Full wwPDB NMR Structure Validation Report (i)

Apr 21, 2024 – 01:06 PM EDT

PDB ID	:	2L1G
Title	:	RDC refined solution structure of the THAP zinc finger of THAP1 in complex with its 16bp RRM1 DNA target
Authors	:	Campagne, S.; Gervais, V.; Saurel, O.; Milon, A.
Deposited on	:	2010-07-28

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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

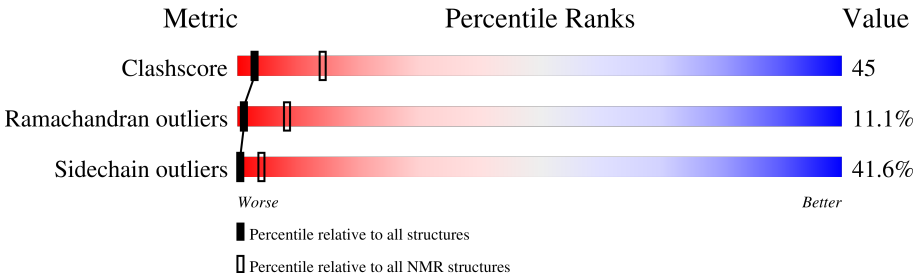
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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	87	23% 52% 16% • 8%
2	B	16	88% 6% 6%
3	C	16	12% 81% 6%

2 Ensemble composition and analysis (i)

This entry contains 17 models. Model 11 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:3-A:82 (80)	0.23	11

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 1 clusters and 3 single-model clusters were found.

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

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 DNA (5'-D(*GP*CP*TP*TP*GP*TP*GP*TP*GP*GP*GP*CP*AP*GP*CP*G)-3').

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 DNA (5'-D(P*CP*GP*CP*TP*GP*CP*CP*CP*AP*CP*AP*CP*AP*AP*GP*C)-3').

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 (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: THAP domain-containing protein 1

Chain A: 23% 52% 16% • 8%

M1 V2 Q3 S4 C5 S6 A7 Y8 R13 Y14 D15 K16 D17 K18 F22 H23 K24 F25 P26 R29 P30 S31 L32 C33 K34 E35 W36 V40 R41 R42 K43 N44 F45 K46 P47 T48 K49 Y50 S51 S52 I53 C54 S55 E56 H57 F58 T59 P60 D61 S62 F63 K64 R65 E66 S67 N68

L71 L72 K73 E74 N75 A76 V77 P78 T79 I80 F81 L82 E83 L84 V85 P86 R87

• Molecule 2: DNA (5'-D(*GP*CP*TP*TP*GP*TP*GP*TP*GP*GP*GP*CP*AP*GP*CP*G)-3')

Chain B: 88% 6% 6%

G1 C2 T3 T4 G5 T6 G7 T8 G9 G10 G11 C12 A13 G14 C15 G16

• Molecule 3: DNA (5'-D(P*CP*GP*CP*TP*GP*CP*CP*CP*AP*CP*AP*CP*AP*AP*GP*C)-3')

Chain C: 12% 81% 6%

C17 G18 C19 T20 G21 C22 C23 C24 A25 C26 A27 C28 A29 A30 G31 C32

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

Chain A: 26% 46% 18% • 8%

M1 V2 Q3 S4 C5 S6 A7 Y8 R13 Y14 D15 K16 D17 K18 S21 F22 H23 K24 F25 P26 R29 P30 S31 L32 C33 K34 E35 W36 V40 R41 R42 K43 N44 F45 K46 P47 T48 K49 Y50 S51 S52 I53 C54 S55 E56 H57 F58 T59 P60 D61 S62 F63 K64 R65 E66 S67

N68 L71 L72 K73 E74 N75 A76 V77 P78 T79 I80 F81 L82 E83 L84 V85 P86 R87

• Molecule 2: DNA (5'-D(*GP*CP*TP*TP*GP*TP*GP*TP*GP*GP*GP*CP*AP*GP*CP*G)-3')

Chain B: 12% 81% 6%

G1 C2 T3 T4 G5 T6 G7 T8 G9 G10 A13 G14 C15 G16

• Molecule 3: DNA (5'-D(P*CP*GP*CP*TP*GP*CP*CP*CP*AP*CP*AP*CP*AP*AP*GP*C)-3')

Chain C: 19% 75% 6%

C17 G18 C19 T20 G21 C22 C23 C26 A27 C28 A29 A30 G31 C32

4.2.2 Score per residue for model 2

• Molecule 1: THAP domain-containing protein 1

Chain A: 26% 47% 17% • 8%

M1 V2 S6 A7 Y8 G9 C10 R13 Y14 D15 K16 D17 K18 P19 V20 S21 F22 H23 K24 F25 P26 R29 P30 S31 L32 C33 K34 E35 W36 V40 R41 N44 F45 K46 P47 T48 K49 Y50 S51 S52 I53 C54 S55 E56 H57 F58 T59 P60 D61 S62 F63 K64 R65 E66 S67

N68 L71 L72 K73 E74 N75 A76 V77 P78 T79 I80 F81 L82 E83 L84 V85 P86 R87

• Molecule 2: DNA (5'-D(*GP*CP*TP*TP*GP*TP*GP*TP*GP*GP*GP*CP*AP*GP*CP*G)-3')

Chain B: 88% 6% 6%

G1 C2 T3 T4 G5 T6 G7 T8 G9 G10 G11 C12 A13 G14 C15 G16

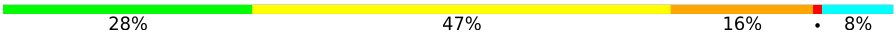
• Molecule 3: DNA (5'-D(P*CP*GP*CP*TP*GP*CP*CP*CP*AP*CP*AP*CP*AP*AP*GP*C)-3')

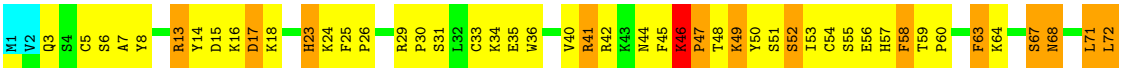
Chain C: 12% 81% 6%

4.2.3 Score per residue for model 3

• Molecule 1: THAP domain-containing protein 1

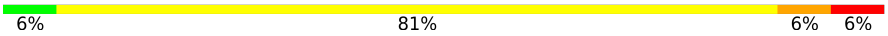
Chain A:

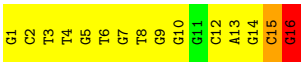




• Molecule 2: DNA (5'-D(*GP*CP*TP*TP*GP*TP*GP*TP*GP*GP*GP*CP*AP*GP*CP*G)-3')

