



Full wwPDB NMR Structure Validation Report ⓘ

Mar 25, 2026 – 02:41 AM UTC

PDB ID : 1HHN / pdb_00001hhn
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 ⓘ 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

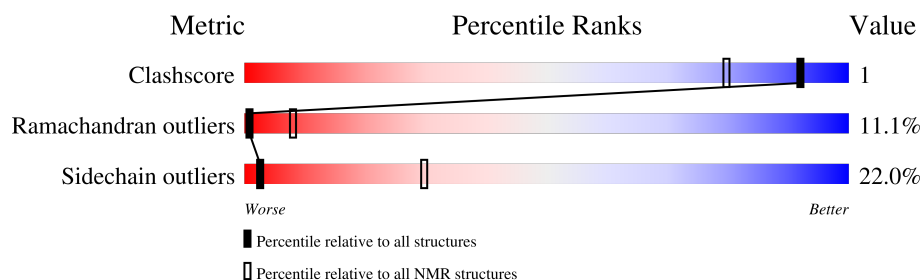
1 Overall quality at a glance

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	101	

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)	1.43	18
2	A:221-A:253 (33)	0.50	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 5 clusters and 5 single-model clusters were found.

Cluster number	Models
1	2, 11, 14, 20
2	5, 17, 18
3	1, 12, 15
4	6, 7, 16
5	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
1	A	101	Total	C	H	N	O	S		0
			1595	528	754	135	177	1		

There is a discrepancy between the modelled and reference sequences:

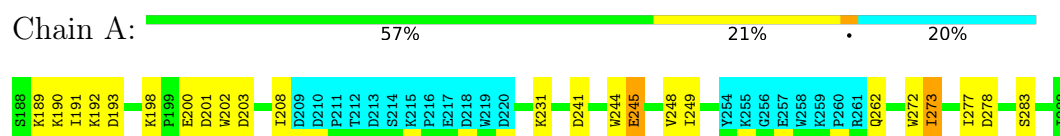
Chain	Residue	Modelled	Actual	Comment	Reference
A	188	SER	PRO	cloning artifact	UNP P18418

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, 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: CALRETICULIN

