



# Full wwPDB NMR Structure Validation Report ⓘ

Nov 1, 2021 – 02:18 AM EDT

PDB ID : 2KO0  
Title : Solution structure of the THAP zinc finger of THAP1 in complex with its DNA target  
Authors : Campagne, S.; Gervais, V.; Saurel, O.; Milon, A.  
Deposited on : 2009-09-08

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

We welcome your comments at [validation@mail.wwpdb.org](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 : 2.23.2  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

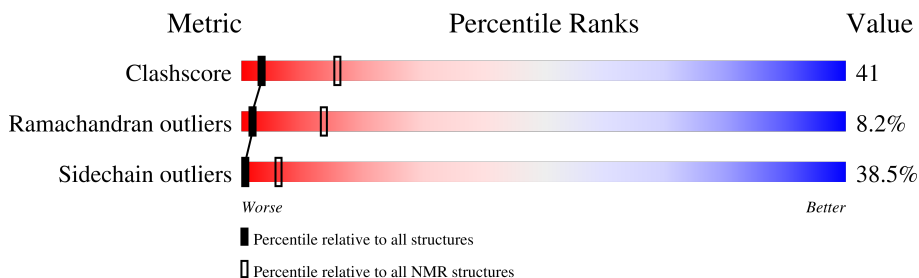
# 1 Overall quality at a glance

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	87	 33% 40% 16% 10%
2	B	16	 6% 88% 6%
3	C	16	 25% 69% 6%

## 2 Ensemble composition and analysis

This entry contains 15 models. Model 9 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:5-A:82 (78)	0.15	9

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 2 clusters and 3 single-model clusters were found.

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

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

There are 4 unique types of molecules in this entry. The entry contains 2447 atoms, of which 1078 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called THAP domain-containing protein 1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	87	1434	455	719	127	128	5	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	62	SER	CYS	engineered mutation	UNP Q9NVV9
A	67	SER	CYS	engineered mutation	UNP Q9NVV9
A	83	GLU	-	expression tag	UNP Q9NVV9
A	84	LEU	-	expression tag	UNP Q9NVV9
A	85	VAL	-	expression tag	UNP Q9NVV9
A	86	PRO	-	expression tag	UNP Q9NVV9
A	87	ARG	-	expression tag	UNP Q9NVV9

- Molecule 2 is a DNA chain called RRM1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
2	B	16	512	157	181	62	97	15	0

- Molecule 3 is a DNA chain called ZINC ION.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
3	C	16	500	152	178	61	93	16	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

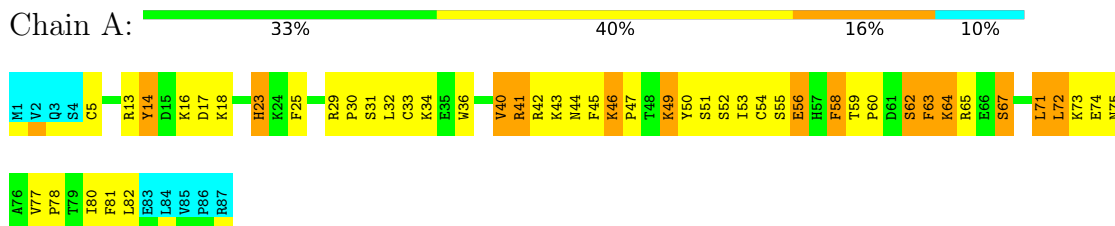
Mol	Chain	Residues	Atoms	
			Total	Zn
4	A	1	1	1

## 4 Residue-property plots

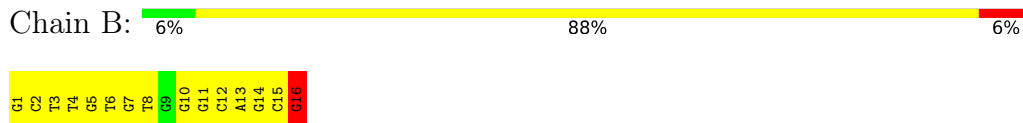
### 4.1 Average score per residue in the NMR ensemble

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: THAP domain-containing protein 1



- Molecule 2: RRM1



- Molecule 3: ZINC ION



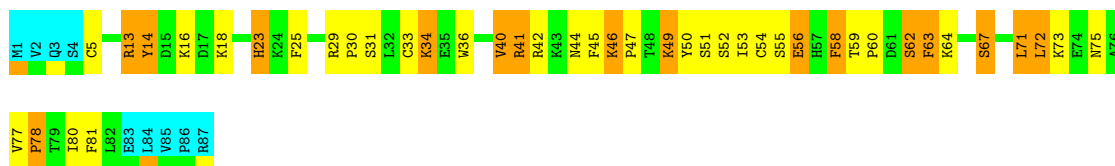
### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

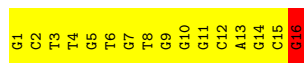
- Molecule 1: THAP domain-containing protein 1





- Molecule 2: RRM1

Chain B: 94% 6%



- Molecule 3: ZINC ION

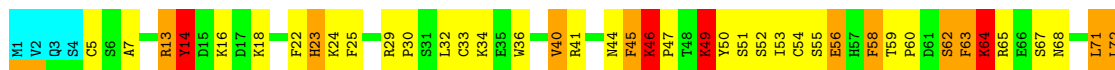
Chain C: 25% 69% 6%



#### 4.2.2 Score per residue for model 2

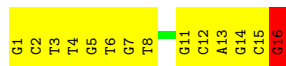
- Molecule 1: THAP domain-containing protein 1

