



Full wwPDB NMR Structure Validation Report ⓘ

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PDB ID : 1MO7
Title : ATPase
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Deposited on : 2002-09-08

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
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

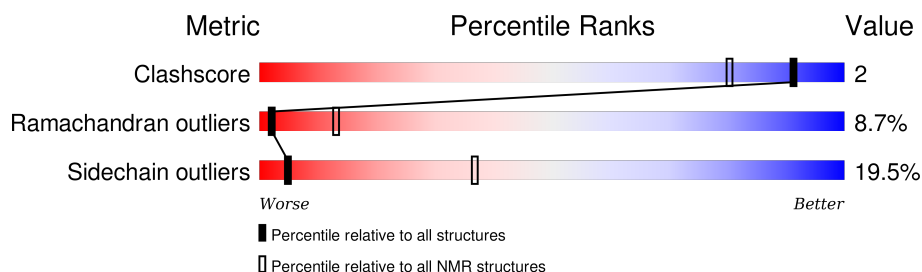
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 78%.

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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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	213	 63% 18% • 17%

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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:386-A:398, A:416-A:434, A:442-A:481, A:487-A:546, A:552-A:595 (176)	0.54	3

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 3 clusters and 3 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3303 atoms, of which 1632 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Sodium/Potassium-transporting ATPase alpha-1 chain.

Mol	Chain	Residues	Atoms						Trace
1	A	213	Total	C	H	N	O	S	0
			3303	1056	1632	282	320	13	

There is a discrepancy between the modelled and reference sequences:

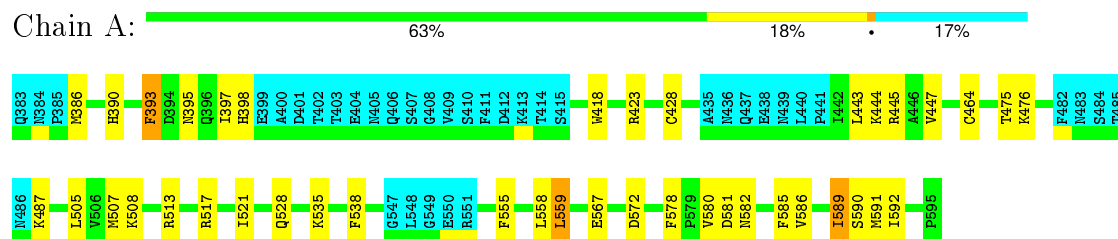
Chain	Residue	Modelled	Actual	Comment	Reference
A	385	PRO	ARG	CLONING ARTIFACT	UNP P06685

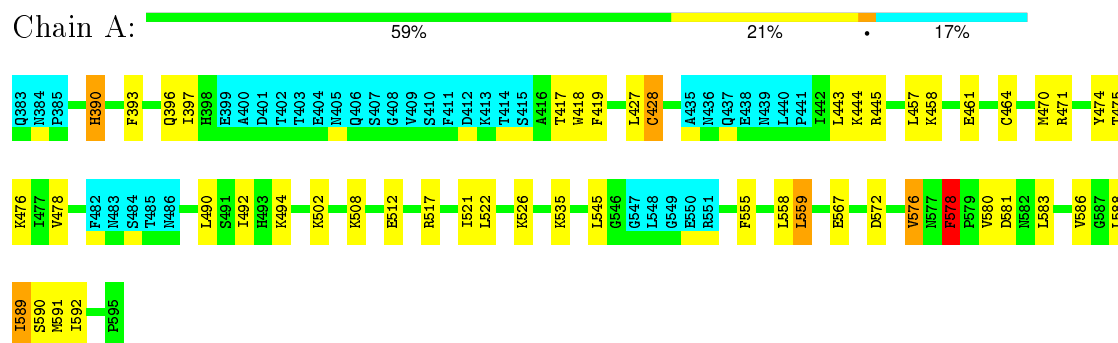
4 Residue-property plots

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.

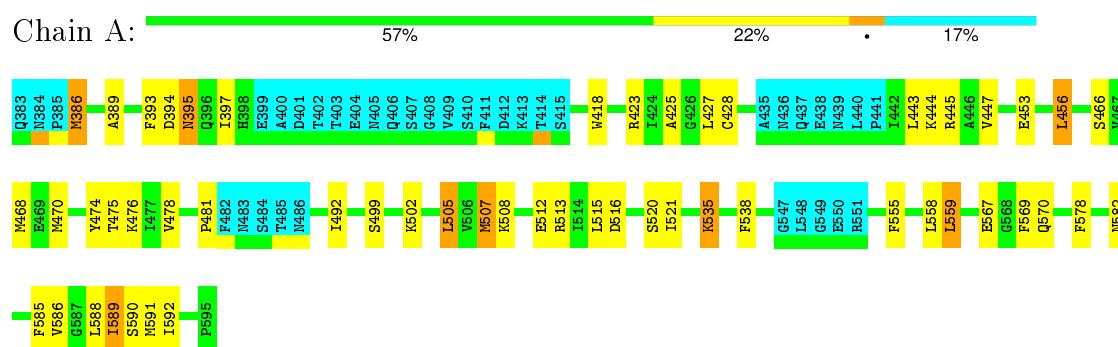
- Molecule 1: Sodium/Potassium-transporting ATPase alpha-1 chain