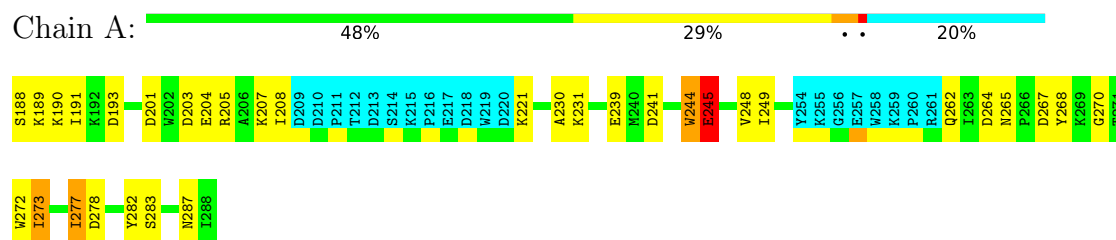


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

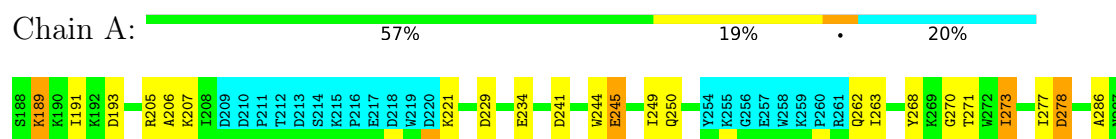
4.2.1 Score per residue for model 1

• Molecule 1: CALRETICULIN



4.2.2 Score per residue for model 2

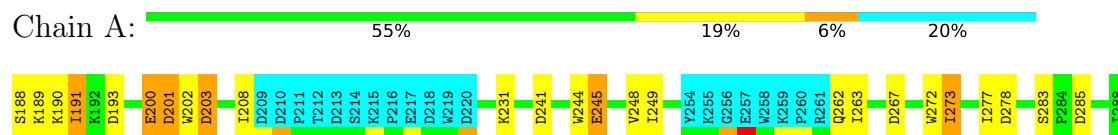
• Molecule 1: CALRETICULIN



I288

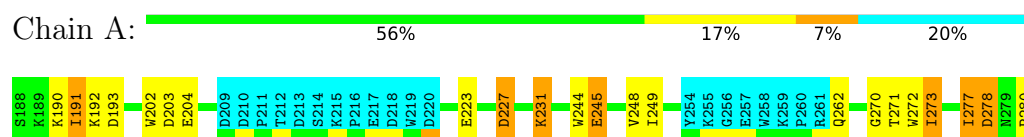
4.2.3 Score per residue for model 3

- Molecule 1: CALRETICULIN



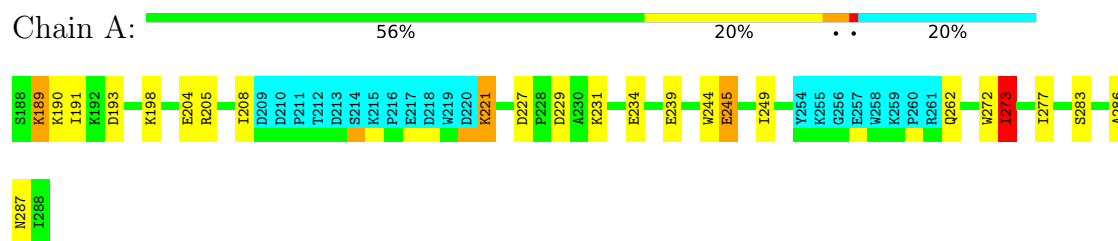
4.2.4 Score per residue for model 4

- Molecule 1: CALRETICULIN



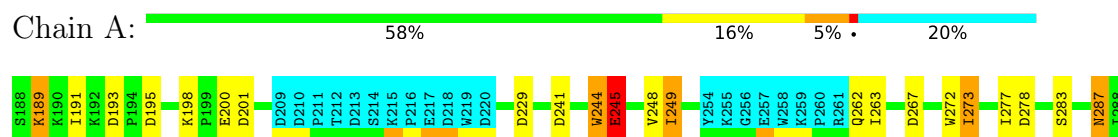
4.2.5 Score per residue for model 5

- Molecule 1: CALRETICULIN

W287
I288

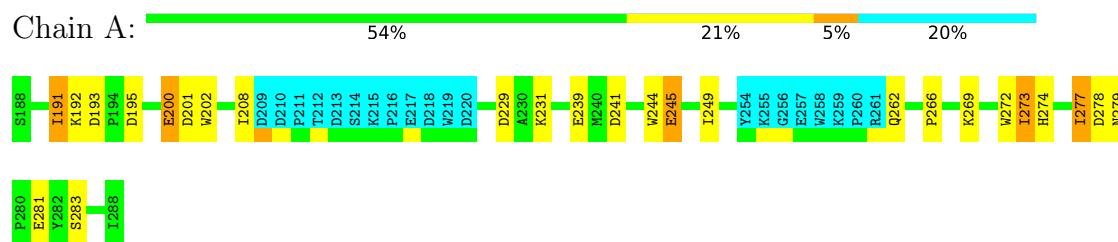
4.2.6 Score per residue for model 6

- Molecule 1: CALRETICULIN



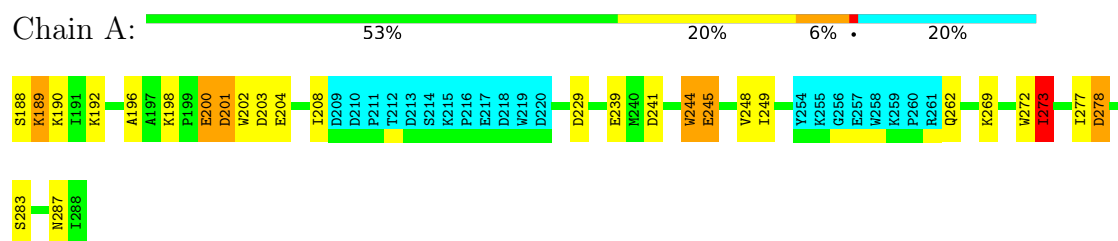
4.2.7 Score per residue for model 7

• Molecule 1: CALRETICULIN



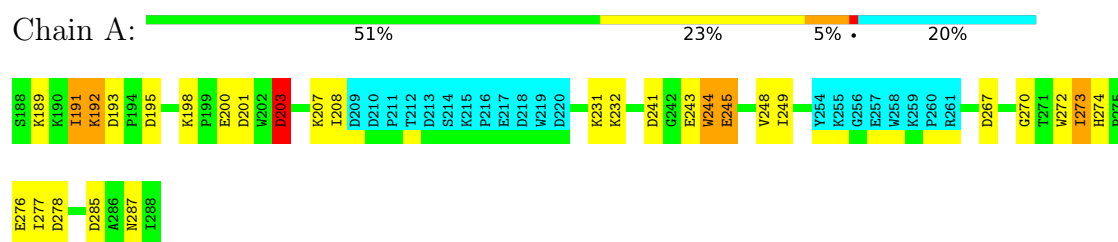
4.2.8 Score per residue for model 8

• Molecule 1: CALRETICULIN



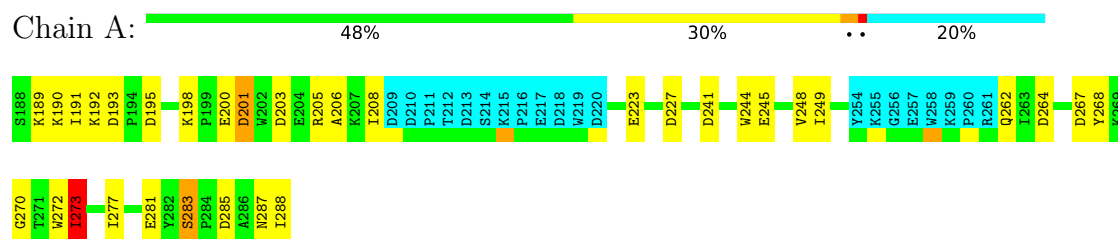
4.2.9 Score per residue for model 9

• Molecule 1: CALRETICULIN



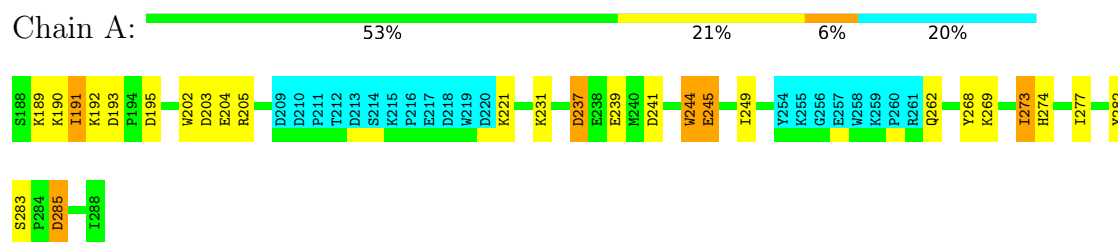
4.2.10 Score per residue for model 10

• Molecule 1: CALRETICULIN