Chain A: 36% 37% 13% 5% 10%



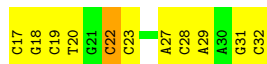
- Molecule 2: RRM1

Chain B: 12% 81% 6%



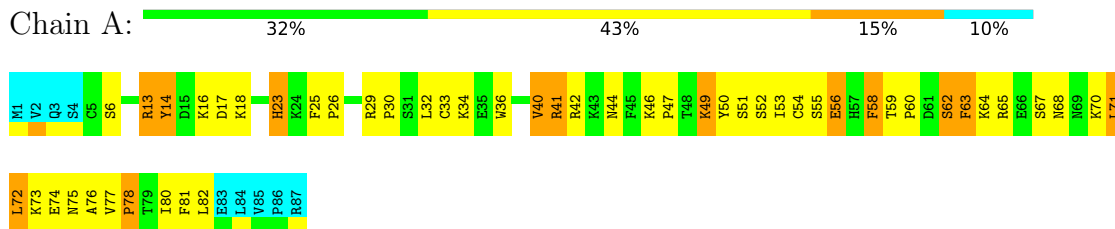
- Molecule 3: ZINC ION

Chain C: 31% 62% 6%



#### 4.2.3 Score per residue for model 3

- Molecule 1: THAP domain-containing protein 1



- Molecule 2: RRM1

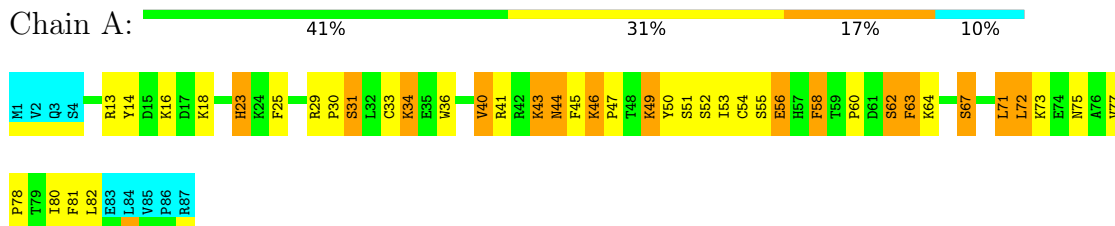


- Molecule 3: ZINC ION



#### 4.2.4 Score per residue for model 4

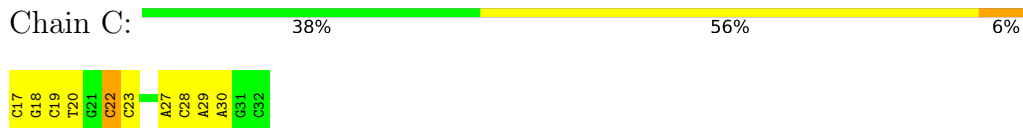
- Molecule 1: THAP domain-containing protein 1



