



Full wwPDB NMR Structure Validation Report ⓘ

Mar 19, 2026 – 09:33 PM UTC

PDB ID : 1MO7 / pdb_00001mo7
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

<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

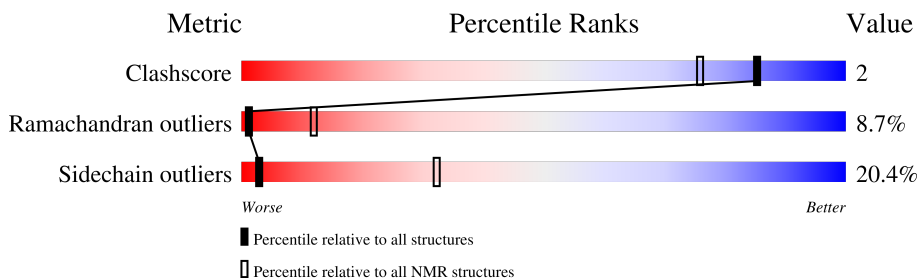
1 Overall quality at a glance

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	213	 62% 19% • 17%

2 Ensemble composition and analysis i

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)	0.93	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 4 clusters and 5 single-model clusters were found.

Cluster number	Models
1	3, 9, 18, 20
2	5, 7, 16, 17
3	1, 4, 6, 12
4	11, 13, 14
Single-model clusters	2; 8; 10; 15; 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
			Total	C	H	N	O	S	
1	A	213	3303	1056	1632	282	320	13	0

There is a discrepancy between the modelled and reference sequences:

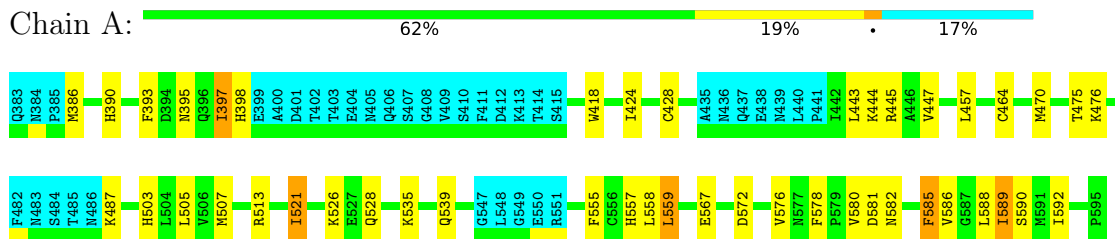
Chain	Residue	Modelled	Actual	Comment	Reference
A	385	PRO	ARG	cloning artifact	UNP P06685