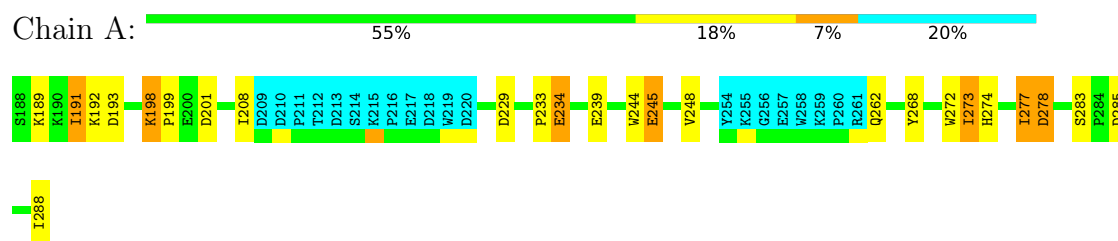
4.2.11 Score per residue for model 11

- Molecule 1: CALRETICULIN



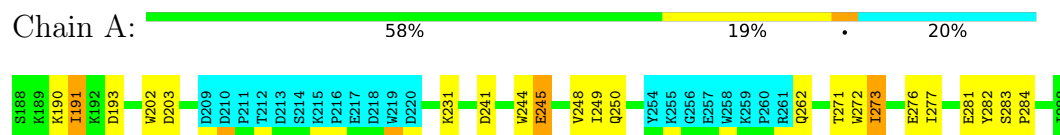
4.2.12 Score per residue for model 12

- Molecule 1: CALRETICULIN



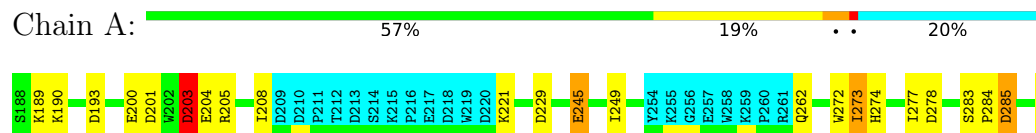
4.2.13 Score per residue for model 13

- Molecule 1: CALRETICULIN



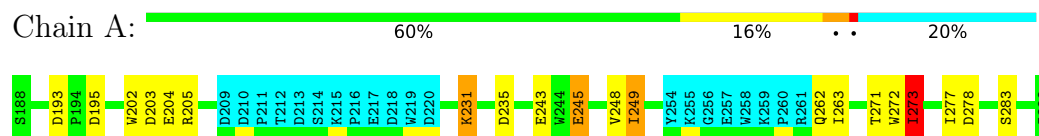
4.2.14 Score per residue for model 14

- Molecule 1: CALRETICULIN



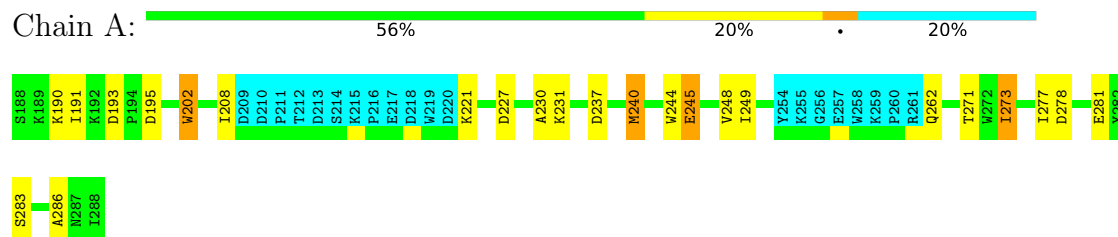
4.2.15 Score per residue for model 15

- Molecule 1: CALRETICULIN



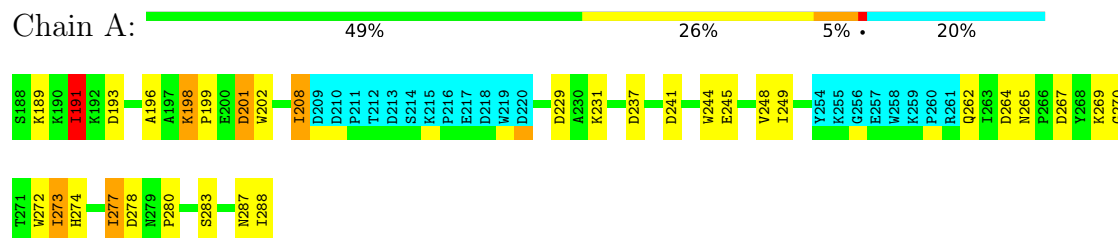
4.2.16 Score per residue for model 16

- Molecule 1: CALRETICULIN



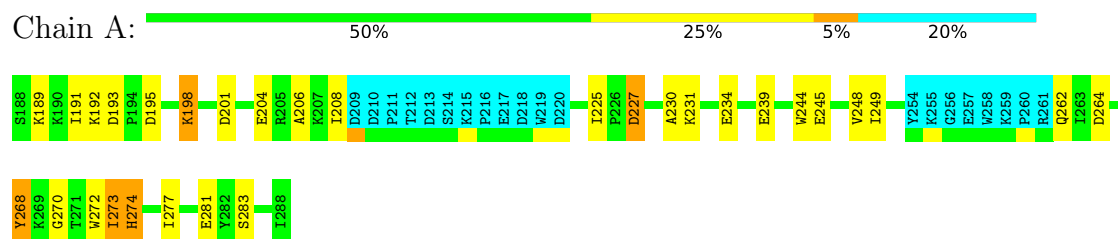
4.2.17 Score per residue for model 17

- Molecule 1: CALRETICULIN



4.2.18 Score per residue for model 18 (medoid)

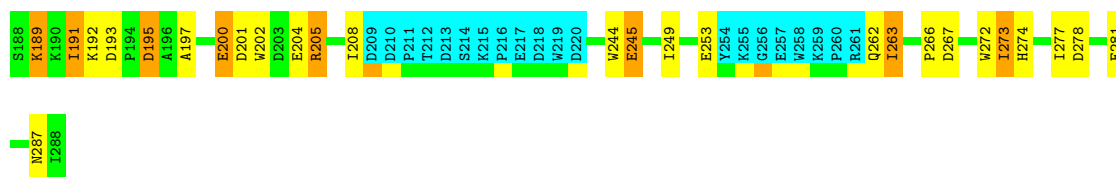
- Molecule 1: CALRETICULIN



4.2.19 Score per residue for model 19

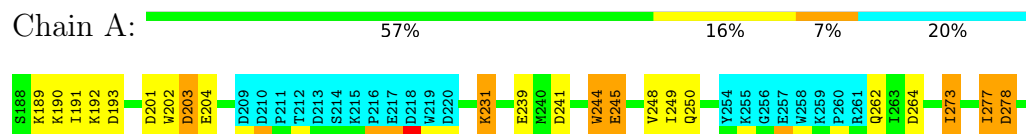
- Molecule 1: CALRETICULIN





4.2.20 Score per residue for model 20

- Molecule 1: CALRETICULIN



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.