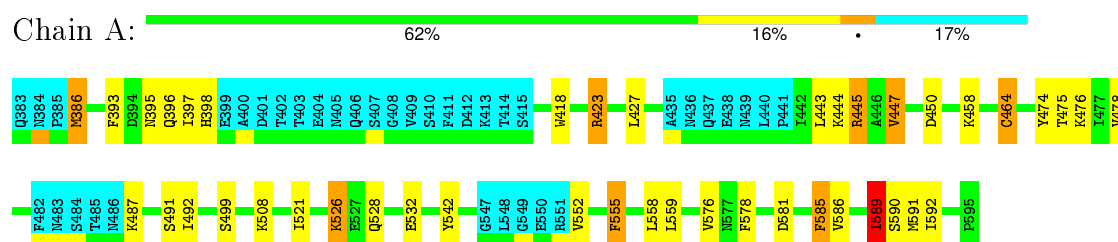
4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: Sodium/Potassium-transporting ATPase alpha-1 chain



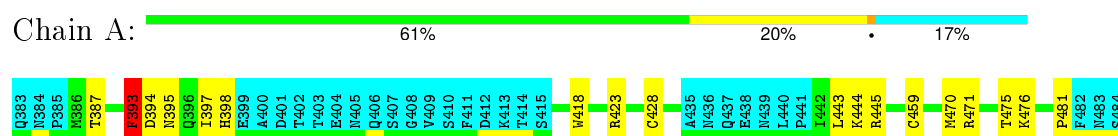
4.2.4 Score per residue for model 4

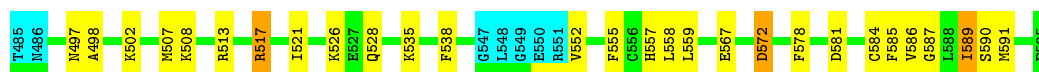
- Molecule 1: Sodium/Potassium-transporting ATPase alpha-1 chain



