Score per residue for model 14

- Molecule 1: NHE1 isoform of Na⁺/H⁺ exchanger 1



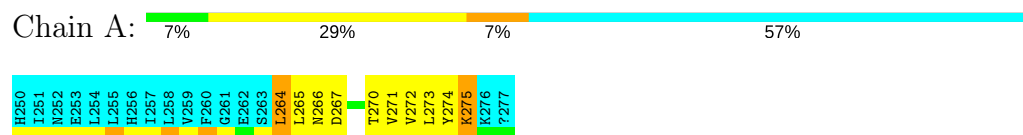
4.2.15 Score per residue for model 15

- Molecule 1: NHE1 isoform of Na⁺/H⁺ exchanger 1



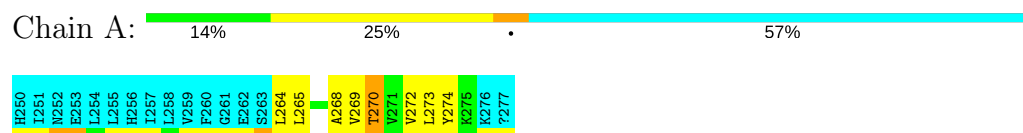
4.2.16 Score per residue for model 16

- Molecule 1: NHE1 isoform of Na⁺/H⁺ exchanger 1



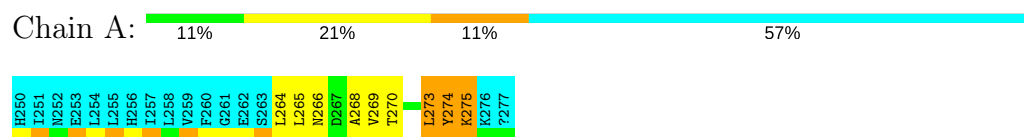
4.2.17 Score per residue for model 17

- Molecule 1: NHE1 isoform of Na⁺/H⁺ exchanger 1



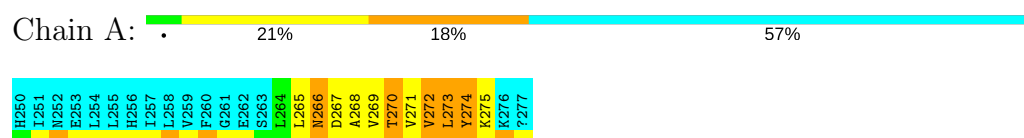
4.2.18 Score per residue for model 18

- Molecule 1: NHE1 isoform of Na⁺/H⁺ exchanger 1



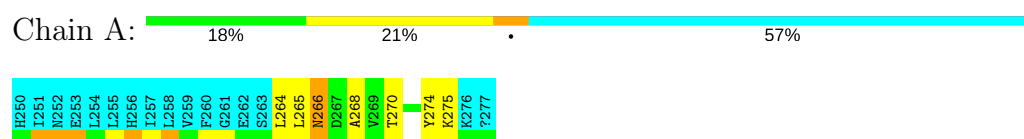
4.2.19 Score per residue for model 19

- Molecule 1: NHE1 isoform of Na⁺/H⁺ exchanger 1



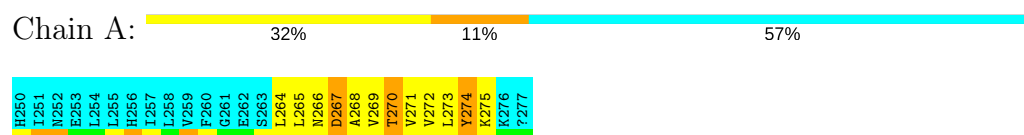
4.2.20 Score per residue for model 20

- Molecule 1: NHE1 isoform of Na⁺/H⁺ exchanger 1



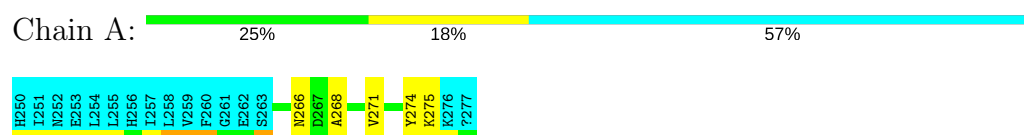
4.2.21 Score per residue for model 21

- Molecule 1: NHE1 isoform of Na⁺/H⁺ exchanger 1



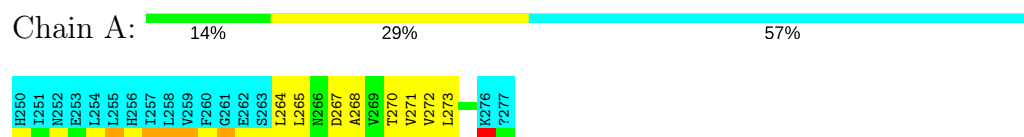
4.2.22 Score per residue for model 22

- Molecule 1: NHE1 isoform of Na⁺/H⁺ exchanger 1



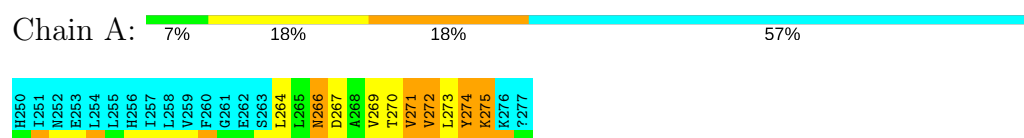
4.2.23 Score per residue for model 23

- Molecule 1: NHE1 isoform of Na⁺/H⁺ exchanger 1



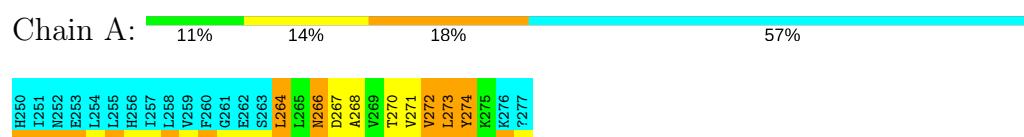
4.2.24 Score per residue for model 24

- Molecule 1: NHE1 isoform of Na⁺/H⁺ exchanger 1