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	0.70±0.02	0±0/691 (0.0± 0.0%)	1.54±0.06	4±2/946 (0.5± 0.3%)
All	All	0.70	0/13820 (0.0%)	1.54	89/18920 (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	0.3±0.6
All	All	0	7

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	227	ASP	CA-CB-CG	9.73	122.33	112.60	4	2
1	A	274	HIS	CB-CG-CD2	-8.01	120.78	131.20	19	8
1	A	278	ASP	CA-CB-CG	7.98	120.58	112.60	15	2
1	A	241	ASP	CA-CB-CG	-7.56	105.04	112.60	2	10
1	A	237	ASP	CA-CB-CG	7.14	119.74	112.60	11	2
1	A	201	ASP	CA-C-N	6.62	134.19	121.54	17	1
1	A	201	ASP	C-N-CA	6.62	134.19	121.54	17	1
1	A	272	TRP	CA-C-N	6.55	133.76	121.97	10	8
1	A	272	TRP	C-N-CA	6.55	133.76	121.97	10	8
1	A	274	HIS	CA-CB-CG	6.43	120.23	113.80	19	1
1	A	235	ASP	CA-CB-CG	6.29	118.89	112.60	15	1
1	A	200	GLU	CA-C-N	6.19	133.36	121.54	10	3
1	A	200	GLU	C-N-CA	6.19	133.36	121.54	10	3
1	A	204	GLU	CA-C-N	6.18	133.35	121.54	11	1
1	A	204	GLU	C-N-CA	6.18	133.35	121.54	11	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	249	ILE	CA-CB-CG1	5.78	120.23	110.40	6	2
1	A	273	ILE	CA-CB-CG2	5.75	120.28	110.50	10	4
1	A	203	ASP	CA-C-N	5.70	132.43	121.54	20	3
1	A	203	ASP	C-N-CA	5.70	132.43	121.54	20	3
1	A	198	LYS	CA-C-N	5.68	126.95	119.84	17	1
1	A	198	LYS	C-N-CA	5.68	126.95	119.84	17	1
1	A	248	VAL	CA-C-N	5.62	130.76	122.94	12	2
1	A	248	VAL	C-N-CA	5.62	130.76	122.94	12	2
1	A	277	ILE	CA-CB-CG1	5.58	119.88	110.40	20	1
1	A	198	LYS	CB-CA-C	5.53	116.67	108.87	18	1
1	A	227	ASP	N-CA-CB	5.49	118.59	109.98	4	1
1	A	221	LYS	CA-C-N	5.48	125.47	120.21	5	1
1	A	221	LYS	C-N-CA	5.48	125.47	120.21	5	1
1	A	240	MET	CA-CB-CG	5.47	125.04	114.10	16	1
1	A	267	ASP	CA-CB-CG	5.45	118.05	112.60	19	1
1	A	202	TRP	CB-CA-C	5.33	118.37	111.50	16	1
1	A	191	ILE	CA-C-N	5.24	128.20	120.82	17	1
1	A	191	ILE	C-N-CA	5.24	128.20	120.82	17	1
1	A	202	TRP	CA-C-N	5.23	131.52	121.54	11	1
1	A	202	TRP	C-N-CA	5.23	131.52	121.54	11	1
1	A	233	PRO	N-CA-CB	5.14	107.88	103.31	12	1
1	A	189	LYS	CB-CA-C	5.09	120.55	110.42	8	1
1	A	207	LYS	CA-C-N	5.05	128.87	121.80	2	1
1	A	207	LYS	C-N-CA	5.05	128.87	121.80	2	1
1	A	284	PRO	CA-C-N	5.02	131.12	121.54	14	1
1	A	284	PRO	C-N-CA	5.02	131.12	121.54	14	1
1	A	191	ILE	CB-CA-C	5.00	118.15	110.55	3	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	268	TYR	Sidechain	2
1	A	200	GLU	Peptide	1
1	A	266	PRO	Peptide	1
1	A	188	SER	Peptide	1
1	A	273	ILE	Peptide	1
1	A	205	ARG	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	667	605	604	2±1
All	All	13340	12100	12080	38

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	5
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:234:GLU:CD	1:A:234:GLU:H	0.46	2.18	12	1
1:A:277:ILE:HD12	1:A:278:ASP:C	0.45	2.36	7	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
1:A:277:ILE:HD12	1:A:277:ILE:C	0.44	2.38	12	1
1:A:277:ILE:HD11	1:A:280:PRO:HD3	0.44	1.90	4	2
1:A:202:TRP:O	1:A:202:TRP:CG	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:N	1:A:231:LYS:HE2	0.42	2.29	18	1
1:A:230:ALA:C	1:A:231:LYS:HE2	0.41	2.39	18	1
1:A:200:GLU:O	1:A:201:ASP:CB	0.41	2.69	8	1
1:A:195:ASP:C	1:A:197:ALA:H	0.41	2.23	19	1
1:A:277:ILE:C	1:A:277:ILE:HD12	0.41	2.41	1	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

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	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	245	GLU	20
1	A	273	ILE	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	270	GLY	7
1	A	189	LYS	7
1	A	205	ARG	6
1	A	278	ASP	6
1	A	203	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	267	ASP	3
1	A	286	ALA	3
1	A	196	ALA	2
1	A	276	GLU	2
1	A	204	GLU	2
1	A	230	ALA	1
1	A	271	THR	1
1	A	279	ASN	1
1	A	284	PRO	1
1	A	199	PRO	1

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Mol	Chain	Res	Type	Models (Total)
1	A	263	ILE	1
1	A	266	PRO	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	74/93 (80%)	58±2 (78±3%)	16±2 (22±3%)	2	30
All	All	1480/1860 (80%)	1154 (78%)	326 (22%)	2	30

All 51 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	277	ILE	20
1	A	193	ASP	19
1	A	249	ILE	19
1	A	262	GLN	19
1	A	191	ILE	17
1	A	208	ILE	13
1	A	245	GLU	13
1	A	231	LYS	12
1	A	248	VAL	12
1	A	189	LYS	10
1	A	278	ASP	10
1	A	195	ASP	9
1	A	203	ASP	8
1	A	239	GLU	8
1	A	229	ASP	8
1	A	198	LYS	8
1	A	192	LYS	7
1	A	204	GLU	6
1	A	221	LYS	6
1	A	281	GLU	6
1	A	264	ASP	5
1	A	263	ILE	5

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Mol	Chain	Res	Type	Models (Total)
1	A	287	ASN	4
1	A	234	GLU	4
1	A	201	ASP	4
1	A	271	THR	4
1	A	288	ILE	4
1	A	269	LYS	4
1	A	250	GLN	3
1	A	200	GLU	3
1	A	285	ASP	3
1	A	227	ASP	3
1	A	267	ASP	3
1	A	202	TRP	3
1	A	188	SER	2
1	A	207	LYS	2
1	A	268	TYR	2
1	A	205	ARG	2
1	A	223	GLU	2
1	A	243	GLU	2
1	A	237	ASP	2
1	A	241	ASP	2
1	A	265	ASN	1
1	A	190	LYS	1
1	A	283	SER	1
1	A	282	TYR	1
1	A	240	MET	1
1	A	225	ILE	1
1	A	274	HIS	1
1	A	253	GLU	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 oligosaccharides 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

No chemical shift data were provided