4.2.5 Score per residue for model 5

- Molecule 1: Sodium/Potassium-transporting ATPase alpha-1 chain

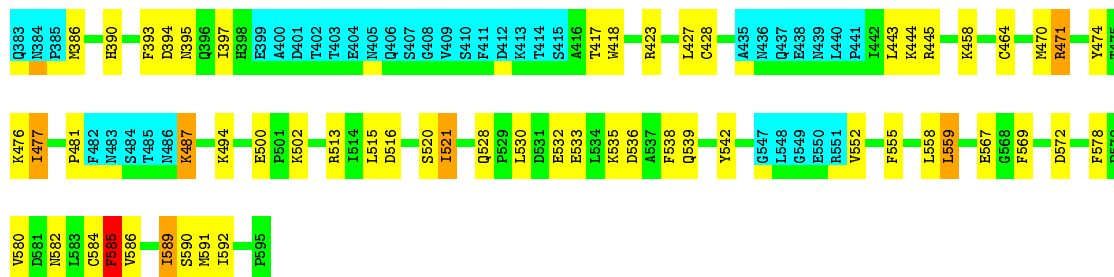




4.2.6 Score per residue for model 6

- Molecule 1: Sodium/Potassium-transporting ATPase alpha-1 chain

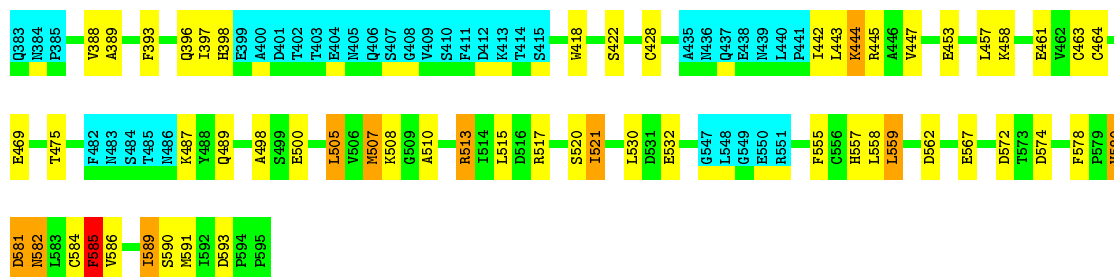
Chain A: 56% 23% 17%



4.2.7 Score per residue for model 7

- Molecule 1: Sodium/Potassium-transporting ATPase alpha-1 chain

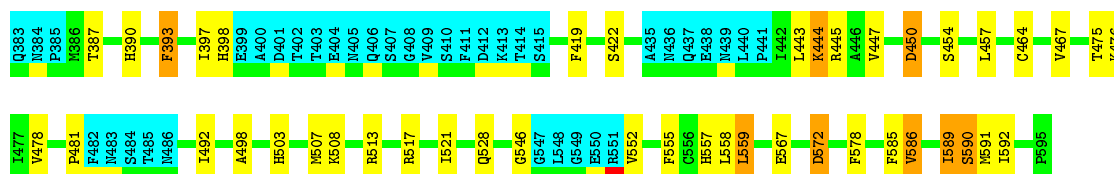
Chain A: 56% 21% 5% 17%



4.2.8 Score per residue for model 8

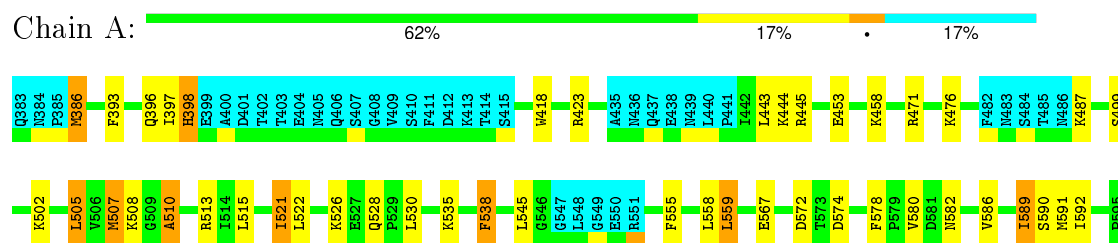
- Molecule 1: Sodium/Potassium-transporting ATPase alpha-1 chain