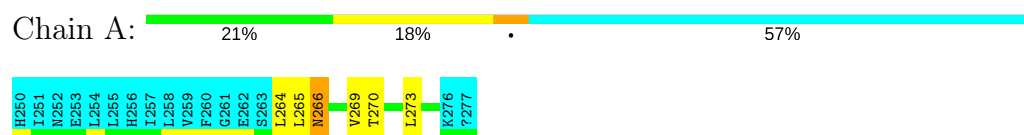
4.2.25 Score per residue for model 25

- Molecule 1: NHE1 isoform of Na⁺/H⁺ exchanger 1



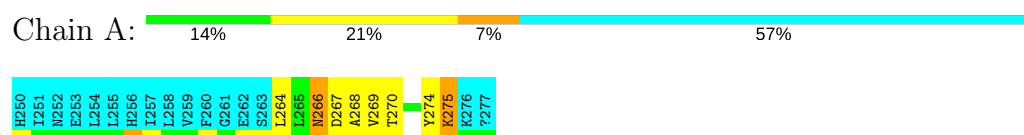
4.2.26 Score per residue for model 26

- Molecule 1: NHE1 isoform of Na⁺/H⁺ exchanger 1



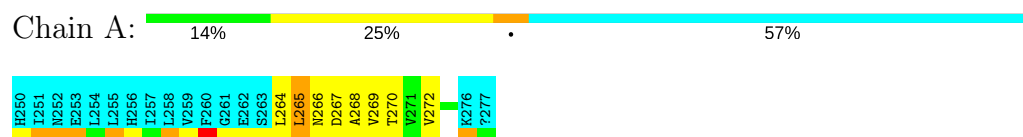
4.2.27 Score per residue for model 27

- Molecule 1: NHE1 isoform of Na⁺/H⁺ exchanger 1



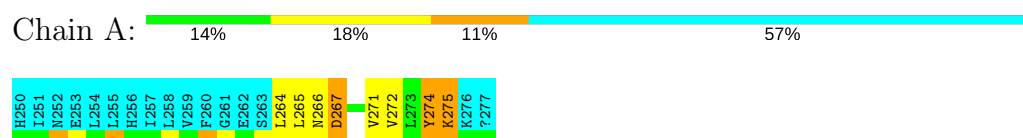
4.2.28 Score per residue for model 28

- Molecule 1: NHE1 isoform of Na⁺/H⁺ exchanger 1



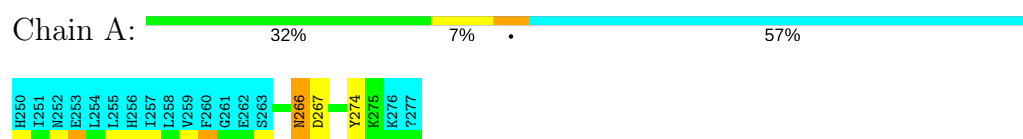
4.2.29 Score per residue for model 29

- Molecule 1: NHE1 isoform of Na⁺/H⁺ exchanger 1



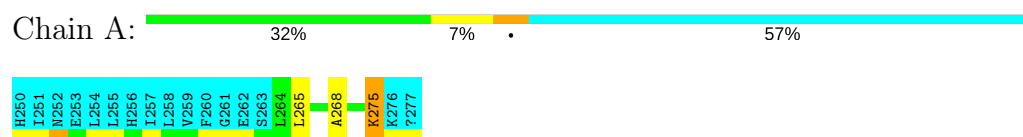
4.2.30 Score per residue for model 30

- Molecule 1: NHE1 isoform of Na⁺/H⁺ exchanger 1



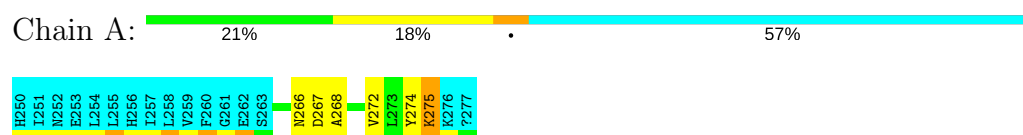
4.2.31 Score per residue for model 31

- Molecule 1: NHE1 isoform of Na⁺/H⁺ exchanger 1



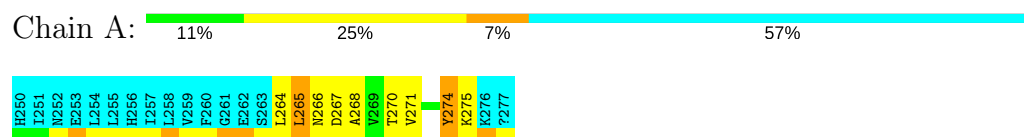
4.2.32 Score per residue for model 32

- Molecule 1: NHE1 isoform of Na⁺/H⁺ exchanger 1



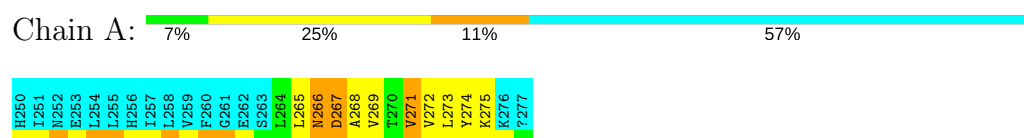
4.2.33 Score per residue for model 33

- Molecule 1: NHE1 isoform of Na⁺/H⁺ exchanger 1



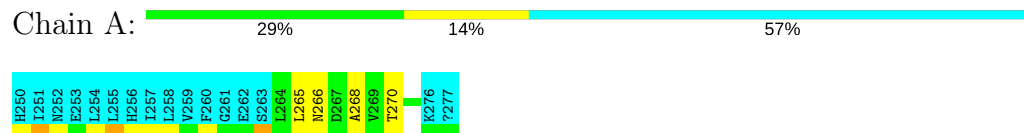
4.2.34 Score per residue for model 34

- Molecule 1: NHE1 isoform of Na⁺/H⁺ exchanger 1



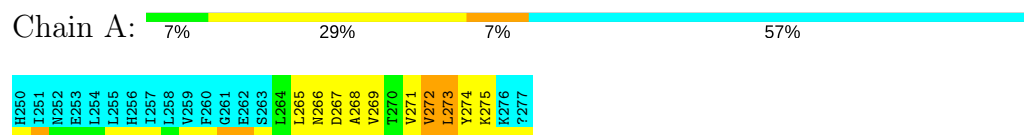
4.2.35 Score per residue for model 35 (medoid)

