



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 27, 2016 – 04:38 AM BST

PDB ID : 2OFG  
Title : Solution structure of the n-terminal domain of the zinc(II) ATPase ziaa in its apo form  
Authors : Banci, L.; Bertini, I.; Ciofi-Baffoni, S.; Poggi, L.; Robinson, N.J.; Vanarotti, M.  
Deposited on : 2007-01-03

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  
<http://wwpdb.org/validation/2016/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:

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

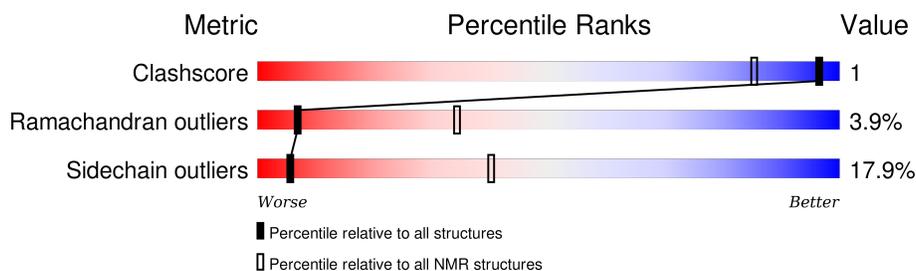
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment 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	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  $\geq 3$ , 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	X	111	

## 2 Ensemble composition and analysis

This entry contains 30 models. The atoms present in the NMR models are not consistent. Some calculations may have failed as a result. All residues are included in the validation scores. Model 24 is the overall representative, medoid model (most similar to other models).

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	X:6-X:75 (70)	0.53	24

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

NmrClust was unable to cluster the ensemble.

Error message: Inconsistent models in file

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1613 atoms, of which 806 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Zinc-transporting ATPase.

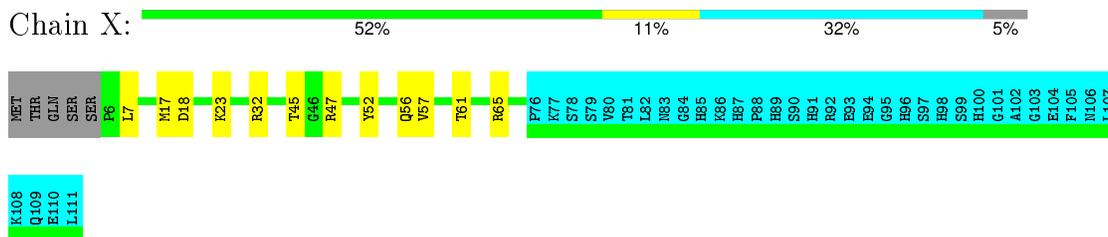
Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	X	106	1613	496	806	148	159	4	0

## 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: Zinc-transporting ATPase

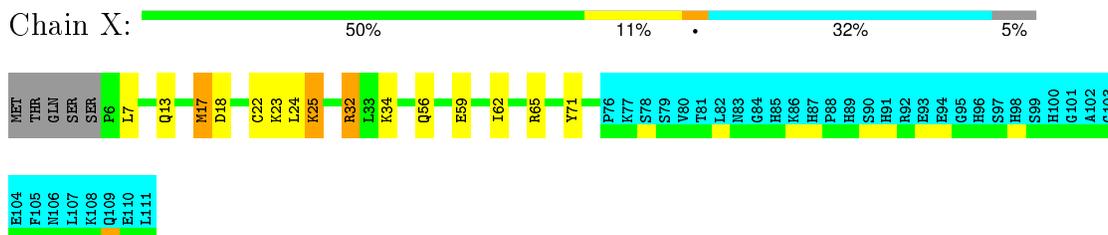


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

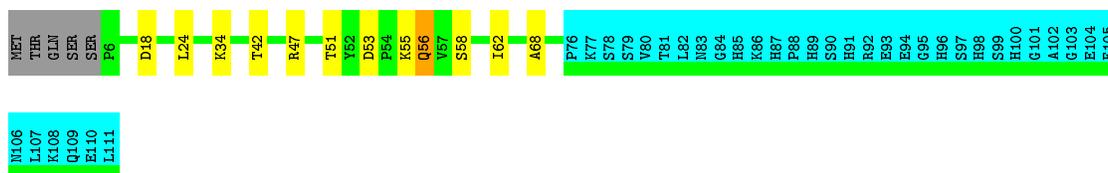
- Molecule 1: Zinc-transporting ATPase



#### 4.2.2 Score per residue for model 2

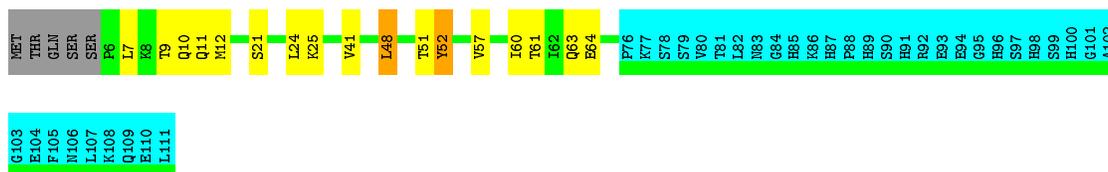
- Molecule 1: Zinc-transporting ATPase





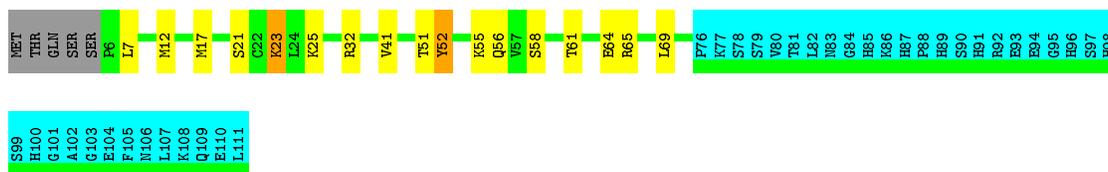
#### 4.2.3 Score per residue for model 3

- Molecule 1: Zinc-transporting ATPase



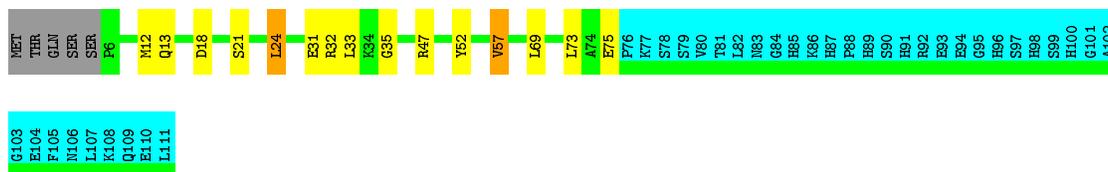
#### 4.2.4 Score per residue for model 4

- Molecule 1: Zinc-transporting ATPase



#### 4.2.5 Score per residue for model 5

- Molecule 1: Zinc-transporting ATPase



#### 4.2.6 Score per residue for model 6

- Molecule 1: Zinc-transporting ATPase





#### 4.2.14 Score per residue for model 14

- Molecule 1: Zinc-transporting ATPase

Chain X: 

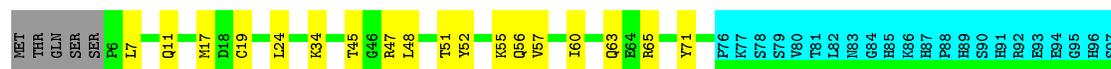


L111

#### 4.2.15 Score per residue for model 15

- Molecule 1: Zinc-transporting ATPase

Chain X: 



H98  
S99  
H100  
G101  
A102  
G103  
E104  
M106  
L107  
K108  
Q109  
E110  
L111

#### 4.2.16 Score per residue for model 16

- Molecule 1: Zinc-transporting ATPase

Chain X: 



M106  
L107  
K108  
Q109  
E110  
L111

#### 4.2.17 Score per residue for model 17

- Molecule 1: Zinc-transporting ATPase

Chain X: 



H100  
G101  
A102  
G103  
E104  
F105  
M106  
L107  
K108  
Q109  
E110  
L111

### 4.2.18 Score per residue for model 18

- Molecule 1: Zinc-transporting ATPase

Chain X: 53% 9% 32% 5%

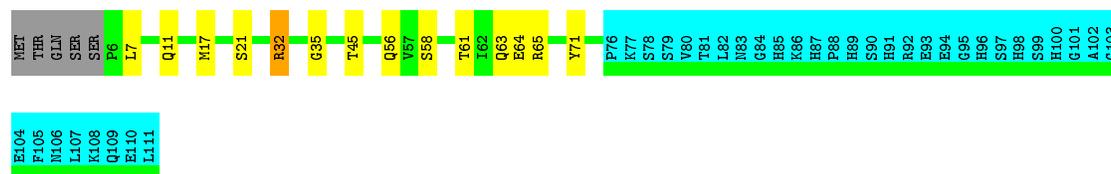


E110  
L111

### 4.2.19 Score per residue for model 19

- Molecule 1: Zinc-transporting ATPase

Chain X: 50% 12% 32% 5%

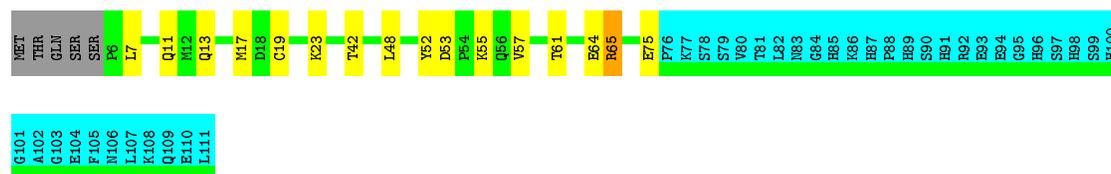


E104  
F105  
M106  
L107  
K108  
Q109  
E110  
E110  
L111

### 4.2.20 Score per residue for model 20

- Molecule 1: Zinc-transporting ATPase

Chain X: 49% 14% 32% 5%

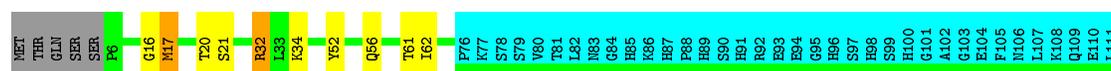


G101  
A102  
G103  
E104  
F105  
M106  
L107  
K108  
Q109  
E110  
L111

### 4.2.21 Score per residue for model 21

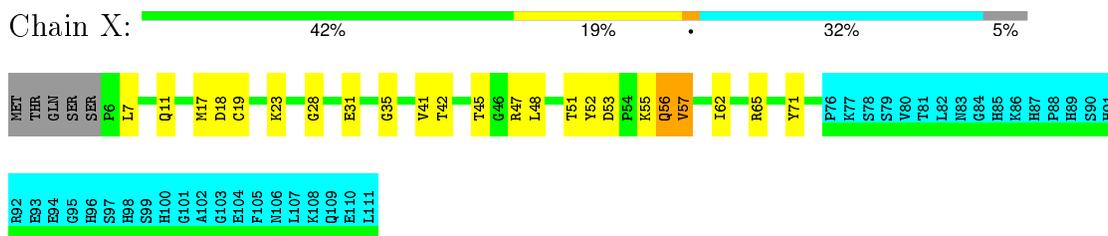
- Molecule 1: Zinc-transporting ATPase

Chain X: 54% 7% 32% 5%



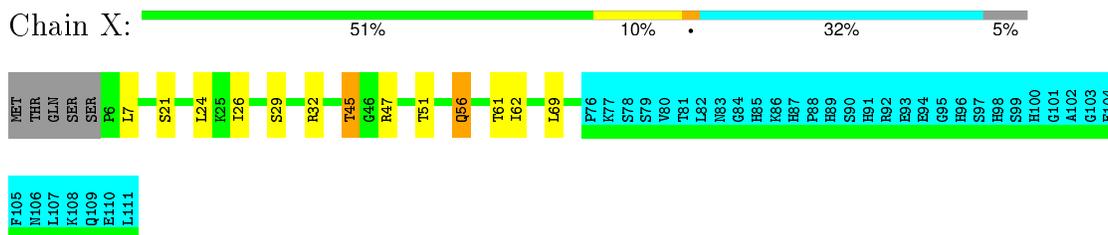
### 4.2.22 Score per residue for model 22

- Molecule 1: Zinc-transporting ATPase



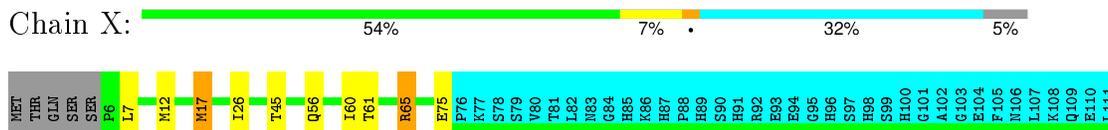
### 4.2.23 Score per residue for model 23

- Molecule 1: Zinc-transporting ATPase



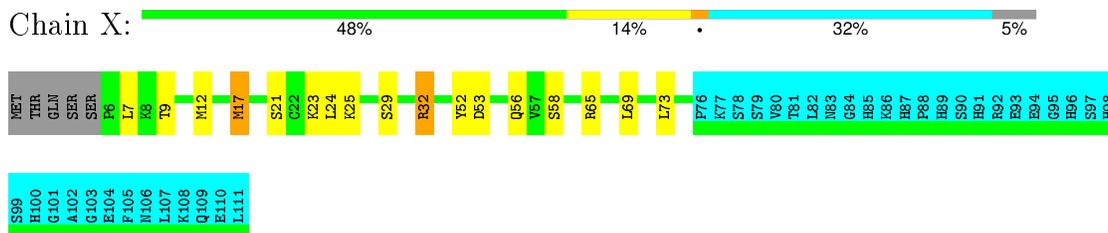
### 4.2.24 Score per residue for model 24 (medoid)

- Molecule 1: Zinc-transporting ATPase



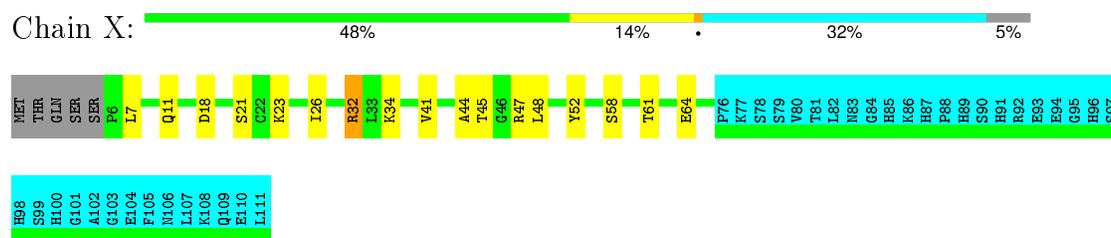
### 4.2.25 Score per residue for model 25

- Molecule 1: Zinc-transporting ATPase



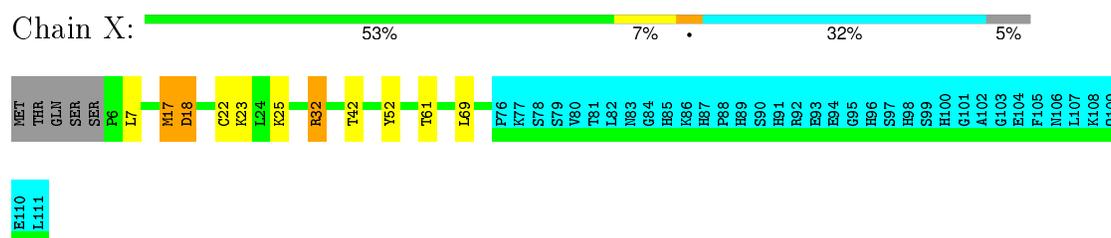
## 4.2.26 Score per residue for model 26

- Molecule 1: Zinc-transporting ATPase



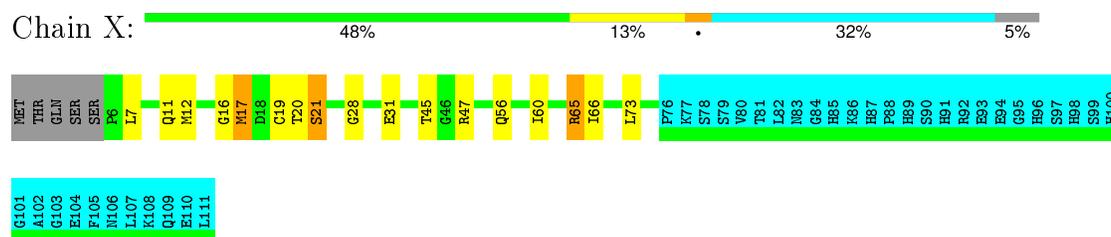
## 4.2.27 Score per residue for model 27

- Molecule 1: Zinc-transporting ATPase



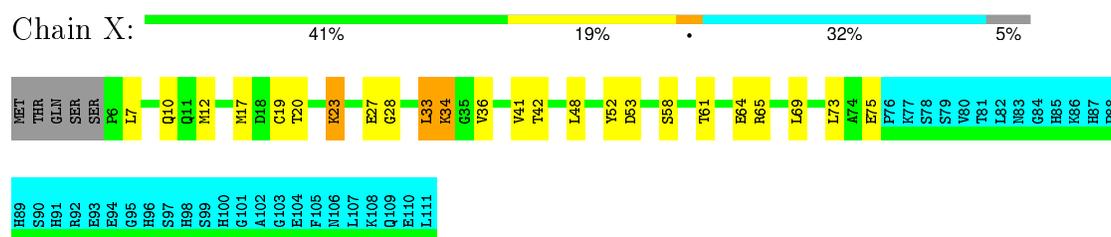
## 4.2.28 Score per residue for model 28

- Molecule 1: Zinc-transporting ATPase



## 4.2.29 Score per residue for model 29

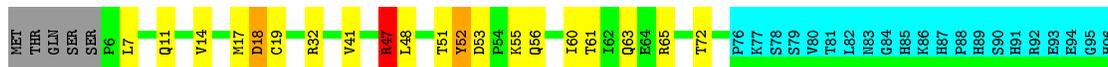
- Molecule 1: Zinc-transporting ATPase



### 4.2.30 Score per residue for model 30

- Molecule 1: Zinc-transporting ATPase

Chain X: 



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *Simulated Annealing in TAD followed by Restrained Energy Minimization*.

Of the 300 calculated structures, 30 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CYANA	structure solution	2.1
AMBER	refinement	8

No chemical shift data was provided. 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	X	0.61±0.01	0±0/527 (0.0±0.0%)	1.15±0.05	2±1/712 (0.2±0.2%)
All	All	0.61	0/15810 (0.0%)	1.15	48/21360 (0.2%)

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	X	0.0±0.0	1.2±1.1
All	All	0	36

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	X	65	ARG	NE-CZ-NH1	11.82	126.21	120.30	28	7
1	X	32	ARG	NE-CZ-NH1	8.65	124.62	120.30	21	9
1	X	47	ARG	NE-CZ-NH2	-7.12	116.74	120.30	2	5
1	X	47	ARG	NE-CZ-NH1	6.87	123.74	120.30	2	9
1	X	71	TYR	CB-CG-CD2	-6.86	116.89	121.00	22	4
1	X	32	ARG	NE-CZ-NH2	-6.55	117.02	120.30	30	3
1	X	32	ARG	CD-NE-CZ	5.86	131.81	123.60	14	1
1	X	65	ARG	NE-CZ-NH2	-5.84	117.38	120.30	9	1
1	X	52	TYR	CB-CG-CD2	-5.69	117.59	121.00	4	2
1	X	59	GLU	N-CA-CB	-5.31	101.04	110.60	6	1
1	X	18	ASP	C-N-CA	5.22	134.76	121.70	10	1
1	X	65	ARG	NH1-CZ-NH2	-5.11	113.78	119.40	28	1
1	X	57	VAL	CG1-CB-CG2	-5.11	102.73	110.90	7	1
1	X	31	GLU	CA-CB-CG	5.03	124.46	113.40	5	1
1	X	65	ARG	CD-NE-CZ	5.02	130.63	123.60	28	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	X	57	VAL	CA-CB-CG2	5.00	118.41	110.90	22	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	X	65	ARG	Sidechain	9
1	X	28	GLY	Peptide	5
1	X	17	MET	Peptide	4
1	X	52	TYR	Sidechain	3
1	X	47	ARG	Sidechain	3
1	X	32	ARG	Sidechain	3
1	X	71	TYR	Sidechain	2
1	X	18	ASP	Peptide	2
1	X	21	SER	Peptide	2
1	X	35	GLY	Peptide	1
1	X	33	LEU	Peptide	1
1	X	56	GLN	Peptide	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	X	523	547	547	1±2
All	All	15690	16410	16410	35

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:X:41:VAL:HB	1:X:48:LEU:HD22	0.64	1.70	30	2
1:X:33:LEU:HD12	1:X:34:LYS:H	0.62	1.54	29	1
1:X:33:LEU:HD12	1:X:34:LYS:N	0.62	2.10	29	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:X:14:VAL:HG21	1:X:48:LEU:HD21	0.56	1.78	30	1
1:X:23:LYS:CG	1:X:41:VAL:HG21	0.55	2.32	13	2
1:X:33:LEU:HD21	1:X:36:VAL:HG21	0.52	1.82	29	1
1:X:48:LEU:HD13	1:X:62:ILE:CG2	0.51	2.35	6	1
1:X:23:LYS:HE3	1:X:41:VAL:HG11	0.51	1.83	4	1
1:X:23:LYS:HG3	1:X:41:VAL:HG21	0.50	1.82	7	1
1:X:66:ILE:HG21	1:X:73:LEU:HB3	0.49	1.84	28	1
1:X:41:VAL:HG13	1:X:48:LEU:HD22	0.48	1.85	12	1
1:X:41:VAL:HG22	1:X:48:LEU:HD22	0.47	1.86	26	2
1:X:25:LYS:HE3	1:X:69:LEU:CD2	0.46	2.41	25	1
1:X:25:LYS:HE3	1:X:69:LEU:HD22	0.45	1.88	4	3
1:X:41:VAL:HG12	1:X:48:LEU:HD22	0.45	1.88	29	1
1:X:8:LYS:HE3	1:X:52:TYR:CE1	0.45	2.46	11	1
1:X:26:ILE:HG21	1:X:48:LEU:HD11	0.45	1.88	6	1
1:X:27:GLU:CD	1:X:41:VAL:HG13	0.44	2.32	29	1
1:X:23:LYS:CB	1:X:41:VAL:HG11	0.43	2.43	29	1
1:X:24:LEU:HD12	1:X:25:LYS:N	0.43	2.28	1	1
1:X:21:SER:H	1:X:24:LEU:CD1	0.43	2.26	5	1
1:X:17:MET:CE	1:X:66:ILE:HG23	0.42	2.44	28	1
1:X:60:ILE:HD12	1:X:60:ILE:H	0.42	1.74	6	1
1:X:66:ILE:HG23	1:X:71:TYR:CE2	0.42	2.50	17	1
1:X:36:VAL:HG22	1:X:52:TYR:HB3	0.41	1.92	7	1
1:X:23:LYS:HB3	1:X:41:VAL:HG11	0.41	1.90	29	1
1:X:22:CYS:HA	1:X:25:LYS:HE2	0.41	1.92	6	1
1:X:47:ARG:C	1:X:48:LEU:HD23	0.40	2.36	30	1
1:X:59:GLU:CD	1:X:59:GLU:H	0.40	2.20	1	1
1:X:23:LYS:CD	1:X:41:VAL:HG11	0.40	2.46	22	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	X	69/111 (62%)	55±2 (80±4%)	11±2 (16±3%)	3±1 (4±2%)	7	34
All	All	2071/3330 (62%)	1658 (80%)	333 (16%)	80 (4%)	7	34

All 16 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	X	19	CYS	12
1	X	18	ASP	9
1	X	56	GLN	8
1	X	21	SER	8
1	X	17	MET	7
1	X	22	CYS	5
1	X	58	SER	5
1	X	45	THR	4
1	X	57	VAL	4
1	X	35	GLY	4
1	X	26	ILE	3
1	X	20	THR	3
1	X	16	GLY	3
1	X	68	ALA	2
1	X	44	ALA	2
1	X	55	LYS	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	X	58/94 (62%)	48±3 (82±4%)	10±3 (18±4%)	5	40
All	All	1740/2820 (62%)	1429 (82%)	311 (18%)	5	40

All 43 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	X	7	LEU	23
1	X	61	THR	19
1	X	17	MET	15
1	X	64	GLU	13
1	X	23	LYS	13
1	X	52	TYR	13
1	X	45	THR	12
1	X	12	MET	12

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Mol	Chain	Res	Type	Models (Total)
1	X	56	GLN	11
1	X	57	VAL	10
1	X	11	GLN	10
1	X	51	THR	10
1	X	24	LEU	10
1	X	75	GLU	10
1	X	53	ASP	9
1	X	55	LYS	9
1	X	65	ARG	9
1	X	34	LYS	9
1	X	32	ARG	9
1	X	63	GLN	8
1	X	48	LEU	7
1	X	62	ILE	7
1	X	60	ILE	7
1	X	42	THR	6
1	X	58	SER	5
1	X	18	ASP	5
1	X	73	LEU	4
1	X	10	GLN	4
1	X	13	GLN	4
1	X	29	SER	3
1	X	47	ARG	3
1	X	69	LEU	3
1	X	31	GLU	3
1	X	8	LYS	2
1	X	72	THR	2
1	X	9	THR	2
1	X	26	ILE	2
1	X	25	LYS	2
1	X	21	SER	2
1	X	22	CYS	1
1	X	49	THR	1
1	X	59	GLU	1
1	X	33	LEU	1

### 6.3.3 RNA

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 carbohydrates 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