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

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

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

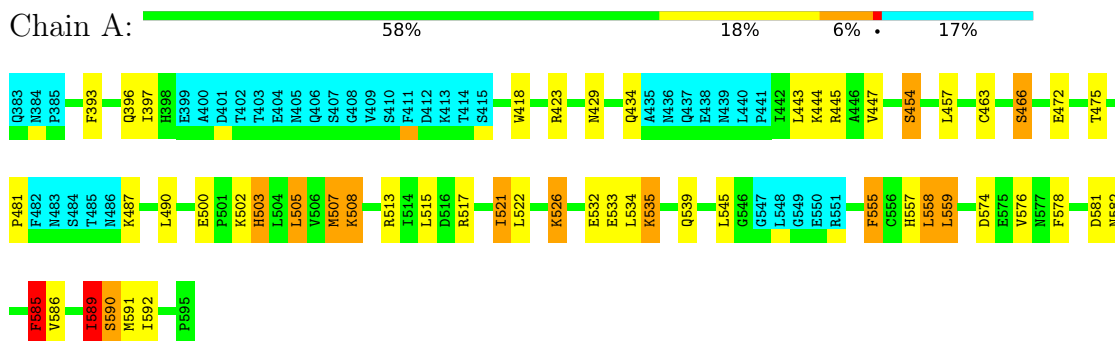


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

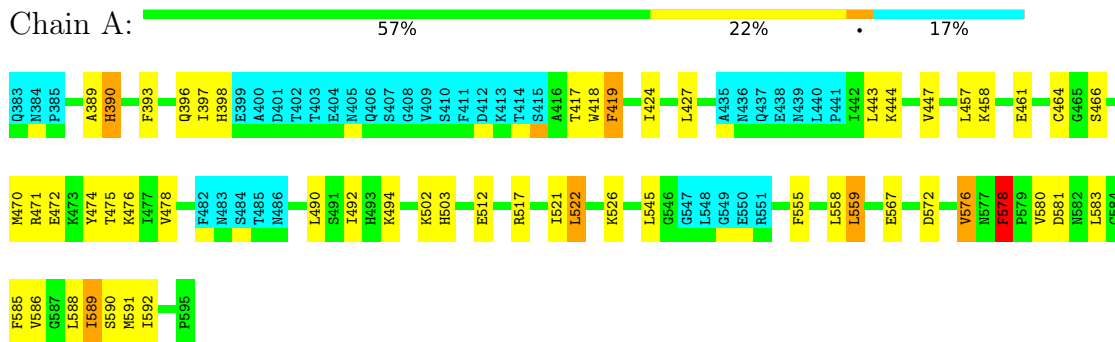
4.2.1 Score per residue for model 1

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



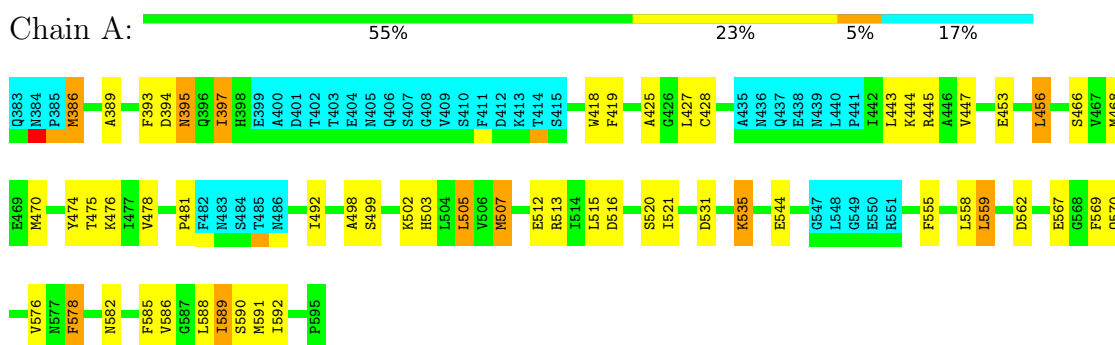
4.2.2 Score per residue for model 2

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



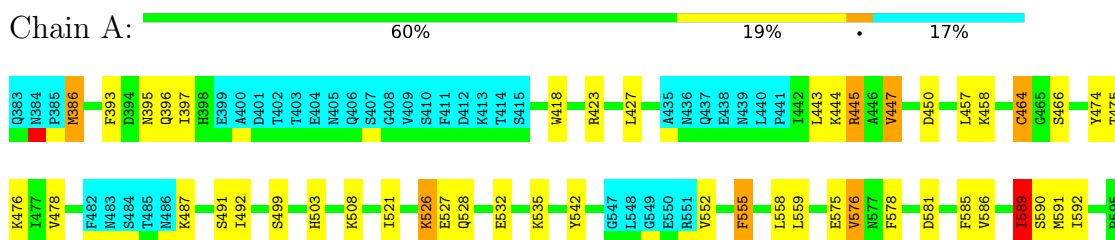
4.2.3 Score per residue for model 3 (medoid)