- Molecule 1: NHE1 isoform of Na⁺/H⁺ exchanger 1



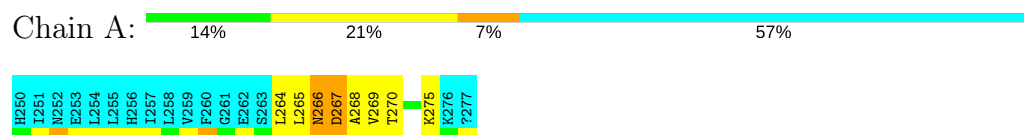
4.2.36 Score per residue for model 36

- Molecule 1: NHE1 isoform of Na⁺/H⁺ exchanger 1



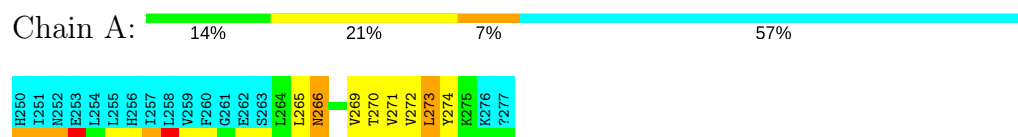
4.2.37 Score per residue for model 37

- Molecule 1: NHE1 isoform of Na⁺/H⁺ exchanger 1



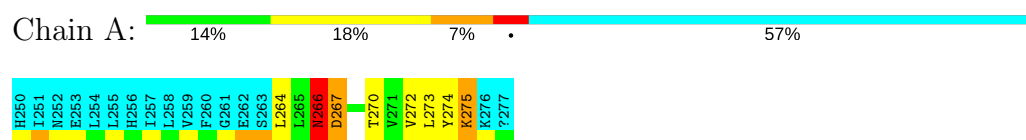
4.2.38 Score per residue for model 38

- Molecule 1: NHE1 isoform of Na⁺/H⁺ exchanger 1



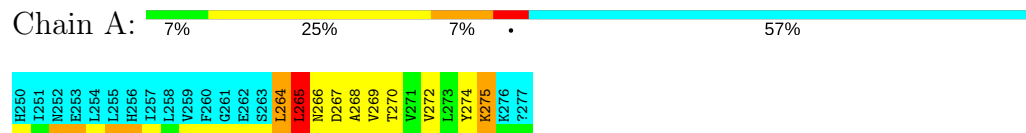
4.2.39 Score per residue for model 39

- Molecule 1: NHE1 isoform of Na⁺/H⁺ exchanger 1



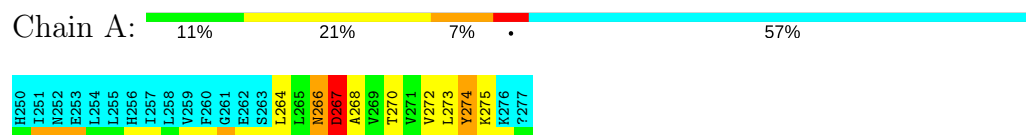
4.2.40 Score per residue for model 40

- Molecule 1: NHE1 isoform of Na⁺/H⁺ exchanger 1



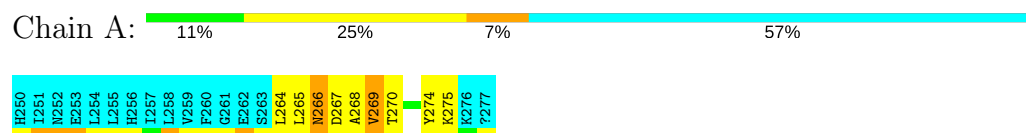
4.2.41 Score per residue for model 41

- Molecule 1: NHE1 isoform of Na⁺/H⁺ exchanger 1



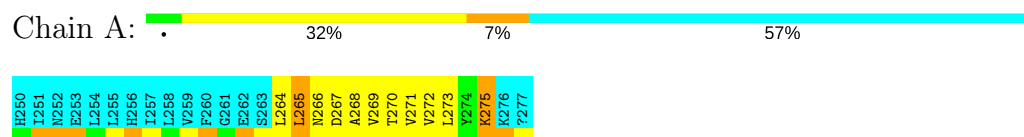
4.2.42 Score per residue for model 42

- Molecule 1: NHE1 isoform of Na⁺/H⁺ exchanger 1



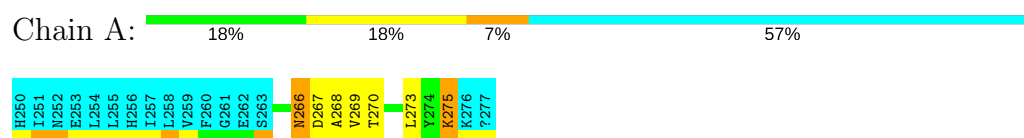
4.2.43 Score per residue for model 43

- Molecule 1: NHE1 isoform of Na⁺/H⁺ exchanger 1