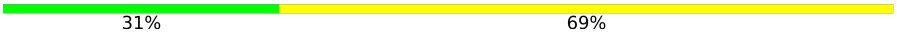
Chain B:

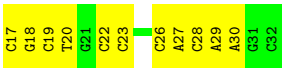




• Molecule 3: DNA (5'-D(P*CP*GP*CP*TP*GP*CP*CP*CP*AP*CP*AP*CP*AP*AP*GP*C)-3')

Chain C:

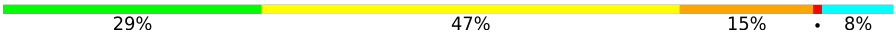


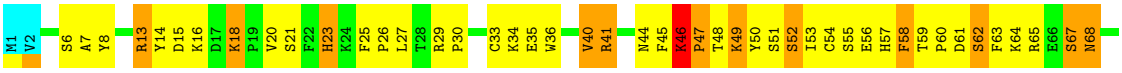


4.2.4 Score per residue for model 4

• Molecule 1: THAP domain-containing protein 1

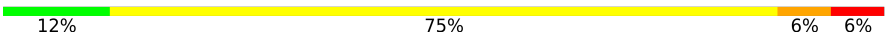
Chain A:

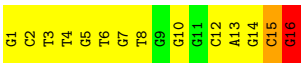




• Molecule 2: DNA (5'-D(*GP*CP*TP*TP*GP*TP*GP*TP*GP*GP*GP*CP*AP*GP*CP*G)-3')

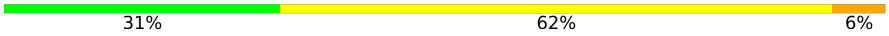
Chain B:

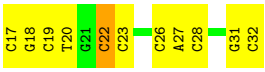




• Molecule 3: DNA (5'-D(P*CP*GP*CP*TP*GP*CP*CP*CP*AP*CP*AP*CP*AP*AP*GP*C)-3')

Chain C:

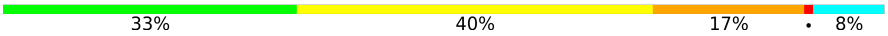


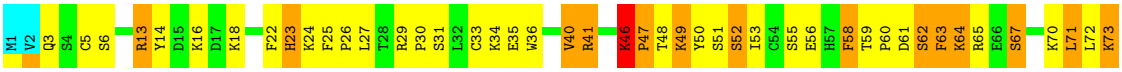


4.2.5 Score per residue for model 5

• Molecule 1: THAP domain-containing protein 1

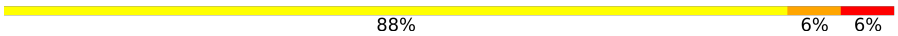
Chain A:

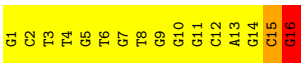




• Molecule 2: DNA (5'-D(*GP*CP*TP*TP*GP*TP*GP*TP*GP*GP*GP*CP*AP*GP*CP*G)-3')

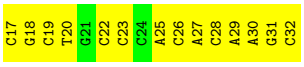
Chain B:





• Molecule 3: DNA (5'-D(P*CP*GP*CP*TP*GP*CP*CP*CP*AP*CP*AP*CP*AP*AP*GP*C)-3')

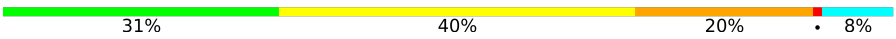
Chain C:

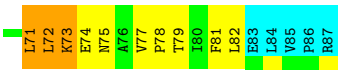


4.2.6 Score per residue for model 6

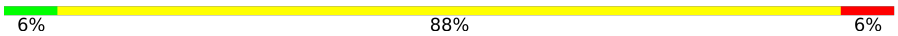
• Molecule 1: THAP domain-containing protein 1

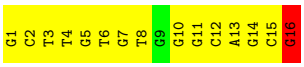
Chain A:



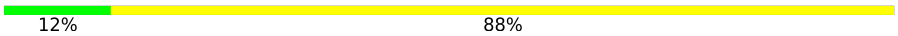


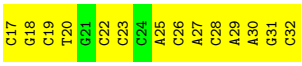
• Molecule 2: DNA (5'-D(*GP*CP*TP*TP*GP*TP*GP*TP*GP*GP*GP*CP*AP*GP*CP*G)-3')

Chain B: 



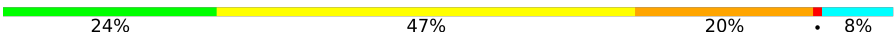
• Molecule 3: DNA (5'-D(P*CP*GP*CP*TP*GP*CP*CP*CP*AP*CP*AP*CP*AP*AP*GP*C)-3')

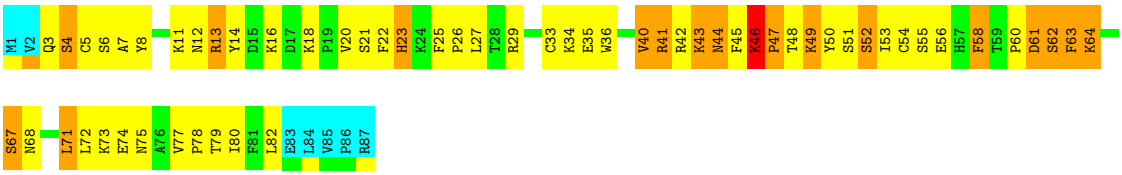
Chain C: 



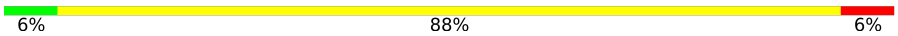
4.2.7 Score per residue for model 7

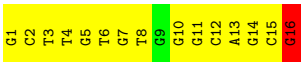
• Molecule 1: THAP domain-containing protein 1

Chain A: 



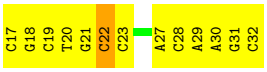
• Molecule 2: DNA (5'-D(*GP*CP*TP*TP*GP*TP*GP*TP*GP*GP*GP*CP*AP*GP*CP*G)-3')

Chain B: 



• Molecule 3: DNA (5'-D(P*CP*GP*CP*TP*GP*CP*CP*CP*AP*CP*AP*CP*AP*AP*GP*C)-3')

Chain C:



4.2.8 Score per residue for model 8

• Molecule 1: THAP domain-containing protein 1

Chain A: 25% 47% 16% • 8%

M1 V2 Q3 S4 C5 S6 A7 Y8 N12 R13 Y14 D15 K16 D17 K18 F22 H23 K24 F25 P26 R29 P30 S31 L32 C33 K34 E35 W36 V40 R41 R42 K46 P47 T48 K49 Y50 S51 S52 I53 C54 S55 E56 H57 F58 T59 P60 D61 S62 F63 K64 S67 N68 L71