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



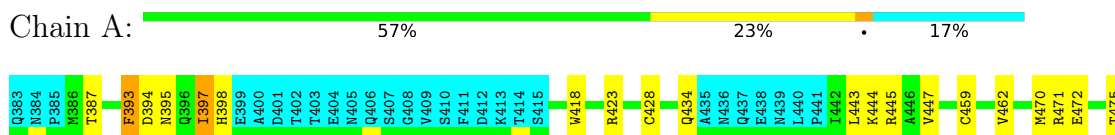
4.2.4 Score per residue for model 4

- 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

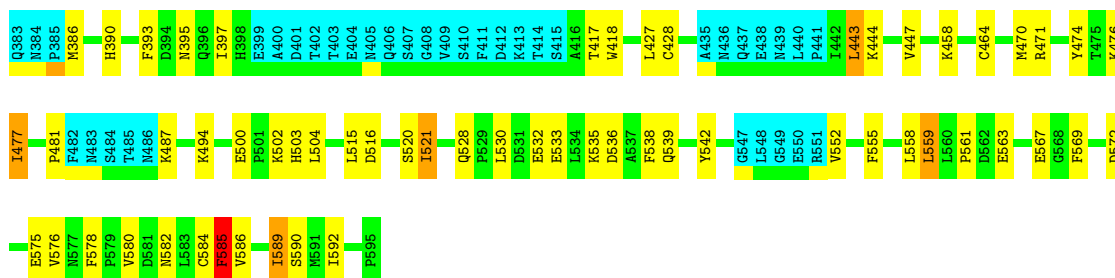




4.2.6 Score per residue for model 6

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

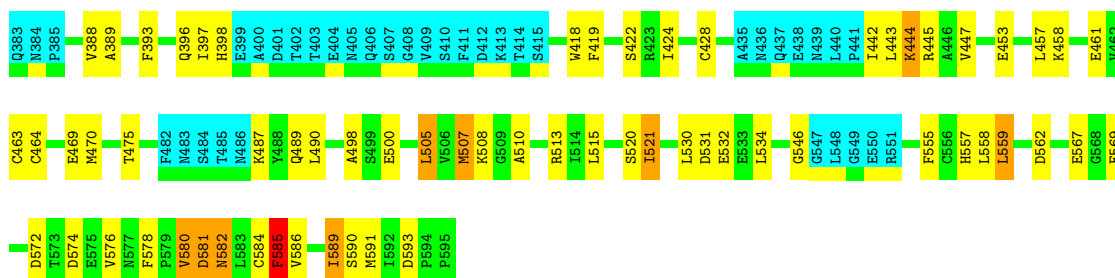
Chain A: 55% 25% 17%



4.2.7 Score per residue for model 7

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

Chain A: 53% 25% 17%

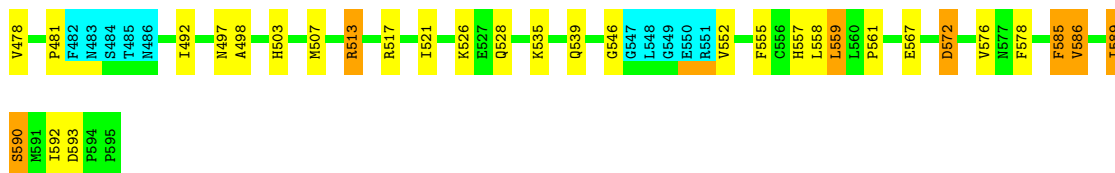


4.2.8 Score per residue for model 8

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

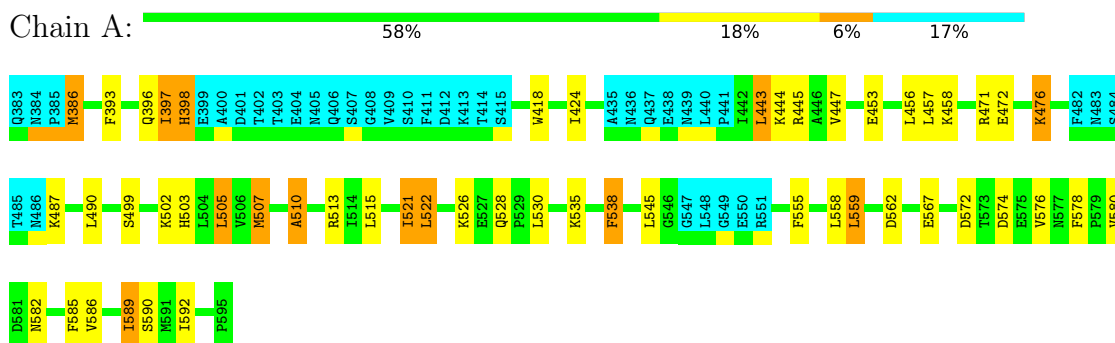
Chain A: 60% 18% 5% 17%





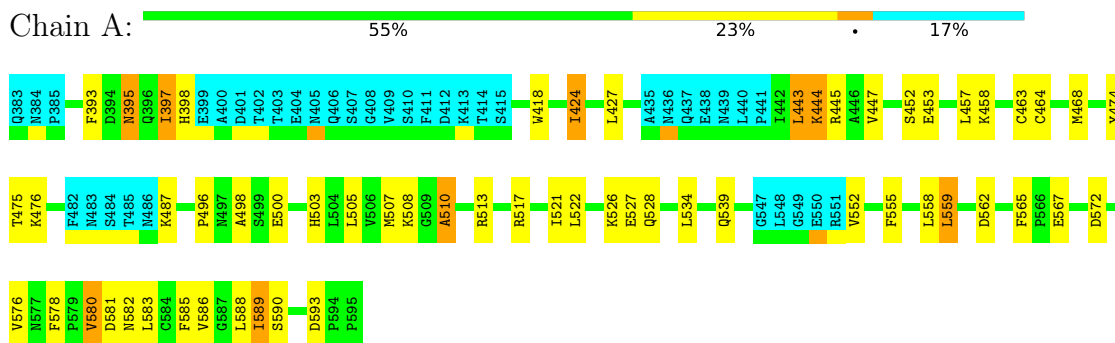
4.2.9 Score per residue for model 9

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



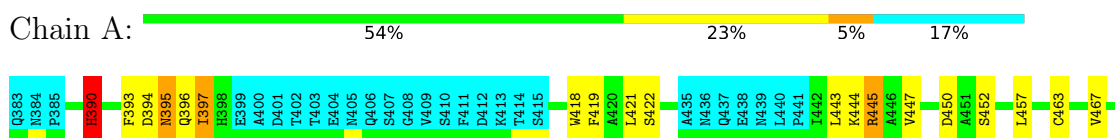
4.2.10 Score per residue for model 10

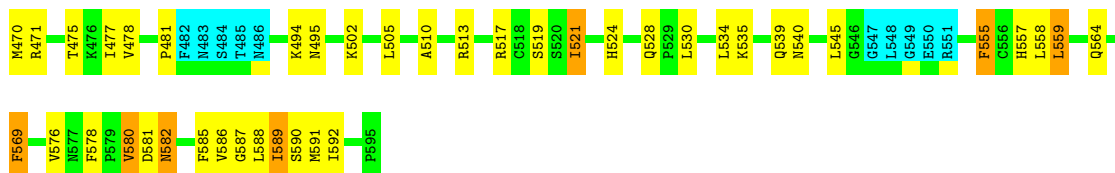
- Molecule 1: Sodium/Potassium-transporting ATPase alpha-1 chain



4.2.11 Score per residue for model 11

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

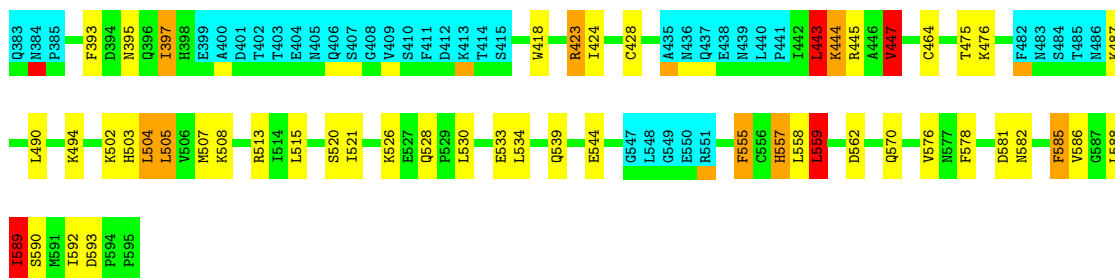




4.2.12 Score per residue for model 12

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

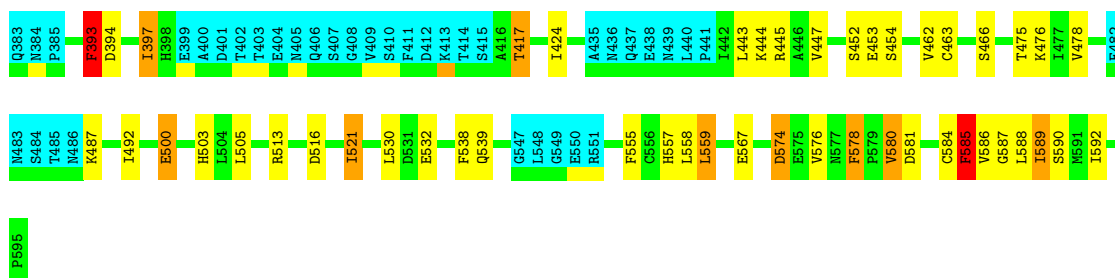
Chain A: 59% 18% 17%



4.2.13 Score per residue for model 13

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

Chain A: 60% 17% 17%

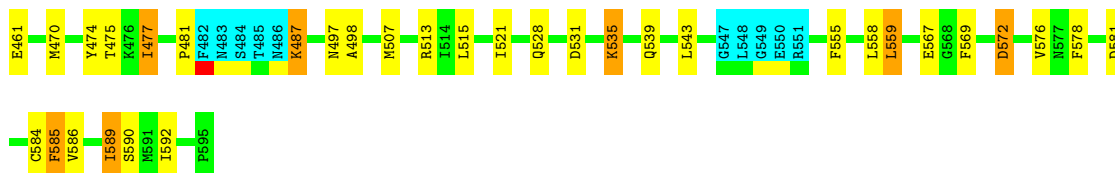


4.2.14 Score per residue for model 14

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

Chain A: 58% 19% 6% 17%

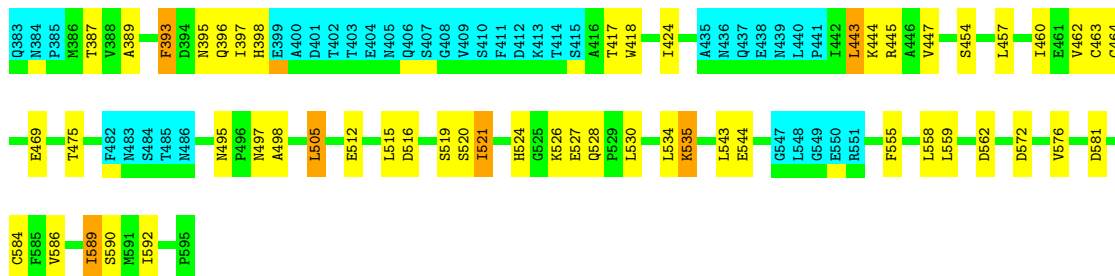




4.2.15 Score per residue for model 15

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

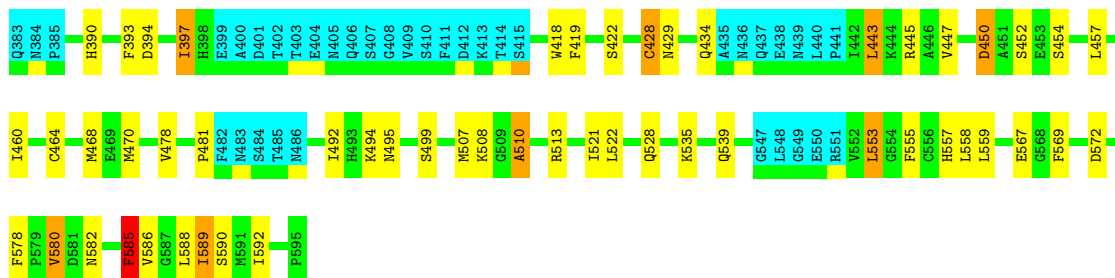
Chain A: 58% 22% 17%



4.2.16 Score per residue for model 16

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

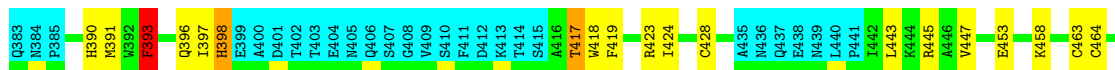
Chain A: 58% 21% 17%

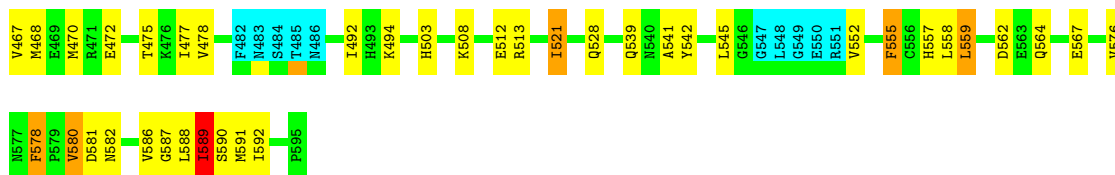


4.2.17 Score per residue for model 17

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

Chain A: 55% 23% 17%





4.2.18 Score per residue for model 18

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

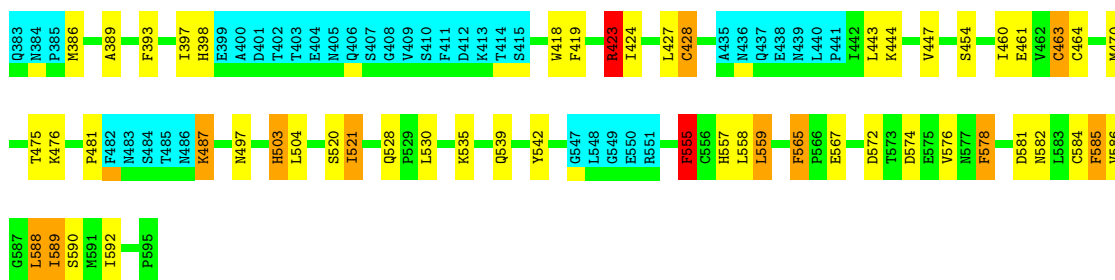
Chain A: 57% 20% 5% 17%



4.2.19 Score per residue for model 19

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

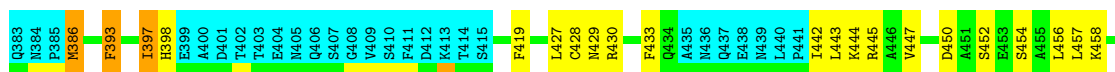
Chain A: 58% 19% 5% 17%

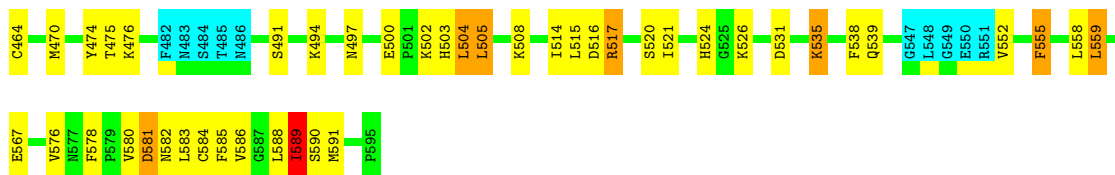


4.2.20 Score per residue for model 20

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

Chain A: 52% 25% 5% 17%





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

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	0.69±0.01	0±0/1423 (0.0± 0.0%)	1.55±0.03	10±3/1926 (0.5± 0.2%)
All	All	0.69	0/28460 (0.0%)	1.55	196/38520 (0.5%)

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	CA-CB-CG	10.74	124.54	113.80	17	4
1	A	593	ASP	CA-CB-CG	8.27	120.87	112.60	8	3
1	A	578	PHE	CA-CB-CG	7.97	121.77	113.80	2	5
1	A	508	LYS	CA-C-N	7.61	131.40	120.91	1	1
1	A	508	LYS	C-N-CA	7.61	131.40	120.91	1	1
1	A	588	LEU	CB-CA-C	7.51	122.79	111.76	11	2
1	A	562	ASP	CA-C-N	7.48	130.62	120.44	10	6
1	A	562	ASP	C-N-CA	7.48	130.62	120.44	10	6
1	A	557	HIS	CA-CB-CG	7.43	121.23	113.80	16	7
1	A	390	HIS	CA-CB-CG	7.29	121.09	113.80	11	1
1	A	391	MET	CA-C-N	6.69	132.74	122.11	17	1
1	A	391	MET	C-N-CA	6.69	132.74	122.11	17	1
1	A	503	HIS	CB-CG-CD2	-6.69	122.51	131.20	1	10
1	A	585	PHE	CA-C-N	6.33	133.37	121.97	8	9
1	A	585	PHE	C-N-CA	6.33	133.37	121.97	8	9

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	544	GLU	CA-C-N	6.33	129.63	120.38	5	4
1	A	544	GLU	C-N-CA	6.33	129.63	120.38	5	4
1	A	397	ILE	CA-C-N	6.27	133.51	121.54	9	1
1	A	397	ILE	C-N-CA	6.27	133.51	121.54	9	1
1	A	443	LEU	CA-C-N	6.27	133.51	121.54	12	5
1	A	443	LEU	C-N-CA	6.27	133.51	121.54	12	5
1	A	468	MET	CA-C-N	6.16	128.81	120.44	17	2
1	A	468	MET	C-N-CA	6.16	128.81	120.44	17	2
1	A	419	PHE	CA-CB-CG	6.15	119.95	113.80	3	8
1	A	462	VAL	CB-CA-C	6.15	117.69	110.93	5	1
1	A	423	ARG	CD-NE-CZ	6.12	132.97	124.40	19	1
1	A	397	ILE	CB-CA-C	6.06	121.22	111.29	5	8
1	A	575	GLU	CA-C-N	6.01	132.79	121.97	4	2
1	A	575	GLU	C-N-CA	6.01	132.79	121.97	4	2
1	A	466	SER	CA-C-N	6.01	128.63	121.84	2	1
1	A	466	SER	C-N-CA	6.01	128.63	121.84	2	1
1	A	497	ASN	CA-C-N	5.95	132.90	121.54	8	3
1	A	497	ASN	C-N-CA	5.95	132.90	121.54	8	3
1	A	452	SER	CA-C-N	5.94	128.52	120.38	11	1
1	A	452	SER	C-N-CA	5.94	128.52	120.38	11	1
1	A	516	ASP	CA-CB-CG	5.94	118.54	112.60	13	1
1	A	424	ILE	N-CA-C	-5.83	105.44	110.74	10	2
1	A	531	ASP	CA-CB-CG	5.82	118.42	112.60	7	2
1	A	531	ASP	CA-C-N	5.76	128.28	120.38	14	1
1	A	531	ASP	C-N-CA	5.76	128.28	120.38	14	1
1	A	569	PHE	CA-CB-CG	5.70	119.50	113.80	16	4
1	A	541	ALA	CA-C-N	5.70	128.19	120.38	17	1
1	A	541	ALA	C-N-CA	5.70	128.19	120.38	17	1
1	A	565	PHE	CA-CB-CG	-5.68	108.12	113.80	19	1
1	A	398	HIS	CA-CB-CG	5.65	119.45	113.80	8	2
1	A	395	ASN	OD1-CG-ND2	-5.64	116.96	122.60	18	1
1	A	389	ALA	CA-C-N	5.58	132.19	121.54	2	1
1	A	389	ALA	C-N-CA	5.58	132.19	121.54	2	1
1	A	423	ARG	CA-C-N	5.57	127.68	120.88	1	1
1	A	423	ARG	C-N-CA	5.57	127.68	120.88	1	1
1	A	572	ASP	CA-CB-CG	-5.57	107.03	112.60	10	2
1	A	463	CYS	CA-C-N	5.55	132.13	121.54	10	3
1	A	463	CYS	C-N-CA	5.55	132.13	121.54	10	3
1	A	543	LEU	CA-C-N	5.54	128.50	120.79	14	2
1	A	543	LEU	C-N-CA	5.54	128.50	120.79	14	2
1	A	591	MET	CA-C-N	5.54	128.20	122.27	17	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	591	MET	C-N-CA	5.54	128.20	122.27	17	1
1	A	526	LYS	CA-C-N	5.49	130.98	121.64	8	1
1	A	526	LYS	C-N-CA	5.49	130.98	121.64	8	1
1	A	447	VAL	CA-CB-CG1	5.48	119.72	110.40	12	1
1	A	494	LYS	CA-C-N	5.46	128.85	121.20	11	1
1	A	494	LYS	C-N-CA	5.46	128.85	121.20	11	1
1	A	532	GLU	CA-C-N	5.35	127.45	120.28	1	1
1	A	532	GLU	C-N-CA	5.35	127.45	120.28	1	1
1	A	394	ASP	CA-CB-CG	5.34	117.94	112.60	14	1
1	A	424	ILE	CA-C-N	5.32	127.67	120.38	2	2
1	A	424	ILE	C-N-CA	5.32	127.67	120.38	2	2
1	A	454	SER	CA-C-N	5.30	128.16	120.79	1	1
1	A	454	SER	C-N-CA	5.30	128.16	120.79	1	1
1	A	472	GLU	CA-C-N	5.30	128.15	120.79	2	1
1	A	472	GLU	C-N-CA	5.30	128.15	120.79	2	1
1	A	521	ILE	CB-CA-C	5.28	118.57	110.55	17	1
1	A	498	ALA	CA-C-N	5.27	131.61	121.54	3	1
1	A	498	ALA	C-N-CA	5.27	131.61	121.54	3	1
1	A	561	PRO	CA-C-N	5.22	129.03	120.63	6	2
1	A	561	PRO	C-N-CA	5.22	129.03	120.63	6	2
1	A	460	ILE	N-CA-C	-5.19	106.60	111.48	15	1
1	A	506	VAL	CB-CA-C	5.17	116.89	110.73	18	1
1	A	398	HIS	CB-CG-CD2	-5.12	124.55	131.20	2	2
1	A	470	MET	CA-C-N	5.11	127.38	120.38	11	1
1	A	470	MET	C-N-CA	5.11	127.38	120.38	11	1
1	A	574	ASP	N-CA-C	-5.11	104.76	111.96	13	1
1	A	540	ASN	CA-CB-CG	5.11	117.70	112.60	11	1
1	A	585	PHE	CA-CB-CG	5.10	118.90	113.80	19	2
1	A	476	LYS	CB-CA-C	5.06	119.50	112.11	9	1
1	A	450	ASP	CA-CB-CG	5.06	117.66	112.60	16	1
1	A	546	GLY	CA-C-N	5.05	131.31	121.41	7	1
1	A	546	GLY	C-N-CA	5.05	131.31	121.41	7	1
1	A	589	ILE	CB-CA-C	5.04	119.56	111.29	1	1
1	A	581	ASP	CA-CB-CG	5.03	117.62	112.60	20	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

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

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	1391	1384	1384	6±2
All	All	27820	27680	27680	121

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:386:MET:HE1	1:A:592:ILE:O	0.57	2.00	19	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:515:LEU:HD13	1:A:585:PHE:CE2	0.52	2.39	7	3
1:A:478:VAL:CG2	1:A:492:ILE:HD12	0.52	2.35	13	7
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:397:ILE:HG23	0.48	2.44	14	1
1:A:390:HIS:CD2	1:A:391:MET:H	0.48	2.26	14	1
1:A:423:ARG:NH2	1:A:427:LEU:HD13	0.48	2.23	19	1
1:A:505:LEU:HD23	1:A:505:LEU:C	0.48	2.33	1	6
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:CD1	1:A:555:PHE:N	0.47	2.81	19	1
1:A:552:VAL:HG22	1:A:590:SER:OG	0.47	2.09	8	1
1:A:395:ASN:ND2	1:A:534:LEU:HD22	0.47	2.25	10	2
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
1:A:578:PHE:CZ	1:A:580:VAL:CG1	0.44	3.01	10	1
1:A:530:LEU:HA	1:A:534:LEU:HD12	0.44	1.89	12	1
1:A:423:ARG:NE	1:A:427:LEU:HD13	0.44	2.28	19	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:545:LEU:HD13	1:A:590:SER:HB3	0.43	1.90	1	1
1:A:490:LEU:HD12	1:A:490:LEU:C	0.43	2.38	9	3
1:A:390:HIS:CE1	1:A:397:ILE:HG23	0.43	2.48	11	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:589:ILE:HB	1:A:591:MET:HE1	0.42	1.92	20	1
1:A:443:LEU:HD23	1:A:444:LYS:CA	0.41	2.45	12	1
1:A:433:PHE:CZ	1:A:442:ILE:HD11	0.41	2.50	20	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:588:LEU:C	1:A:588:LEU:HD13	0.41	2.41	5	1
1:A:521:ILE:HG21	1:A:534:LEU:HD13	0.40	1.92	1	1
1:A:423:ARG:HH21	1:A:557:HIS:CE1	0.40	2.34	17	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	175/213 (82%)	127±5 (73±3%)	32±6 (18±3%)	15±2 (9±1%)	1	12
All	All	3500/4260 (82%)	2549 (73%)	645 (18%)	306 (9%)	1	12

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	393	PHE	20
1	A	555	PHE	20
1	A	586	VAL	20
1	A	589	ILE	20
1	A	590	SER	20
1	A	397	ILE	19
1	A	559	LEU	16
1	A	444	LYS	15

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Mol	Chain	Res	Type	Models (Total)
1	A	464	CYS	13
1	A	581	ASP	12
1	A	502	LYS	10
1	A	481	PRO	9
1	A	580	VAL	9
1	A	572	ASP	9
1	A	428	CYS	8
1	A	396	GLN	7
1	A	487	LYS	6
1	A	386	MET	6
1	A	552	VAL	6
1	A	498	ALA	6
1	A	395	ASN	5
1	A	576	VAL	4
1	A	389	ALA	4
1	A	499	SER	4
1	A	445	ARG	4
1	A	477	ILE	4
1	A	510	ALA	4
1	A	500	GLU	3
1	A	466	SER	2
1	A	390	HIS	2
1	A	447	VAL	2
1	A	398	HIS	2
1	A	459	CYS	1
1	A	388	VAL	1
1	A	442	ILE	1
1	A	387	THR	1
1	A	450	ASP	1
1	A	503	HIS	1
1	A	546	GLY	1
1	A	496	PRO	1
1	A	524	HIS	1
1	A	443	LEU	1
1	A	452	SER	1
1	A	463	CYS	1
1	A	553	LEU	1
1	A	460	ILE	1
1	A	497	ASN	1

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	154/186 (83%)	123±4 (80±2%)	31±4 (20±2%)	3	32
All	All	3080/3720 (83%)	2453 (80%)	627 (20%)	3	32

All 103 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	443	LEU	20
1	A	447	VAL	20
1	A	521	ILE	20
1	A	558	LEU	20
1	A	559	LEU	20
1	A	589	ILE	20
1	A	578	PHE	18
1	A	418	TRP	17
1	A	475	THR	17
1	A	576	VAL	17
1	A	535	LYS	14
1	A	592	ILE	14
1	A	567	GLU	14
1	A	445	ARG	13
1	A	539	GLN	13
1	A	528	GLN	13
1	A	457	LEU	12
1	A	505	LEU	12
1	A	476	LYS	12
1	A	507	MET	10
1	A	585	PHE	10
1	A	458	LYS	10
1	A	424	ILE	10
1	A	588	LEU	9
1	A	454	SER	8
1	A	508	LYS	8
1	A	584	CYS	8
1	A	591	MET	7
1	A	520	SER	7

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Mol	Chain	Res	Type	Models (Total)
1	A	398	HIS	7
1	A	574	ASP	6
1	A	494	LYS	6
1	A	386	MET	6
1	A	453	GLU	6
1	A	450	ASP	6
1	A	487	LYS	6
1	A	580	VAL	6
1	A	582	ASN	5
1	A	390	HIS	5
1	A	461	GLU	5
1	A	545	LEU	5
1	A	572	ASP	5
1	A	394	ASP	5
1	A	513	ARG	5
1	A	444	LYS	5
1	A	526	LYS	5
1	A	470	MET	5
1	A	422	SER	5
1	A	463	CYS	4
1	A	472	GLU	4
1	A	500	GLU	4
1	A	512	GLU	4
1	A	516	ASP	4
1	A	423	ARG	4
1	A	532	GLU	4
1	A	417	THR	4
1	A	428	CYS	4
1	A	504	LEU	4
1	A	452	SER	4
1	A	429	ASN	3
1	A	434	GLN	3
1	A	466	SER	3
1	A	490	LEU	3
1	A	533	GLU	3
1	A	522	LEU	3
1	A	581	ASP	3
1	A	583	LEU	3
1	A	395	ASN	3
1	A	456	LEU	3
1	A	468	MET	3
1	A	527	GLU	3

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Mol	Chain	Res	Type	Models (Total)
1	A	497	ASN	3
1	A	467	VAL	3
1	A	495	ASN	3
1	A	570	GLN	2
1	A	491	SER	2
1	A	387	THR	2
1	A	471	ARG	2
1	A	469	GLU	2
1	A	538	PHE	2
1	A	519	SER	2
1	A	555	PHE	2
1	A	564	GLN	2
1	A	503	HIS	2
1	A	462	VAL	2
1	A	524	HIS	2
1	A	464	CYS	1
1	A	536	ASP	1
1	A	563	GLU	1
1	A	489	GLN	1
1	A	534	LEU	1
1	A	562	ASP	1
1	A	593	ASP	1
1	A	569	PHE	1
1	A	396	GLN	1
1	A	460	ILE	1
1	A	553	LEU	1
1	A	393	PHE	1
1	A	459	CYS	1
1	A	586	VAL	1
1	A	557	HIS	1
1	A	517	ARG	1
1	A	531	ASP	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