



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2022 – 11:42 AM EST

PDB ID : 2KFT  
Title : NMR Solution structure of the first PHD finger domain of human Autoimmune Regulator (AIRE) in complex with Histone H3(1-20Cys) Peptide  
Authors : Chakravarty, S.; Zeng, L.; Zhou, M.  
Deposited on : 2009-02-27

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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 : 2.27  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.27

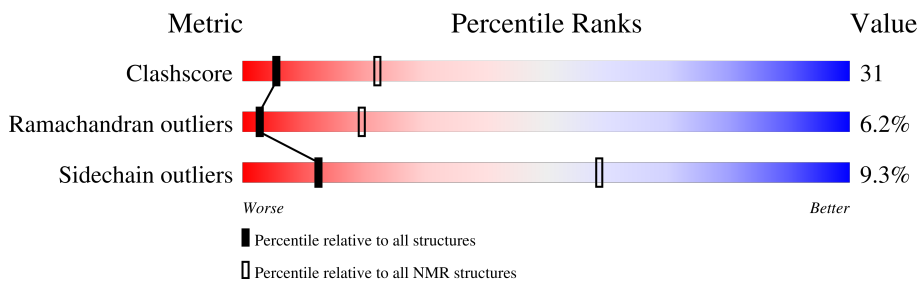
# 1 Overall quality at a glance

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  $\geq 3$ , 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	56	
2	B	21	

## 2 Ensemble composition and analysis i

This entry contains 20 models. Model 8 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:295-A:341, B:1-B:6 (53)	0.29	8

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 2 single-model clusters were found.

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

### 3 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 1141 atoms, of which 566 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Autoimmune regulator.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	56	801	248	387	75	83	8	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP O43918
A	-1	SER	-	expression tag	UNP O43918

- Molecule 2 is a protein called Histone H3.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	21	338	94	179	36	28	1	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

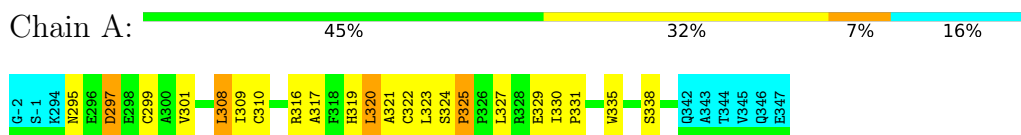
Mol	Chain	Residues	Atoms	
			Total	Zn
3	A	2	2	2