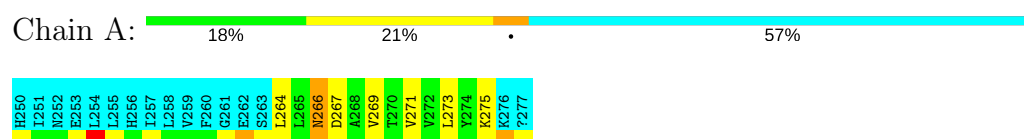
4.2.44 Score per residue for model 44

- Molecule 1: NHE1 isoform of Na⁺/H⁺ exchanger 1



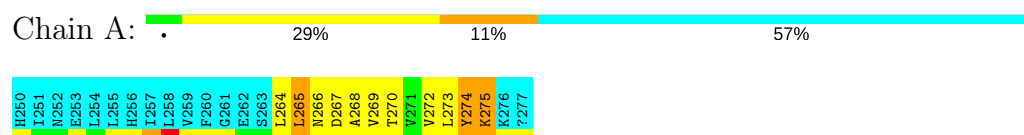
4.2.45 Score per residue for model 45

- Molecule 1: NHE1 isoform of Na⁺/H⁺ exchanger 1



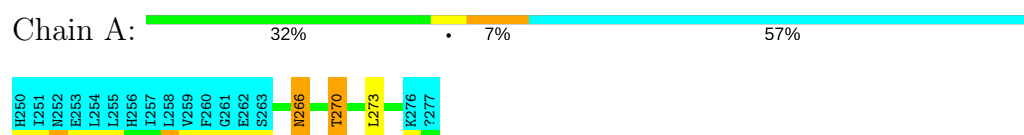
4.2.46 Score per residue for model 46

- Molecule 1: NHE1 isoform of Na⁺/H⁺ exchanger 1



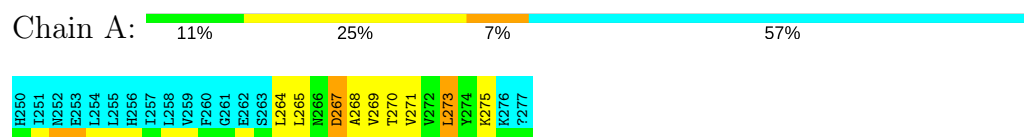
4.2.47 Score per residue for model 47

- Molecule 1: NHE1 isoform of Na⁺/H⁺ exchanger 1



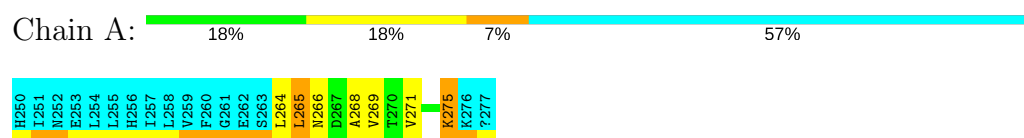
4.2.48 Score per residue for model 48

- Molecule 1: NHE1 isoform of Na⁺/H⁺ exchanger 1



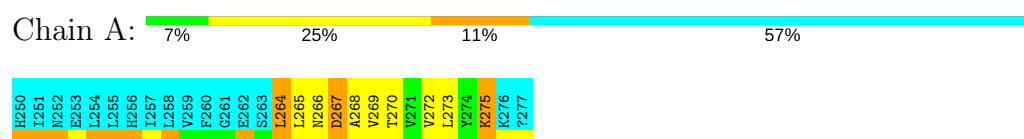
4.2.49 Score per residue for model 49

- Molecule 1: NHE1 isoform of Na⁺/H⁺ exchanger 1



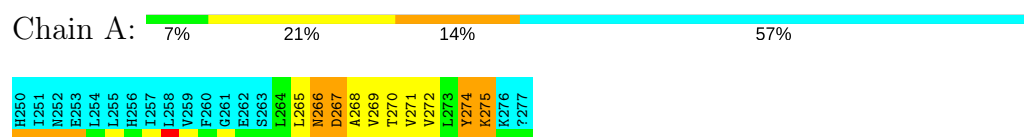
4.2.50 Score per residue for model 50

- Molecule 1: NHE1 isoform of Na⁺/H⁺ exchanger 1



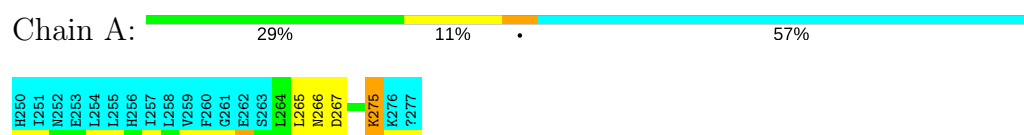
4.2.51 Score per residue for model 51

- Molecule 1: NHE1 isoform of Na⁺/H⁺ exchanger 1



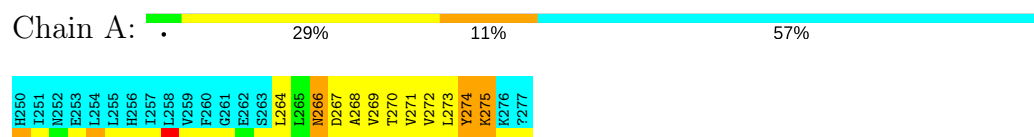
4.2.52 Score per residue for model 52