Chain A: 62% 17% 17%



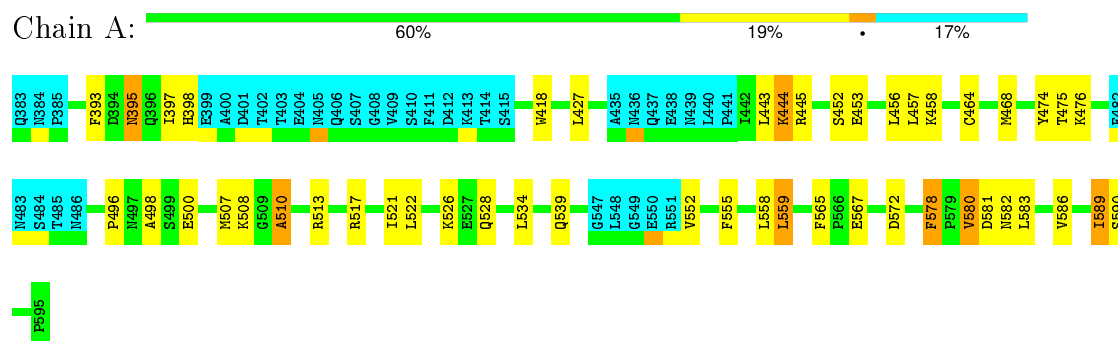
4.2.9 Score per residue for model 9

- Molecule 1: Sodium/Potassium-transporting ATPase alpha-1 chain



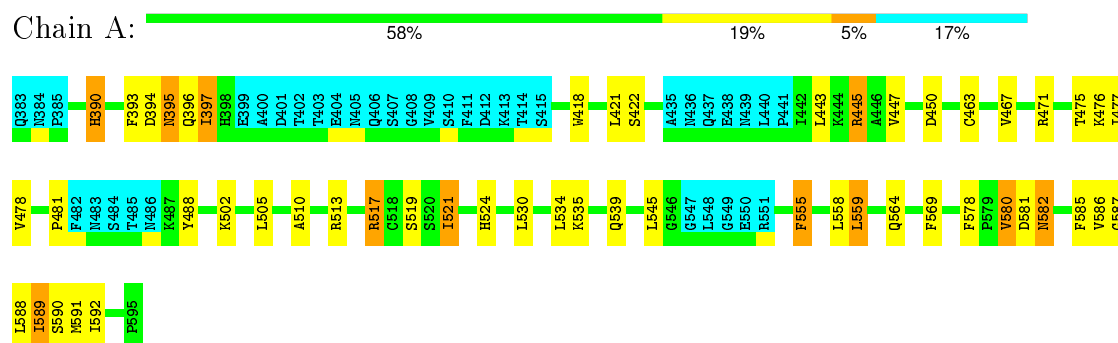
4.2.10 Score per residue for model 10

- Molecule 1: Sodium/Potassium-transporting ATPase alpha-1 chain



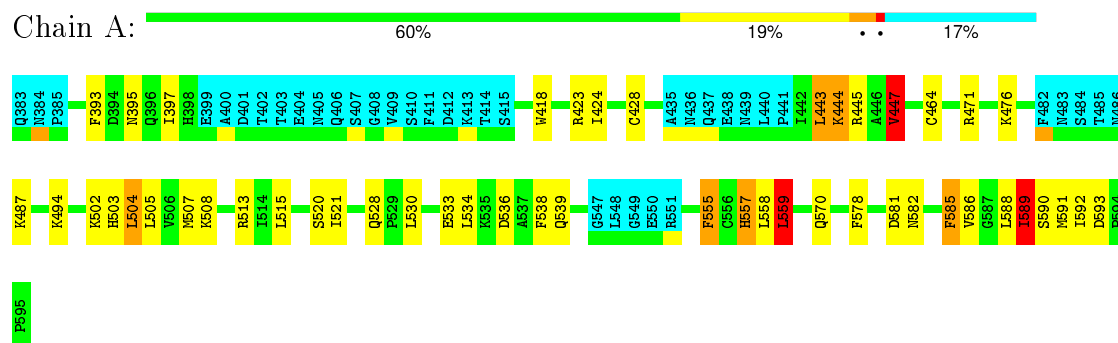
4.2.11 Score per residue for model 11

- Molecule 1: Sodium/Potassium-transporting ATPase alpha-1 chain



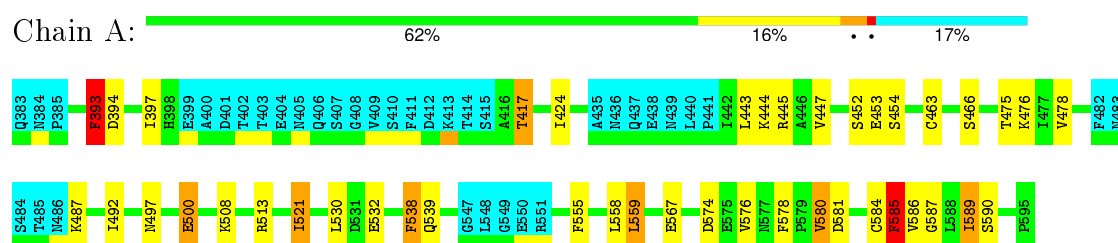
4.2.12 Score per residue for model 12

- Molecule 1: Sodium/Potassium-transporting ATPase alpha-1 chain



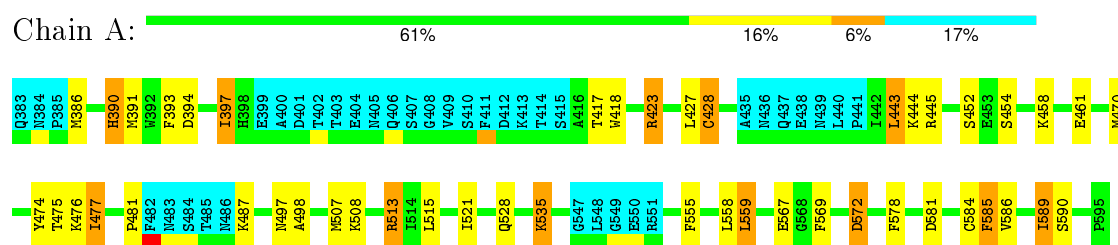
4.2.13 Score per residue for model 13

- Molecule 1: Sodium/Potassium-transporting ATPase alpha-1 chain



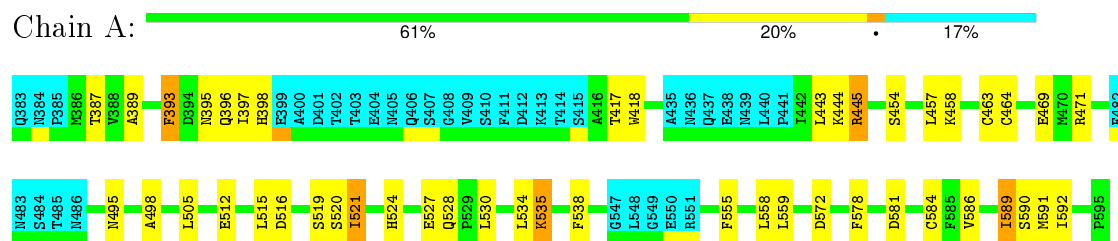
4.2.14 Score per residue for model 14

- Molecule 1: Sodium/Potassium-transporting ATPase alpha-1 chain



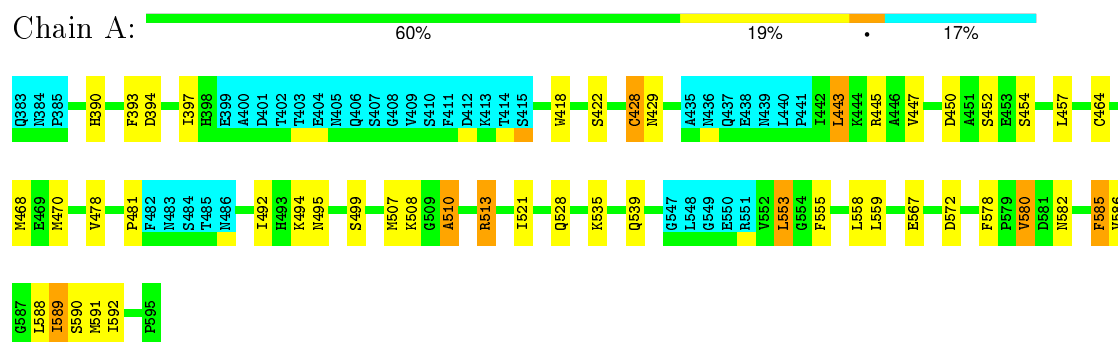
4.2.15 Score per residue for model 15

- Molecule 1: Sodium/Potassium-transporting ATPase alpha-1 chain



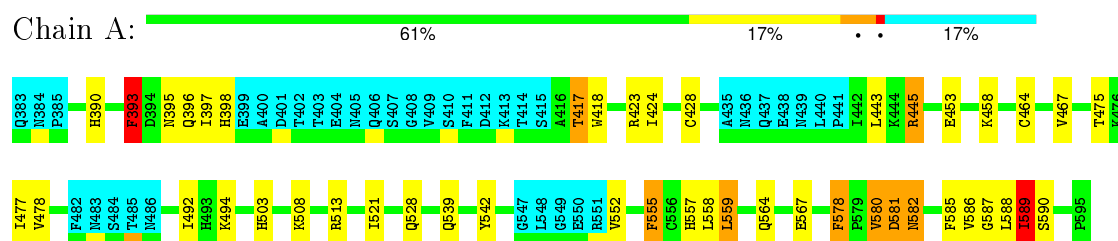
4.2.16 Score per residue for model 16

- Molecule 1: Sodium/Potassium-transporting ATPase alpha-1 chain



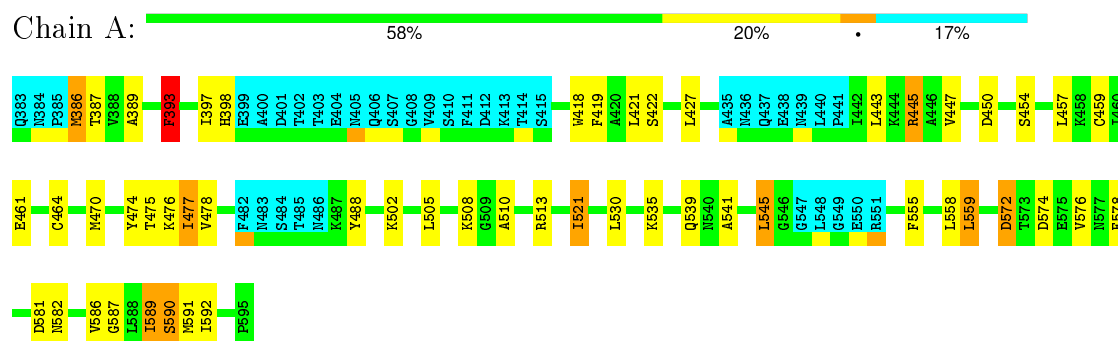
4.2.17 Score per residue for model 17

- Molecule 1: Sodium/Potassium-transporting ATPase alpha-1 chain



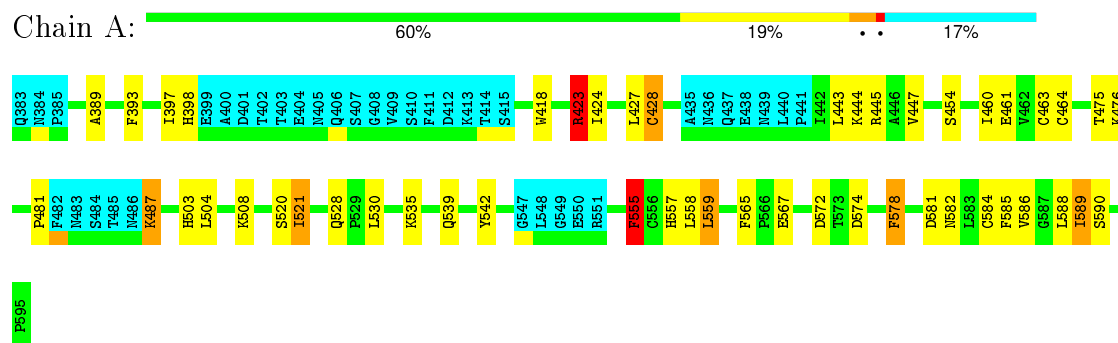
4.2.18 Score per residue for model 18

- Molecule 1: Sodium/Potassium-transporting ATPase alpha-1 chain



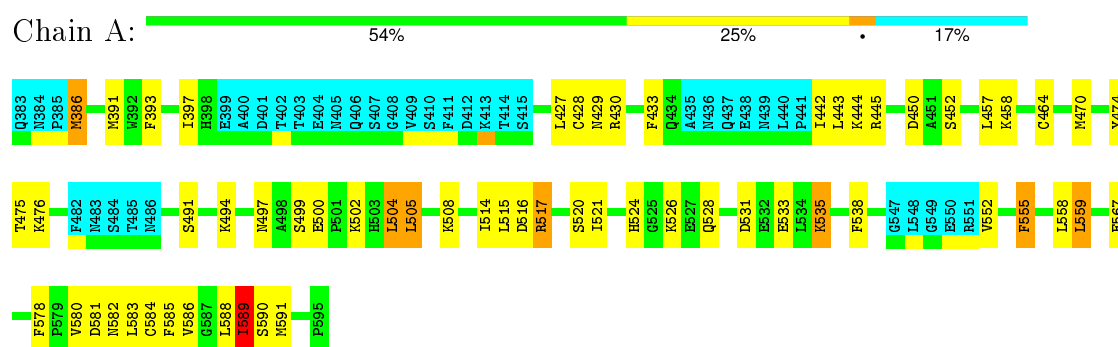
4.2.19 Score per residue for model 19

- Molecule 1: Sodium/Potassium-transporting ATPase alpha-1 chain



4.2.20 Score per residue for model 20

- Molecule 1: Sodium/Potassium-transporting ATPase alpha-1 chain



5 Refinement protocol and experimental data overview

The models were refined using the following method: *automated NOESY cross peak assignment*.

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy, target function*.

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

Software name	Classification	Version
CYANA	structure solution	1.0.5
OPALp	refinement	1.0

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	BMRB entry 5577
Number of chemical shift lists	1
Total number of shifts	2159
Number of shifts mapped to atoms	2159
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	78%

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

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	0.59±0.01	0±0/1423 (0.0±0.0%)	1.14±0.03	2±1/1926 (0.1±0.1%)
All	All	0.59	0/28460 (0.0%)	1.14	30/38520 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	2.5±1.0
All	All	0	50

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	393	PHE	CB-CG-CD2	-7.79	115.35	120.80	17	3
1	A	423	ARG	CD-NE-CZ	6.70	132.97	123.60	19	1
1	A	588	LEU	CB-CA-C	6.63	122.79	110.20	11	2
1	A	513	ARG	NE-CZ-NH2	-6.43	117.08	120.30	7	3
1	A	445	ARG	NE-CZ-NH1	6.23	123.42	120.30	15	2
1	A	471	ARG	NE-CZ-NH2	-5.98	117.31	120.30	12	1
1	A	447	VAL	CA-CB-CG1	5.88	119.72	110.90	12	1
1	A	517	ARG	NE-CZ-NH2	-5.84	117.38	120.30	1	2
1	A	578	PHE	CB-CG-CD2	-5.53	116.93	120.80	2	3
1	A	419	PHE	CB-CG-CD2	-5.49	116.96	120.80	1	1
1	A	513	ARG	NE-CZ-NH1	5.46	123.03	120.30	7	1
1	A	428	CYS	CA-CB-SG	-5.33	104.41	114.00	2	1
1	A	423	ARG	NE-CZ-NH1	5.30	122.95	120.30	14	1
1	A	517	ARG	CD-NE-CZ	5.22	130.91	123.60	7	1
1	A	423	ARG	NE-CZ-NH2	-5.12	117.74	120.30	6	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	585	PHE	CB-CG-CD2	-5.10	117.23	120.80	7	2
1	A	578	PHE	CB-CG-CD1	5.09	124.37	120.80	17	1
1	A	488	TYR	CB-CG-CD2	-5.01	117.99	121.00	11	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	582	ASN	Peptide	10
1	A	585	PHE	Peptide,Sidechain	7
1	A	517	ARG	Sidechain	6
1	A	513	ARG	Sidechain	5
1	A	587	GLY	Peptide	3
1	A	471	ARG	Sidechain	3
1	A	503	HIS	Sidechain	2
1	A	565	PHE	Sidechain	2
1	A	542	TYR	Sidechain	2
1	A	526	LYS	Peptide	2
1	A	423	ARG	Sidechain	2
1	A	569	PHE	Sidechain	1
1	A	430	ARG	Sidechain	1
1	A	488	TYR	Peptide	1
1	A	445	ARG	Sidechain	1
1	A	581	ASP	Mainchain	1
1	A	390	HIS	Sidechain	1

6.2 Too-close contacts ⓘ

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	1391	1384	1384	6±2
All	All	27820	27680	27680	110

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 2.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:423:ARG:CZ	1:A:427:LEU:HD13	0.60	2.27	19	1
1:A:514:ILE:HG23	1:A:517:ARG:NH1	0.59	2.11	20	1
1:A:397:ILE:HD11	1:A:541:ALA:HA	0.56	1.77	18	1
1:A:555:PHE:CD2	1:A:589:ILE:HD11	0.56	2.36	20	3
1:A:395:ASN:HD21	1:A:534:LEU:HD22	0.55	1.60	10	2
1:A:427:LEU:HD21	1:A:474:TYR:CD1	0.54	2.37	3	7
1:A:515:LEU:HD11	1:A:535:LYS:HG3	0.53	1.81	1	5
1:A:521:ILE:HB	1:A:530:LEU:HD13	0.53	1.80	6	8
1:A:515:LEU:HD13	1:A:585:PHE:CZ	0.52	2.39	3	2
1:A:478:VAL:CG2	1:A:492:ILE:HD12	0.52	2.35	13	7
1:A:515:LEU:HD13	1:A:585:PHE:CE2	0.52	2.39	7	3
1:A:504:LEU:HD12	1:A:505:LEU:N	0.52	2.20	12	2
1:A:555:PHE:CE2	1:A:589:ILE:HD11	0.51	2.41	17	3
1:A:510:ALA:HB3	1:A:513:ARG:HG2	0.51	1.82	9	4
1:A:477:ILE:HD12	1:A:569:PHE:HB2	0.51	1.82	6	2
1:A:505:LEU:HD22	1:A:558:LEU:HG	0.50	1.83	1	1
1:A:393:PHE:CD1	1:A:417:THR:HG21	0.50	2.42	15	1
1:A:393:PHE:CE2	1:A:421:LEU:HD13	0.50	2.41	18	1
1:A:505:LEU:HD21	1:A:507:MET:SD	0.50	2.47	3	4
1:A:393:PHE:CZ	1:A:417:THR:HG22	0.50	2.42	13	2
1:A:425:ALA:HB1	1:A:456:LEU:CD1	0.49	2.36	3	1
1:A:522:LEU:HD13	1:A:526:LYS:O	0.49	2.06	2	4
1:A:538:PHE:CD1	1:A:585:PHE:CZ	0.49	3.00	6	2
1:A:555:PHE:CD1	1:A:589:ILE:HD11	0.49	2.43	1	1
1:A:443:LEU:HD23	1:A:444:LYS:N	0.49	2.23	12	1
1:A:557:HIS:NE2	1:A:586:VAL:HG21	0.49	2.23	8	1
1:A:427:LEU:HD23	1:A:470:MET:HB3	0.48	1.84	2	6
1:A:477:ILE:HG22	1:A:478:VAL:HG22	0.48	1.85	11	2
1:A:515:LEU:HD22	1:A:538:PHE:CE1	0.48	2.44	9	1
1:A:390:HIS:CD2	1:A:391:MET:H	0.48	2.26	14	1
1:A:390:HIS:CD2	1:A:397:ILE:HG23	0.48	2.44	14	1
1:A:423:ARG:NH2	1:A:427:LEU:HD13	0.48	2.23	19	1
1:A:421:LEU:HD13	1:A:587:GLY:CA	0.47	2.39	11	1
1:A:393:PHE:CE2	1:A:417:THR:HG22	0.47	2.45	13	2
1:A:555:PHE:N	1:A:555:PHE:CD1	0.47	2.81	19	1
1:A:395:ASN:ND2	1:A:534:LEU:HD22	0.47	2.25	10	2
1:A:552:VAL:HG22	1:A:590:SER:OG	0.47	2.09	8	1
1:A:427:LEU:HD11	1:A:474:TYR:CZ	0.46	2.45	10	1
1:A:545:LEU:HD13	1:A:590:SER:CB	0.45	2.42	18	1
1:A:576:VAL:CG1	1:A:578:PHE:CD2	0.44	3.00	2	1
1:A:387:THR:HG23	1:A:389:ALA:H	0.44	1.71	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:578:PHE:CZ	1:A:580:VAL:CG1	0.44	3.01	10	1
1:A:423:ARG:NE	1:A:427:LEU:HD13	0.44	2.28	19	1
1:A:530:LEU:HA	1:A:534:LEU:HD12	0.44	1.89	12	1
1:A:393:PHE:CD2	1:A:587:GLY:HA3	0.43	2.48	18	1
1:A:557:HIS:CE1	1:A:559:LEU:HD21	0.43	2.49	12	1
1:A:545:LEU:HD13	1:A:590:SER:HB3	0.43	1.90	1	1
1:A:390:HIS:CE1	1:A:397:ILE:HG23	0.43	2.48	11	1
1:A:505:LEU:HD23	1:A:505:LEU:C	0.43	2.33	1	1
1:A:428:CYS:SG	1:A:508:LYS:HE2	0.42	2.53	16	1
1:A:443:LEU:CD2	1:A:445:ARG:H	0.42	2.27	9	1
1:A:443:LEU:HD23	1:A:444:LYS:HA	0.42	1.90	12	1
1:A:433:PHE:CZ	1:A:442:ILE:HD11	0.41	2.50	20	1
1:A:443:LEU:HD23	1:A:444:LYS:CA	0.41	2.45	12	1
1:A:490:LEU:HD21	1:A:578:PHE:CE2	0.41	2.51	2	1
1:A:443:LEU:HD22	1:A:445:ARG:H	0.41	1.75	16	1
1:A:423:ARG:HH21	1:A:557:HIS:CE1	0.40	2.34	17	1
1:A:521:ILE:HG21	1:A:534:LEU:HD13	0.40	1.92	1	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	175/213 (82%)	127±5 (73±3%)	32±6 (18±3%)	15±2 (9±1%)	2	13
All	All	3500/4260 (82%)	2549 (73%)	645 (18%)	306 (9%)	2	13

All 47 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	586	VAL	20
1	A	589	ILE	20
1	A	393	PHE	20
1	A	555	PHE	20
1	A	590	SER	20

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Mol	Chain	Res	Type	Models (Total)
1	A	397	ILE	19
1	A	559	LEU	16
1	A	444	LYS	15
1	A	464	CYS	13
1	A	581	ASP	12
1	A	502	LYS	10
1	A	572	ASP	9
1	A	580	VAL	9
1	A	481	PRO	9
1	A	428	CYS	8
1	A	396	GLN	7
1	A	386	MET	6
1	A	487	LYS	6
1	A	552	VAL	6
1	A	498	ALA	6
1	A	395	ASN	5
1	A	477	ILE	4
1	A	510	ALA	4
1	A	576	VAL	4
1	A	499	SER	4
1	A	445	ARG	4
1	A	389	ALA	4
1	A	500	GLU	3
1	A	398	HIS	2
1	A	466	SER	2
1	A	447	VAL	2
1	A	390	HIS	2
1	A	459	CYS	1
1	A	387	THR	1
1	A	460	ILE	1
1	A	463	CYS	1
1	A	503	HIS	1
1	A	496	PRO	1
1	A	546	GLY	1
1	A	442	ILE	1
1	A	497	ASN	1
1	A	443	LEU	1
1	A	524	HIS	1
1	A	450	ASP	1
1	A	452	SER	1
1	A	553	LEU	1
1	A	388	VAL	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	154/186 (83%)	124±4 (80±2%)	30±4 (20±2%)	5	37
All	All	3080/3720 (83%)	2479 (80%)	601 (20%)	5	37

All 98 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	558	LEU	20
1	A	559	LEU	20
1	A	589	ILE	20
1	A	521	ILE	20
1	A	578	PHE	20
1	A	443	LEU	19
1	A	418	TRP	17
1	A	445	ARG	17
1	A	508	LYS	16
1	A	475	THR	15
1	A	591	MET	15
1	A	476	LYS	15
1	A	567	GLU	14
1	A	535	LYS	13
1	A	528	GLN	13
1	A	585	PHE	12
1	A	592	ILE	11
1	A	507	MET	10
1	A	539	GLN	10
1	A	447	VAL	10
1	A	458	LYS	10
1	A	457	LEU	9
1	A	505	LEU	8
1	A	538	PHE	8
1	A	584	CYS	8
1	A	454	SER	8
1	A	398	HIS	8
1	A	572	ASP	7
1	A	394	ASP	7

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Mol	Chain	Res	Type	Models (Total)
1	A	520	SER	7
1	A	582	ASN	6
1	A	580	VAL	6
1	A	450	ASP	6
1	A	494	LYS	6
1	A	453	GLU	6
1	A	386	MET	6
1	A	588	LEU	6
1	A	574	ASP	6
1	A	513	ARG	6
1	A	461	GLU	5
1	A	487	LYS	5
1	A	557	HIS	5
1	A	422	SER	5
1	A	428	CYS	5
1	A	390	HIS	5
1	A	417	THR	4
1	A	532	GLU	4
1	A	533	GLU	4
1	A	471	ARG	4
1	A	500	GLU	4
1	A	395	ASN	4
1	A	424	ILE	4
1	A	423	ARG	4
1	A	463	CYS	4
1	A	452	SER	4
1	A	545	LEU	4
1	A	516	ASP	4
1	A	581	ASP	4
1	A	444	LYS	4
1	A	526	LYS	3
1	A	429	ASN	3
1	A	497	ASN	3
1	A	468	MET	3
1	A	393	PHE	3
1	A	467	VAL	3
1	A	512	GLU	3
1	A	504	LEU	3
1	A	583	LEU	3
1	A	495	ASN	2
1	A	564	GLN	2
1	A	470	MET	2

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Mol	Chain	Res	Type	Models (Total)
1	A	503	HIS	2
1	A	456	LEU	2
1	A	517	ARG	2
1	A	491	SER	2
1	A	570	GLN	2
1	A	593	ASP	2
1	A	387	THR	2
1	A	419	PHE	2
1	A	466	SER	2
1	A	524	HIS	2
1	A	536	ASP	2
1	A	555	PHE	2
1	A	469	GLU	2
1	A	519	SER	2
1	A	396	GLN	1
1	A	569	PHE	1
1	A	489	GLN	1
1	A	459	CYS	1
1	A	391	MET	1
1	A	527	GLU	1
1	A	499	SER	1
1	A	553	LEU	1
1	A	490	LEU	1
1	A	562	ASP	1
1	A	464	CYS	1
1	A	434	GLN	1
1	A	531	ASP	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 78% for the well-defined parts and 73% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 5577

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	2159
Number of shifts mapped to atoms	2159
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	189	-0.14 ± 0.09	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	186	0.04 ± 0.09	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	—
^{15}N	175	-0.09 ± 0.33	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 78%, i.e. 1699 atoms were assigned a chemical shift out of a possible 2180. 32 out of 32 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	654/860 (76%)	332/342 (97%)	163/352 (46%)	159/166 (96%)
Sidechain	951/1140 (83%)	570/670 (85%)	372/428 (87%)	9/42 (21%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	94/180 (52%)	53/98 (54%)	39/74 (53%)	2/8 (25%)
Overall	1699/2180 (78%)	955/1110 (86%)	574/854 (67%)	170/216 (79%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 73%, i.e. 1895 atoms were assigned a chemical shift out of a possible 2598. 35 out of 35 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	739/1041 (71%)	375/414 (91%)	189/426 (44%)	175/201 (87%)
Sidechain	1055/1359 (78%)	634/798 (79%)	411/506 (81%)	10/55 (18%)
Aromatic	101/198 (51%)	57/108 (53%)	42/82 (51%)	2/8 (25%)
Overall	1895/2598 (73%)	1066/1320 (81%)	642/1014 (63%)	187/264 (71%)

7.1.4 Statistically unusual chemical shifts ⓘ

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	422	SER	HB2	1.78	5.18 – 2.58	-8.1

7.1.5 Random Coil Index (RCI) plots ⓘ

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:

