



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 04:31 AM UTC

PDB ID : 2KRG / pdb_00002krq
Title : Solution Structure of human sodium/ hydrogen exchange regulatory factor 1(150-358)
Authors : Bhattacharya, S.; Dai, Z.; Li, J.; Baxter, S.; Callaway, D.J.E.; Cowburn, D.; Bu, Z.
Deposited on : 2009-12-17

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

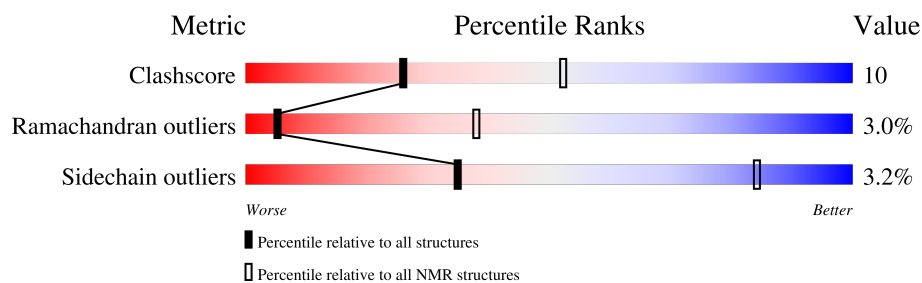
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

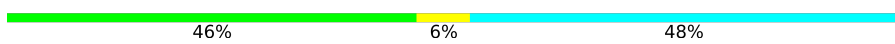
The overall completeness of chemical shifts assignment was not calculated.

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	216	

2 Ensemble composition and analysis

This entry contains 20 models. Model 13 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:147-A:168, A:177-A:255 (101)	0.70	13
2	A:325-A:336 (12)	1.06	20

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 5 clusters. No single-model clusters were found.

Cluster number	Models
1	6, 8, 14, 17, 18, 20
2	1, 4, 5, 7, 10, 15
3	2, 3, 12
4	11, 13, 19
5	9, 16

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3293 atoms, of which 1636 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Na(+)/H(+) exchange regulatory cofactor NHE-RF1.

Mol	Chain	Residues	Atoms						Trace
1	A	216	Total	C	H	N	O	S	0
			3293	1016	1636	300	333	8	

There are 7 discrepancies between the modelled and reference sequences:

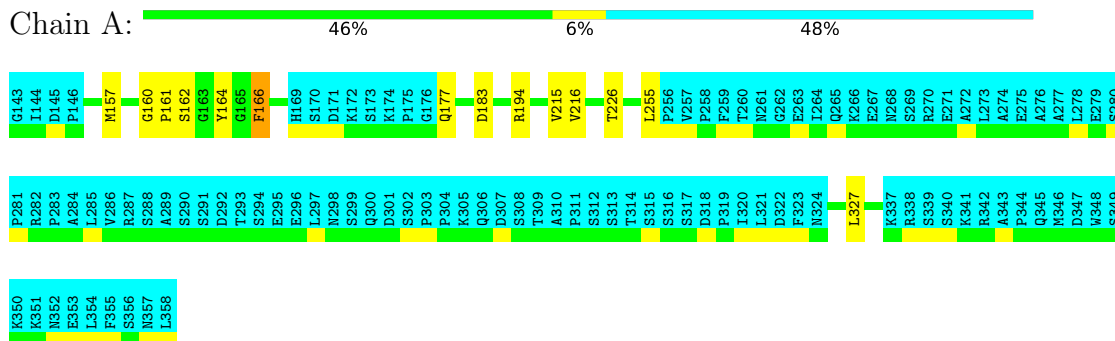
Chain	Residue	Modelled	Actual	Comment	Reference
A	143	GLY	-	expression tag	UNP O14745
A	144	ILE	-	expression tag	UNP O14745
A	145	ASP	-	expression tag	UNP O14745
A	146	PRO	-	expression tag	UNP O14745
A	147	PHE	-	expression tag	UNP O14745
A	148	THR	-	expression tag	UNP O14745
A	149	MET	-	expression tag	UNP O14745

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: Na(+)/H(+) exchange regulatory cofactor NHE-RF1

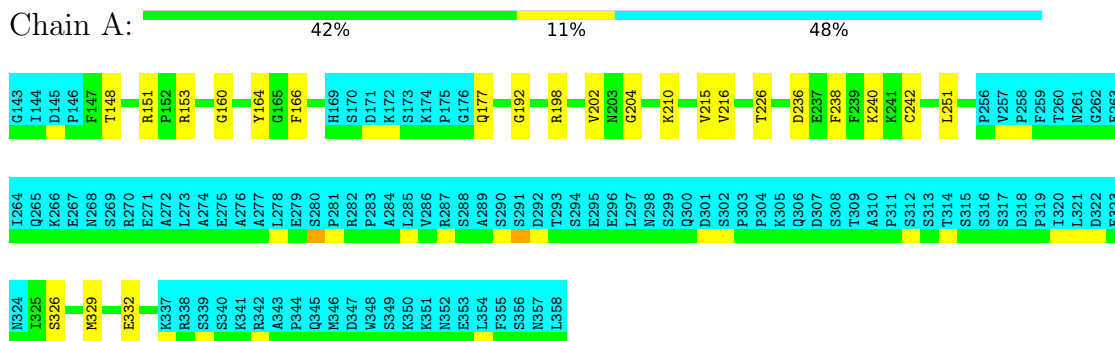


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

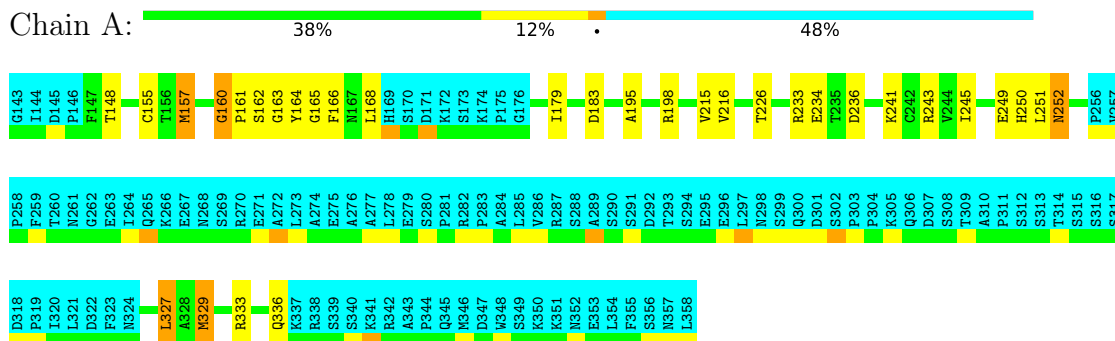
4.2.1 Score per residue for model 1

- Molecule 1: Na(+)/H(+) exchange regulatory cofactor NHE-RF1



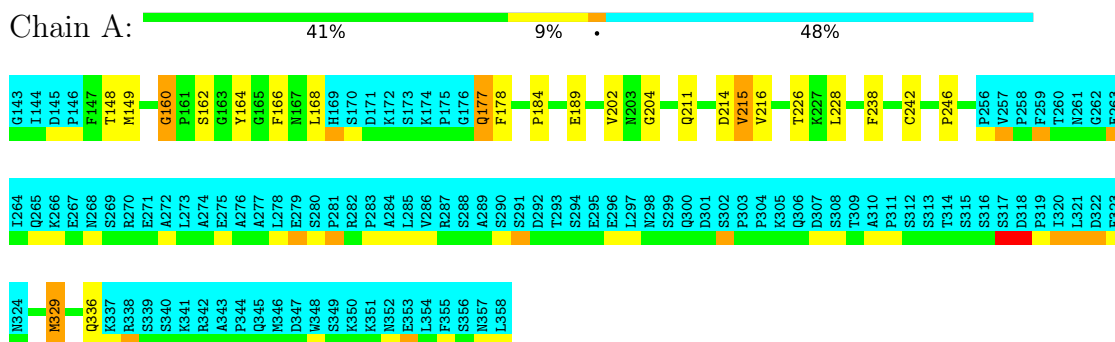
4.2.2 Score per residue for model 2

- Molecule 1: Na(+)/H(+) exchange regulatory cofactor NHE-RF1



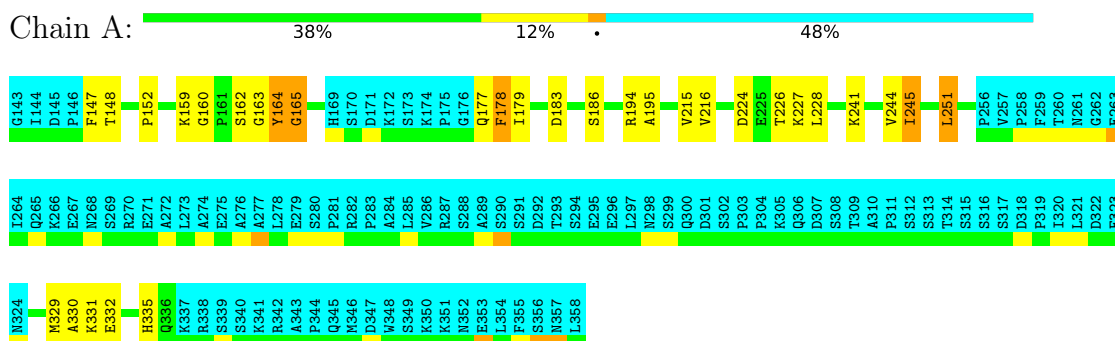
4.2.3 Score per residue for model 3

- Molecule 1: Na(+)/H(+) exchange regulatory cofactor NHE-RF1



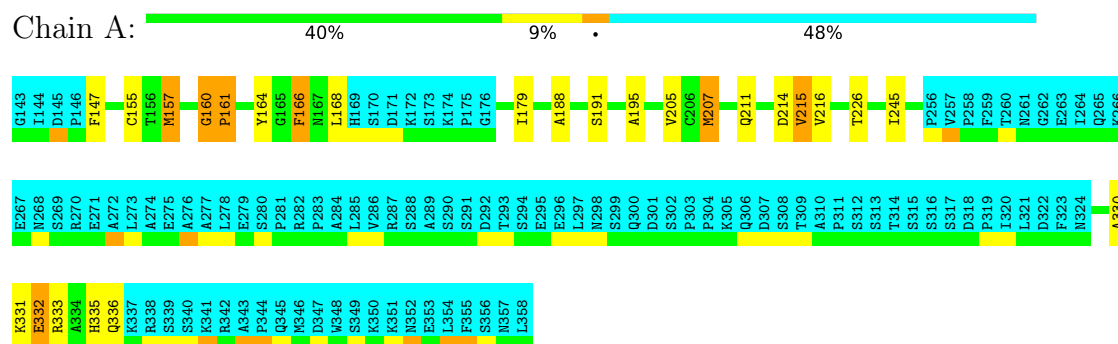
4.2.4 Score per residue for model 4

- Molecule 1: Na(+)/H(+) exchange regulatory cofactor NHE-RF1



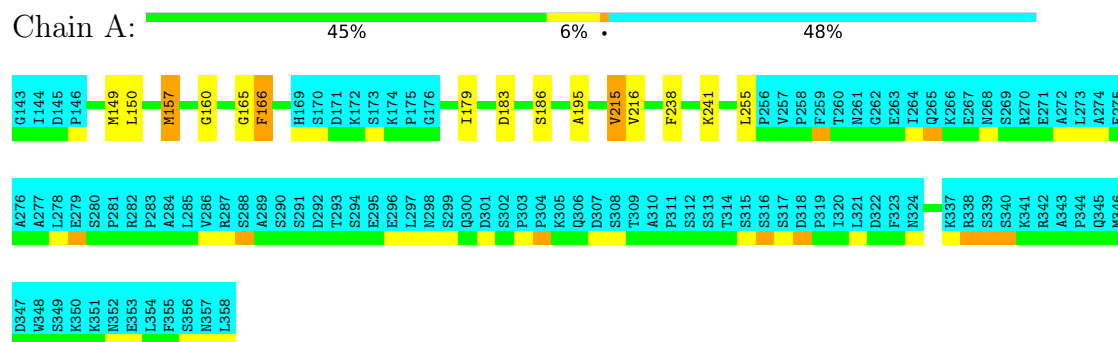
4.2.5 Score per residue for model 5

- Molecule 1: Na(+)/H(+) exchange regulatory cofactor NHE-RF1



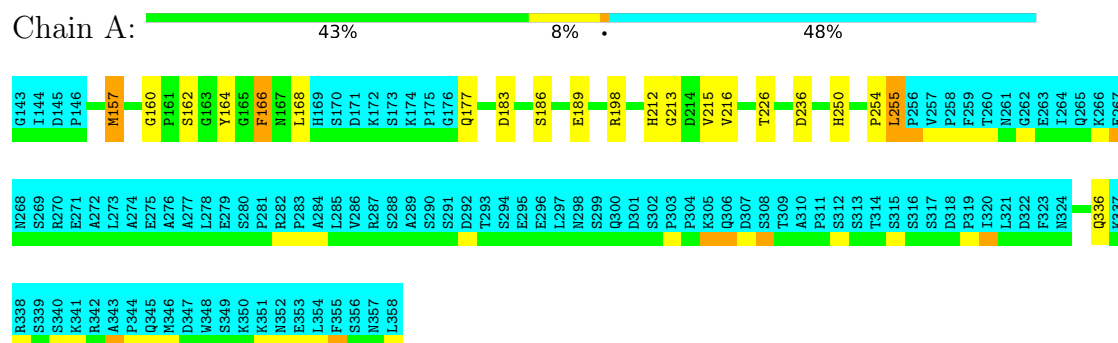
4.2.6 Score per residue for model 6

- Molecule 1: Na(+)/H(+) exchange regulatory cofactor NHE-RF1



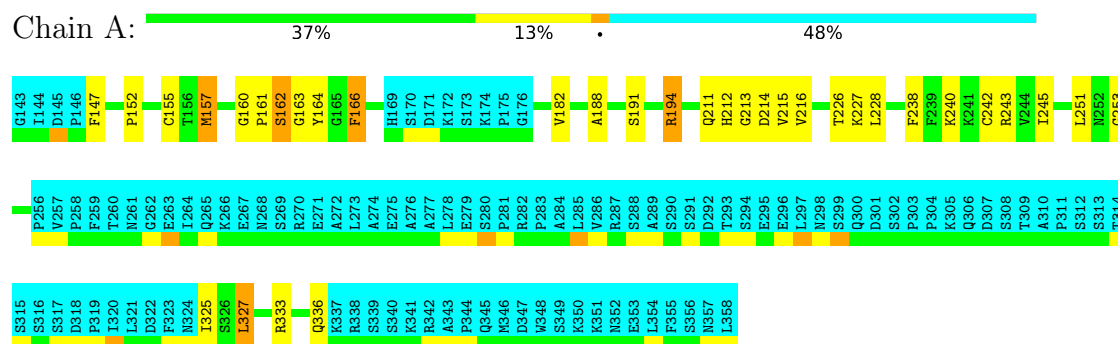
4.2.7 Score per residue for model 7

- Molecule 1: Na(+)/H(+) exchange regulatory cofactor NHE-RF1



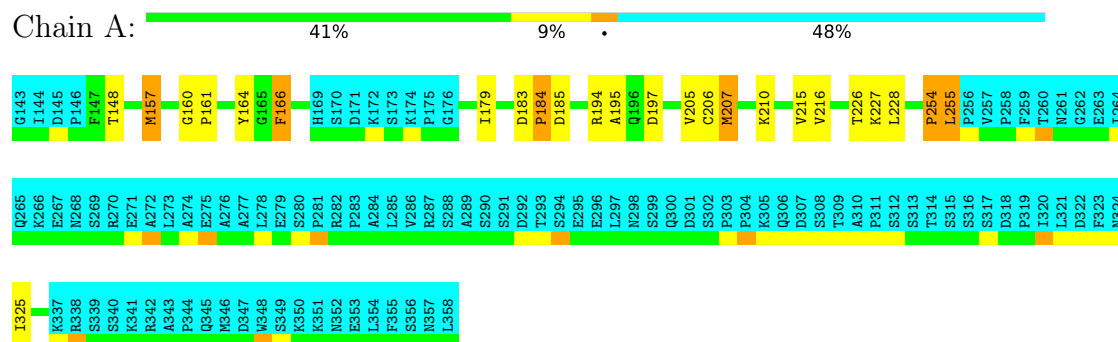
4.2.8 Score per residue for model 8

- Molecule 1: Na(+)/H(+) exchange regulatory cofactor NHE-RF1



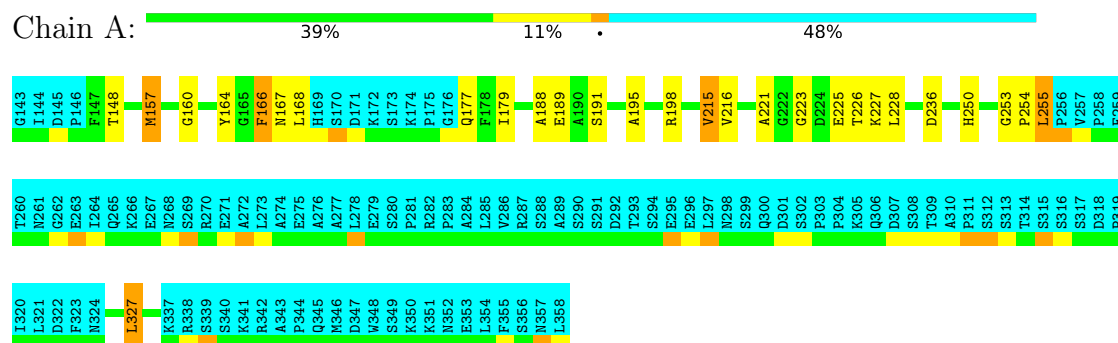
4.2.9 Score per residue for model 9

- Molecule 1: Na(+)/H(+) exchange regulatory cofactor NHE-RF1



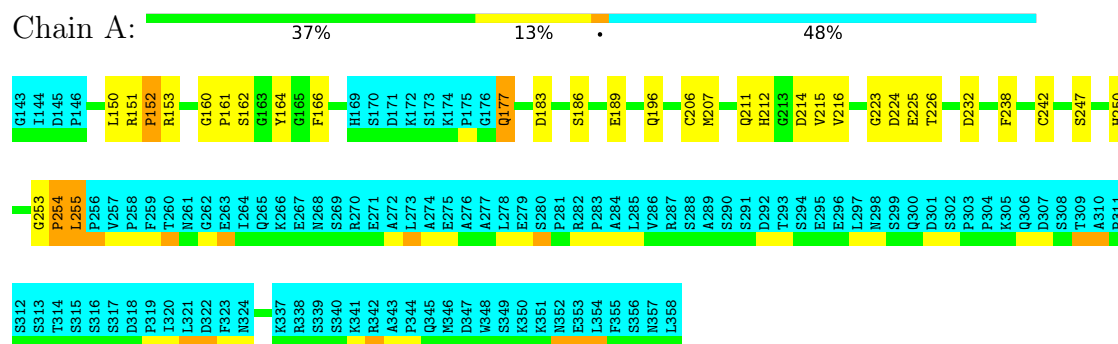
4.2.10 Score per residue for model 10

- Molecule 1: Na(+)/H(+) exchange regulatory cofactor NHE-RF1



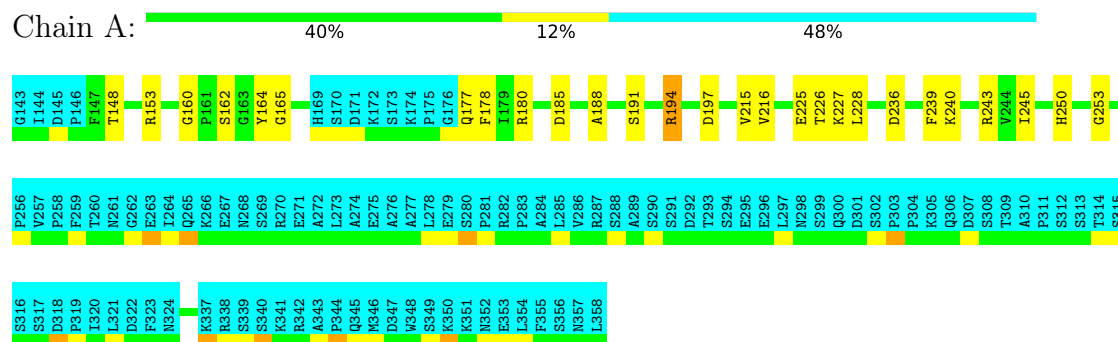
4.2.11 Score per residue for model 11

- Molecule 1: Na(+)/H(+) exchange regulatory cofactor NHE-RF1



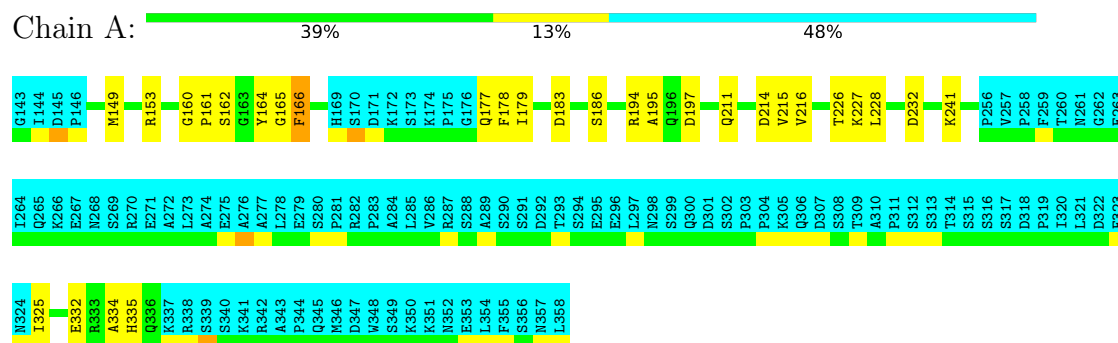
4.2.12 Score per residue for model 12

- Molecule 1: Na(+)/H(+) exchange regulatory cofactor NHE-RF1



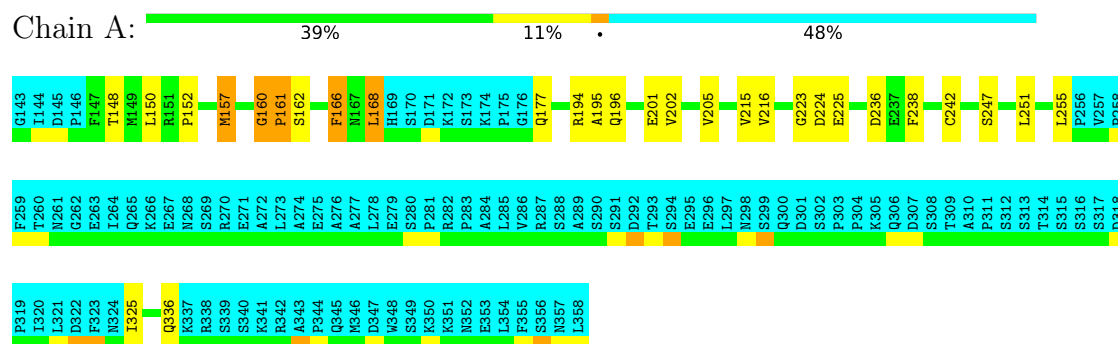
4.2.13 Score per residue for model 13 (medoid)

- Molecule 1: Na(+)/H(+) exchange regulatory cofactor NHE-RF1



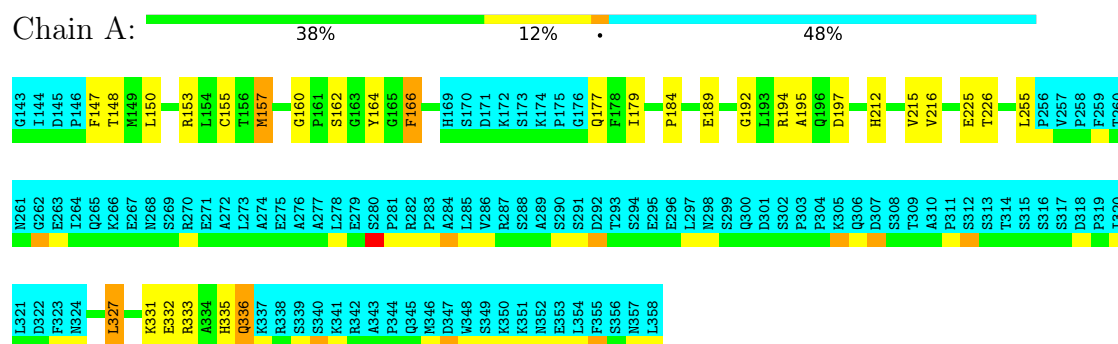
4.2.17 Score per residue for model 17

- Molecule 1: Na(+)/H(+) exchange regulatory cofactor NHE-RF1



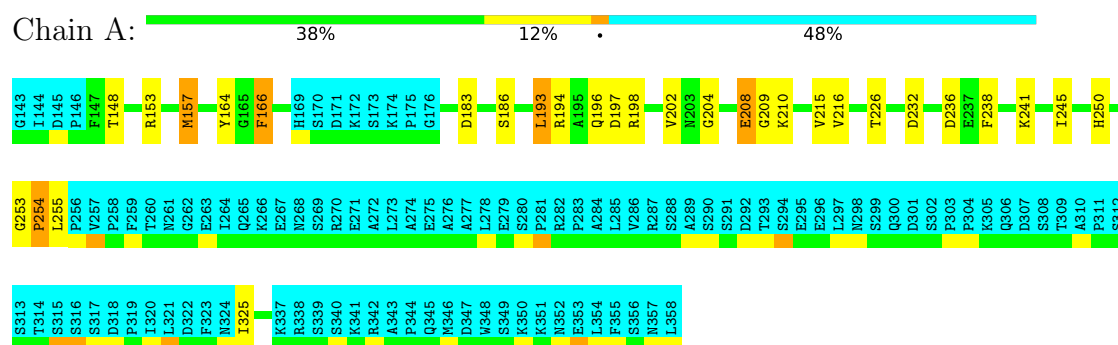
4.2.18 Score per residue for model 18

- Molecule 1: Na(+)/H(+) exchange regulatory cofactor NHE-RF1



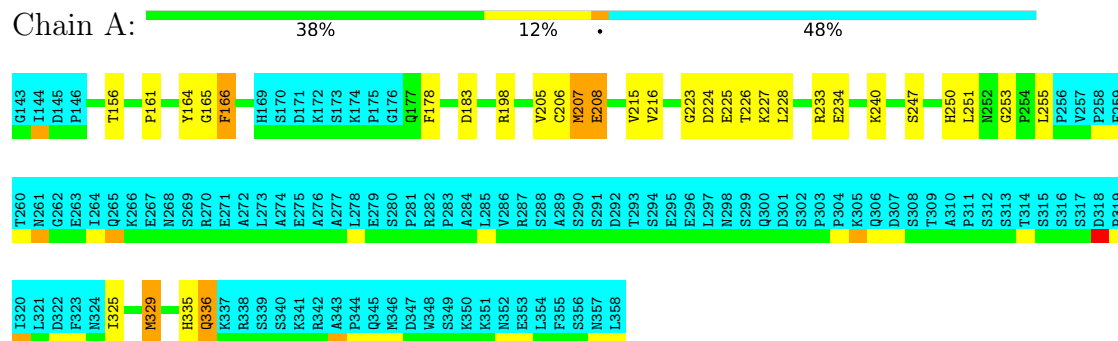
4.2.19 Score per residue for model 19

- Molecule 1: Na(+)/H(+) exchange regulatory cofactor NHE-RF1



4.2.20 Score per residue for model 20

- Molecule 1: Na(+)/H(+) exchange regulatory cofactor NHE-RF1



5 Refinement protocol and experimental data overview

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

Of the 500 calculated structures, 20 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
CYANA	structure solution	2.1
X-PLOR NIH	structure solution	2.24
X-PLOR NIH	refinement	2.24

No chemical shift data was provided.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.67±0.01	0±0/888 (0.0± 0.0%)	1.02±0.01	0±1/1195 (0.0± 0.1%)
All	All	0.67	0/17760 (0.0%)	1.02	9/23900 (0.0%)

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	194	ARG	CB-CA-C	-5.94	108.52	117.07	4	3
1	A	147	PHE	CA-CB-CG	-5.66	108.14	113.80	5	1
1	A	245	ILE	N-CA-C	5.58	113.68	108.15	4	1
1	A	194	ARG	CA-C-O	5.58	121.17	117.94	8	2
1	A	250	HIS	CA-CB-CG	-5.40	108.40	113.80	15	2

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	873	881	878	18±6
All	All	17460	17620	17560	358

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 10.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:168:LEU:HD22	1:A:168:LEU:N	0.76	1.94	17	1
1:A:166:PHE:CE2	1:A:168:LEU:HD11	0.67	2.24	5	2
1:A:157:MET:SD	1:A:157:MET:N	0.63	2.72	7	10
1:A:178:PHE:CD1	1:A:178:PHE:N	0.62	2.67	4	4
1:A:150:LEU:O	1:A:255:LEU:HD21	0.62	1.94	17	3
1:A:325:ILE:HD12	1:A:325:ILE:N	0.61	2.11	19	1
1:A:238:PHE:CD2	1:A:241:LYS:NZ	0.58	2.71	6	1
1:A:147:PHE:CD1	1:A:148:THR:N	0.58	2.72	4	2
1:A:238:PHE:CD1	1:A:241:LYS:NZ	0.58	2.71	19	1
1:A:147:PHE:C	1:A:147:PHE:CD1	0.58	2.82	18	2
1:A:147:PHE:CG	1:A:148:THR:N	0.56	2.74	4	2
1:A:177:GLN:N	1:A:177:GLN:CD	0.56	2.64	3	8
1:A:254:PRO:O	1:A:255:LEU:O	0.55	2.25	9	3
1:A:207:MET:SD	1:A:207:MET:N	0.55	2.80	5	4
1:A:329:MET:N	1:A:329:MET:SD	0.55	2.80	20	1
1:A:255:LEU:N	1:A:255:LEU:CD2	0.54	2.70	19	2
1:A:177:GLN:O	1:A:178:PHE:CD1	0.54	2.60	3	2
1:A:147:PHE:CD1	1:A:147:PHE:C	0.54	2.85	4	1
1:A:223:GLY:C	1:A:225:GLU:H	0.54	2.10	11	3
1:A:247:SER:OG	1:A:250:HIS:CE1	0.54	2.61	11	3
1:A:153:ARG:NH1	1:A:232:ASP:OD1	0.54	2.41	19	2
1:A:210:LYS:CD	1:A:210:LYS:N	0.54	2.71	19	1
1:A:327:LEU:HD23	1:A:327:LEU:O	0.54	2.03	15	1
1:A:198:ARG:NH2	1:A:236:ASP:OD1	0.54	2.41	19	2
1:A:236:ASP:OD1	1:A:240:LYS:NZ	0.53	2.41	12	1
1:A:198:ARG:NH1	1:A:236:ASP:OD1	0.53	2.42	2	1
1:A:194:ARG:N	1:A:197:ASP:OD2	0.53	2.42	9	4
1:A:153:ARG:NH2	1:A:232:ASP:OD2	0.53	2.42	11	1
1:A:329:MET:SD	1:A:330:ALA:N	0.53	2.82	4	1
1:A:249:GLU:OE2	1:A:250:HIS:NE2	0.53	2.42	2	1
1:A:211:GLN:N	1:A:214:ASP:OD2	0.53	2.42	13	6
1:A:332:GLU:O	1:A:335:HIS:ND1	0.53	2.41	13	2
1:A:168:LEU:N	1:A:168:LEU:CD2	0.53	2.66	17	1
1:A:335:HIS:O	1:A:335:HIS:CG	0.53	2.62	18	1
1:A:153:ARG:NH1	1:A:192:GLY:O	0.53	2.42	18	1
1:A:164:TYR:CE1	1:A:226:THR:HG22	0.52	2.39	15	16
1:A:205:VAL:O	1:A:207:MET:SD	0.52	2.67	20	2
1:A:198:ARG:NH1	1:A:236:ASP:OD2	0.52	2.43	10	1
1:A:208:GLU:H	1:A:208:GLU:CD	0.52	2.11	20	1
1:A:152:PRO:O	1:A:251:LEU:HD23	0.52	2.04	4	1
1:A:166:PHE:CD1	1:A:166:PHE:O	0.52	2.63	8	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:249:GLU:OE2	1:A:250:HIS:CD2	0.51	2.63	2	1
1:A:331:LYS:C	1:A:333:ARG:N	0.51	2.67	18	2
1:A:194:ARG:NE	1:A:197:ASP:OD1	0.51	2.43	12	1
1:A:183:ASP:N	1:A:183:ASP:OD1	0.51	2.41	14	1
1:A:153:ARG:NH2	1:A:192:GLY:O	0.51	2.44	18	3
1:A:166:PHE:CD1	1:A:166:PHE:C	0.51	2.88	10	8
1:A:208:GLU:C	1:A:210:LYS:N	0.51	2.68	19	1
1:A:251:LEU:C	1:A:253:GLY:N	0.50	2.68	8	2
1:A:193:LEU:C	1:A:193:LEU:HD13	0.50	2.30	19	2
1:A:240:LYS:O	1:A:243:ARG:NH1	0.50	2.44	8	1
1:A:206:CYS:C	1:A:207:MET:SD	0.50	2.94	11	3
1:A:329:MET:SD	1:A:329:MET:C	0.50	2.94	4	3
1:A:193:LEU:HD13	1:A:194:ARG:N	0.50	2.22	15	2
1:A:151:ARG:NH2	1:A:251:LEU:O	0.50	2.44	1	1
1:A:251:LEU:C	1:A:253:GLY:H	0.50	2.15	8	1
1:A:333:ARG:O	1:A:336:GLN:NE2	0.49	2.45	2	1
1:A:163:GLY:C	1:A:165:GLY:H	0.49	2.16	2	1
1:A:215:VAL:CG2	1:A:216:VAL:N	0.49	2.76	7	20
1:A:182:VAL:CG2	1:A:194:ARG:O	0.49	2.60	8	1
1:A:329:MET:SD	1:A:332:GLU:OE2	0.49	2.71	1	1
1:A:330:ALA:C	1:A:332:GLU:N	0.49	2.70	4	2
1:A:223:GLY:C	1:A:225:GLU:N	0.49	2.71	20	3
1:A:215:VAL:HG23	1:A:216:VAL:N	0.48	2.23	7	18
1:A:238:PHE:O	1:A:242:CYS:SG	0.48	2.70	1	5
1:A:163:GLY:O	1:A:165:GLY:N	0.48	2.46	4	1
1:A:161:PRO:O	1:A:162:SER:CB	0.48	2.61	17	1
1:A:198:ARG:HH12	1:A:240:LYS:NZ	0.48	2.06	1	1
1:A:327:LEU:O	1:A:327:LEU:HD13	0.48	2.09	8	5
1:A:179:ILE:O	1:A:195:ALA:O	0.48	2.32	6	8
1:A:200:VAL:HG21	1:A:246:PRO:HG2	0.48	1.85	16	1
1:A:208:GLU:O	1:A:210:LYS:N	0.48	2.47	19	1
1:A:247:SER:OG	1:A:250:HIS:ND1	0.48	2.47	20	1
1:A:255:LEU:N	1:A:255:LEU:HD22	0.48	2.24	20	2
1:A:244:VAL:HG12	1:A:245:ILE:N	0.48	2.24	4	1
1:A:168:LEU:HD12	1:A:168:LEU:N	0.48	2.24	5	1
1:A:160:GLY:O	1:A:161:PRO:C	0.47	2.56	5	2
1:A:228:LEU:CD1	1:A:228:LEU:N	0.47	2.78	20	5
1:A:249:GLU:O	1:A:252:ASN:O	0.47	2.33	15	1
1:A:207:MET:SD	1:A:214:ASP:CG	0.47	2.97	16	1
1:A:331:LYS:C	1:A:333:ARG:H	0.47	2.15	5	2
1:A:198:ARG:CZ	1:A:236:ASP:CG	0.47	2.88	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:153:ARG:NH1	1:A:155:CYS:SG	0.47	2.88	18	1
1:A:153:ARG:CZ	1:A:192:GLY:O	0.47	2.62	18	1
1:A:155:CYS:O	1:A:157:MET:SD	0.47	2.73	5	3
1:A:184:PRO:O	1:A:189:GLU:OE1	0.47	2.32	3	2
1:A:330:ALA:C	1:A:332:GLU:H	0.46	2.16	4	1
1:A:160:GLY:C	1:A:162:SER:H	0.46	2.17	17	1
1:A:202:VAL:C	1:A:204:GLY:N	0.46	2.72	1	4
1:A:250:HIS:O	1:A:253:GLY:O	0.46	2.34	10	4
1:A:249:GLU:OE2	1:A:250:HIS:CE1	0.46	2.68	2	1
1:A:227:LYS:C	1:A:228:LEU:HD12	0.46	2.36	4	6
1:A:239:PHE:O	1:A:243:ARG:N	0.46	2.48	14	2
1:A:325:ILE:N	1:A:325:ILE:CD1	0.46	2.78	19	1
1:A:207:MET:O	1:A:208:GLU:C	0.46	2.58	15	1
1:A:166:PHE:CE2	1:A:168:LEU:HD22	0.46	2.46	3	1
1:A:164:TYR:CE2	1:A:226:THR:HG22	0.46	2.46	9	2
1:A:212:HIS:CD2	1:A:213:GLY:N	0.45	2.84	8	2
1:A:198:ARG:NH2	1:A:236:ASP:OD2	0.45	2.49	2	1
1:A:335:HIS:O	1:A:336:GLN:O	0.45	2.35	20	2
1:A:193:LEU:C	1:A:193:LEU:CD1	0.45	2.90	19	2
1:A:183:ASP:O	1:A:186:SER:OG	0.45	2.33	11	5
1:A:161:PRO:O	1:A:163:GLY:N	0.45	2.50	8	1
1:A:335:HIS:O	1:A:336:GLN:C	0.45	2.60	5	1
1:A:208:GLU:C	1:A:210:LYS:H	0.45	2.20	19	1
1:A:200:VAL:O	1:A:207:MET:C	0.45	2.60	16	1
1:A:198:ARG:NH1	1:A:236:ASP:CG	0.44	2.75	2	1
1:A:251:LEU:O	1:A:252:ASN:O	0.44	2.35	2	1
1:A:159:LYS:NZ	1:A:224:ASP:OD1	0.44	2.49	4	2
1:A:156:THR:HG23	1:A:227:LYS:HG2	0.44	1.89	20	1
1:A:331:LYS:O	1:A:333:ARG:N	0.44	2.50	18	2
1:A:325:ILE:HD12	1:A:325:ILE:H	0.44	1.72	19	1
1:A:165:GLY:O	1:A:183:ASP:CG	0.44	2.61	2	1
1:A:198:ARG:NH1	1:A:240:LYS:NZ	0.44	2.65	20	1
1:A:153:ARG:HH22	1:A:232:ASP:CG	0.44	2.21	13	1
1:A:183:ASP:O	1:A:184:PRO:C	0.44	2.59	9	1
1:A:202:VAL:O	1:A:205:VAL:N	0.44	2.50	14	2
1:A:195:ALA:O	1:A:196:GLN:OE1	0.44	2.36	17	1
1:A:161:PRO:O	1:A:162:SER:C	0.43	2.61	11	3
1:A:200:VAL:HG13	1:A:201:GLU:N	0.43	2.28	15	1
1:A:249:GLU:OE1	1:A:249:GLU:C	0.43	2.61	2	1
1:A:168:LEU:N	1:A:168:LEU:HD23	0.43	2.29	3	1
1:A:177:GLN:C	1:A:178:PHE:CD1	0.43	2.96	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:151:ARG:O	1:A:152:PRO:O	0.43	2.37	11	2
1:A:327:LEU:HD23	1:A:327:LEU:C	0.43	2.37	15	1
1:A:198:ARG:CZ	1:A:236:ASP:OD2	0.43	2.66	2	1
1:A:196:GLN:OE1	1:A:196:GLN:O	0.43	2.36	11	1
1:A:196:GLN:O	1:A:197:ASP:OD1	0.43	2.35	15	2
1:A:188:ALA:O	1:A:191:SER:OG	0.43	2.36	8	4
1:A:249:GLU:C	1:A:249:GLU:CD	0.43	2.87	2	1
1:A:160:GLY:O	1:A:162:SER:N	0.43	2.49	3	1
1:A:189:GLU:CD	1:A:189:GLU:C	0.43	2.87	11	3
1:A:333:ARG:O	1:A:336:GLN:O	0.43	2.37	8	1
1:A:253:GLY:O	1:A:254:PRO:O	0.43	2.36	19	1
1:A:223:GLY:O	1:A:225:GLU:N	0.42	2.52	20	3
1:A:165:GLY:C	1:A:183:ASP:CG	0.42	2.87	20	1
1:A:251:LEU:O	1:A:253:GLY:N	0.42	2.53	8	1
1:A:185:ASP:OD1	1:A:185:ASP:O	0.42	2.37	12	1
1:A:201:GLU:OE2	1:A:247:SER:OG	0.42	2.36	17	1
1:A:151:ARG:O	1:A:152:PRO:C	0.42	2.63	11	1
1:A:165:GLY:C	1:A:183:ASP:OD2	0.42	2.62	6	2
1:A:202:VAL:O	1:A:204:GLY:N	0.42	2.52	19	1
1:A:152:PRO:O	1:A:251:LEU:CD2	0.42	2.68	17	1
1:A:335:HIS:O	1:A:335:HIS:CD2	0.42	2.72	18	1
1:A:177:GLN:CD	1:A:212:HIS:ND1	0.42	2.77	11	1
1:A:233:ARG:H	1:A:233:ARG:CD	0.41	2.28	16	1
1:A:202:VAL:C	1:A:204:GLY:H	0.41	2.21	19	1
1:A:330:ALA:O	1:A:332:GLU:N	0.41	2.53	4	1
1:A:253:GLY:O	1:A:255:LEU:N	0.41	2.53	11	1
1:A:245:ILE:O	1:A:246:PRO:C	0.41	2.63	15	1
1:A:161:PRO:C	1:A:163:GLY:N	0.41	2.75	8	1
1:A:225:GLU:CD	1:A:225:GLU:N	0.41	2.79	18	1
1:A:236:ASP:C	1:A:236:ASP:OD1	0.41	2.62	17	2
1:A:233:ARG:CG	1:A:234:GLU:N	0.41	2.84	20	1
1:A:167:ASN:OD1	1:A:168:LEU:O	0.41	2.38	10	1
1:A:221:ALA:C	1:A:223:GLY:N	0.41	2.79	10	1
1:A:163:GLY:C	1:A:165:GLY:N	0.41	2.79	2	1
1:A:232:ASP:OD1	1:A:233:ARG:N	0.41	2.53	14	1
1:A:198:ARG:NH1	1:A:240:LYS:HZ1	0.41	2.14	20	1
1:A:183:ASP:O	1:A:185:ASP:N	0.40	2.54	9	1
1:A:236:ASP:OD1	1:A:236:ASP:C	0.40	2.62	1	1
1:A:233:ARG:NH1	1:A:234:GLU:OE2	0.40	2.55	2	1
1:A:241:LYS:O	1:A:243:ARG:NH1	0.40	2.54	2	1
1:A:212:HIS:C	1:A:214:ASP:N	0.40	2.78	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:206:CYS:O	1:A:210:LYS:NZ	0.40	2.53	9	1
1:A:177:GLN:CD	1:A:177:GLN:N	0.40	2.79	13	1
1:A:254:PRO:O	1:A:255:LEU:C	0.40	2.64	14	1
1:A:233:ARG:CD	1:A:233:ARG:N	0.40	2.84	16	1
1:A:212:HIS:O	1:A:215:VAL:HG22	0.40	2.16	18	1
1:A:211:GLN:CD	1:A:211:GLN:N	0.40	2.79	16	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	113/216 (52%)	104±2 (92±2%)	6±2 (5±2%)	3±1 (3±1%)	5	38
All	All	2260/4320 (52%)	2080 (92%)	112 (5%)	68 (3%)	5	38

All 20 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	160	GLY	17
1	A	162	SER	6
1	A	245	ILE	6
1	A	161	PRO	5
1	A	336	GLN	4
1	A	254	PRO	4
1	A	255	LEU	4
1	A	152	PRO	3
1	A	224	ASP	3
1	A	208	GLU	3
1	A	246	PRO	2
1	A	165	GLY	2
1	A	332	GLU	2
1	A	252	ASN	1
1	A	164	TYR	1
1	A	251	LEU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	331	LYS	1
1	A	184	PRO	1
1	A	150	LEU	1
1	A	209	GLY	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	95/187 (51%)	92±1 (97±1%)	3±1 (3±1%)	35 84
All	All	1900/3740 (51%)	1839 (97%)	61 (3%)	35 84

All 22 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	166	PHE	16
1	A	157	MET	10
1	A	327	LEU	5
1	A	215	VAL	4
1	A	329	MET	3
1	A	207	MET	3
1	A	177	GLN	2
1	A	186	SER	2
1	A	225	GLU	2
1	A	193	LEU	2
1	A	178	PHE	1
1	A	183	ASP	1
1	A	205	VAL	1
1	A	153	ARG	1
1	A	194	ARG	1
1	A	241	LYS	1
1	A	180	ARG	1
1	A	238	PHE	1
1	A	255	LEU	1
1	A	229	LEU	1
1	A	168	LEU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	208	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 [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided