



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2022 – 11:33 PM EST

PDB ID : 2KOM  
Title : Solution structure of humar Par-3b PDZ2 (residues 451-549)  
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Deposited on : 2009-09-24

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : 2.27  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.27

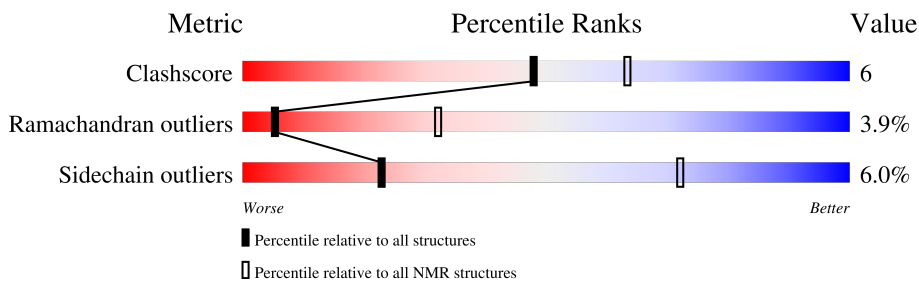
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	121	

## 2 Ensemble composition and analysis i

This entry contains 20 models. Model 16 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:458-A:477, A:487-A:546 (80)	0.35	16

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

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

The models can be grouped into 3 clusters. No single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1576 atoms, of which 810 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Partitioning defective 3 homolog.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	101	1576	478	810	139	148	1	0

There are 22 discrepancies between the modelled and reference sequences:

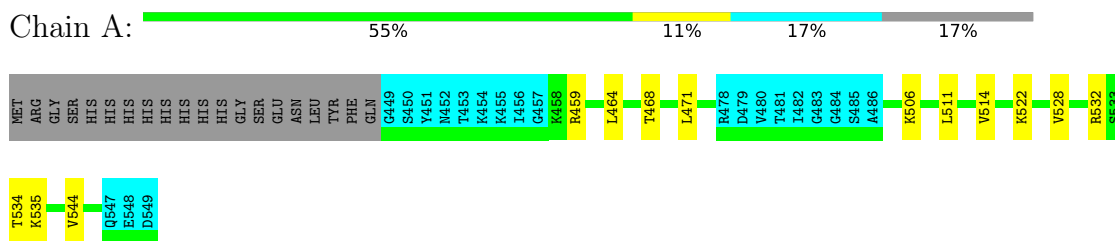
Chain	Residue	Modelled	Actual	Comment	Reference
A	429	MET	-	expression tag	UNP Q8TEW0
A	430	ARG	-	expression tag	UNP Q8TEW0
A	431	GLY	-	expression tag	UNP Q8TEW0
A	432	SER	-	expression tag	UNP Q8TEW0
A	433	HIS	-	expression tag	UNP Q8TEW0
A	434	HIS	-	expression tag	UNP Q8TEW0
A	435	HIS	-	expression tag	UNP Q8TEW0
A	436	HIS	-	expression tag	UNP Q8TEW0
A	437	HIS	-	expression tag	UNP Q8TEW0
A	438	HIS	-	expression tag	UNP Q8TEW0
A	439	HIS	-	expression tag	UNP Q8TEW0
A	440	HIS	-	expression tag	UNP Q8TEW0
A	441	GLY	-	expression tag	UNP Q8TEW0
A	442	SER	-	expression tag	UNP Q8TEW0
A	443	GLU	-	expression tag	UNP Q8TEW0
A	444	ASN	-	expression tag	UNP Q8TEW0
A	445	LEU	-	expression tag	UNP Q8TEW0
A	446	TYR	-	expression tag	UNP Q8TEW0
A	447	PHE	-	expression tag	UNP Q8TEW0
A	448	GLN	-	expression tag	UNP Q8TEW0
A	449	GLY	-	expression tag	UNP Q8TEW0
A	450	SER	-	expression tag	UNP Q8TEW0

## 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: Partitioning defective 3 homolog

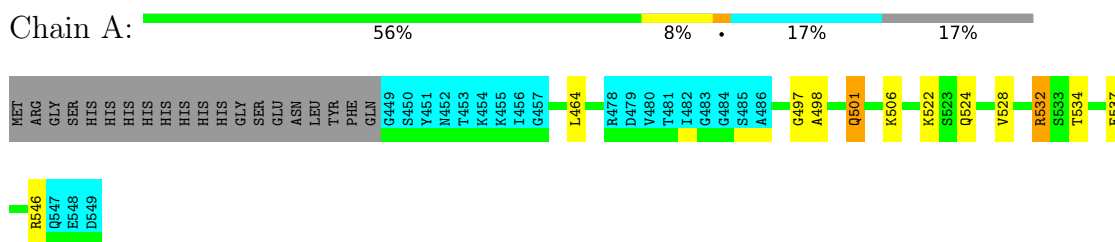


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

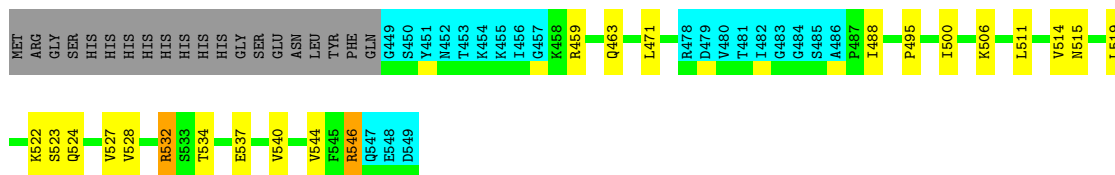
- Molecule 1: Partitioning defective 3 homolog



#### 4.2.2 Score per residue for model 2

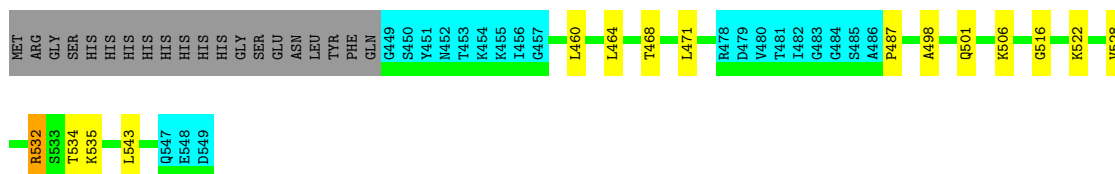
- Molecule 1: Partitioning defective 3 homolog





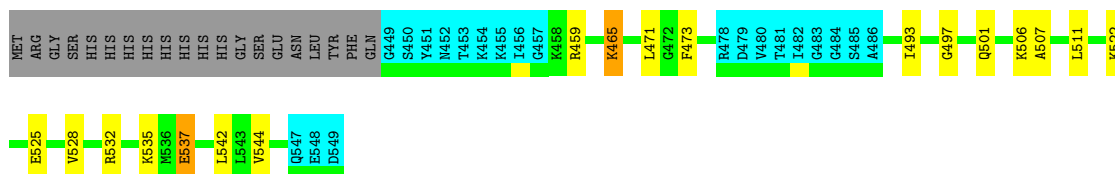
### 4.2.3 Score per residue for model 3

- Molecule 1: Partitioning defective 3 homolog



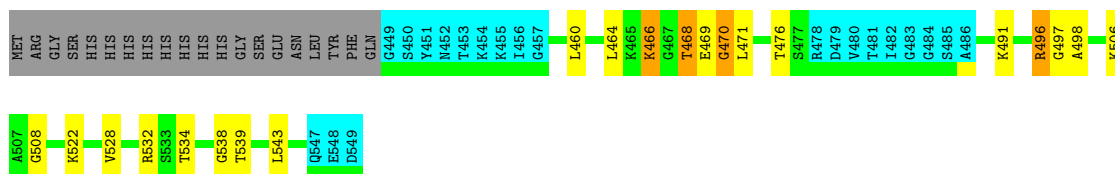
### 4.2.4 Score per residue for model 4

- Molecule 1: Partitioning defective 3 homolog



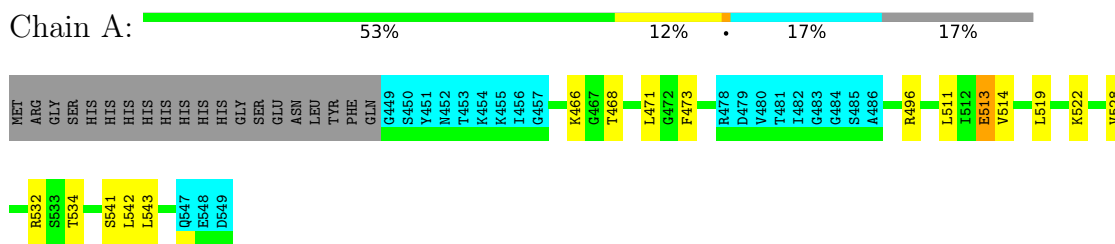
### 4.2.5 Score per residue for model 5

- Molecule 1: Partitioning defective 3 homolog



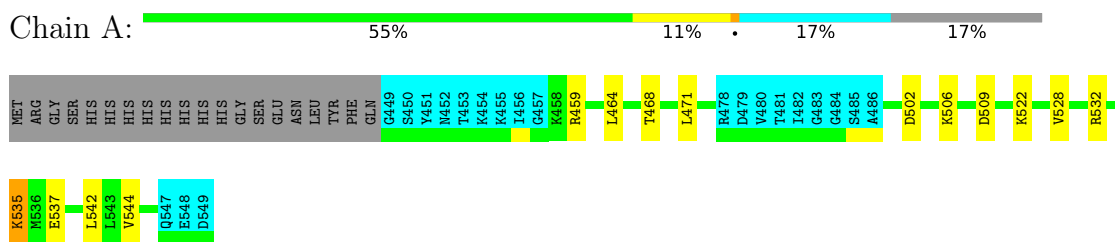
### 4.2.6 Score per residue for model 6

- Molecule 1: Partitioning defective 3 homolog



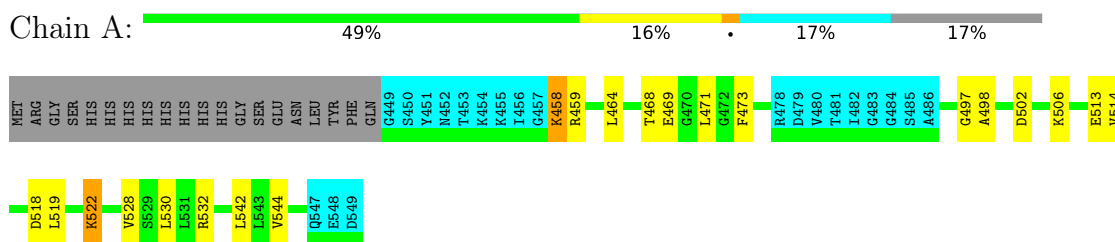
#### 4.2.7 Score per residue for model 7

- Molecule 1: Partitioning defective 3 homolog



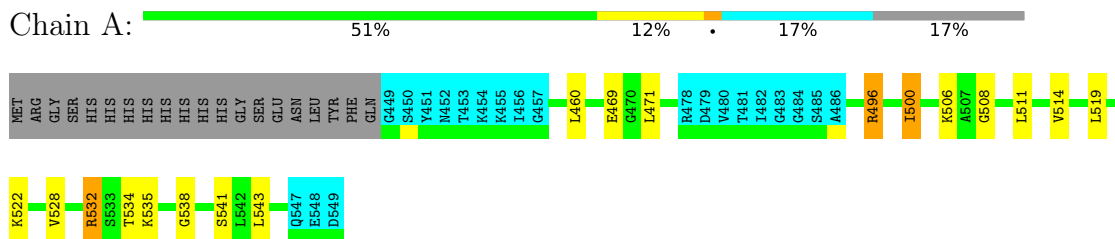
#### 4.2.8 Score per residue for model 8

- Molecule 1: Partitioning defective 3 homolog



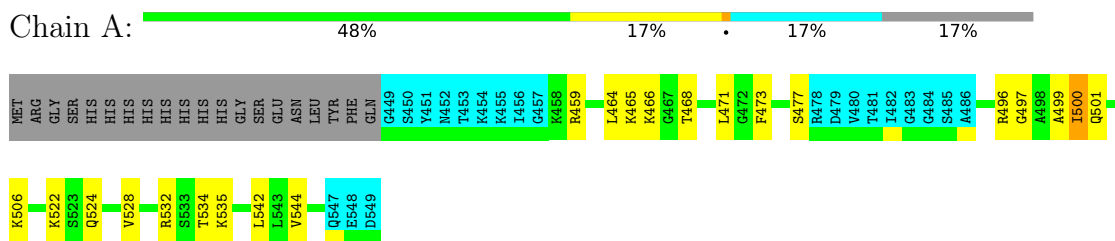
#### 4.2.9 Score per residue for model 9

- Molecule 1: Partitioning defective 3 homolog



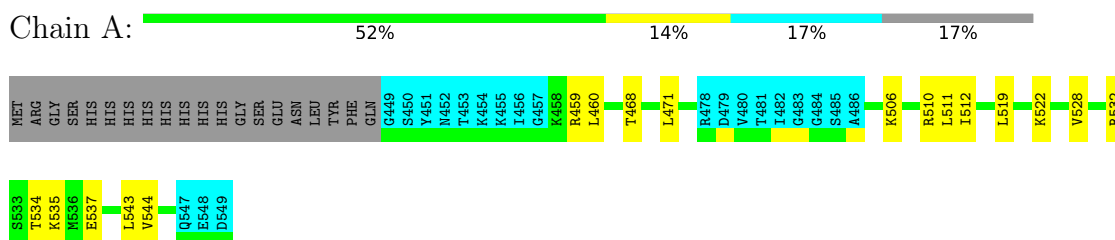
#### 4.2.10 Score per residue for model 10

- Molecule 1: Partitioning defective 3 homolog



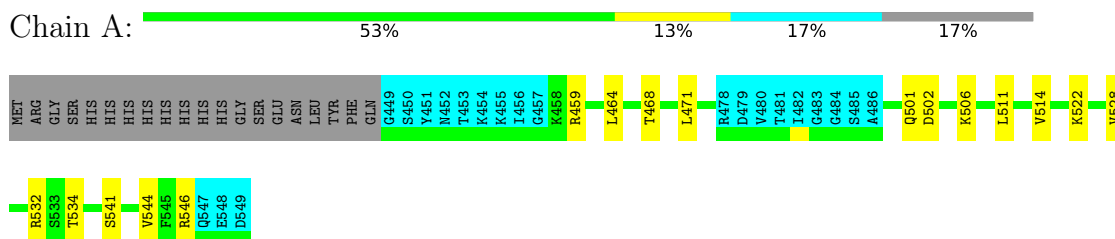
#### 4.2.11 Score per residue for model 11

- Molecule 1: Partitioning defective 3 homolog



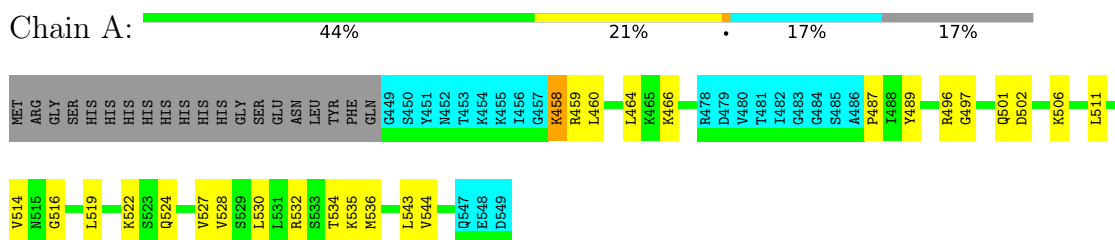
#### 4.2.12 Score per residue for model 12

- Molecule 1: Partitioning defective 3 homolog



#### 4.2.13 Score per residue for model 13

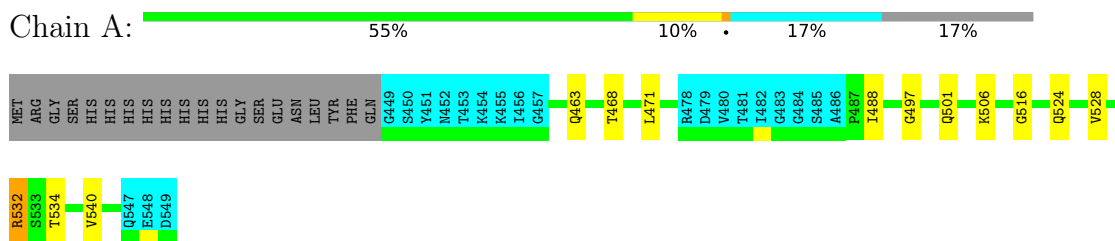
- Molecule 1: Partitioning defective 3 homolog





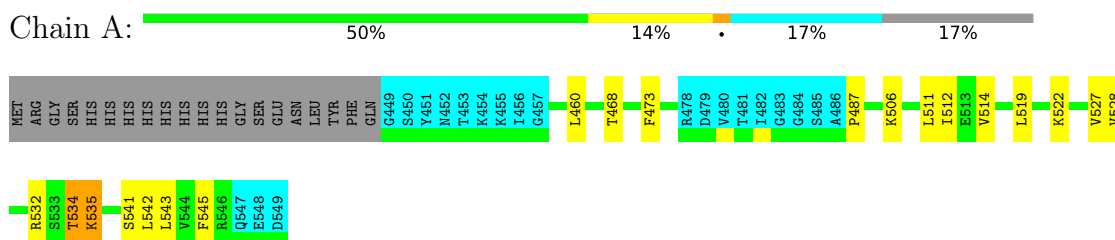
#### 4.2.14 Score per residue for model 14

- Molecule 1: Partitioning defective 3 homolog



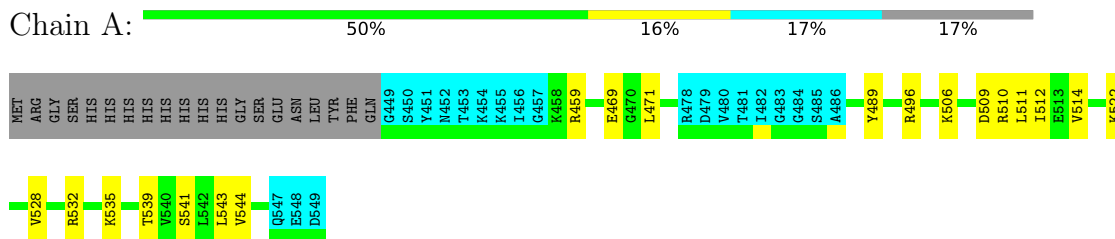
#### 4.2.15 Score per residue for model 15

- Molecule 1: Partitioning defective 3 homolog



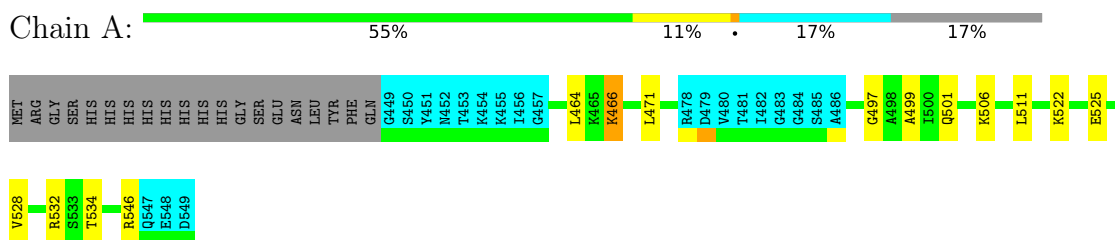
#### 4.2.16 Score per residue for model 16 (medoid)

- Molecule 1: Partitioning defective 3 homolog



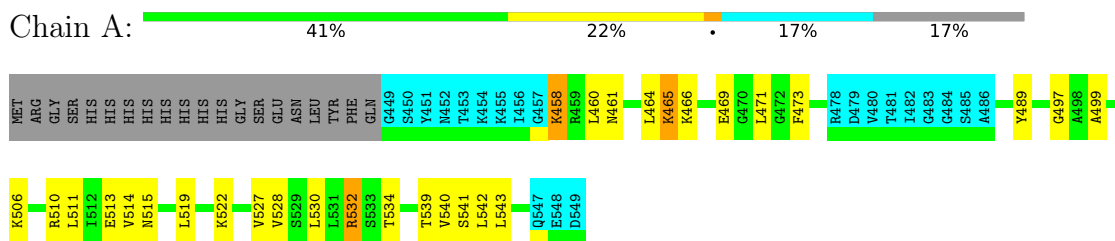
#### 4.2.17 Score per residue for model 17

- Molecule 1: Partitioning defective 3 homolog



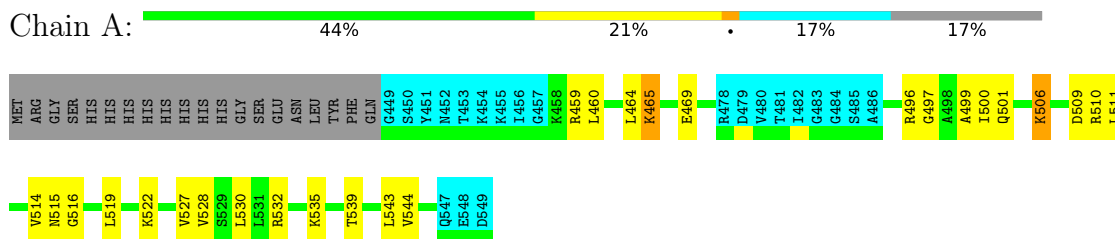
### 4.2.18 Score per residue for model 18

- Molecule 1: Partitioning defective 3 homolog



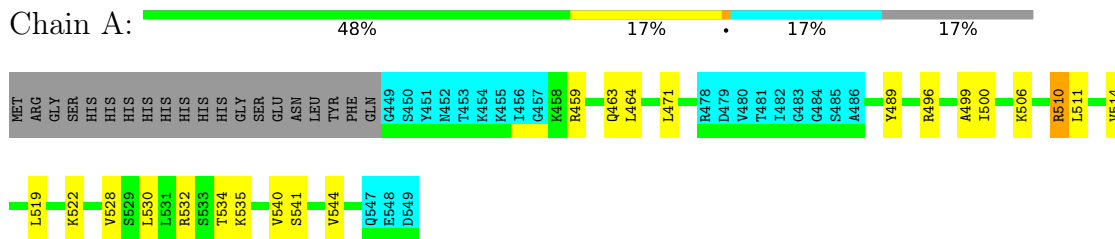
### 4.2.19 Score per residue for model 19

- Molecule 1: Partitioning defective 3 homolog



### 4.2.20 Score per residue for model 20

- Molecule 1: Partitioning defective 3 homolog



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *AUTOMATED METHODS WERE USED FOR BACKBONE CHEMICAL SHIFT ASSIGNMENT AND ITERATIVE NOE REFINEMENT. FINAL STRUCTURES WERE OBTAINED BY MOLECULAR DYNAMICS IN EXPLICIT SOLVENT.*

Of the 100 calculated structures, 20 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
Xplor-NIH	refinement	2.9.3

No chemical shift data was provided.

## 6 Model quality i

### 6.1 Standard geometry i

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts i

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	612	662	662	8±4
All	All	12240	13240	13240	160

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 6.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:465:LYS:HE3	1:A:465:LYS:N	0.67	2.05	4	3
1:A:535:LYS:HE2	1:A:539:THR:O	0.62	1.94	16	1
1:A:511:LEU:HB3	1:A:519:LEU:CD1	0.61	2.25	18	8
1:A:528:VAL:O	1:A:532:ARG:HG3	0.61	1.96	16	2
1:A:468:THR:HB	1:A:496:ARG:O	0.61	1.95	5	2
1:A:514:VAL:HA	1:A:541:SER:O	0.60	1.97	18	7
1:A:528:VAL:O	1:A:532:ARG:HG2	0.59	1.98	12	18
1:A:514:VAL:HG13	1:A:530:LEU:HD11	0.58	1.73	19	5
1:A:464:LEU:HD21	1:A:499:ALA:HA	0.56	1.77	17	1
1:A:458:LYS:H	1:A:458:LYS:HE2	0.55	1.60	13	1
1:A:514:VAL:HG12	1:A:519:LEU:HD21	0.54	1.78	20	6
1:A:511:LEU:HB3	1:A:519:LEU:HD12	0.54	1.80	2	3
1:A:469:GLU:HB3	1:A:497:GLY:CA	0.53	2.34	8	1
1:A:509:ASP:OD1	1:A:544:VAL:HB	0.53	2.03	16	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:477:SER:HB3	1:A:524:GLN:OE1	0.53	2.03	10	1
1:A:473:PHE:CZ	1:A:542:LEU:HD11	0.53	2.38	10	5
1:A:510:ARG:O	1:A:544:VAL:HA	0.52	2.05	19	1
1:A:515:ASN:ND2	1:A:540:VAL:HG13	0.52	2.20	18	1
1:A:471:LEU:H	1:A:498:ALA:CB	0.51	2.19	5	1
1:A:464:LEU:HD13	1:A:502:ASP:HB2	0.50	1.83	8	4
1:A:496:ARG:HA	1:A:500:ILE:HG21	0.50	1.82	20	2
1:A:489:TYR:CE1	1:A:510:ARG:HD3	0.50	2.41	16	1
1:A:460:LEU:O	1:A:543:LEU:HA	0.49	2.07	13	8
1:A:497:GLY:O	1:A:501:GLN:HG2	0.49	2.06	14	6
1:A:527:VAL:O	1:A:530:LEU:HG	0.49	2.07	19	3
1:A:473:PHE:CE2	1:A:542:LEU:HD11	0.48	2.44	8	1
1:A:464:LEU:CD2	1:A:499:ALA:HA	0.48	2.37	19	3
1:A:535:LYS:HE3	1:A:537:GLU:OE1	0.48	2.09	4	1
1:A:488:ILE:HD12	1:A:524:GLN:HE21	0.47	1.69	2	1
1:A:469:GLU:HB3	1:A:497:GLY:HA2	0.47	1.86	8	1
1:A:459:ARG:HA	1:A:544:VAL:O	0.47	2.09	10	11
1:A:476:THR:HB	1:A:491:LYS:HE3	0.47	1.87	5	1
1:A:535:LYS:HE3	1:A:535:LYS:HA	0.47	1.86	7	1
1:A:487:PRO:HB2	1:A:489:TYR:CE2	0.47	2.45	13	1
1:A:518:ASP:O	1:A:522:LYS:HE2	0.47	2.10	8	1
1:A:458:LYS:HE2	1:A:458:LYS:N	0.46	2.24	13	1
1:A:496:ARG:N	1:A:500:ILE:HG21	0.46	2.26	10	2
1:A:510:ARG:NH1	1:A:512:ILE:HD13	0.46	2.26	11	1
1:A:489:TYR:CE2	1:A:510:ARG:HB2	0.45	2.46	20	1
1:A:525:GLU:HA	1:A:528:VAL:HG22	0.45	1.88	4	2
1:A:463:GLN:HA	1:A:540:VAL:O	0.45	2.12	20	3
1:A:468:THR:O	1:A:497:GLY:HA2	0.44	2.11	8	1
1:A:523:SER:O	1:A:527:VAL:HG23	0.44	2.12	2	1
1:A:493:ILE:HG12	1:A:507:ALA:HB2	0.44	1.90	4	1
1:A:469:GLU:HB2	1:A:497:GLY:HA2	0.44	1.89	5	3
1:A:512:ILE:O	1:A:519:LEU:HG	0.44	2.12	11	2
1:A:512:ILE:HB	1:A:543:LEU:HD12	0.44	1.90	16	1
1:A:466:LYS:HG3	1:A:470:GLY:HA3	0.44	1.89	5	1
1:A:546:ARG:O	1:A:546:ARG:HD3	0.43	2.13	2	1
1:A:471:LEU:H	1:A:498:ALA:HB2	0.43	1.73	8	1
1:A:506:LYS:HD2	1:A:509:ASP:OD2	0.43	2.14	19	1
1:A:496:ARG:HA	1:A:500:ILE:CG2	0.43	2.44	20	1
1:A:466:LYS:HE3	1:A:534:THR:HG21	0.43	1.89	18	1
1:A:512:ILE:CG1	1:A:545:PHE:HB2	0.43	2.44	15	1
1:A:524:GLN:O	1:A:528:VAL:HG13	0.43	2.13	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:519:LEU:HD22	1:A:527:VAL:HG13	0.42	1.90	15	1
1:A:464:LEU:HD12	1:A:498:ALA:O	0.42	2.15	3	1
1:A:489:TYR:CE1	1:A:510:ARG:HB2	0.42	2.50	18	1
1:A:515:ASN:HD21	1:A:535:LYS:HB2	0.42	1.75	19	1
1:A:458:LYS:HA	1:A:458:LYS:HE3	0.42	1.92	18	2
1:A:488:ILE:HD12	1:A:524:GLN:OE1	0.42	2.15	14	1
1:A:464:LEU:HD23	1:A:542:LEU:HD23	0.41	1.92	7	1
1:A:534:THR:O	1:A:535:LYS:HB2	0.41	2.15	15	1
1:A:495:PRO:O	1:A:500:ILE:HD13	0.41	2.15	2	1
1:A:464:LEU:CD1	1:A:499:ALA:HA	0.41	2.45	10	1
1:A:497:GLY:O	1:A:501:GLN:HB2	0.41	2.15	1	1
1:A:464:LEU:HB3	1:A:498:ALA:HB1	0.41	1.92	1	1
1:A:464:LEU:O	1:A:539:THR:HA	0.41	2.15	5	1
1:A:532:ARG:HE	1:A:532:ARG:HA	0.41	1.76	1	1
1:A:513:GLU:HG3	1:A:543:LEU:CB	0.40	2.46	6	1
1:A:466:LYS:HE2	1:A:534:THR:HG21	0.40	1.93	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	80/121 (66%)	70±2 (88±2%)	6±2 (8±2%)	3±2 (4±2%)	5	32
All	All	1600/2420 (66%)	1407 (88%)	130 (8%)	63 (4%)	5	32

All 11 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	471	LEU	14
1	A	534	THR	13
1	A	468	THR	8
1	A	535	LYS	8
1	A	466	LYS	5
1	A	496	ARG	5

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Mol	Chain	Res	Type	Models (Total)
1	A	516	GLY	4
1	A	508	GLY	2
1	A	538	GLY	2
1	A	470	GLY	1
1	A	537	GLU	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	68/102 (67%)	64±2 (94±2%)	4±2 (6±2%)	23 72
All	All	1360/2040 (67%)	1279 (94%)	81 (6%)	23 72

All 18 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	506	LYS	19
1	A	522	LYS	19
1	A	532	ARG	6
1	A	511	LEU	5
1	A	537	GLU	4
1	A	546	ARG	4
1	A	465	LYS	4
1	A	501	GLN	3
1	A	513	GLU	3
1	A	458	LYS	3
1	A	469	GLU	2
1	A	500	ILE	2
1	A	539	THR	2
1	A	515	ASN	1
1	A	487	PRO	1
1	A	536	MET	1
1	A	461	ASN	1
1	A	510	ARG	1

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

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

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