- Molecule 1: NHE1 isoform of Na⁺/H⁺ exchanger 1



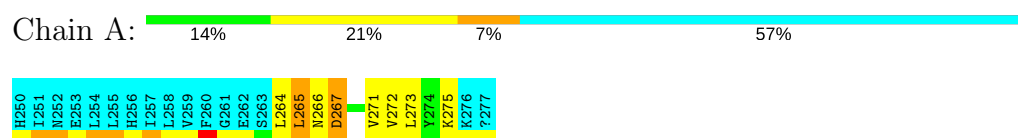
4.2.53 Score per residue for model 53

- Molecule 1: NHE1 isoform of Na⁺/H⁺ exchanger 1



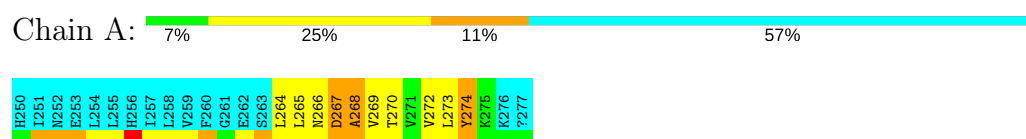
4.2.54 Score per residue for model 54

- Molecule 1: NHE1 isoform of Na⁺/H⁺ exchanger 1



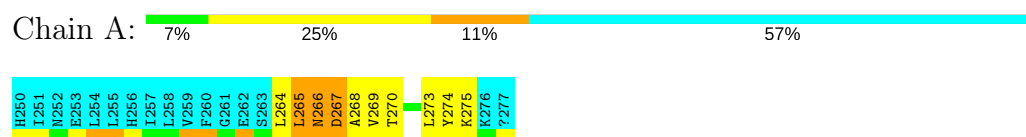
4.2.55 Score per residue for model 55

- Molecule 1: NHE1 isoform of Na⁺/H⁺ exchanger 1



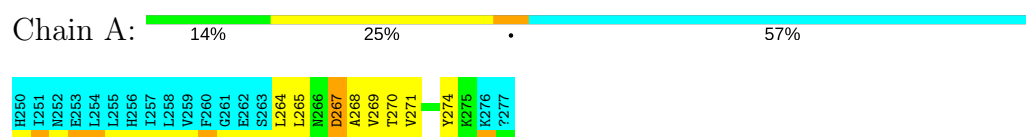
4.2.56 Score per residue for model 56

- Molecule 1: NHE1 isoform of Na⁺/H⁺ exchanger 1



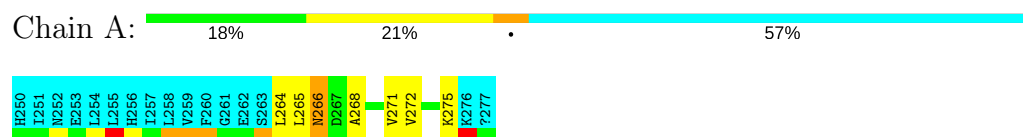
4.2.57 Score per residue for model 57

- Molecule 1: NHE1 isoform of Na⁺/H⁺ exchanger 1



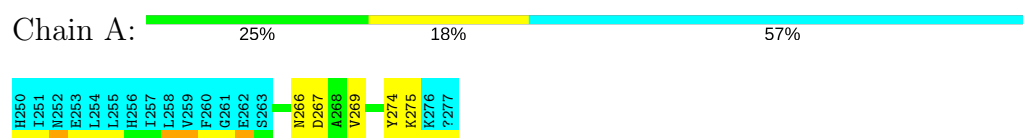
4.2.58 Score per residue for model 58

- Molecule 1: NHE1 isoform of Na⁺/H⁺ exchanger 1



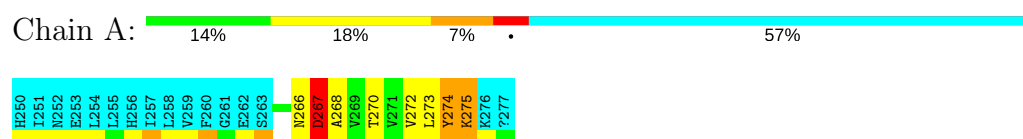
4.2.59 Score per residue for model 59

- Molecule 1: NHE1 isoform of Na⁺/H⁺ exchanger 1



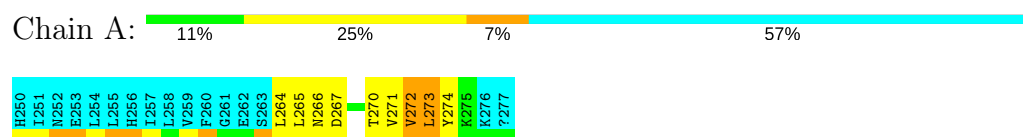
4.2.60 Score per residue for model 60

- Molecule 1: NHE1 isoform of Na⁺/H⁺ exchanger 1



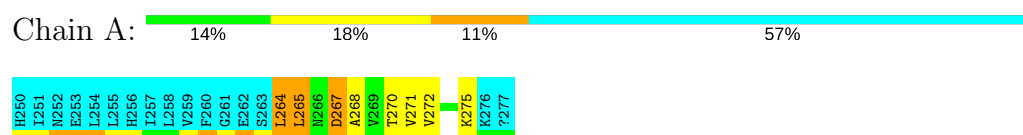
4.2.61 Score per residue for model 61

- Molecule 1: NHE1 isoform of Na⁺/H⁺ exchanger 1



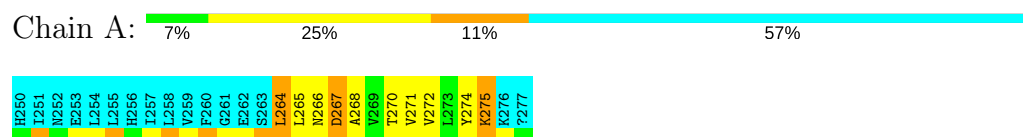
4.2.62 Score per residue for model 62

- Molecule 1: NHE1 isoform of Na⁺/H⁺ exchanger 1



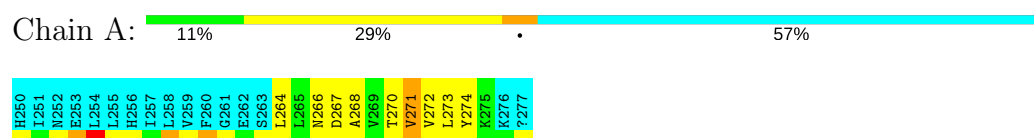
4.2.63 Score per residue for model 63

- Molecule 1: NHE1 isoform of Na⁺/H⁺ exchanger 1



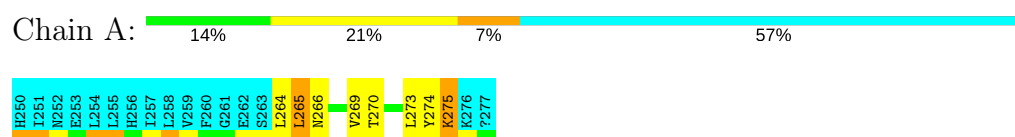
4.2.64 Score per residue for model 64

- Molecule 1: NHE1 isoform of Na⁺/H⁺ exchanger 1



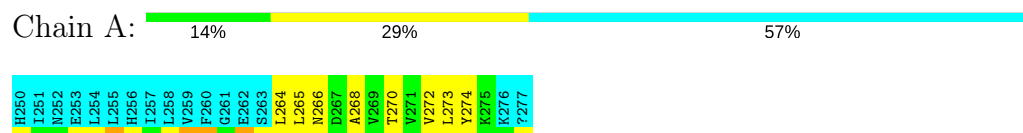
4.2.65 Score per residue for model 65

- Molecule 1: NHE1 isoform of Na⁺/H⁺ exchanger 1



4.2.66 Score per residue for model 66

- Molecule 1: NHE1 isoform of Na⁺/H⁺ exchanger 1



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing; torsion angle dynamics*.

Of the 120 calculated structures, 66 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
XPLOR-NIH	structure solution	2.13
XPLOR-NIH	refinement	2.13

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NH2

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	94	104	104	6±3
All	All	6204	6864	6864	405

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 31.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:264:LEU:HD13	1:A:265:LEU:N	0.90	1.82	62	1
1:A:264:LEU:HD22	1:A:264:LEU:O	0.79	1.77	62	1
1:A:265:LEU:HD12	1:A:265:LEU:N	0.76	1.95	10	1
1:A:267:ASP:O	1:A:270:THR:HG22	0.74	1.81	16	7
1:A:268:ALA:O	1:A:272:VAL:HG12	0.71	1.84	62	1
1:A:265:LEU:O	1:A:269:VAL:HG23	0.71	1.85	26	6
1:A:270:THR:HG23	1:A:271:VAL:HG23	0.70	1.64	16	3
1:A:265:LEU:O	1:A:269:VAL:HG13	0.68	1.89	21	2
1:A:268:ALA:O	1:A:272:VAL:HG23	0.65	1.91	63	3
1:A:274:TYR:CD1	1:A:275:LYS:N	0.64	2.66	65	12
1:A:274:TYR:CG	1:A:275:LYS:N	0.62	2.68	11	8
1:A:274:TYR:CD2	1:A:275:LYS:N	0.62	2.67	39	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:266:ASN:O	1:A:270:THR:HG22	0.60	1.96	6	3
1:A:266:ASN:HD22	1:A:266:ASN:N	0.60	1.93	39	2
1:A:264:LEU:HD13	1:A:264:LEU:C	0.60	2.16	62	1
1:A:264:LEU:HD22	1:A:264:LEU:C	0.59	2.15	62	1
1:A:264:LEU:HD23	1:A:264:LEU:N	0.59	2.12	16	1
1:A:265:LEU:HD23	1:A:265:LEU:N	0.59	2.13	28	1
1:A:266:ASN:N	1:A:266:ASN:ND2	0.58	2.47	39	1
1:A:272:VAL:O	1:A:272:VAL:HG22	0.58	1.98	28	1
1:A:272:VAL:O	1:A:272:VAL:HG12	0.58	1.98	11	3
1:A:268:ALA:O	1:A:271:VAL:HG22	0.58	1.98	53	1
1:A:272:VAL:HG12	1:A:272:VAL:O	0.57	2.00	50	4
1:A:266:ASN:H	1:A:266:ASN:ND2	0.56	1.98	27	1
1:A:264:LEU:N	1:A:264:LEU:HD12	0.56	2.16	26	1
1:A:269:VAL:HG12	1:A:269:VAL:O	0.55	2.02	59	5
1:A:265:LEU:CD1	1:A:265:LEU:N	0.55	2.67	10	1
1:A:264:LEU:O	1:A:268:ALA:N	0.54	2.41	49	13
1:A:266:ASN:ND2	1:A:267:ASP:N	0.54	2.56	56	7
1:A:264:LEU:O	1:A:266:ASN:N	0.54	2.41	28	9
1:A:266:ASN:ND2	1:A:267:ASP:H	0.53	2.01	39	1
1:A:264:LEU:O	1:A:267:ASP:N	0.53	2.42	37	8
1:A:270:THR:O	1:A:273:LEU:N	0.53	2.42	23	18
1:A:270:THR:O	1:A:274:TYR:N	0.53	2.42	33	3
1:A:270:THR:O	1:A:274:TYR:CD1	0.52	2.63	14	3
1:A:271:VAL:O	1:A:271:VAL:HG12	0.52	2.04	63	2
1:A:266:ASN:ND2	1:A:267:ASP:OD1	0.52	2.42	45	1
1:A:267:ASP:O	1:A:270:THR:N	0.52	2.42	39	3
1:A:268:ALA:O	1:A:270:THR:N	0.52	2.42	42	11
1:A:273:LEU:N	1:A:273:LEU:CD2	0.52	2.72	53	1
1:A:265:LEU:O	1:A:268:ALA:N	0.52	2.42	31	6
1:A:269:VAL:O	1:A:273:LEU:N	0.52	2.42	56	5
1:A:270:THR:O	1:A:272:VAL:N	0.52	2.42	24	7
1:A:267:ASP:O	1:A:269:VAL:N	0.52	2.43	55	3
1:A:265:LEU:N	1:A:265:LEU:HD12	0.52	2.20	52	1
1:A:273:LEU:N	1:A:273:LEU:HD22	0.52	2.19	53	1
1:A:268:ALA:O	1:A:271:VAL:N	0.52	2.42	6	7
1:A:266:ASN:O	1:A:268:ALA:N	0.52	2.42	10	5
1:A:265:LEU:N	1:A:265:LEU:CD2	0.52	2.73	28	1
1:A:268:ALA:O	1:A:272:VAL:N	0.52	2.43	32	4
1:A:264:LEU:N	1:A:264:LEU:CD2	0.52	2.72	29	3
1:A:264:LEU:CD2	1:A:264:LEU:N	0.52	2.72	16	1
1:A:264:LEU:HD23	1:A:264:LEU:O	0.51	2.05	12	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:271:VAL:O	1:A:273:LEU:N	0.51	2.42	61	9
1:A:266:ASN:O	1:A:269:VAL:N	0.51	2.44	38	3
1:A:267:ASP:N	1:A:267:ASP:OD1	0.50	2.43	54	3
1:A:264:LEU:N	1:A:264:LEU:HD22	0.50	2.21	15	3
1:A:269:VAL:HG22	1:A:269:VAL:O	0.48	2.07	37	2
1:A:266:ASN:ND2	1:A:266:ASN:H	0.48	2.06	11	2
1:A:267:ASP:O	1:A:271:VAL:HG23	0.48	2.08	29	2
1:A:270:THR:C	1:A:272:VAL:N	0.48	2.67	39	10
1:A:274:TYR:N	1:A:274:TYR:CD1	0.48	2.75	41	3
1:A:274:TYR:CD1	1:A:274:TYR:C	0.48	2.86	18	5
1:A:264:LEU:N	1:A:264:LEU:CD1	0.48	2.77	26	1
1:A:274:TYR:CG	1:A:274:TYR:O	0.48	2.64	5	1
1:A:267:ASP:O	1:A:270:THR:CG2	0.48	2.62	21	1
1:A:271:VAL:C	1:A:273:LEU:N	0.47	2.68	54	10
1:A:268:ALA:C	1:A:270:THR:N	0.47	2.67	42	20
1:A:265:LEU:O	1:A:269:VAL:N	0.47	2.42	65	6
1:A:266:ASN:C	1:A:268:ALA:N	0.47	2.66	10	7
1:A:274:TYR:C	1:A:274:TYR:CD1	0.47	2.88	24	5
1:A:267:ASP:OD1	1:A:267:ASP:N	0.46	2.46	39	1
1:A:269:VAL:O	1:A:269:VAL:HG12	0.46	2.10	57	4
1:A:274:TYR:CD1	1:A:274:TYR:N	0.46	2.82	59	2
1:A:264:LEU:C	1:A:266:ASN:N	0.46	2.67	28	9
1:A:266:ASN:CG	1:A:267:ASP:N	0.46	2.69	28	4
1:A:270:THR:HG22	1:A:271:VAL:N	0.46	2.25	15	7
1:A:269:VAL:C	1:A:271:VAL:N	0.46	2.69	21	3
1:A:266:ASN:ND2	1:A:266:ASN:C	0.46	2.68	30	3
1:A:271:VAL:O	1:A:275:LYS:N	0.46	2.47	62	1
1:A:266:ASN:O	1:A:270:THR:CG2	0.46	2.64	19	1
1:A:265:LEU:HA	1:A:268:ALA:HB3	0.46	1.88	40	3
1:A:265:LEU:N	1:A:265:LEU:CD1	0.46	2.79	52	1
1:A:269:VAL:HG23	1:A:270:THR:N	0.46	2.26	21	1
1:A:269:VAL:O	1:A:273:LEU:HD23	0.45	2.12	8	2
1:A:267:ASP:C	1:A:269:VAL:N	0.45	2.68	2	3
1:A:272:VAL:O	1:A:272:VAL:CG1	0.45	2.63	11	2
1:A:265:LEU:O	1:A:269:VAL:CG2	0.45	2.63	46	4
1:A:270:THR:O	1:A:274:TYR:CE2	0.45	2.70	42	2
1:A:272:VAL:C	1:A:274:TYR:N	0.45	2.69	9	1
1:A:273:LEU:HD23	1:A:273:LEU:C	0.44	2.32	65	1
1:A:269:VAL:CG1	1:A:269:VAL:O	0.44	2.66	7	4
1:A:271:VAL:O	1:A:275:LYS:CG	0.44	2.65	22	2
1:A:269:VAL:O	1:A:269:VAL:CG1	0.44	2.65	34	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:267:ASP:O	1:A:271:VAL:CG1	0.44	2.66	34	1
1:A:266:ASN:O	1:A:270:THR:N	0.44	2.49	50	1
1:A:269:VAL:O	1:A:271:VAL:N	0.44	2.51	49	2
1:A:269:VAL:O	1:A:272:VAL:N	0.44	2.51	46	1
1:A:274:TYR:O	1:A:274:TYR:CG	0.43	2.71	24	2
1:A:270:THR:C	1:A:272:VAL:H	0.43	2.17	12	1
1:A:264:LEU:O	1:A:267:ASP:OD1	0.43	2.37	5	1
1:A:267:ASP:O	1:A:270:THR:OG1	0.43	2.37	41	1
1:A:266:ASN:O	1:A:269:VAL:HG22	0.43	2.14	36	1
1:A:273:LEU:C	1:A:275:LYS:H	0.43	2.16	24	1
1:A:264:LEU:CD2	1:A:264:LEU:C	0.43	2.84	62	1
1:A:272:VAL:CG1	1:A:272:VAL:O	0.42	2.67	50	2
1:A:264:LEU:O	1:A:265:LEU:C	0.42	2.58	40	4
1:A:266:ASN:N	1:A:266:ASN:HD22	0.42	2.12	2	1
1:A:269:VAL:C	1:A:271:VAL:H	0.42	2.18	49	3
1:A:271:VAL:C	1:A:273:LEU:H	0.42	2.18	25	4
1:A:266:ASN:ND2	1:A:266:ASN:N	0.42	2.68	20	1
1:A:268:ALA:C	1:A:270:THR:H	0.42	2.18	40	8
1:A:269:VAL:CG1	1:A:270:THR:N	0.42	2.83	4	1
1:A:271:VAL:HG12	1:A:272:VAL:N	0.42	2.28	19	1
1:A:269:VAL:O	1:A:273:LEU:CB	0.42	2.68	48	1
1:A:272:VAL:CG2	1:A:272:VAL:O	0.42	2.67	28	1
1:A:268:ALA:O	1:A:272:VAL:HG22	0.41	2.15	36	1
1:A:272:VAL:HG22	1:A:272:VAL:O	0.41	2.16	29	1
1:A:273:LEU:C	1:A:275:LYS:N	0.41	2.74	24	1
1:A:264:LEU:O	1:A:266:ASN:ND2	0.40	2.55	39	1
1:A:264:LEU:CD1	1:A:264:LEU:C	0.40	2.85	62	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	12/28 (43%)	8±2 (66±17%)	3±2 (27±14%)	1±1 (7±7%)	3	17
All	All	792/1848 (43%)	524 (66%)	212 (27%)	56 (7%)	3	17

All 11 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	265	LEU	9
1	A	272	VAL	8
1	A	274	TYR	7
1	A	269	VAL	6
1	A	275	LYS	6
1	A	267	ASP	5
1	A	264	LEU	5
1	A	271	VAL	3
1	A	268	ALA	3
1	A	266	ASN	2
1	A	273	LEU	2

6.3.2 Protein sidechains [i](#)

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	11/25 (44%)	9±1 (77±13%)	2±1 (23±13%)	3	30
All	All	726/1650 (44%)	562 (77%)	164 (23%)	3	30

All 11 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	266	ASN	37
1	A	267	ASP	31
1	A	275	LYS	27
1	A	274	TYR	20
1	A	264	LEU	13
1	A	265	LEU	13
1	A	273	LEU	11
1	A	270	THR	6
1	A	269	VAL	3
1	A	272	VAL	2
1	A	271	VAL	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided