Full wwPDB NMR Structure Validation Report (i)

May 28, 2020 – 07:43 pm BST

PDB ID	:	1HHN
Title	:	Calreticulin P-domain
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Deposited on	:	2000-12-22

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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

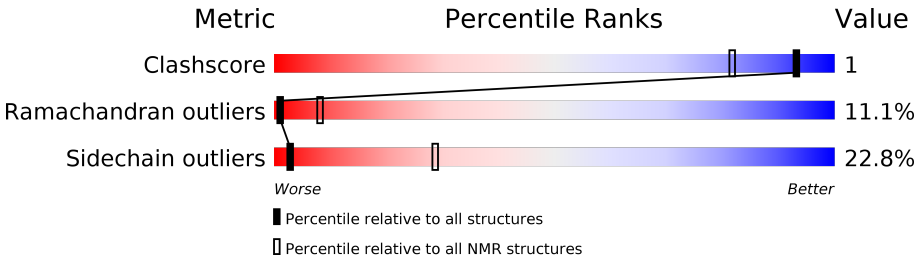
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	101	59% 19% • 20%

2 Ensemble composition and analysis

This entry contains 20 models. Model 18 is the overall representative, medoid model (most similar to other models). The authors have identified model 4 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:188-A:208, A:262-A:288 (48)	0.83	18
2	A:221-A:253 (33)	0.29	15

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1595 atoms, of which 754 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called CALRETICULIN.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	101	1595	528	754	135	177	1	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	188	SER	PRO	cloning artifact	UNP P18418

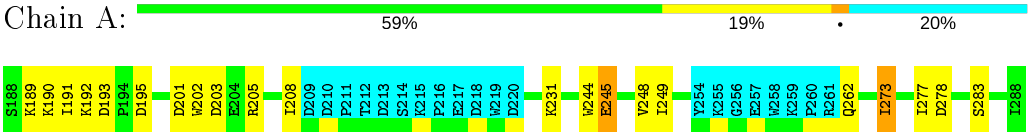
4 Residue-property plots (i)

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: CALRETICULIN

Chain A:



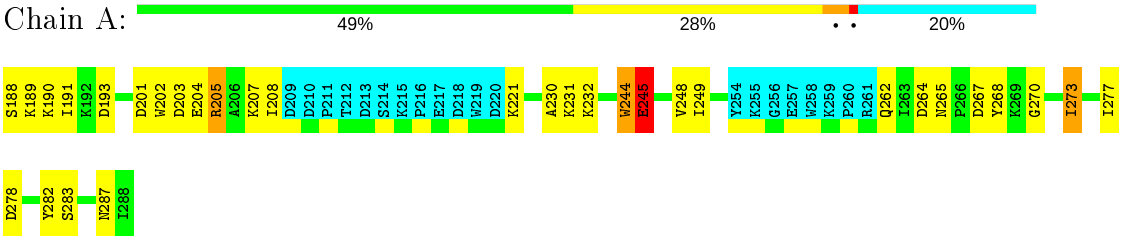
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: CALRETICULIN

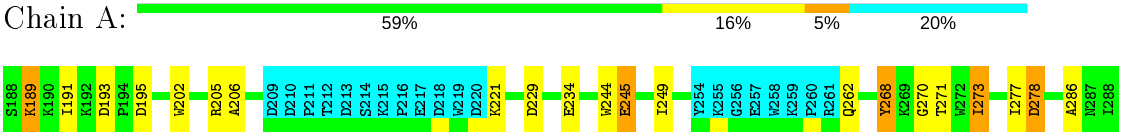
Chain A:



4.2.2 Score per residue for model 2

• Molecule 1: CALRETICULIN

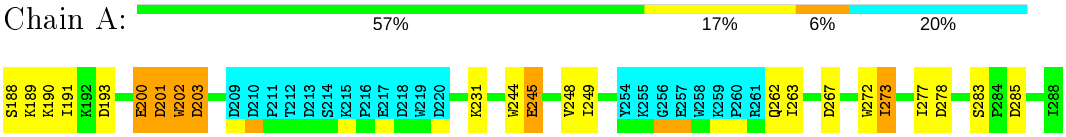
Chain A:



4.2.3 Score per residue for model 3

- Molecule 1: CALRETICULIN

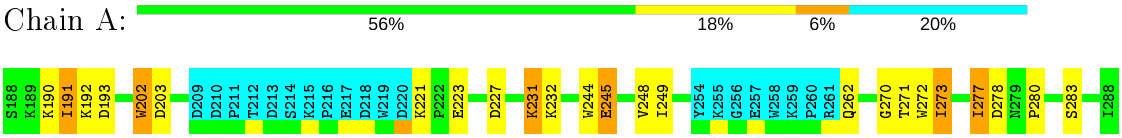
Chain A:



4.2.4 Score per residue for model 4

- Molecule 1: CALRETICULIN

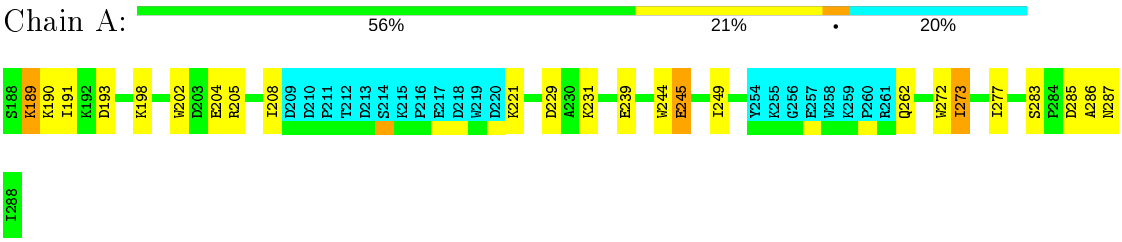
Chain A:



4.2.5 Score per residue for model 5

- Molecule 1: CALRETICULIN

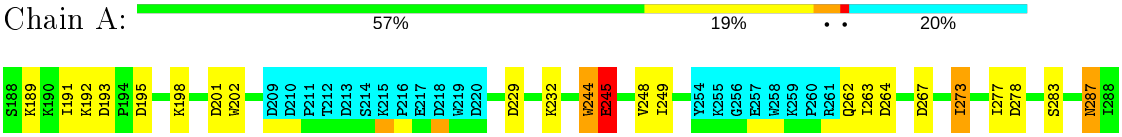
Chain A:



4.2.6 Score per residue for model 6

- Molecule 1: CALRETICULIN

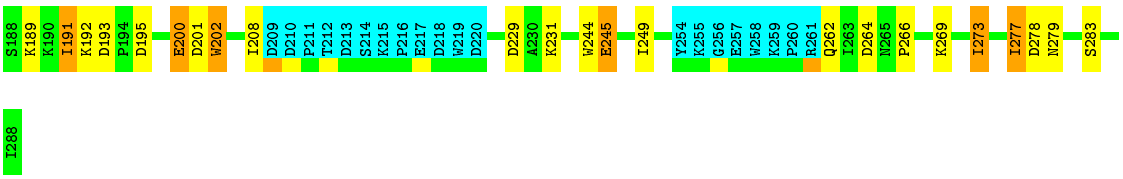
Chain A:



4.2.7 Score per residue for model 7

- Molecule 1: CALRETICULIN

Chain A:



4.2.8 Score per residue for model 8

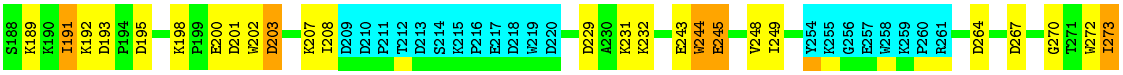
- Molecule 1: CALRETICULIN

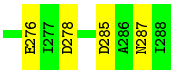
Chain A:

4.2.9 Score per residue for model 9

- Molecule 1: CALRETICULIN

Chain A:





4.2.10 Score per residue for model 10

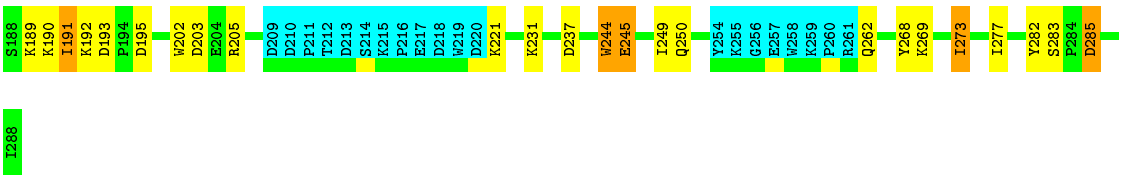
- Molecule 1: CALRETICULIN

Chain A:

4.2.11 Score per residue for model 11

- Molecule 1: CALRETICULIN

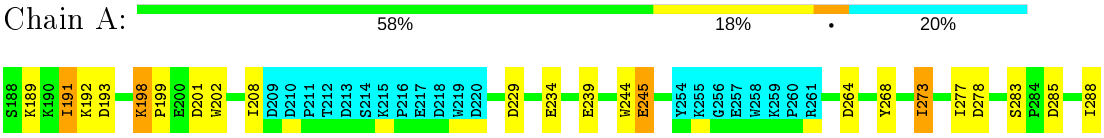
Chain A:



4.2.12 Score per residue for model 12

- Molecule 1: CALRETICULIN

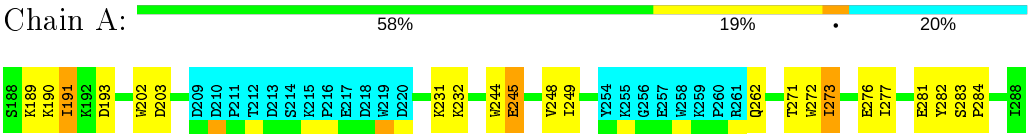
Chain A:



4.2.13 Score per residue for model 13

- Molecule 1: CALRETICULIN

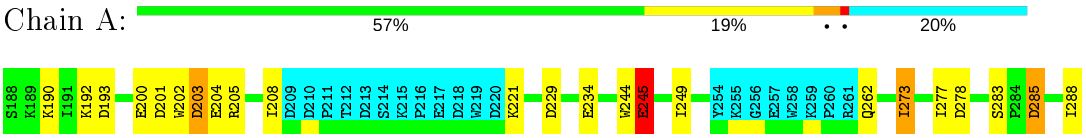
Chain A:



4.2.14 Score per residue for model 14

- Molecule 1: CALRETICULIN

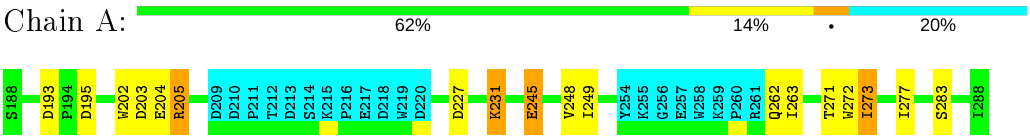
Chain A:



4.2.15 Score per residue for model 15

- Molecule 1: CALRETICULIN

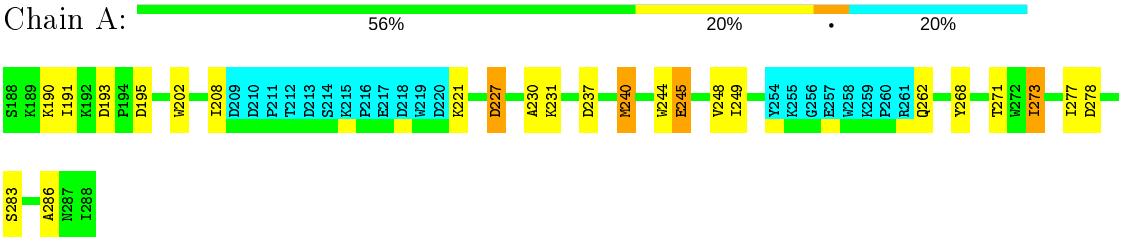
Chain A:



4.2.16 Score per residue for model 16

• Molecule 1: CALRETICULIN

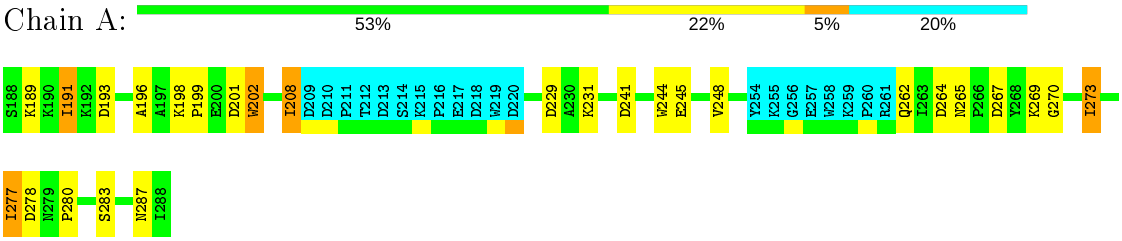
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: CALRETICULIN

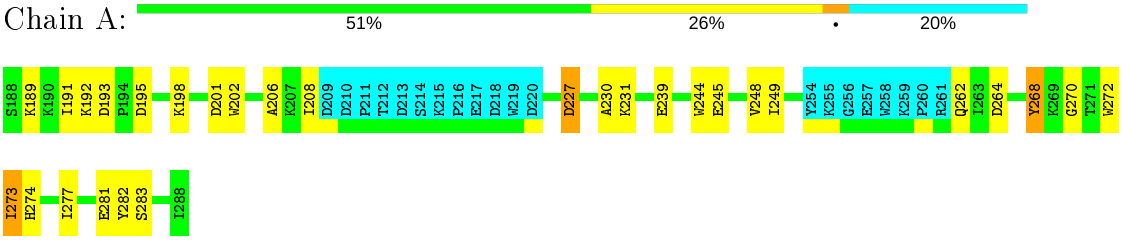
Chain A:



4.2.18 Score per residue for model 18 (medoid)

• Molecule 1: CALRETICULIN

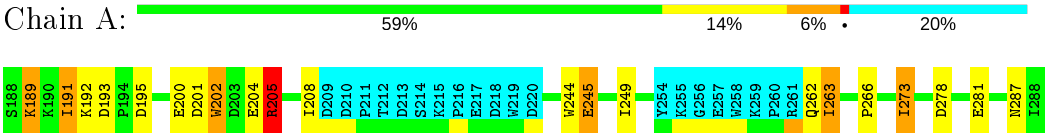
Chain A:



4.2.19 Score per residue for model 19

• Molecule 1: CALRETICULIN

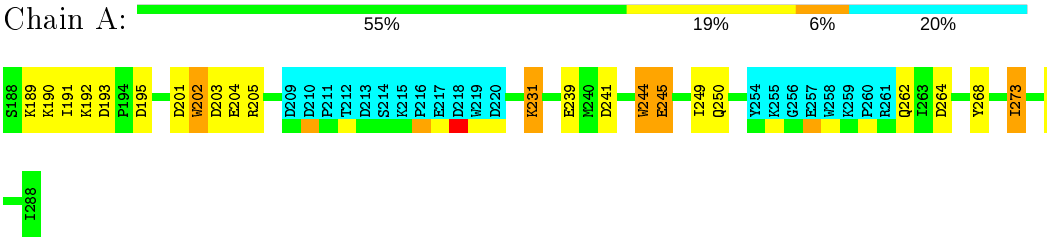
Chain A:



4.2.20 Score per residue for model 20

- Molecule 1: CALRETICULIN

Chain A:



5 Refinement protocol and experimental data overview

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

Of the ? calculated structures, 20 were deposited, based on the following criterion: *?*.

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

Software name	Classification	Version
OPALP	refinement	
DYANA	structure solution	

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

COVALENT-GEOMETRY INFOmissingINFO

5.1 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	667	605	604	2±1
All	All	13340	12100	12080	34

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 1.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:227:ASP:HB2	1:A:230:ALA:HB2	0.57	1.77	16	2
1:A:191:ILE:HD13	1:A:192:LYS:H	0.54	1.62	11	4
1:A:208:ILE:HD12	1:A:265:ASN:HB2	0.54	1.78	17	1
1:A:189:LYS:HE2	1:A:282:TYR:CD2	0.53	2.37	1	1
1:A:231:LYS:HE3	1:A:231:LYS:H	0.48	1.68	20	2
1:A:244:TRP:CG	1:A:245:GLU:N	0.48	2.82	6	6
1:A:189:LYS:HE3	1:A:282:TYR:CD2	0.47	2.44	11	1
1:A:206:ALA:HB2	1:A:268:TYR:CE2	0.47	2.45	2	1
1:A:206:ALA:HA	1:A:268:TYR:CG	0.46	2.45	10	2
1:A:231:LYS:N	1:A:231:LYS:HE3	0.45	2.25	4	1
1:A:232:LYS:HB3	1:A:244:TRP:CD2	0.45	2.46	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:277:ILE:HD11	1:A:280:PRO:HD3	0.44	1.90	4	2
1:A:202:TRP:CG	1:A:202:TRP:O	0.43	2.71	4	1
1:A:198:LYS:HE3	1:A:199:PRO:O	0.43	2.14	12	1
1:A:244:TRP:CD1	1:A:245:GLU:HG3	0.42	2.49	2	1
1:A:283:SER:H	1:A:288:ILE:HD12	0.42	1.73	10	1
1:A:231:LYS:HE2	1:A:231:LYS:N	0.42	2.29	18	1
1:A:200:GLU:O	1:A:201:ASP:CB	0.41	2.69	8	1
1:A:234:GLU:H	1:A:234:GLU:CD	0.41	2.18	12	1
1:A:277:ILE:HD12	1:A:278:ASP:C	0.41	2.36	7	1
1:A:202:TRP:CD1	1:A:204:GLU:HB2	0.41	2.51	8	1
1:A:231:LYS:H	1:A:231:LYS:CE	0.40	2.29	20	1

5.2 Torsion angles (i)

5.2.1 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	79/101 (78%)	56±2 (71±3%)	14±3 (17±4%)	9±2 (11±2%)	1	8
All	All	1580/2020 (78%)	1129 (71%)	275 (17%)	176 (11%)	1	8

All 29 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	273	ILE	20
1	A	245	GLU	20
1	A	244	TRP	17
1	A	283	SER	16
1	A	201	ASP	11
1	A	190	LYS	10
1	A	272	TRP	8
1	A	189	LYS	7
1	A	270	GLY	7
1	A	203	ASP	6
1	A	205	ARG	6

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Mol	Chain	Res	Type	Models (Total)
1	A	278	ASP	6
1	A	202	TRP	5
1	A	287	ASN	5
1	A	285	ASP	5
1	A	200	GLU	4
1	A	191	ILE	4
1	A	286	ALA	3
1	A	267	ASP	3
1	A	196	ALA	2
1	A	204	GLU	2
1	A	276	GLU	2
1	A	263	ILE	1
1	A	230	ALA	1
1	A	266	PRO	1
1	A	279	ASN	1
1	A	271	THR	1
1	A	284	PRO	1
1	A	199	PRO	1

5.2.2 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	74/93 (80%)	57±2 (77±3%)	17±2 (23±3%)	3	29
All	All	1480/1860 (80%)	1142 (77%)	338 (23%)	3	29

All 50 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	273	ILE	20
1	A	202	TRP	20
1	A	193	ASP	19
1	A	277	ILE	18
1	A	262	GLN	18
1	A	191	ILE	17
1	A	249	ILE	17

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Mol	Chain	Res	Type	Models (Total)
1	A	245	GLU	14
1	A	231	LYS	12
1	A	208	ILE	12
1	A	195	ASP	11
1	A	248	VAL	11
1	A	189	LYS	10
1	A	278	ASP	10
1	A	229	ASP	9
1	A	192	LYS	8
1	A	203	ASP	8
1	A	264	ASP	8
1	A	221	LYS	7
1	A	198	LYS	6
1	A	227	ASP	5
1	A	239	GLU	5
1	A	268	TYR	5
1	A	232	LYS	4
1	A	263	ILE	4
1	A	287	ASN	4
1	A	204	GLU	4
1	A	205	ARG	4
1	A	271	THR	4
1	A	201	ASP	4
1	A	285	ASP	4
1	A	269	LYS	3
1	A	200	GLU	3
1	A	281	GLU	3
1	A	267	ASP	3
1	A	241	ASP	2
1	A	288	ILE	2
1	A	282	TYR	2
1	A	188	SER	2
1	A	250	GLN	2
1	A	234	GLU	2
1	A	207	LYS	2
1	A	237	ASP	2
1	A	223	GLU	2
1	A	265	ASN	1
1	A	274	HIS	1
1	A	283	SER	1
1	A	243	GLU	1
1	A	190	LYS	1

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Mol	Chain	Res	Type	Models (Total)
1	A	240	MET	1

5.2.3 RNA

There are no RNA molecules in this entry.

5.3 Non-standard residues in protein, DNA, RNA chains

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

5.4 Carbohydrates

There are no carbohydrates in this entry.

5.5 Ligand geometry

There are no ligands in this entry.

5.6 Other polymers

There are no such molecules in this entry.

5.7 Polymer linkage issues

There are no chain breaks in this entry.

6 Chemical shift validation

No chemical shift data were provided