L72 K73 E74 N75 A76 V77 P78 T79 I80 F81 L82 E83 L84 V85 P86 R87

• Molecule 2: DNA (5'-D(*GP*CP*TP*TP*GP*TP*GP*TP*GP*GP*GP*CP*AP*GP*CP*G)-3')

Chain B: 88% 6% 6%

G1 C2 T3 T4 G5 T6 G7 T8 G9 G10 G11 C12 A13 G14 C15 G16

• Molecule 3: DNA (5'-D(P*CP*GP*CP*TP*GP*CP*CP*CP*AP*CP*AP*CP*AP*AP*GP*C)-3')

Chain C: 19% 69% 12%

C17 G18 C19 T20 G21 C22 C23 C24 A25 C26 A27 C28 A29 A30 G31 C32

4.2.9 Score per residue for model 9

• Molecule 1: THAP domain-containing protein 1

Chain A: 30% 43% 18% • 8%

M1 V2 Q3 S4 C5 S6 A7 Y8 R13 Y14 D15 K16 D17 K18 S21 F22 H23 K24 F25 P26 R29 P30 S31 L32 C33 K34 E35 W36 V40 R41 R42 K43 N44 F45 K46 P47 T48 K49 Y50 S51 S52 I53 C54 S55 E56 H57 F58 T59 P60 D61 S62 F63 K64 S67 N68

L71 L72 K73 E74 N75 A76 V77 P78 T79 I80 F81 L82 E83 L84 V85 P86 R87

• Molecule 2: DNA (5'-D(*GP*CP*TP*TP*GP*TP*GP*TP*GP*GP*GP*CP*AP*GP*CP*G)-3')

Chain B: 6% 81% 6% 6%

G1 C2 T3 T4 G5 T6 G7 T8 G9 G10 G11 C12 A13 G14 C15 G16

• Molecule 3: DNA (5'-D(P*CP*GP*CP*TP*GP*CP*CP*CP*AP*CP*AP*CP*AP*AP*GP*C)-3')

Chain C: 12% 81% 6%

C17 G18 C19 T20 G21 C22 C23 C24 A25 C26 A27 C28 A29 A30 G31 C32

4.2.10 Score per residue for model 10

• Molecule 1: THAP domain-containing protein 1

Chain A: 26% 45% 18% • 8%

M1 V2 Q3 S4 C5 S6 A7 Y8 R13 Y14 D15 K16 D17 K18 F22 H23 K24 F25 P26 L27 T28 R29 P30 S31 L32 C33 K34 E35 W36 V40 R41 R42 K43 N44 F45 K46 P47 T48 K49 Y50 S51 S52 I53 C54 S55 E56 H57 F58 T59 P60 D61 S62 F63 K64 R65 E66 S67

N68 N69 K70 L71 L72 K73 E74 N75 A76 V77 P78 T79 I80 F81 L82 E83 L84 V85 P86 R87

• Molecule 2: DNA (5'-D(*GP*CP*TP*TP*GP*TP*GP*TP*GP*GP*GP*CP*AP*GP*CP*G)-3')

Chain B: 94% 6%

G1 C2 T3 T4 G5 T6 G7 T8 G9 G10 G11 C12 A13 G14 C15 G16

• Molecule 3: DNA (5'-D(P*CP*GP*CP*TP*GP*CP*CP*CP*AP*CP*AP*CP*AP*AP*GP*C)-3')

Chain C: 6% 88% 6%

C17 G18 C19 T20 G21 C22 C23 C24 A25 C26 A27 C28 A29 A30 G31 C32

4.2.11 Score per residue for model 11 (medoid)

• Molecule 1: THAP domain-containing protein 1

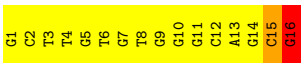
Chain A: 29% 44% 18% • 8%

M1 V2 Q3 S4 C5 S6 A7 N12 R13 Y14 D15 K16 D17 K18 S21 F22 H23 K24 F25 R29 P30 S31 L32 C33 K34 E35 W36 V40 R41 R42 K43 N44 F45 K46 P47 T48 K49 Y50 S51 S52 I53 C54 S55 E56 H57 F58 T59 P60 D61 S62 F63 K64 S67 N68

L71 L72 K73 E74 N75 A76 V77 P78 T79 I80 F81 L82 E83 L84 V85 P86 R87

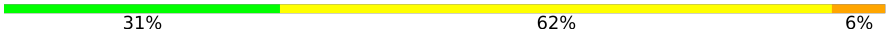
• Molecule 2: DNA (5'-D(*GP*CP*TP*TP*GP*TP*GP*TP*GP*GP*GP*CP*AP*GP*CP*G)-3')

Chain B: 88% 6% 6%



• Molecule 3: DNA (5'-D(P*CP*GP*CP*TP*GP*CP*CP*CP*AP*CP*AP*CP*AP*AP*GP*C)-3')

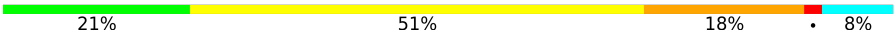
Chain C:

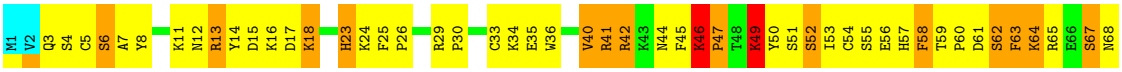


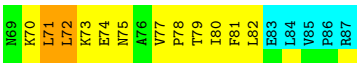
4.2.12 Score per residue for model 12

• Molecule 1: THAP domain-containing protein 1

Chain A:

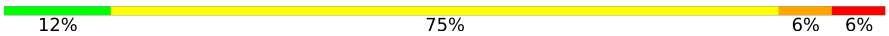


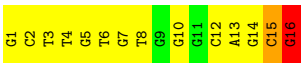




• Molecule 2: DNA (5'-D(*GP*CP*TP*TP*GP*TP*GP*TP*GP*GP*GP*CP*AP*GP*CP*G)-3')

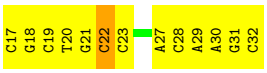
Chain B:





• Molecule 3: DNA (5'-D(P*CP*GP*CP*TP*GP*CP*CP*CP*AP*CP*AP*CP*AP*AP*GP*C)-3')

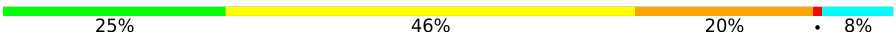
Chain C:

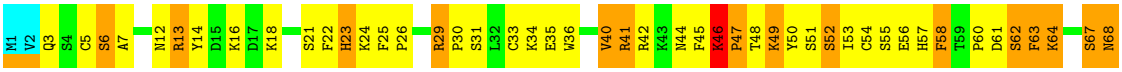


4.2.13 Score per residue for model 13

• Molecule 1: THAP domain-containing protein 1

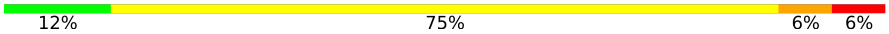
Chain A:

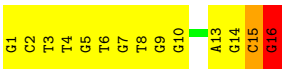




• Molecule 2: DNA (5'-D(*GP*CP*TP*TP*GP*TP*GP*TP*GP*GP*GP*CP*AP*GP*CP*G)-3')

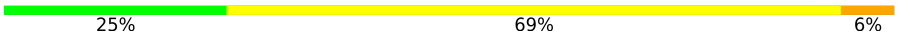
Chain B:





• Molecule 3: DNA (5'-D(P*CP*GP*CP*TP*GP*CP*CP*CP*AP*CP*AP*CP*AP*AP*GP*C)-3')

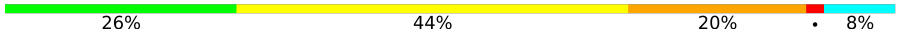
Chain C:

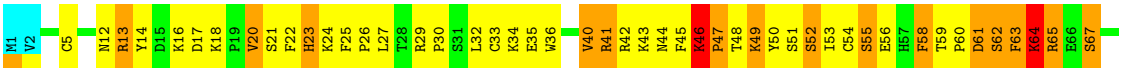


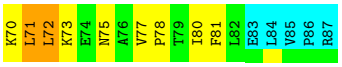
4.2.14 Score per residue for model 14

• Molecule 1: THAP domain-containing protein 1

Chain A:

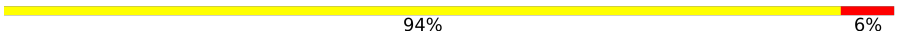


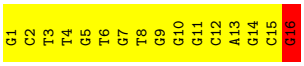




• Molecule 2: DNA (5'-D(*GP*CP*TP*TP*GP*TP*GP*TP*GP*GP*GP*CP*AP*GP*CP*G)-3')

Chain B:





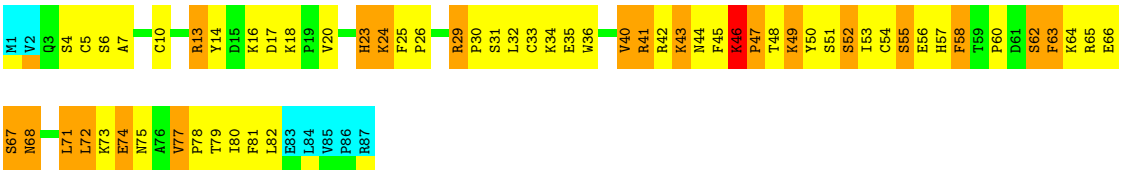
• Molecule 3: DNA (5'-D(P*CP*GP*CP*TP*GP*CP*CP*CP*AP*CP*AP*CP*AP*AP*GP*C)-3')

Chain C:

4.2.15 Score per residue for model 15

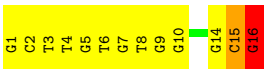
• Molecule 1: THAP domain-containing protein 1

Chain A: 22% 46% 23% • 8%



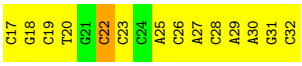
• Molecule 2: DNA (5'-D(*GP*CP*TP*TP*GP*TP*GP*TP*GP*GP*GP*CP*AP*GP*CP*G)-3')

Chain B: 19% 69% 6% 6%



• Molecule 3: DNA (5'-D(P*CP*GP*CP*TP*GP*CP*CP*CP*AP*CP*AP*CP*AP*AP*GP*C)-3')

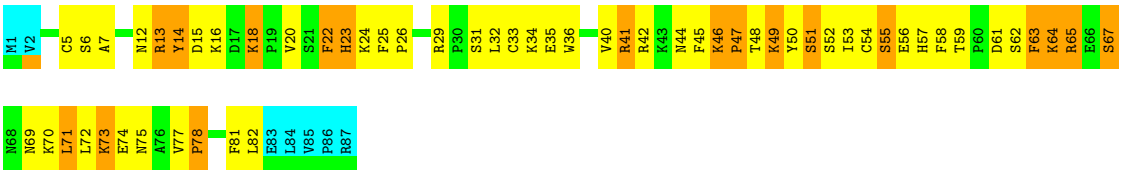
Chain C: 12% 81% 6%



4.2.16 Score per residue for model 16

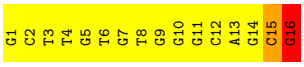
• Molecule 1: THAP domain-containing protein 1

Chain A: 25% 46% 21% 8%



• Molecule 2: DNA (5'-D(*GP*CP*TP*TP*GP*TP*GP*TP*GP*GP*GP*CP*AP*GP*CP*G)-3')

Chain B: 88% 6% 6%



• Molecule 3: DNA (5'-D(P*CP*GP*CP*TP*GP*CP*CP*CP*AP*CP*AP*CP*AP*AP*GP*C)-3')

Chain C: 19% 75% 6%

C17 G18 C19 T20 G21 C22 C23 A27 C28 A29 A30 G31 C32

4.2.17 Score per residue for model 17

• Molecule 1: THAP domain-containing protein 1

Chain A: 22% 49% 18% • 8%

M1 V2 Q3 S4 C5 S6 A7 Y8 G9 C10 R13 Y14 D15 K16 D17 K18 F22 H23 K24 F25 P26 L27 T28 R29 P30 S31 L32 C33 K34 E35 W36 V40 R41 R42 K43 N44 F45 K46 P47 T48 K49 Y50 S51 S52 I53 C54 S55 E56 H57 F58 T59 P60 D61 S62 F63 K64

S67 N68 N69 K70 L71 L72 K73 E74 N75 A76 V77 P78 T79 I80 F81 L82 E83 L84 V85 P86 R87

• Molecule 2: DNA (5'-D(*GP*CP*TP*TP*GP*TP*GP*TP*GP*GP*GP*CP*AP*GP*CP*G)-3')

Chain B: 12% 81% 6%

G1 C2 T3 T4 G5 T6 G7 T8 G9 G10 A13 G14 C15 G16

• Molecule 3: DNA (5'-D(P*CP*GP*CP*TP*GP*CP*CP*CP*AP*CP*AP*CP*AP*AP*GP*C)-3')

Chain C: 19% 81%

C17 G18 C19 T20 G21 C22 C23 C26 A27 C28 A29 A30 G31 C32

5 Refinement protocol and experimental data overview (i)

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

Of the 200 calculated structures, 17 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
CNS	refinement	1.21

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	0.50±0.02	0±0/676 (0.0± 0.0%)	0.78±0.02	0±0/910 (0.0± 0.0%)
2	B	0.42±0.02	0±0/371 (0.0± 0.0%)	0.84±0.01	2±0/573 (0.3± 0.0%)
3	C	0.31±0.02	0±0/360 (0.0± 0.0%)	0.69±0.01	0±0/551 (0.0± 0.0%)
All	All	0.44	0/23919 (0.0%)	0.77	34/34578 (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	1.6±0.5
3	C	0.0±0.0	0.8±0.5
All	All	0	42

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(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	16	DG	O4'-C4'-C3'	-6.70	101.82	104.50	1	17
2	B	16	DG	O4'-C1'-N9	6.46	112.52	108.00	7	17

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	17

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Mol	Chain	Res	Type	Group	Models (Total)
2	B	15	DC	Sidechain	11
3	C	22	DC	Sidechain	11
3	C	23	DC	Sidechain	3

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	657	653	652	40±5
2	B	331	181	182	47±2
3	C	322	178	178	25±3
All	All	22287	17204	17204	1781

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 45.

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	1.12	1.60	7	17
2:B:7:DG:C2'	2:B:8:DT:H71	0.94	1.91	5	10
2:B:14:DG:H2"	2:B:15:DC:C5	0.91	1.99	16	17
2:B:7:DG:H2'	2:B:8:DT:H72	0.91	1.41	6	7
1:A:25:PHE:HD2	1:A:33:CYS:HG	0.89	1.11	7	17
2:B:15:DC:C1'	2:B:16:DG:N7	0.88	2.35	12	17
2:B:1:DG:H2"	2:B:2:DC:C5	0.86	2.04	5	17
3:C:19:DC:C2'	3:C:20:DT:H72	0.84	2.03	11	7
3:C:19:DC:H2"	3:C:20:DT:C5	0.84	2.06	1	17
1:A:71:LEU:HD13	1:A:72:LEU:HD12	0.82	1.52	4	17
2:B:7:DG:H2'	2:B:8:DT:H71	0.82	1.50	15	10
3:C:18:DG:H2"	3:C:19:DC:C5	0.82	2.10	9	17
2:B:3:DT:H2"	2:B:4:DT:H71	0.81	1.50	9	17
2:B:7:DG:H2"	2:B:8:DT:H71	0.76	1.57	12	10
2:B:7:DG:C2'	2:B:8:DT:H72	0.76	2.09	9	7
1:A:67:SER:HB3	1:A:71:LEU:O	0.75	1.81	7	17
2:B:1:DG:H2"	2:B:2:DC:C6	0.75	2.15	5	17
2:B:11:DG:H2"	2:B:12:DC:C5	0.73	2.18	14	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:1:DG:C2'	2:B:2:DC:C5	0.73	2.72	5	17
3:C:27:DA:H2"	3:C:28:DC:C5	0.73	2.19	17	17
1:A:55:SER:HB3	1:A:63:PHE:CE1	0.72	2.19	14	1
3:C:19:DC:H2'	3:C:20:DT:H72	0.72	1.60	11	7
2:B:14:DG:C2'	2:B:15:DC:C5	0.72	2.71	16	17
1:A:62:SER:HA	1:A:73:LYS:CD	0.72	2.15	16	1
3:C:18:DG:H2"	3:C:19:DC:C6	0.71	2.21	9	17
2:B:6:DT:H1'	2:B:7:DG:C8	0.70	2.21	11	17
2:B:3:DT:H2"	2:B:4:DT:C7	0.70	2.17	9	17
2:B:2:DC:H2"	2:B:3:DT:H71	0.70	1.63	9	17
2:B:5:DG:H2"	2:B:6:DT:C5	0.69	2.22	17	16
2:B:7:DG:C2'	2:B:8:DT:C7	0.69	2.69	13	17
1:A:67:SER:OG	1:A:73:LYS:HD2	0.69	1.88	14	16
2:B:5:DG:H2"	2:B:6:DT:C7	0.69	2.17	17	17
2:B:15:DC:C2'	2:B:16:DG:N7	0.69	2.55	1	17
3:C:19:DC:H2"	3:C:20:DT:C7	0.69	2.18	5	17
2:B:5:DG:H2"	2:B:6:DT:H71	0.68	1.64	17	17
1:A:47:PRO:HB2	1:A:51:SER:OG	0.68	1.88	10	16
2:B:15:DC:H2"	2:B:16:DG:N7	0.68	2.02	1	17
2:B:3:DT:C2'	2:B:4:DT:H71	0.68	2.19	9	17
2:B:14:DG:H2"	2:B:15:DC:C6	0.68	2.24	7	17
2:B:16:DG:O5'	2:B:16:DG:C8	0.67	2.47	1	16
1:A:23:HIS:HE1	1:A:55:SER:N	0.67	1.88	15	17
1:A:25:PHE:CD1	1:A:53:ILE:HD11	0.66	2.26	16	15
2:B:7:DG:H2'	2:B:8:DT:C7	0.65	2.22	13	16
1:A:25:PHE:HD2	1:A:33:CYS:SG	0.65	2.14	12	17
1:A:24:LYS:HD3	2:B:8:DT:H72	0.65	1.67	5	4
2:B:15:DC:H1'	2:B:16:DG:C8	0.65	2.26	12	17
3:C:17:DC:H2"	3:C:18:DG:C8	0.64	2.26	2	17
3:C:18:DG:C2'	3:C:19:DC:C5	0.64	2.80	9	15
2:B:16:DG:C8	2:B:16:DG:O5'	0.64	2.50	12	1
3:C:19:DC:H2"	3:C:20:DT:H72	0.64	1.68	15	7
3:C:19:DC:C2'	3:C:20:DT:C7	0.63	2.75	5	16
3:C:26:DC:H2"	3:C:27:DA:C8	0.63	2.28	15	9
2:B:15:DC:C2	2:B:16:DG:O6	0.63	2.51	13	17
3:C:19:DC:H2"	3:C:20:DT:C6	0.62	2.29	5	15
1:A:50:TYR:CD2	3:C:22:DC:H2'	0.62	2.29	8	16
2:B:2:DC:C2'	2:B:3:DT:H71	0.62	2.24	8	17
1:A:48:THR:HG21	3:C:22:DC:OP2	0.62	1.95	1	14
1:A:50:TYR:HB2	3:C:22:DC:C5	0.62	2.29	12	17
1:A:36:TRP:O	1:A:40:VAL:HG23	0.61	1.95	14	17

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:5:DG:C2'	2:B:6:DT:H71	0.61	2.25	14	17
2:B:2:DC:H2"	2:B:3:DT:C7	0.61	2.26	6	17
2:B:7:DG:H2"	2:B:8:DT:C6	0.61	2.31	13	17
2:B:16:DG:O5'	2:B:16:DG:H8	0.60	1.79	3	17
1:A:40:VAL:HG22	1:A:81:PHE:HE2	0.60	1.56	16	2
1:A:60:PRO:HA	1:A:63:PHE:CD2	0.60	2.30	7	12
3:C:27:DA:H2"	3:C:28:DC:C6	0.60	2.31	15	17
1:A:62:SER:O	1:A:72:LEU:HD23	0.60	1.97	13	12
1:A:55:SER:HB2	1:A:63:PHE:CE1	0.60	2.31	5	10
1:A:6:SER:HA	1:A:46:LYS:CB	0.60	2.27	9	14
1:A:23:HIS:CE1	1:A:58:PHE:HE2	0.59	2.15	14	4
3:C:19:DC:H2"	3:C:20:DT:H71	0.59	1.74	6	10
1:A:50:TYR:CD1	3:C:23:DC:H5	0.59	2.15	13	16
2:B:6:DT:H2"	2:B:7:DG:C8	0.59	2.31	11	17
2:B:12:DC:H2"	2:B:13:DA:C8	0.59	2.31	6	11
2:B:3:DT:C2'	2:B:4:DT:C7	0.59	2.80	9	15
1:A:42:ARG:HG3	1:A:43:LYS:O	0.59	1.97	14	2
2:B:6:DT:C1'	2:B:7:DG:C8	0.58	2.86	11	17
3:C:28:DC:H2"	3:C:29:DA:C8	0.58	2.33	13	13
1:A:5:CYS:O	1:A:46:LYS:HD3	0.58	1.98	15	4
1:A:64:LYS:O	1:A:67:SER:HB3	0.58	1.99	14	2
1:A:52:SER:C	1:A:53:ILE:HD12	0.57	2.20	6	16
2:B:6:DT:C2	2:B:7:DG:C5	0.57	2.92	11	17
1:A:24:LYS:HG3	2:B:8:DT:H72	0.57	1.74	16	1
2:B:5:DG:C2'	2:B:6:DT:C7	0.57	2.82	17	16
1:A:26:PRO:HB3	1:A:72:LEU:CD1	0.57	2.29	8	12
3:C:19:DC:C2'	3:C:20:DT:C5	0.57	2.86	1	10
1:A:43:LYS:HG2	1:A:44:ASN:N	0.57	2.14	7	2
3:C:29:DA:H2"	3:C:30:DA:C8	0.56	2.36	5	10
2:B:13:DA:H2"	2:B:14:DG:C8	0.56	2.36	6	14
2:B:7:DG:H2"	2:B:8:DT:C7	0.55	2.29	7	12
3:C:27:DA:C2'	3:C:28:DC:C5	0.55	2.89	16	15
1:A:61:ASP:O	1:A:73:LYS:HD3	0.55	2.01	7	6
2:B:2:DC:C2'	2:B:3:DT:C7	0.55	2.84	8	17
1:A:49:LYS:HD2	1:A:49:LYS:H	0.55	1.62	14	1
1:A:47:PRO:HB2	1:A:51:SER:CB	0.55	2.31	8	2
1:A:3:GLN:NE2	3:C:20:DT:H71	0.55	2.17	12	3
3:C:19:DC:C2'	3:C:20:DT:H71	0.54	2.32	5	4
1:A:36:TRP:CE2	1:A:78:PRO:HD2	0.54	2.38	17	17
1:A:23:HIS:HE1	1:A:54:CYS:C	0.54	2.05	17	13
1:A:50:TYR:CE2	3:C:22:DC:H2'	0.54	2.38	8	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:31:DG:H2"	3:C:32:DC:C5	0.54	2.38	2	14
1:A:64:LYS:HD3	2:B:8:DT:OP1	0.54	2.02	7	4
1:A:23:HIS:CE1	1:A:55:SER:N	0.54	2.75	15	17
1:A:27:LEU:HD21	1:A:49:LYS:HG3	0.53	1.79	5	6
1:A:50:TYR:CD2	3:C:23:DC:H5	0.53	2.21	14	1
1:A:45:PHE:HD1	1:A:46:LYS:O	0.53	1.87	14	15
2:B:2:DC:H2"	2:B:3:DT:C5	0.53	2.39	2	16
1:A:25:PHE:CD2	1:A:49:LYS:HB3	0.53	2.39	9	9
1:A:26:PRO:HB3	1:A:72:LEU:HD13	0.53	1.81	2	12
2:B:15:DC:C2	2:B:16:DG:C6	0.52	2.97	1	17
2:B:2:DC:H2"	2:B:3:DT:C6	0.52	2.39	16	12
1:A:15:ASP:OD2	1:A:17:ASP:HB2	0.52	2.05	17	1
3:C:31:DG:H2"	3:C:32:DC:C6	0.52	2.40	17	9
1:A:67:SER:HB2	1:A:73:LYS:CE	0.52	2.34	16	1
3:C:17:DC:OP2	3:C:17:DC:C5	0.52	2.63	16	1
2:B:3:DT:H2"	2:B:4:DT:C5	0.51	2.40	5	8
2:B:9:DG:H2"	2:B:10:DG:OP2	0.51	2.05	8	13
1:A:60:PRO:O	1:A:63:PHE:HB2	0.51	2.04	10	2
1:A:15:ASP:O	1:A:18:LYS:HG2	0.51	2.04	12	3
1:A:57:HIS:O	1:A:78:PRO:HA	0.51	2.06	15	11
3:C:20:DT:H71	3:C:20:DT:OP2	0.51	2.05	16	4
1:A:61:ASP:O	1:A:67:SER:HA	0.50	2.07	14	1
1:A:30:PRO:O	1:A:33:CYS:HB3	0.50	2.07	2	12
3:C:17:DC:OP2	3:C:17:DC:C6	0.49	2.65	16	1
2:B:11:DG:H2"	2:B:12:DC:C6	0.49	2.42	14	1
2:B:5:DG:H2"	2:B:6:DT:C6	0.49	2.41	17	8
2:B:12:DC:H2"	2:B:13:DA:N7	0.49	2.22	6	2
2:B:11:DG:C2'	2:B:12:DC:C5	0.49	2.93	14	2
3:C:28:DC:C4	3:C:29:DA:N6	0.49	2.80	1	9
1:A:15:ASP:OD1	1:A:17:ASP:HB2	0.49	2.07	3	2
3:C:17:DC:H2"	3:C:18:DG:N7	0.49	2.22	6	5
1:A:33:CYS:SG	1:A:49:LYS:HD3	0.49	2.47	15	2
1:A:24:LYS:HB2	2:B:8:DT:H72	0.49	1.84	15	3
3:C:20:DT:H2"	3:C:21:DG:C8	0.49	2.43	12	1
1:A:32:LEU:HD21	1:A:76:ALA:O	0.49	2.07	17	1
1:A:8:TYR:CE1	1:A:42:ARG:HD3	0.49	2.43	6	2
2:B:14:DG:C4	2:B:15:DC:C4	0.48	3.01	13	6
1:A:67:SER:OG	1:A:68:ASN:N	0.48	2.47	13	14
1:A:8:TYR:CE1	1:A:82:LEU:HB2	0.48	2.44	10	1
1:A:65:ARG:HA	1:A:70:LYS:C	0.48	2.27	10	2
1:A:78:PRO:HB2	1:A:81:PHE:CE1	0.48	2.44	14	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:6:DT:C2'	2:B:7:DG:C8	0.48	2.96	11	7
1:A:23:HIS:CE1	1:A:58:PHE:CE2	0.48	3.02	1	3
1:A:65:ARG:HA	1:A:70:LYS:O	0.48	2.09	14	1
2:B:5:DG:C2'	2:B:6:DT:C5	0.48	2.96	17	2
1:A:4:SER:HB2	1:A:11:LYS:HA	0.47	1.86	7	3
1:A:23:HIS:HB3	2:B:8:DT:OP1	0.47	2.09	7	4
1:A:64:LYS:HG2	1:A:65:ARG:N	0.47	2.24	14	2
1:A:62:SER:OG	1:A:73:LYS:HG2	0.47	2.09	17	4
1:A:25:PHE:HD1	1:A:53:ILE:HD11	0.47	1.68	16	1
1:A:64:LYS:HG3	1:A:66:GLU:OE1	0.47	2.08	1	1
1:A:23:HIS:CE1	1:A:58:PHE:HE1	0.47	2.27	9	9
1:A:46:LYS:HG3	3:C:20:DT:OP1	0.47	2.10	7	2
1:A:47:PRO:HA	3:C:21:DG:OP2	0.47	2.09	16	2
1:A:62:SER:HA	1:A:73:LYS:HD3	0.47	1.87	16	1
1:A:61:ASP:C	1:A:73:LYS:HD3	0.47	2.30	12	5
2:B:10:DG:H2"	2:B:11:DG:OP2	0.47	2.10	6	2
1:A:29:ARG:HG2	1:A:32:LEU:CB	0.47	2.40	10	3
1:A:6:SER:HA	1:A:46:LYS:HB3	0.47	1.85	16	1
1:A:25:PHE:CE1	1:A:53:ILE:HD11	0.46	2.45	17	6
1:A:20:VAL:HB	1:A:55:SER:OG	0.46	2.10	14	5
1:A:62:SER:CB	1:A:73:LYS:HG2	0.46	2.40	1	3
1:A:23:HIS:CE1	1:A:58:PHE:CE1	0.46	3.03	13	10
1:A:25:PHE:CD1	1:A:49:LYS:HA	0.46	2.45	10	7
3:C:27:DA:C4	3:C:28:DC:C4	0.46	3.04	6	2
1:A:18:LYS:HZ2	1:A:20:VAL:HG22	0.46	1.71	14	1
1:A:49:LYS:HD2	1:A:49:LYS:N	0.46	2.25	14	1
1:A:10:CYS:SG	1:A:10:CYS:O	0.46	2.73	15	1
3:C:25:DA:H2"	3:C:26:DC:OP2	0.46	2.11	6	9
1:A:40:VAL:O	1:A:40:VAL:HG12	0.46	2.10	3	2
1:A:25:PHE:CD2	1:A:33:CYS:SG	0.46	3.08	13	5
1:A:8:TYR:CE2	1:A:42:ARG:HD3	0.45	2.45	12	1
1:A:49:LYS:H	1:A:49:LYS:CD	0.45	2.22	14	1
1:A:6:SER:O	1:A:40:VAL:HG13	0.45	2.11	2	3
2:B:1:DG:HO5'	2:B:1:DG:H8	0.45	1.53	15	1
1:A:72:LEU:HD12	1:A:72:LEU:H	0.45	1.71	12	7
1:A:62:SER:HA	1:A:73:LYS:HD2	0.45	1.88	16	1
1:A:23:HIS:O	1:A:53:ILE:N	0.45	2.46	8	2
2:B:6:DT:H2"	2:B:7:DG:OP2	0.45	2.12	9	5
1:A:10:CYS:O	1:A:10:CYS:SG	0.45	2.75	2	2
1:A:14:TYR:CD2	1:A:22:PHE:HD2	0.45	2.30	16	2
1:A:25:PHE:CG	1:A:49:LYS:HB3	0.44	2.47	3	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:6:DT:C1'	2:B:7:DG:N7	0.44	2.81	2	7
1:A:29:ARG:HG2	1:A:32:LEU:HB3	0.44	1.89	10	1
2:B:7:DG:H2"	2:B:8:DT:C5	0.44	2.47	13	3
1:A:64:LYS:HG2	1:A:65:ARG:H	0.44	1.72	14	1
1:A:50:TYR:CD2	3:C:22:DC:C6	0.43	3.06	6	4
1:A:60:PRO:HA	1:A:63:PHE:CE2	0.43	2.47	7	1
1:A:62:SER:HA	1:A:73:LYS:NZ	0.43	2.28	16	1
1:A:59:THR:O	1:A:62:SER:N	0.43	2.51	16	2
3:C:30:DA:H2"	3:C:31:DG:C8	0.43	2.49	16	4
1:A:3:GLN:HE22	3:C:20:DT:H73	0.43	1.73	5	1
1:A:60:PRO:HA	1:A:63:PHE:CG	0.43	2.48	11	4
1:A:71:LEU:CD1	1:A:72:LEU:HD12	0.43	2.40	13	1
1:A:46:LYS:HG3	3:C:20:DT:P	0.43	2.53	2	2
1:A:65:ARG:HD2	2:B:7:DG:H4'	0.43	1.88	16	2
1:A:46:LYS:CB	1:A:47:PRO:CD	0.43	2.97	3	17
1:A:3:GLN:NE2	3:C:20:DT:H73	0.42	2.29	7	3
3:C:21:DG:H2"	3:C:22:DC:C6	0.42	2.48	10	2
3:C:26:DC:C4	3:C:27:DA:N6	0.42	2.87	15	1
1:A:25:PHE:CD1	1:A:53:ILE:CD1	0.42	3.02	13	2
1:A:69:ASN:CG	1:A:70:LYS:N	0.42	2.72	16	1
1:A:48:THR:O	1:A:50:TYR:N	0.42	2.52	10	2
1:A:60:PRO:HA	1:A:63:PHE:CD1	0.42	2.50	17	1
2:B:15:DC:N3	2:B:16:DG:O6	0.42	2.51	9	1
1:A:23:HIS:HB3	2:B:8:DT:P	0.42	2.54	15	1
1:A:48:THR:HG23	3:C:21:DG:H2'	0.42	1.92	9	1
1:A:81:PHE:O	1:A:82:LEU:HG	0.42	2.15	10	1
1:A:50:TYR:HB3	3:C:23:DC:H41	0.41	1.75	16	1
1:A:77:VAL:O	1:A:79:THR:HG23	0.41	2.15	17	1
1:A:50:TYR:O	3:C:23:DC:N4	0.41	2.52	12	1
3:C:19:DC:H2'	3:C:20:DT:C7	0.41	2.45	5	1
1:A:45:PHE:O	3:C:20:DT:H3'	0.41	2.15	10	1
1:A:29:ARG:HD3	1:A:32:LEU:CB	0.41	2.45	15	1
1:A:47:PRO:HB2	1:A:51:SER:HB2	0.41	1.91	16	1
1:A:47:PRO:HB3	3:C:22:DC:N4	0.41	2.30	8	1
1:A:26:PRO:HB3	1:A:72:LEU:HD11	0.41	1.92	8	1
1:A:8:TYR:CZ	1:A:42:ARG:HD3	0.41	2.49	9	1
1:A:29:ARG:HD2	1:A:74:GLU:HB2	0.41	1.92	17	1
2:B:6:DT:C2	2:B:7:DG:N7	0.41	2.89	16	1
1:A:71:LEU:HD23	1:A:71:LEU:HA	0.41	1.77	6	2
1:A:64:LYS:HD2	2:B:8:DT:OP1	0.41	2.16	5	1
2:B:3:DT:H2"	2:B:4:DT:C6	0.41	2.50	11	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:TRP:CE2	1:A:78:PRO:CD	0.41	3.03	17	1
1:A:29:ARG:N	1:A:30:PRO:CD	0.41	2.83	15	2
1:A:67:SER:OG	1:A:73:LYS:HE3	0.41	2.14	16	1
3:C:21:DG:H2"	3:C:22:DC:C5	0.41	2.51	10	1
1:A:46:LYS:HG3	3:C:20:DT:OP2	0.41	2.15	13	1
1:A:77:VAL:HG23	1:A:78:PRO:HD2	0.41	1.92	15	1
1:A:67:SER:CB	1:A:71:LEU:O	0.41	2.63	16	1
3:C:17:DC:C6	3:C:17:DC:O5'	0.41	2.74	16	1
1:A:57:HIS:HD1	1:A:81:PHE:HA	0.40	1.75	8	1
1:A:50:TYR:CZ	3:C:23:DC:OP2	0.40	2.73	11	1
3:C:17:DC:C5	3:C:17:DC:OP2	0.40	2.75	14	1
1:A:8:TYR:CD1	1:A:42:ARG:HG2	0.40	2.51	12	1
2:B:6:DT:C4	2:B:7:DG:O6	0.40	2.75	2	1
1:A:45:PHE:CD1	1:A:46:LYS:O	0.40	2.72	11	3
1:A:50:TYR:CD1	3:C:23:DC:C5	0.40	3.04	13	1
1:A:67:SER:HB2	1:A:73:LYS:HZ1	0.40	1.76	16	1
1:A:50:TYR:CD2	3:C:22:DC:C2'	0.40	3.04	8	1
1:A:55:SER:HA	1:A:58:PHE:CE1	0.40	2.52	17	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	80/87 (92%)	57±2 (71±2%)	14±2 (18±2%)	9±1 (11±1%)	1 8
All	All	1360/1479 (92%)	970 (71%)	239 (18%)	151 (11%)	1 8

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	41	ARG	17
1	A	46	LYS	17
1	A	47	PRO	17
1	A	64	LYS	17

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Mol	Chain	Res	Type	Models (Total)
1	A	67	SER	17
1	A	13	ARG	16
1	A	7	ALA	15
1	A	74	GLU	14
1	A	40	VAL	11
1	A	72	LEU	6
1	A	49	LYS	3
1	A	63	PHE	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	75/82 (91%)	44±2 (58±3%)	31±2 (42±3%)	0 4
All	All	1275/1394 (91%)	744 (58%)	531 (42%)	0 4

All 53 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	17
1	A	14	TYR	17
1	A	16	LYS	17
1	A	23	HIS	17
1	A	34	LYS	17
1	A	41	ARG	17
1	A	49	LYS	17
1	A	52	SER	17
1	A	56	GLU	17
1	A	58	PHE	17
1	A	71	LEU	17
1	A	75	ASN	17
1	A	77	VAL	17
1	A	18	LYS	16
1	A	35	GLU	16
1	A	63	PHE	16
1	A	46	LYS	15

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Mol	Chain	Res	Type	Models (Total)
1	A	80	ILE	15
1	A	82	LEU	15
1	A	29	ARG	14
1	A	31	SER	13
1	A	44	ASN	13
1	A	22	PHE	12
1	A	62	SER	12
1	A	42	ARG	11
1	A	68	ASN	10
1	A	74	GLU	10
1	A	4	SER	9
1	A	8	TYR	9
1	A	17	ASP	9
1	A	73	LYS	9
1	A	21	SER	8
1	A	65	ARG	8
1	A	79	THR	8
1	A	5	CYS	8
1	A	59	THR	7
1	A	61	ASP	7
1	A	12	ASN	7
1	A	55	SER	4
1	A	70	LYS	4
1	A	25	PHE	3
1	A	45	PHE	3
1	A	64	LYS	3
1	A	66	GLU	2
1	A	43	LYS	2
1	A	6	SER	2
1	A	81	PHE	2
1	A	20	VAL	2
1	A	24	LYS	2
1	A	15	ASP	1
1	A	72	LEU	1
1	A	51	SER	1
1	A	78	PRO	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 (i)

No chemical shift data were provided