- Molecule 2: RRM1

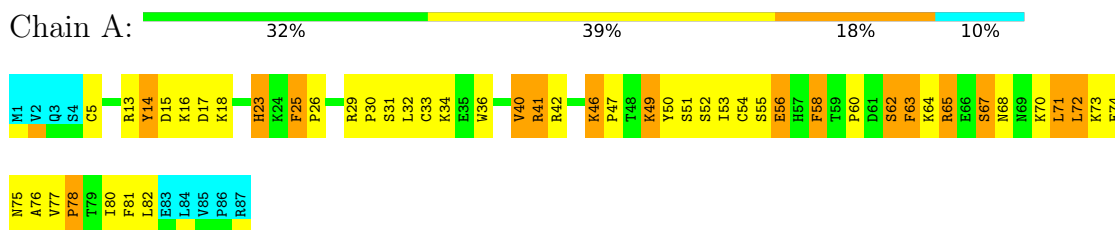


- Molecule 3: ZINC ION



### 4.2.5 Score per residue for model 5

- Molecule 1: THAP domain-containing protein 1



- Molecule 2: RRM1

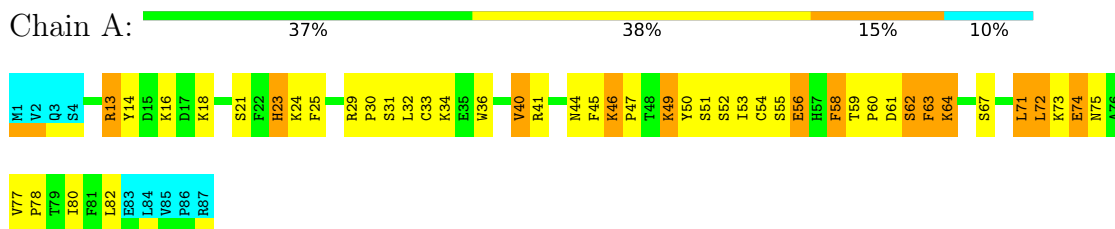


- Molecule 3: ZINC ION



### 4.2.6 Score per residue for model 6

- Molecule 1: THAP domain-containing protein 1



- Molecule 2: RRM1



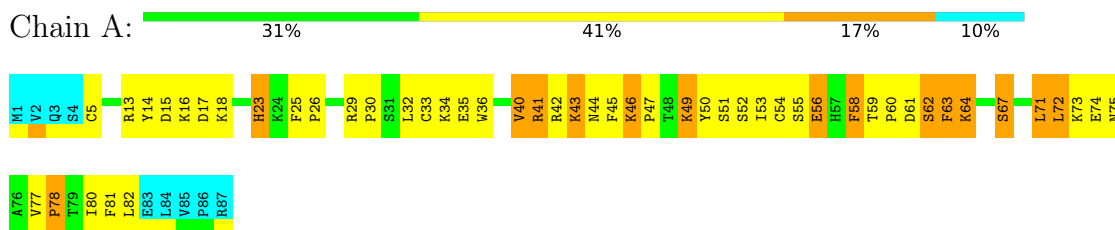
- Molecule 3: ZINC ION



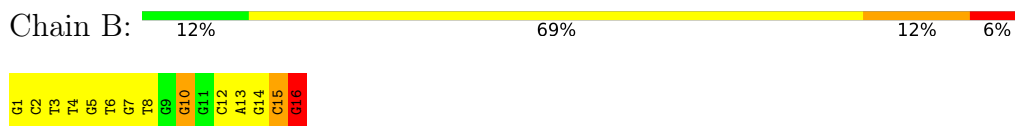


### 4.2.7 Score per residue for model 7

- Molecule 1: THAP domain-containing protein 1



- Molecule 2: RRM1

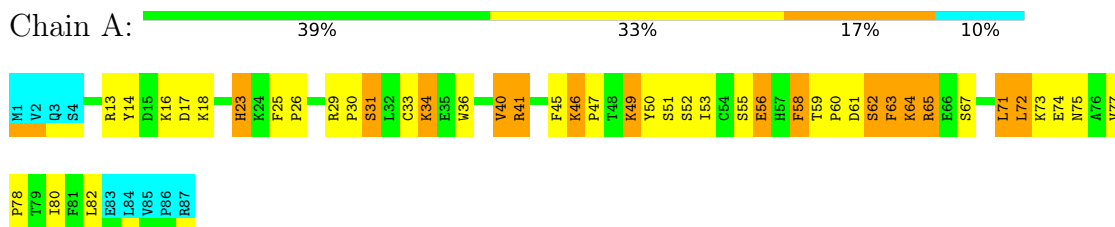


- Molecule 3: ZINC ION

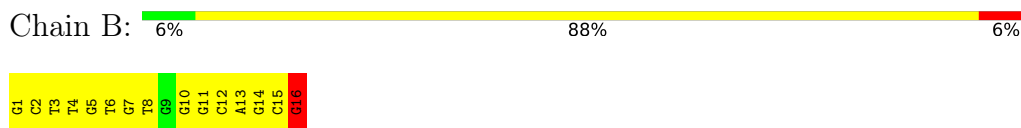


### 4.2.8 Score per residue for model 8

- Molecule 1: THAP domain-containing protein 1



- Molecule 2: RRM1

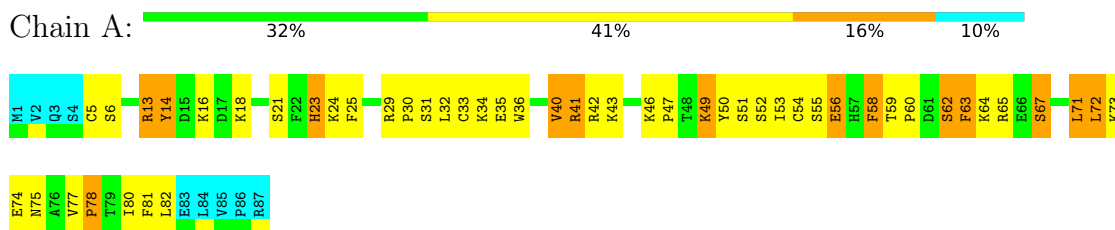


- Molecule 3: ZINC ION

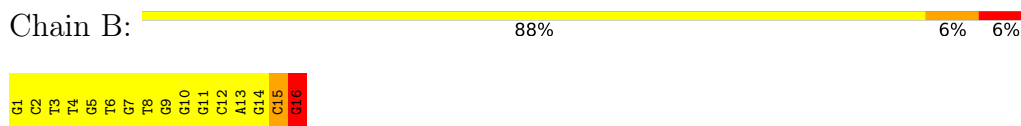


### 4.2.9 Score per residue for model 9 (medoid)

- Molecule 1: THAP domain-containing protein 1



- Molecule 2: RRM1

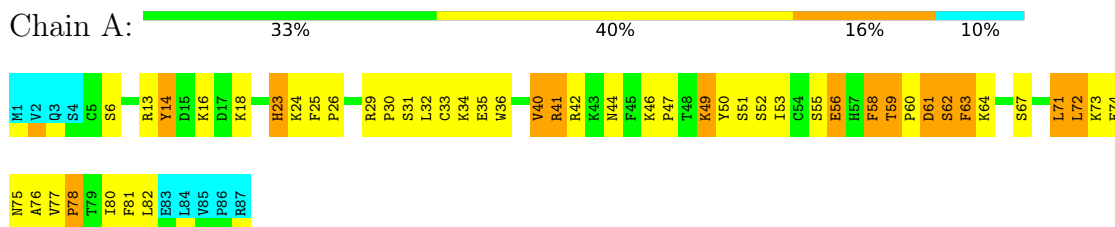


- Molecule 3: ZINC ION

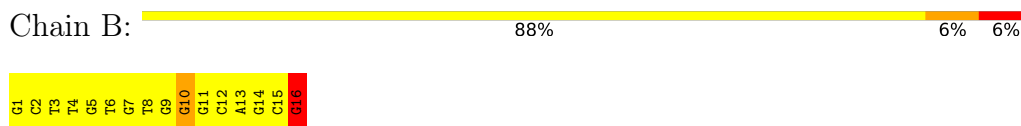


### 4.2.10 Score per residue for model 10

- Molecule 1: THAP domain-containing protein 1



- Molecule 2: RRM1

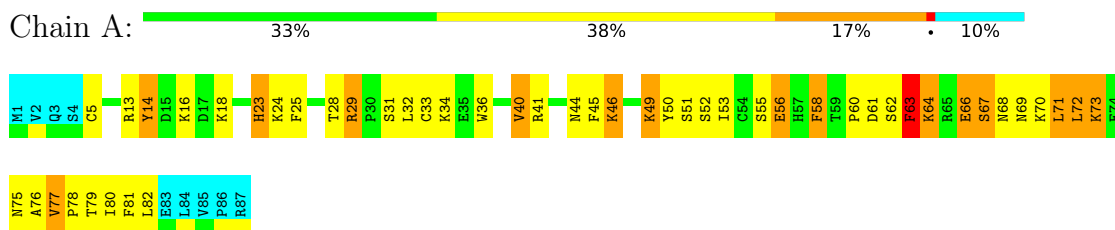


- Molecule 3: ZINC ION



### 4.2.11 Score per residue for model 11

- Molecule 1: THAP domain-containing protein 1



- Molecule 2: RRM1

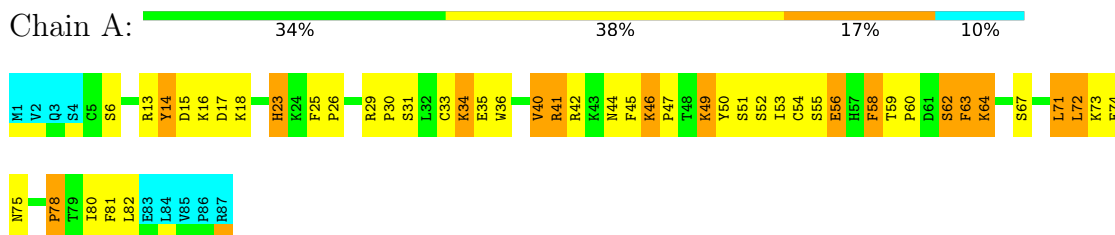


- Molecule 3: ZINC ION



### 4.2.12 Score per residue for model 12

- Molecule 1: THAP domain-containing protein 1



- Molecule 2: RRM1

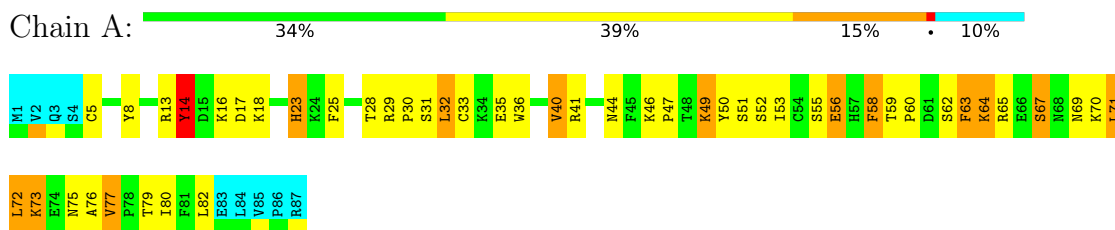


- Molecule 3: ZINC ION

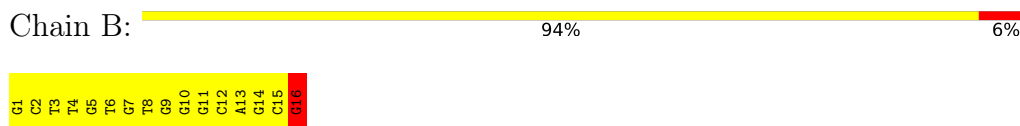


### 4.2.13 Score per residue for model 13

- Molecule 1: THAP domain-containing protein 1



- Molecule 2: RRM1

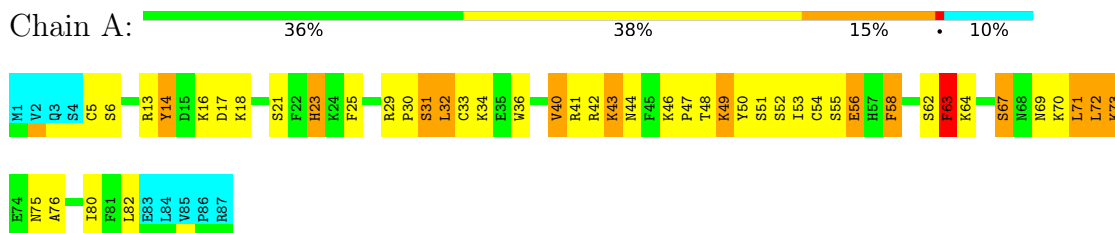


- Molecule 3: ZINC ION

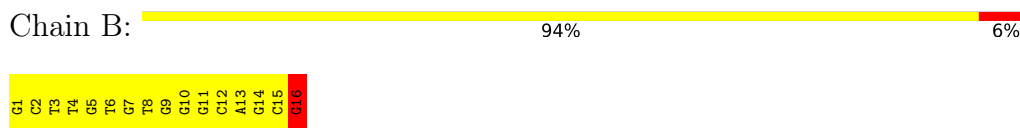


### 4.2.14 Score per residue for model 14

- Molecule 1: THAP domain-containing protein 1



- Molecule 2: RRM1

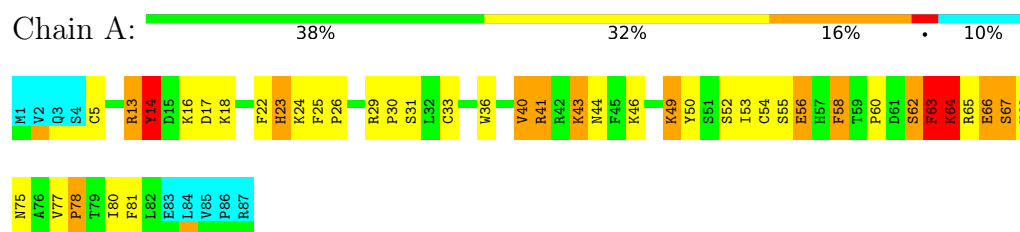


- Molecule 3: ZINC ION

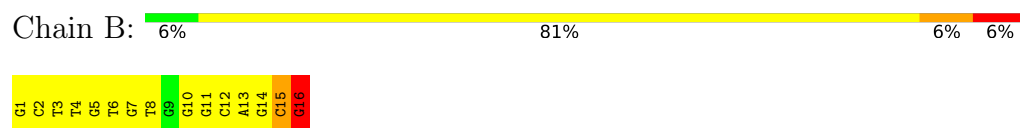


### 4.2.15 Score per residue for model 15

- Molecule 1: THAP domain-containing protein 1



- Molecule 2: RRM1



- Molecule 3: ZINC ION



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *Rigid body docking, Semi flexible simulated annealing, Water refinement.*

Of the 200 calculated structures, 15 were deposited, based on the following criterion: *structures with the least restraint violations.*

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

Software name	Classification	Version
HADDOCK	refinement	2.0

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

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	0.42±0.01	0±0/661 ( 0.0± 0.0%)	0.59±0.01	0±0/890 ( 0.0± 0.0%)
2	B	0.42±0.01	0±0/371 ( 0.0± 0.0%)	0.83±0.01	2±0/573 ( 0.3± 0.0%)
3	C	0.28±0.01	0±0/360 ( 0.0± 0.0%)	0.68±0.01	0±0/551 ( 0.0± 0.0%)
All	All	0.39	0/20880 ( 0.0%)	0.69	30/30210 ( 0.1%)

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
2	B	0.0±0.0	1.5±0.6
3	C	0.0±0.0	0.8±0.5
All	All	0	34

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
2	B	16	DG	O4'-C1'-N9	6.43	112.50	108.00	8	15
2	B	16	DG	O4'-C4'-C3'	-6.41	101.94	104.50	2	15

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)
2	B	16	DG	Sidechain	15

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Mol	Chain	Res	Type	Group	Models (Total)
3	C	22	DC	Sidechain	10
2	B	15	DC	Sidechain	5
2	B	10	DG	Sidechain	2
3	C	23	DC	Sidechain	2

## 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	642	640	639	31±3
2	B	331	181	182	46±3
3	C	322	178	178	23±2
All	All	19440	14985	14985	1410

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 41.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:15:DC:H1'	2:B:16:DG:N7	1.14	1.58	5	15
2:B:14:DG:H2''	2:B:15:DC:C5	0.88	2.03	9	15
2:B:15:DC:C1'	2:B:16:DG:N7	0.88	2.37	4	15
2:B:7:DG:H2'	2:B:8:DT:H72	0.87	1.45	5	10
2:B:7:DG:C2'	2:B:8:DT:H71	0.87	1.99	9	5
2:B:1:DG:H2''	2:B:2:DC:C5	0.84	2.07	10	15
3:C:19:DC:C2'	3:C:20:DT:H72	0.83	2.03	14	10
1:A:25:PHE:CD1	1:A:53:ILE:HD11	0.82	2.09	10	15
3:C:18:DG:H2''	3:C:19:DC:C5	0.80	2.12	10	15
2:B:7:DG:H2'	2:B:8:DT:H71	0.79	1.53	1	5
2:B:3:DT:H2''	2:B:4:DT:H71	0.78	1.52	3	15
3:C:27:DA:H2''	3:C:28:DC:C5	0.77	2.15	12	15
1:A:25:PHE:CD1	1:A:49:LYS:HA	0.75	2.16	1	15
2:B:7:DG:C2'	2:B:8:DT:H72	0.74	2.11	5	10
1:A:25:PHE:CG	1:A:49:LYS:HA	0.73	2.18	1	15
3:C:19:DC:H2''	3:C:20:DT:C5	0.73	2.19	8	15
1:A:25:PHE:HD2	1:A:33:CYS:HG	0.72	1.28	8	14

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:19:DC:H2'	3:C:20:DT:H72	0.72	1.62	10	10
2:B:2:DC:H2''	2:B:3:DT:H71	0.71	1.62	10	15
2:B:11:DG:H2''	2:B:12:DC:C5	0.70	2.21	2	10
2:B:7:DG:H2''	2:B:8:DT:H71	0.69	1.62	11	5
2:B:14:DG:C2'	2:B:15:DC:C5	0.69	2.75	8	15
3:C:19:DC:H2''	3:C:20:DT:C7	0.69	2.18	13	14
1:A:71:LEU:HD13	1:A:72:LEU:HD12	0.68	1.66	15	15
2:B:1:DG:H2''	2:B:2:DC:C6	0.68	2.23	2	15
3:C:19:DC:H2''	3:C:20:DT:H72	0.67	1.66	6	10
1:A:60:PRO:HA	1:A:63:PHE:CD2	0.67	2.24	9	12
2:B:6:DT:H1'	2:B:7:DG:C8	0.67	2.25	9	15
1:A:50:TYR:HB2	3:C:22:DC:C5	0.66	2.24	10	15
2:B:3:DT:H2''	2:B:4:DT:C7	0.66	2.21	3	15
2:B:5:DG:H2''	2:B:6:DT:H71	0.66	1.67	7	15
2:B:16:DG:O5'	2:B:16:DG:C8	0.65	2.49	15	15
1:A:28:THR:HG21	2:B:6:DT:H3'	0.64	1.70	13	2
2:B:7:DG:C2'	2:B:8:DT:C7	0.64	2.75	9	15
1:A:24:LYS:HG3	2:B:8:DT:H72	0.64	1.68	11	1
2:B:14:DG:H2''	2:B:15:DC:C6	0.64	2.27	15	15
2:B:15:DC:C2	2:B:16:DG:O6	0.64	2.51	14	15
2:B:3:DT:C2'	2:B:4:DT:H71	0.63	2.23	3	15
3:C:19:DC:H2''	3:C:20:DT:H71	0.63	1.71	13	5
2:B:5:DG:C2'	2:B:6:DT:H71	0.63	2.23	3	15
2:B:1:DG:C2'	2:B:2:DC:C5	0.62	2.82	15	15
1:A:50:TYR:CD2	3:C:22:DC:H2'	0.62	2.28	1	15
2:B:15:DC:C2'	2:B:16:DG:N7	0.61	2.64	4	15
3:C:17:DC:H2''	3:C:18:DG:C8	0.61	2.31	10	15
2:B:2:DC:H2''	2:B:3:DT:C7	0.61	2.26	9	15
2:B:2:DC:C2'	2:B:3:DT:H71	0.61	2.26	10	15
2:B:5:DG:H2''	2:B:6:DT:C7	0.60	2.26	12	15
2:B:12:DC:H2''	2:B:13:DA:C8	0.60	2.32	10	13
2:B:15:DC:H1'	2:B:16:DG:C8	0.60	2.30	12	15
2:B:5:DG:H2''	2:B:6:DT:C5	0.60	2.32	12	14
3:C:27:DA:C2'	3:C:28:DC:C5	0.59	2.85	12	12
2:B:7:DG:H2'	2:B:8:DT:C7	0.59	2.27	1	11
3:C:18:DG:H2''	3:C:19:DC:C6	0.59	2.32	14	15
1:A:25:PHE:HD2	1:A:33:CYS:SG	0.59	2.21	8	14
1:A:47:PRO:HB2	1:A:51:SER:OG	0.59	1.98	12	11
1:A:60:PRO:O	1:A:63:PHE:HB2	0.58	1.98	2	3
3:C:18:DG:C2'	3:C:19:DC:C5	0.58	2.85	10	15
2:B:2:DC:H2''	2:B:3:DT:C5	0.58	2.34	9	15

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:28:DC:H2''	3:C:29:DA:C8	0.58	2.33	12	14
1:A:43:LYS:HG2	1:A:44:ASN:N	0.58	2.13	14	4
1:A:25:PHE:HD1	1:A:53:ILE:HD11	0.58	1.56	10	9
1:A:36:TRP:O	1:A:40:VAL:HG23	0.58	1.98	14	15
1:A:23:HIS:CE1	1:A:58:PHE:HE1	0.58	2.17	6	11
3:C:27:DA:H2''	3:C:28:DC:C6	0.57	2.34	12	14
2:B:15:DC:H2''	2:B:16:DG:N7	0.57	2.14	2	15
3:C:19:DC:C2'	3:C:20:DT:C7	0.57	2.83	13	10
1:A:50:TYR:CE2	3:C:22:DC:H2'	0.57	2.34	11	15
2:B:5:DG:C2'	2:B:6:DT:C7	0.57	2.83	12	15
1:A:23:HIS:CE1	1:A:58:PHE:HE2	0.57	2.17	15	3
3:C:31:DG:H2''	3:C:32:DC:C5	0.57	2.35	11	14
1:A:62:SER:O	1:A:72:LEU:HD23	0.56	1.99	9	12
2:B:16:DG:O5'	2:B:16:DG:H8	0.56	1.83	15	15
1:A:78:PRO:HB2	1:A:81:PHE:CE1	0.56	2.35	1	11
1:A:22:PHE:CE1	1:A:54:CYS:HB3	0.55	2.36	2	1
1:A:62:SER:HA	1:A:73:LYS:CD	0.54	2.32	14	3
2:B:3:DT:C2'	2:B:4:DT:C7	0.54	2.85	3	15
2:B:6:DT:H2''	2:B:7:DG:C8	0.54	2.37	5	15
2:B:7:DG:H2''	2:B:8:DT:C6	0.54	2.38	6	14
2:B:2:DC:C2'	2:B:3:DT:C7	0.54	2.85	15	15
1:A:50:TYR:CD1	3:C:23:DC:H5	0.53	2.21	11	15
2:B:3:DT:H2''	2:B:4:DT:C5	0.53	2.39	4	8
2:B:13:DA:H2''	2:B:14:DG:C8	0.53	2.39	8	9
1:A:59:THR:HB	1:A:61:ASP:OD1	0.53	2.04	10	1
1:A:25:PHE:CE1	1:A:53:ILE:HD11	0.53	2.38	1	5
2:B:6:DT:C2	2:B:7:DG:C5	0.52	2.97	8	15
2:B:6:DT:C1'	2:B:7:DG:C8	0.52	2.93	13	15
1:A:32:LEU:HD21	1:A:76:ALA:O	0.52	2.04	11	5
3:C:30:DA:H2''	3:C:31:DG:C8	0.52	2.40	12	6
2:B:5:DG:H2''	2:B:6:DT:C6	0.52	2.40	3	10
1:A:23:HIS:HE1	1:A:55:SER:N	0.52	2.02	14	15
2:B:2:DC:H2''	2:B:3:DT:C6	0.52	2.39	15	12
1:A:5:CYS:O	1:A:46:LYS:HD3	0.52	2.05	5	2
3:C:31:DG:H2''	3:C:32:DC:C6	0.52	2.39	11	8
1:A:45:PHE:HD1	1:A:46:LYS:O	0.52	1.88	2	5
3:C:29:DA:H2''	3:C:30:DA:C8	0.51	2.40	12	11
3:C:26:DC:H2''	3:C:27:DA:C8	0.51	2.40	5	5
1:A:63:PHE:O	1:A:64:LYS:HG3	0.51	2.06	15	1
1:A:49:LYS:HD2	1:A:49:LYS:H	0.51	1.66	2	1
2:B:1:DG:HO5'	2:B:1:DG:H8	0.50	1.46	7	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:HIS:CE1	1:A:58:PHE:CE1	0.50	2.99	14	11
1:A:30:PRO:O	1:A:33:CYS:HB3	0.50	2.07	2	14
3:C:19:DC:H2''	3:C:20:DT:C6	0.49	2.43	10	8
1:A:53:ILE:HD12	1:A:53:ILE:N	0.49	2.23	4	15
2:B:7:DG:H2''	2:B:8:DT:C7	0.49	2.38	5	8
1:A:13:ARG:HD2	1:A:13:ARG:C	0.49	2.29	1	1
2:B:11:DG:C2'	2:B:12:DC:C5	0.48	2.95	2	1
1:A:25:PHE:CD2	1:A:33:CYS:SG	0.48	3.07	2	7
1:A:26:PRO:HB3	1:A:72:LEU:CD1	0.48	2.39	3	6
2:B:11:DG:H2''	2:B:12:DC:C6	0.48	2.44	2	2
3:C:19:DC:C2'	3:C:20:DT:H71	0.48	2.37	13	2
2:B:12:DC:H2''	2:B:13:DA:N7	0.47	2.24	10	1
2:B:4:DT:H2''	2:B:5:DG:C8	0.47	2.44	3	6
3:C:28:DC:C4	3:C:29:DA:N6	0.47	2.83	13	10
1:A:29:ARG:HG2	1:A:32:LEU:CB	0.47	2.39	2	4
1:A:67:SER:HB3	1:A:71:LEU:O	0.47	2.10	9	8
1:A:47:PRO:HA	3:C:21:DG:OP2	0.46	2.10	13	3
2:B:15:DC:C2	2:B:16:DG:C6	0.46	3.04	9	15
1:A:13:ARG:HD2	1:A:14:TYR:N	0.46	2.25	15	2
3:C:20:DT:H71	3:C:20:DT:OP2	0.46	2.11	2	1
1:A:8:TYR:CD1	1:A:8:TYR:O	0.46	2.69	13	1
1:A:24:LYS:HB2	2:B:8:DT:H72	0.45	1.88	6	2
1:A:64:LYS:NZ	2:B:8:DT:H5''	0.45	2.26	7	3
2:B:14:DG:C4	2:B:15:DC:C4	0.45	3.04	8	4
1:A:23:HIS:HB3	2:B:8:DT:P	0.45	2.51	7	5
1:A:24:LYS:CG	2:B:8:DT:H72	0.45	2.40	11	1
1:A:14:TYR:CE2	1:A:22:PHE:HB2	0.45	2.47	15	1
1:A:50:TYR:CD2	3:C:22:DC:C6	0.45	3.05	12	10
3:C:19:DC:C2'	3:C:20:DT:C5	0.45	2.98	11	5
1:A:64:LYS:HE3	1:A:66:GLU:OE1	0.45	2.11	15	1
1:A:60:PRO:HA	1:A:63:PHE:CG	0.45	2.46	4	5
3:C:25:DA:H2''	3:C:26:DC:OP2	0.45	2.12	8	3
1:A:73:LYS:HB2	1:A:76:ALA:CB	0.45	2.42	14	3
1:A:50:TYR:O	3:C:23:DC:N4	0.44	2.50	11	5
1:A:25:PHE:CD1	1:A:53:ILE:CD1	0.44	2.99	4	3
1:A:33:CYS:SG	1:A:49:LYS:HD3	0.44	2.52	6	1
1:A:65:ARG:HD2	2:B:7:DG:H4'	0.44	1.89	8	1
2:B:6:DT:H2''	2:B:7:DG:OP2	0.44	2.13	15	2
1:A:24:LYS:HE3	1:A:50:TYR:O	0.44	2.12	15	1
1:A:32:LEU:HG	1:A:74:GLU:HA	0.44	1.89	9	3
1:A:55:SER:HB2	1:A:63:PHE:CE1	0.43	2.48	12	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:67:SER:HB2	1:A:73:LYS:HZ1	0.43	1.73	13	3
1:A:15:ASP:OD2	1:A:17:ASP:HB2	0.43	2.12	12	1
1:A:24:LYS:HD3	2:B:8:DT:H72	0.43	1.90	9	1
1:A:23:HIS:HE1	1:A:54:CYS:C	0.43	2.17	6	9
2:B:9:DG:H2''	2:B:10:DG:OP2	0.43	2.13	1	6
1:A:23:HIS:O	1:A:53:ILE:N	0.43	2.51	10	7
1:A:45:PHE:CD1	1:A:46:LYS:O	0.43	2.71	2	7
1:A:7:ALA:O	1:A:46:LYS:HD3	0.42	2.14	2	1
2:B:2:DC:C2'	2:B:3:DT:C5	0.42	3.02	15	2
2:B:5:DG:C2'	2:B:6:DT:C5	0.42	3.02	12	4
1:A:62:SER:OG	1:A:76:ALA:HB1	0.42	2.14	11	1
1:A:31:SER:O	1:A:34:LYS:HB3	0.42	2.13	4	5
1:A:77:VAL:O	1:A:79:THR:HG23	0.42	2.14	11	2
1:A:26:PRO:HB3	1:A:72:LEU:HD13	0.42	1.90	15	1
1:A:48:THR:HG21	3:C:22:DC:OP2	0.42	2.15	14	1
1:A:45:PHE:O	3:C:20:DT:H3'	0.42	2.15	7	3
3:C:20:DT:H2''	3:C:21:DG:C8	0.42	2.49	3	1
1:A:69:ASN:CG	1:A:70:LYS:N	0.42	2.73	14	3
3:C:17:DC:O5'	3:C:17:DC:C6	0.42	2.73	3	3
1:A:55:SER:HG	1:A:63:PHE:HE1	0.42	1.55	14	1
1:A:23:HIS:CE1	1:A:55:SER:N	0.41	2.87	15	2
1:A:23:HIS:HB3	2:B:8:DT:OP1	0.41	2.14	12	1
1:A:64:LYS:HE3	1:A:66:GLU:OE2	0.41	2.15	11	1
2:B:10:DG:H2''	2:B:11:DG:OP2	0.41	2.15	13	1
1:A:64:LYS:HD3	2:B:8:DT:OP1	0.41	2.15	12	2
1:A:23:HIS:CD2	1:A:64:LYS:HD2	0.41	2.50	15	1
1:A:23:HIS:CE1	1:A:58:PHE:CE2	0.41	3.04	15	3
1:A:53:ILE:HG22	1:A:54:CYS:N	0.41	2.30	2	2
1:A:64:LYS:HG2	1:A:65:ARG:N	0.41	2.31	2	1
3:C:17:DC:H2''	3:C:18:DG:N7	0.41	2.31	13	1
2:B:6:DT:C2'	2:B:7:DG:C8	0.41	3.04	14	1
3:C:17:DC:C6	3:C:17:DC:P	0.41	3.14	3	1
1:A:65:ARG:HA	1:A:70:LYS:O	0.41	2.15	5	1
1:A:62:SER:HA	1:A:73:LYS:NZ	0.40	2.31	13	1
2:B:6:DT:C2	2:B:7:DG:N7	0.40	2.89	7	1
1:A:64:LYS:O	1:A:67:SER:HB3	0.40	2.17	15	1
1:A:71:LEU:HD13	1:A:72:LEU:CD1	0.40	2.46	1	1
1:A:46:LYS:HG3	3:C:20:DT:P	0.40	2.57	7	1
1:A:23:HIS:HB3	2:B:8:DT:OP2	0.40	2.17	11	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	78/87 (90%)	57±1 (73±1%)	15±1 (19±2%)	6±1 (8±1%)	2	13
All	All	1170/1305 (90%)	855 (73%)	219 (19%)	96 (8%)	2	13

All 10 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	40	VAL	15
1	A	56	GLU	15
1	A	64	LYS	15
1	A	67	SER	15
1	A	14	TYR	11
1	A	78	PRO	11
1	A	41	ARG	9
1	A	63	PHE	3
1	A	46	LYS	1
1	A	49	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	A	73/82 (89%)	45±2 (61±2%)	28±2 (39±2%)	0	6
All	All	1095/1230 (89%)	673 (61%)	422 (39%)	0	6

All 45 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	13	ARG	15
1	A	14	TYR	15
1	A	16	LYS	15
1	A	18	LYS	15
1	A	23	HIS	15
1	A	41	ARG	15
1	A	46	LYS	15
1	A	49	LYS	15
1	A	52	SER	15
1	A	56	GLU	15
1	A	58	PHE	15
1	A	63	PHE	15
1	A	71	LEU	15
1	A	72	LEU	15
1	A	73	LYS	15
1	A	75	ASN	15
1	A	80	ILE	15
1	A	77	VAL	13
1	A	29	ARG	12
1	A	34	LYS	12
1	A	62	SER	12
1	A	82	LEU	12
1	A	59	THR	10
1	A	31	SER	10
1	A	44	ASN	9
1	A	42	ARG	8
1	A	5	CYS	7
1	A	17	ASP	7
1	A	65	ARG	6
1	A	74	GLU	6
1	A	68	ASN	5
1	A	6	SER	5
1	A	43	LYS	5
1	A	61	ASP	5
1	A	35	GLU	5
1	A	21	SER	3
1	A	51	SER	3
1	A	64	LYS	2
1	A	15	ASP	2
1	A	66	GLU	2
1	A	32	LEU	2
1	A	24	LYS	1
1	A	45	PHE	1

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Mol	Chain	Res	Type	Models (Total)
1	A	70	LYS	1
1	A	25	PHE	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 1 ligands modelled in this entry, 1 is 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