## 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: Autoimmune regulator



- Molecule 2: Histone H3

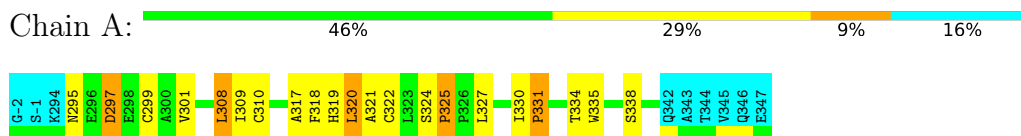


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

- Molecule 1: Autoimmune regulator

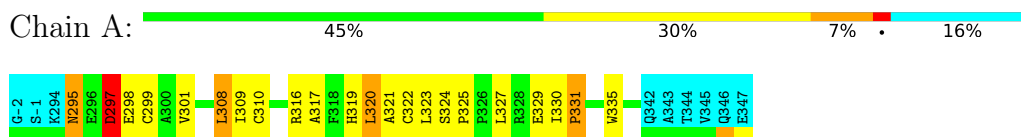


- Molecule 2: Histone H3



### 4.2.2 Score per residue for model 2

- Molecule 1: Autoimmune regulator

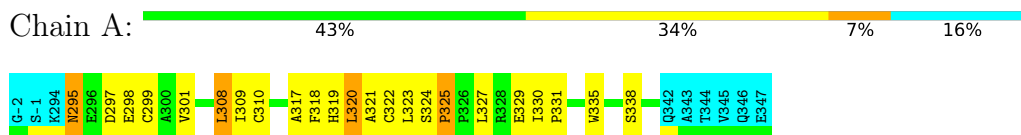


- Molecule 2: Histone H3



### 4.2.3 Score per residue for model 3

- Molecule 1: Autoimmune regulator

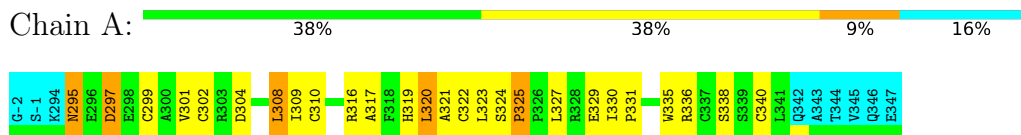


- Molecule 2: Histone H3



### 4.2.4 Score per residue for model 4

- Molecule 1: Autoimmune regulator

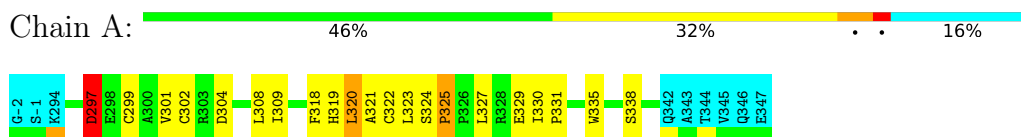


- Molecule 2: Histone H3



### 4.2.5 Score per residue for model 5

- Molecule 1: Autoimmune regulator

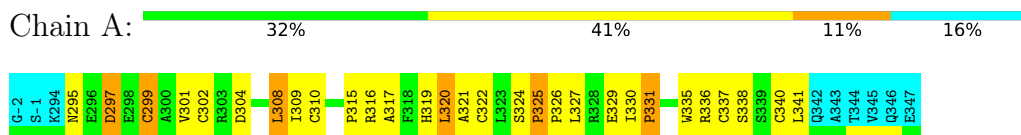


- Molecule 2: Histone H3



### 4.2.6 Score per residue for model 6

- Molecule 1: Autoimmune regulator

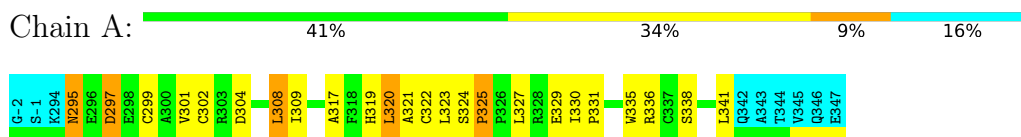


- Molecule 2: Histone H3



### 4.2.7 Score per residue for model 7

- Molecule 1: Autoimmune regulator

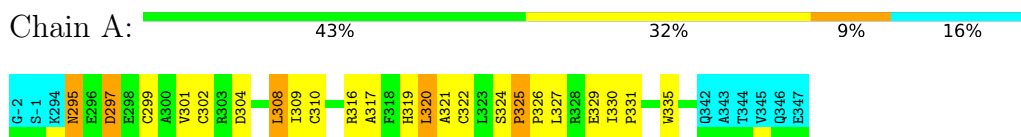


- Molecule 2: Histone H3



### 4.2.8 Score per residue for model 8 (medoid)

- Molecule 1: Autoimmune regulator

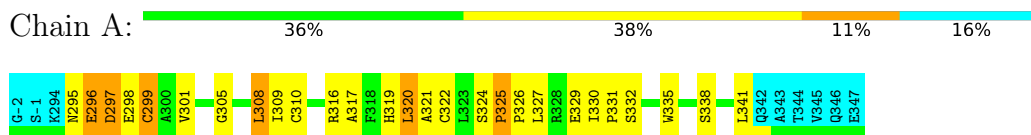


- Molecule 2: Histone H3



### 4.2.9 Score per residue for model 9

- Molecule 1: Autoimmune regulator

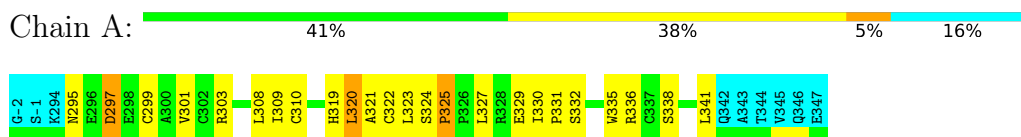


- Molecule 2: Histone H3



### 4.2.10 Score per residue for model 10

- Molecule 1: Autoimmune regulator



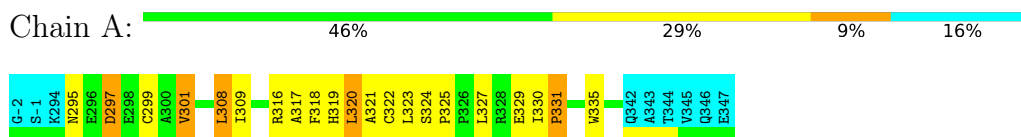
- Molecule 2: Histone H3





### 4.2.11 Score per residue for model 11

- Molecule 1: Autoimmune regulator

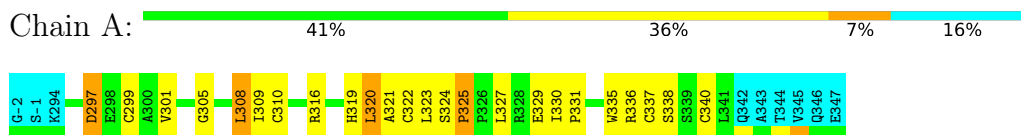


- Molecule 2: Histone H3



### 4.2.12 Score per residue for model 12

- Molecule 1: Autoimmune regulator

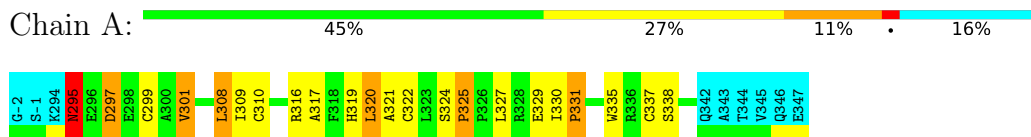


- Molecule 2: Histone H3



### 4.2.13 Score per residue for model 13

- Molecule 1: Autoimmune regulator

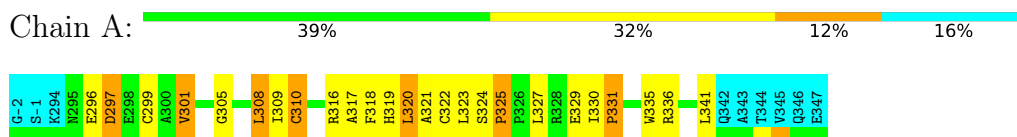


- Molecule 2: Histone H3



#### 4.2.14 Score per residue for model 14

- Molecule 1: Autoimmune regulator

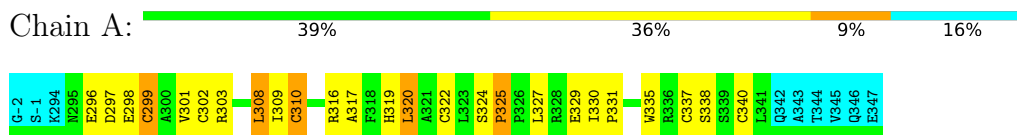


- Molecule 2: Histone H3



#### 4.2.15 Score per residue for model 15

- Molecule 1: Autoimmune regulator

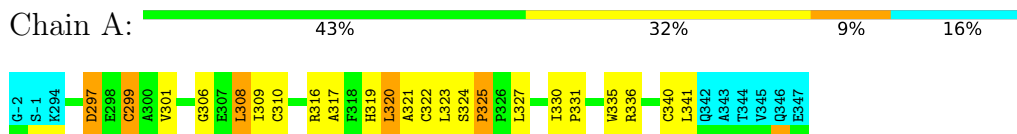


- Molecule 2: Histone H3



#### 4.2.16 Score per residue for model 16

- Molecule 1: Autoimmune regulator

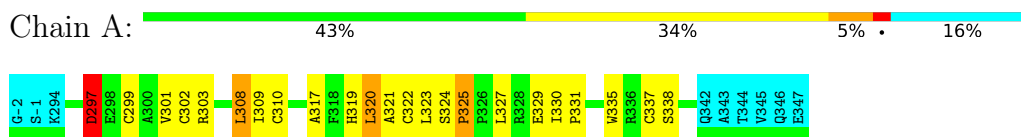


- Molecule 2: Histone H3



### 4.2.17 Score per residue for model 17

- Molecule 1: Autoimmune regulator

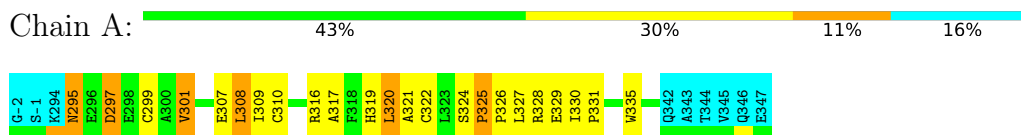


- Molecule 2: Histone H3



### 4.2.18 Score per residue for model 18

- Molecule 1: Autoimmune regulator

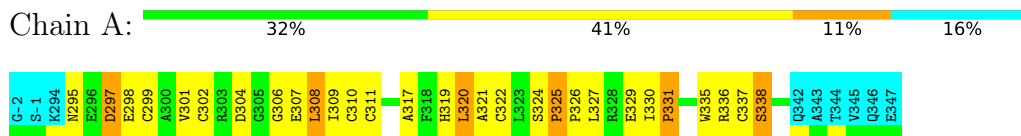


- Molecule 2: Histone H3



### 4.2.19 Score per residue for model 19

- Molecule 1: Autoimmune regulator

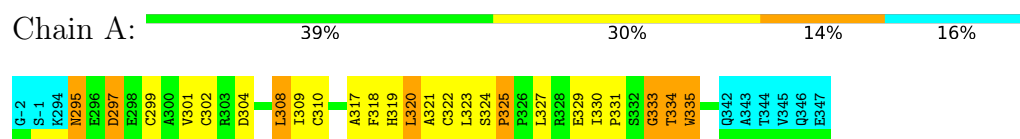


- Molecule 2: Histone H3



### 4.2.20 Score per residue for model 20

- Molecule 1: Autoimmune regulator



- Molecule 2: Histone H3



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 200 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
CNS	structure solution	1.0
CNS	refinement	1.0

No chemical shift data was provided.

## 6 Model quality i

### 6.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section:  
ZN

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

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	348	321	321	24±3
2	B	48	55	55	5±2
All	All	7960	7520	7520	479

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 31.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:330:ILE:HD12	2:B:3:THR:HG21	0.95	1.38	17	19
1:A:336:ARG:HB3	1:A:340:CYS:SG	0.74	2.22	12	1
1:A:308:LEU:HB2	1:A:317:ALA:HB1	0.71	1.62	1	17
1:A:331:PRO:HB2	2:B:1:ALA:HB2	0.70	1.64	2	8
1:A:299:CYS:SG	1:A:301:VAL:HG13	0.69	2.28	18	20
1:A:320:LEU:CD2	1:A:330:ILE:HD11	0.67	2.19	20	13
1:A:324:SER:HB3	1:A:325:PRO:HD3	0.62	1.71	15	10
1:A:324:SER:HB2	1:A:325:PRO:HD3	0.62	1.72	18	10
1:A:319:HIS:HB2	1:A:322:CYS:SG	0.62	2.35	1	20
1:A:331:PRO:HG2	1:A:335:TRP:CD1	0.61	2.29	18	20
1:A:297:ASP:HA	2:B:6:THR:HG21	0.61	1.73	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:296:GLU:HB3	1:A:308:LEU:HD12	0.61	1.73	15	1
1:A:309:ILE:HG13	2:B:3:THR:HG22	0.60	1.73	10	19
1:A:301:VAL:HG11	1:A:322:CYS:HB3	0.59	1.75	3	9
1:A:320:LEU:HD21	1:A:330:ILE:HD11	0.54	1.79	16	19
1:A:330:ILE:CD1	2:B:3:THR:HG21	0.54	2.28	13	16
1:A:305:GLY:O	1:A:319:HIS:NE2	0.54	2.40	12	2
1:A:337:CYS:O	1:A:340:CYS:SG	0.53	2.66	12	1
1:A:319:HIS:HB2	1:A:322:CYS:HB2	0.53	1.81	14	17
1:A:310:CYS:HB3	2:B:2:ARG:HB2	0.52	1.80	3	1
1:A:299:CYS:SG	1:A:301:VAL:HG22	0.52	2.44	11	4
1:A:320:LEU:HD23	1:A:320:LEU:N	0.51	2.20	18	18
1:A:309:ILE:CG1	2:B:3:THR:HG22	0.51	2.36	20	18
1:A:338:SER:HA	1:A:341:LEU:HD12	0.51	1.83	9	4
1:A:296:GLU:O	1:A:298:GLU:N	0.51	2.44	9	1
1:A:310:CYS:HA	1:A:316:ARG:O	0.50	2.04	16	11
1:A:336:ARG:HD3	1:A:340:CYS:HB3	0.49	1.84	4	3
1:A:309:ILE:HA	2:B:3:THR:HA	0.49	1.83	10	7
1:A:295:ASN:HD22	1:A:295:ASN:N	0.49	2.06	8	4
1:A:301:VAL:HG21	1:A:322:CYS:HB3	0.48	1.85	5	6
1:A:337:CYS:N	1:A:340:CYS:SG	0.48	2.86	12	1
1:A:308:LEU:CB	1:A:317:ALA:HB1	0.48	2.38	6	11
1:A:330:ILE:CG2	2:B:1:ALA:HB3	0.48	2.38	13	1
1:A:323:LEU:HB3	1:A:325:PRO:HD2	0.48	1.86	10	12
1:A:330:ILE:HG23	2:B:1:ALA:HB3	0.47	1.84	11	2
1:A:295:ASN:ND2	1:A:297:ASP:H	0.47	2.07	4	1
1:A:296:GLU:HG2	1:A:317:ALA:HB2	0.47	1.86	15	1
1:A:309:ILE:O	1:A:317:ALA:HA	0.46	2.11	1	2
1:A:301:VAL:CG1	1:A:322:CYS:HB3	0.46	2.41	15	9
1:A:320:LEU:HD22	1:A:327:LEU:HD12	0.46	1.87	16	8
1:A:309:ILE:HG23	1:A:309:ILE:O	0.46	2.11	11	4
2:B:2:ARG:N	2:B:2:ARG:HD2	0.45	2.26	1	1
1:A:301:VAL:HG21	1:A:322:CYS:SG	0.45	2.52	3	4
1:A:309:ILE:HD11	2:B:1:ALA:HB1	0.45	1.87	2	3
1:A:327:LEU:C	1:A:329:GLU:N	0.45	2.70	12	18
1:A:319:HIS:O	1:A:321:ALA:N	0.44	2.50	8	19
1:A:305:GLY:O	1:A:308:LEU:HD21	0.44	2.12	12	2
1:A:309:ILE:HG22	1:A:318:PHE:O	0.44	2.12	5	5
1:A:320:LEU:N	1:A:320:LEU:HD23	0.44	2.26	1	1
1:A:320:LEU:HD22	1:A:330:ILE:HD11	0.44	1.86	20	6
1:A:337:CYS:O	1:A:338:SER:C	0.44	2.56	13	5
1:A:319:HIS:HB2	1:A:322:CYS:CB	0.44	2.43	9	16

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:295:ASN:HD22	1:A:316:ARG:N	0.44	2.11	11	1
1:A:302:CYS:O	1:A:303:ARG:C	0.43	2.57	17	2
1:A:302:CYS:SG	1:A:304:ASP:HB2	0.43	2.53	6	7
1:A:299:CYS:HA	1:A:317:ALA:O	0.43	2.14	7	1
1:A:321:ALA:HA	1:A:326:PRO:HB3	0.43	1.91	18	5
1:A:295:ASN:ND2	1:A:310:CYS:HB3	0.43	2.29	10	1
1:A:295:ASN:ND2	1:A:317:ALA:HB2	0.43	2.29	7	1
1:A:295:ASN:ND2	1:A:311:CYS:N	0.43	2.67	19	1
1:A:301:VAL:CG2	1:A:322:CYS:SG	0.42	3.07	13	4
1:A:295:ASN:HD22	1:A:310:CYS:HB3	0.42	1.74	10	1
1:A:295:ASN:HB2	1:A:310:CYS:SG	0.42	2.54	18	1
1:A:309:ILE:CB	2:B:3:THR:HG22	0.42	2.44	10	2
1:A:335:TRP:HB3	2:B:1:ALA:HB1	0.42	1.90	10	1
1:A:295:ASN:OD1	1:A:317:ALA:HB2	0.42	2.14	13	1
2:B:4:LYS:HG2	2:B:5:GLN:N	0.41	2.29	7	1
1:A:324:SER:CB	1:A:325:PRO:HD3	0.41	2.44	19	1
1:A:336:ARG:O	1:A:337:CYS:HB3	0.41	2.15	19	1
1:A:295:ASN:HD22	1:A:315:PRO:HA	0.41	1.75	6	1
1:A:295:ASN:ND2	1:A:310:CYS:SG	0.41	2.93	20	1
1:A:337:CYS:O	1:A:340:CYS:N	0.41	2.53	15	1
1:A:334:THR:HG22	2:B:2:ARG:HH12	0.41	1.75	1	1
1:A:331:PRO:CG	1:A:335:TRP:CD1	0.41	3.02	18	1
1:A:335:TRP:CE2	1:A:336:ARG:O	0.41	2.73	10	1
1:A:330:ILE:HG23	1:A:331:PRO:HD2	0.41	1.91	16	1
1:A:306:GLY:O	2:B:6:THR:HG22	0.41	2.16	19	1
1:A:333:GLY:O	1:A:334:THR:O	0.41	2.38	20	1
1:A:308:LEU:HA	1:A:318:PHE:O	0.41	2.16	1	1
1:A:331:PRO:HG2	1:A:335:TRP:CG	0.41	2.51	19	1
1:A:334:THR:O	1:A:335:TRP:HB2	0.41	2.16	20	1
1:A:306:GLY:O	2:B:6:THR:HB	0.40	2.16	16	1
1:A:309:ILE:O	1:A:309:ILE:HG23	0.40	2.16	16	1
1:A:310:CYS:SG	2:B:2:ARG:HB2	0.40	2.57	14	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	47/56 (84%)	33±2 (69±4%)	11±2 (24±5%)	3±1 (7±2%)	2	18
2	B	5/21 (24%)	4±1 (84±10%)	1±1 (15±11%)	0±0 (1±4%)	20	68
All	All	1040/1540 (68%)	735 (71%)	241 (23%)	64 (6%)	3	19

All 12 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	320	LEU	20
1	A	325	PRO	18
1	A	331	PRO	7
1	A	295	ASN	5
1	A	297	ASP	5
1	A	332	SER	2
1	A	298	GLU	2
2	B	2	ARG	1
1	A	338	SER	1
1	A	333	GLY	1
1	A	334	THR	1
1	A	335	TRP	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	40/47 (85%)	37±1 (92±3%)	3±1 (8±3%)	14	61
2	B	5/16 (31%)	4±1 (84±16%)	1±1 (16±16%)	5	42
All	All	900/1260 (71%)	816 (91%)	84 (9%)	12	59

All 17 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	308	LEU	20
1	A	297	ASP	19
2	B	4	LYS	8
1	A	295	ASN	6

*Continued on next page...*

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Mol	Chain	Res	Type	Models (Total)
1	A	310	CYS	5
2	B	3	THR	5
1	A	299	CYS	4
1	A	301	VAL	4
1	A	298	GLU	2
1	A	296	GLU	2
2	B	2	ARG	2
1	A	307	GLU	2
1	A	303	ARG	1
1	A	336	ARG	1
1	A	341	LEU	1
2	B	5	GLN	1
1	A	328	ARG	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 monosaccharides in this entry.

### 6.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

### 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