



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 05:47 PM BST

PDB ID : 1WID  
Title : Solution Structure of the B3 DNA-Binding Domain of RAV1  
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Deposited on : 2004-05-28

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)  
NmrClust : Kelley et al. (1996)  
MolProbity : 4.02b-467  
Mogul : unknown  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : rb-20027457  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027457

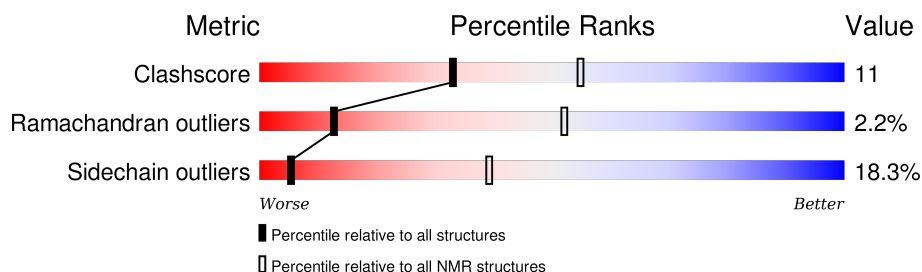
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment was not calculated.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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

Mol	Chain	Length	Quality of chain
1	A	130	

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 13 is the overall representative, medoid model (most similar to other models). The authors have identified model 15 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:184-A:197, A:202-A:215, A:226-A:245, A:249-A:278, A:283-A:290 (86)	0.38	13

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

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

The models can be grouped into 3 clusters and 2 single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1875 atoms, of which 932 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called DNA-binding protein RAV1.

Mol	Chain	Residues	Atoms					Trace
1	A	117	Total	C	H	N	O	0
			1875	599	932	172	172	

There are 13 discrepancies between the modelled and reference sequences:

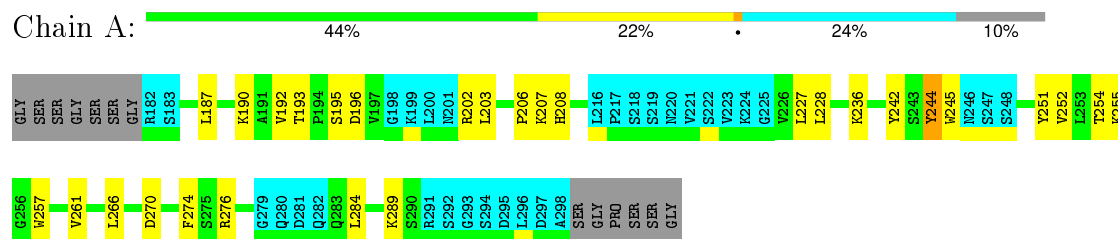
Chain	Residue	Modelled	Actual	Comment	Reference
A	175	GLY	-	CLONING ARTIFACT	UNP Q9ZWM9
A	176	SER	-	CLONING ARTIFACT	UNP Q9ZWM9
A	177	SER	-	CLONING ARTIFACT	UNP Q9ZWM9
A	178	GLY	-	CLONING ARTIFACT	UNP Q9ZWM9
A	179	SER	-	CLONING ARTIFACT	UNP Q9ZWM9
A	180	SER	-	CLONING ARTIFACT	UNP Q9ZWM9
A	181	GLY	-	CLONING ARTIFACT	UNP Q9ZWM9
A	299	SER	-	CLONING ARTIFACT	UNP Q9ZWM9
A	300	GLY	-	CLONING ARTIFACT	UNP Q9ZWM9
A	301	PRO	-	CLONING ARTIFACT	UNP Q9ZWM9
A	302	SER	-	CLONING ARTIFACT	UNP Q9ZWM9
A	303	SER	-	CLONING ARTIFACT	UNP Q9ZWM9
A	304	GLY	-	CLONING ARTIFACT	UNP Q9ZWM9

## 4 Residue-property plots

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

These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: DNA-binding protein RAV1

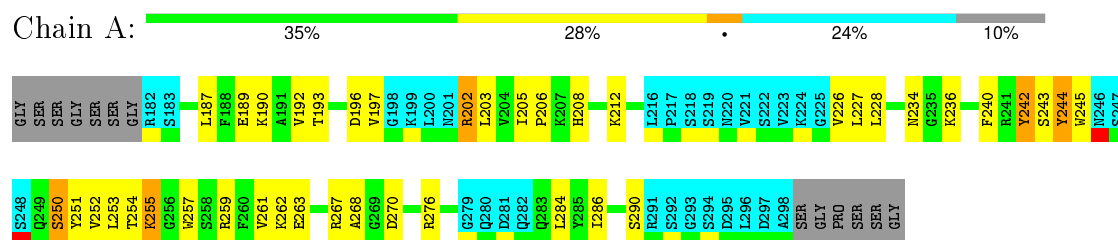


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

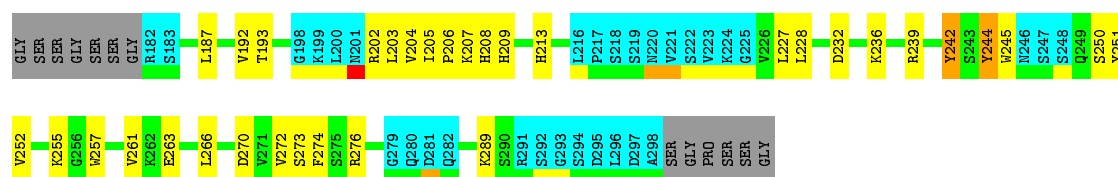
- Molecule 1: DNA-binding protein RAV1



#### 4.2.2 Score per residue for model 2

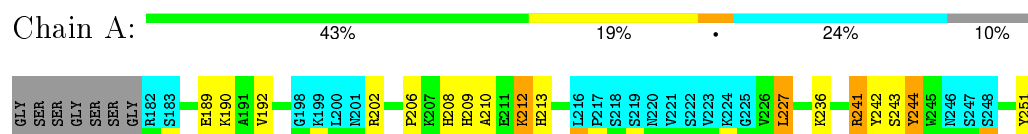
- Molecule 1: DNA-binding protein RAV1





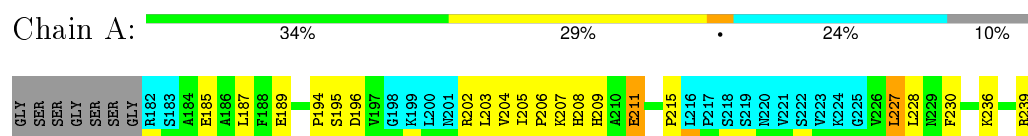
### 4.2.3 Score per residue for model 3

- Molecule 1: DNA-binding protein RAV1



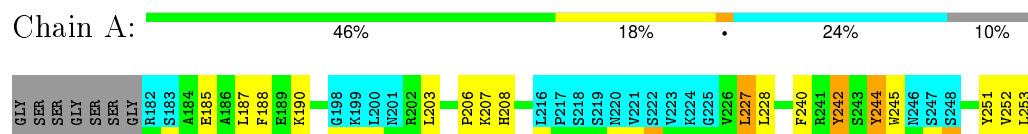
### 4.2.4 Score per residue for model 4

- Molecule 1: DNA-binding protein RAV1



### 4.2.5 Score per residue for model 5

- Molecule 1: DNA-binding protein RAV1



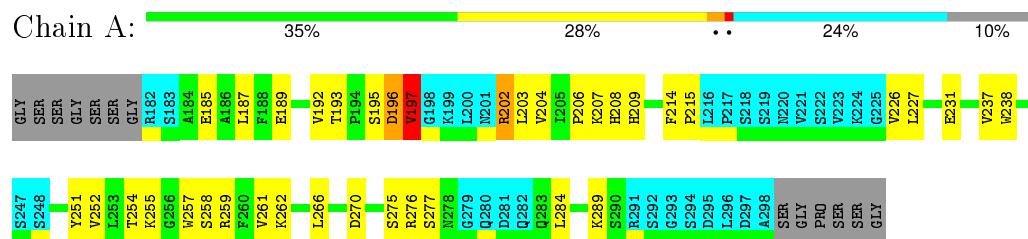
### 4.2.6 Score per residue for model 6

- Molecule 1: DNA-binding protein RAV1



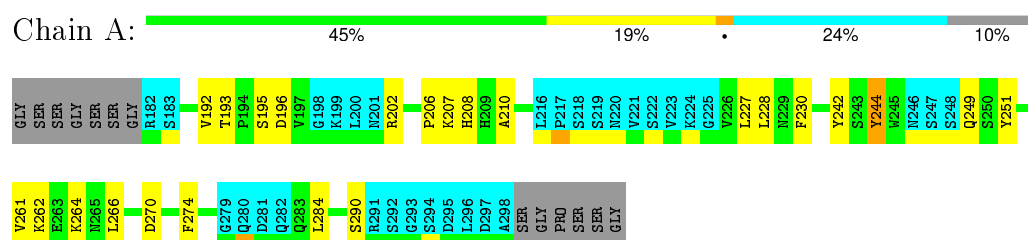
### 4.2.10 Score per residue for model 10

- Molecule 1: DNA-binding protein RAV1



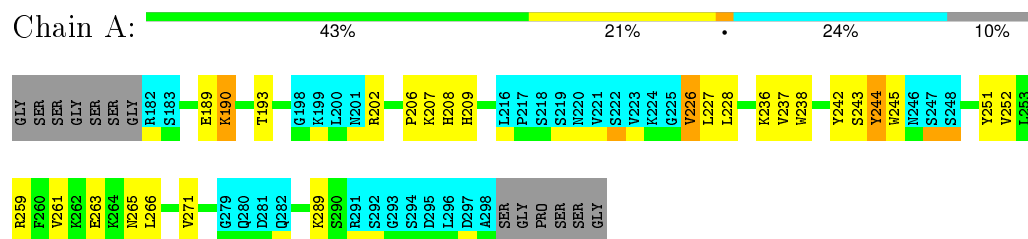
### 4.2.11 Score per residue for model 11

- Molecule 1: DNA-binding protein RAV1



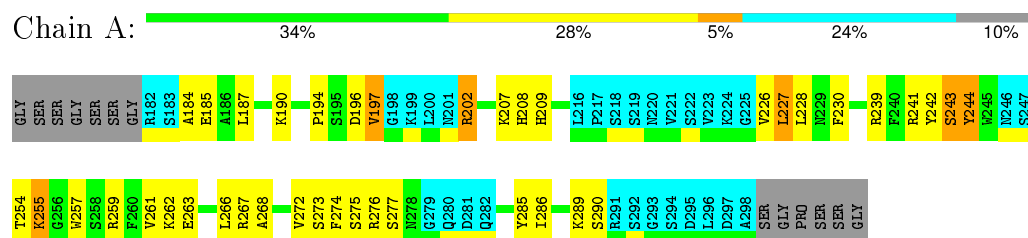
### 4.2.12 Score per residue for model 12

- Molecule 1: DNA-binding protein RAV1



### 4.2.13 Score per residue for model 13 (medoid)

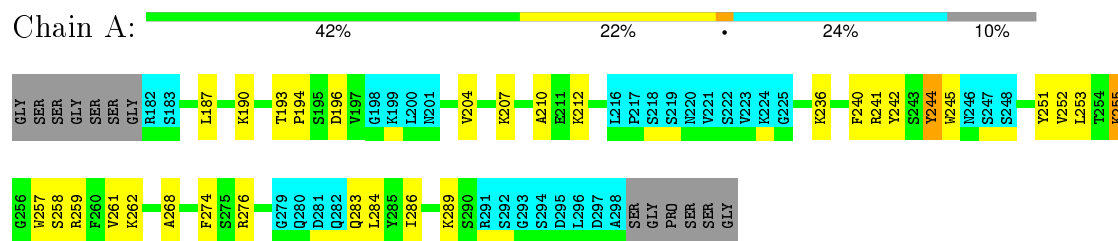
- Molecule 1: DNA-binding protein RAV1





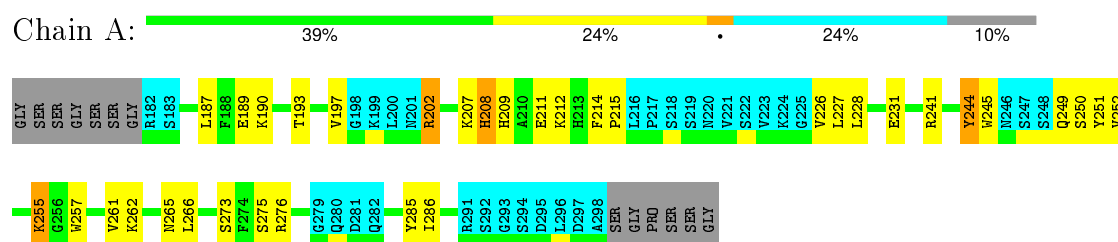
#### 4.2.14 Score per residue for model 14

- Molecule 1: DNA-binding protein RAV1



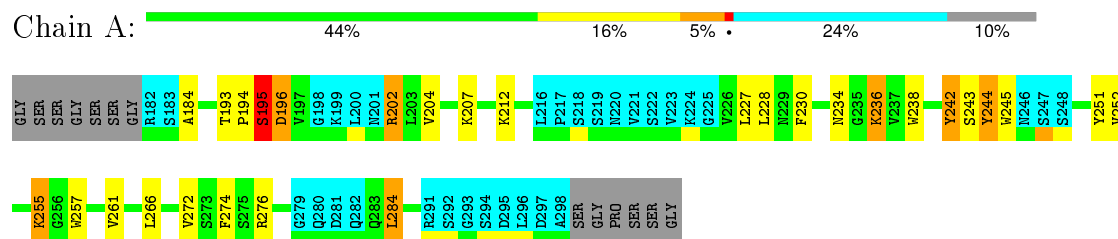
#### 4.2.15 Score per residue for model 15

- Molecule 1: DNA-binding protein RAV1



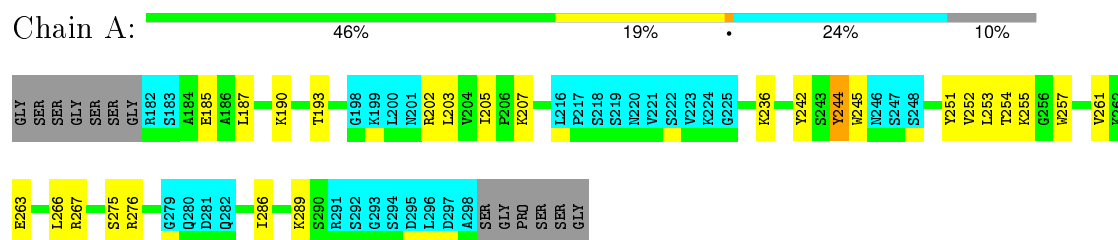
#### 4.2.16 Score per residue for model 16

- Molecule 1: DNA-binding protein RAV1



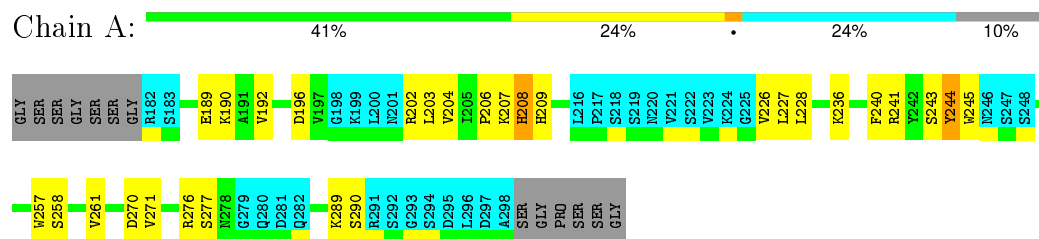
#### 4.2.17 Score per residue for model 17

- Molecule 1: DNA-binding protein RAV1



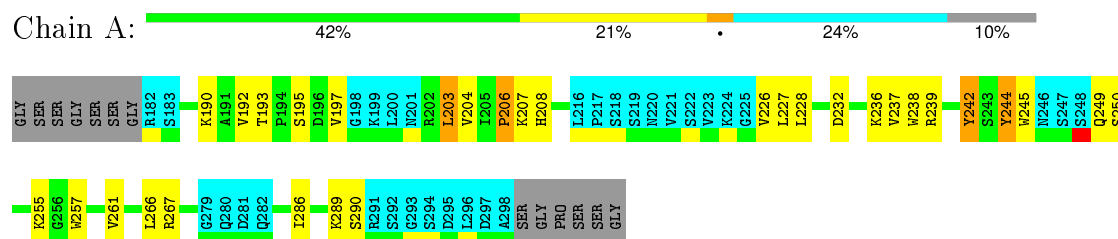
### 4.2.18 Score per residue for model 18

- Molecule 1: DNA-binding protein RAV1



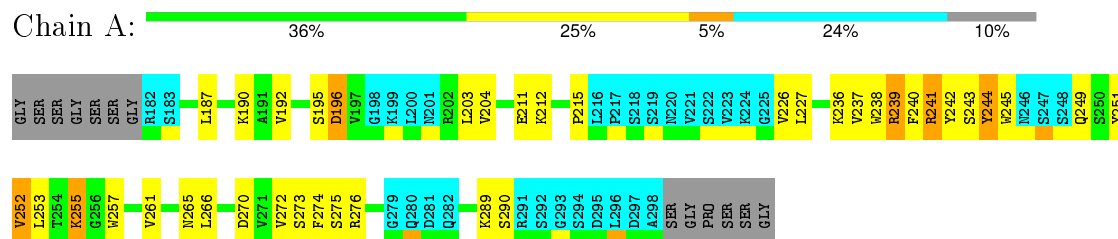
### 4.2.19 Score per residue for model 19

- Molecule 1: DNA-binding protein RAV1



### 4.2.20 Score per residue for model 20

- Molecule 1: DNA-binding protein RAV1



## 5 Refinement protocol and experimental data overview ⓘ

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

Of the 50 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CNS	structure solution	1.1
CNS	refinement	1.1

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

## 6 Model quality ⓘ

### 6.1 Standard geometry ⓘ

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 ⓘ

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	723	719	716	16±4
All	All	14460	14380	14320	317

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 11.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:203:LEU:HD23	1:A:257:TRP:CZ2	0.83	2.09	17	2
1:A:226:VAL:O	1:A:227:LEU:HD13	0.79	1.76	9	1
1:A:203:LEU:HD13	1:A:257:TRP:CZ2	0.75	2.16	2	3
1:A:257:TRP:O	1:A:261:VAL:HG23	0.74	1.81	15	19
1:A:245:TRP:CE2	1:A:252:VAL:HG21	0.74	2.17	8	4
1:A:230:PHE:CE1	1:A:284:LEU:HD22	0.74	2.18	16	1
1:A:203:LEU:HD13	1:A:257:TRP:CH2	0.72	2.18	4	2
1:A:245:TRP:CD1	1:A:252:VAL:HG21	0.72	2.18	14	9
1:A:192:VAL:HG12	1:A:270:ASP:O	0.69	1.87	18	6
1:A:245:TRP:CE3	1:A:252:VAL:HG11	0.68	2.23	17	2
1:A:184:ALA:HB1	1:A:276:ARG:O	0.68	1.89	16	2
1:A:203:LEU:HD23	1:A:253:LEU:HD12	0.67	1.66	7	3
1:A:261:VAL:HG13	1:A:266:LEU:HB3	0.66	1.68	2	17
1:A:202:ARG:HD3	1:A:254:THR:HG22	0.64	1.68	17	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:187:LEU:HD11	1:A:276:ARG:HB2	0.63	1.70	1	8
1:A:187:LEU:HD22	1:A:213:HIS:HB3	0.62	1.71	8	2
1:A:204:VAL:O	1:A:205:ILE:HD13	0.62	1.95	2	2
1:A:202:ARG:HG2	1:A:254:THR:HG22	0.62	1.72	8	4
1:A:272:VAL:HG12	1:A:274:PHE:CE2	0.61	2.30	4	6
1:A:227:LEU:C	1:A:228:LEU:HD12	0.60	2.16	4	4
1:A:227:LEU:N	1:A:227:LEU:HD22	0.60	2.11	9	1
1:A:245:TRP:CD2	1:A:252:VAL:HG11	0.60	2.31	15	2
1:A:227:LEU:O	1:A:228:LEU:HD12	0.59	1.97	2	4
1:A:243:SER:HB2	1:A:254:THR:HG23	0.59	1.74	13	1
1:A:228:LEU:HD13	1:A:253:LEU:CD2	0.59	2.28	9	1
1:A:245:TRP:CG	1:A:252:VAL:HG21	0.58	2.33	20	8
1:A:226:VAL:O	1:A:227:LEU:HD22	0.57	2.00	18	1
1:A:274:PHE:CE1	1:A:286:ILE:HD12	0.57	2.34	13	2
1:A:187:LEU:HD21	1:A:276:ARG:HB2	0.56	1.75	10	4
1:A:241:ARG:O	1:A:253:LEU:HD23	0.56	2.00	20	2
1:A:203:LEU:HD13	1:A:204:VAL:N	0.56	2.15	19	1
1:A:226:VAL:HG22	1:A:227:LEU:H	0.56	1.60	9	1
1:A:210:ALA:HB1	1:A:242:TYR:OH	0.56	2.01	14	2
1:A:227:LEU:HD23	1:A:240:PHE:O	0.55	2.00	5	1
1:A:230:PHE:CZ	1:A:284:LEU:HD23	0.55	2.35	11	1
1:A:196:ASP:OD2	1:A:204:VAL:HG22	0.55	2.01	18	3
1:A:204:VAL:HA	1:A:252:VAL:HG12	0.54	1.77	18	2
1:A:192:VAL:O	1:A:192:VAL:HG13	0.54	2.02	18	5
1:A:197:VAL:HG22	1:A:197:VAL:O	0.54	2.03	15	2
1:A:240:PHE:CB	1:A:253:LEU:HD22	0.53	2.33	5	2
1:A:274:PHE:HE1	1:A:286:ILE:HD12	0.53	1.64	13	2
1:A:286:ILE:HG23	1:A:286:ILE:O	0.53	2.03	8	4
1:A:197:VAL:HG21	1:A:267:ARG:HA	0.53	1.79	6	1
1:A:187:LEU:HD21	1:A:276:ARG:CB	0.52	2.34	10	1
1:A:210:ALA:HB1	1:A:251:TYR:CD2	0.52	2.40	11	1
1:A:203:LEU:O	1:A:252:VAL:HG12	0.52	2.04	7	3
1:A:244:TYR:CZ	1:A:251:TYR:CZ	0.51	2.99	17	3
1:A:240:PHE:HB3	1:A:253:LEU:HD22	0.51	1.82	4	3
1:A:196:ASP:O	1:A:197:VAL:HG13	0.51	2.06	13	2
1:A:196:ASP:CG	1:A:204:VAL:HG22	0.51	2.27	18	1
1:A:205:ILE:CD1	1:A:253:LEU:HD13	0.50	2.36	1	1
1:A:286:ILE:O	1:A:286:ILE:HG23	0.50	2.06	19	3
1:A:192:VAL:HG13	1:A:192:VAL:O	0.50	2.06	7	3
1:A:226:VAL:HG12	1:A:242:TYR:CB	0.50	2.37	9	1
1:A:196:ASP:OD1	1:A:204:VAL:HG22	0.50	2.07	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:187:LEU:HD22	1:A:213:HIS:ND1	0.50	2.21	9	1
1:A:244:TYR:CZ	1:A:251:TYR:CE2	0.50	3.00	10	5
1:A:208:HIS:CD2	1:A:209:HIS:CD2	0.50	3.00	4	6
1:A:242:TYR:CE2	1:A:251:TYR:CD2	0.50	2.99	4	3
1:A:228:LEU:HD13	1:A:253:LEU:HD21	0.49	1.84	9	1
1:A:251:TYR:CD1	1:A:251:TYR:N	0.49	2.80	18	4
1:A:197:VAL:HG21	1:A:268:ALA:N	0.49	2.22	1	1
1:A:245:TRP:CD2	1:A:252:VAL:HG21	0.49	2.41	8	2
1:A:227:LEU:HD23	1:A:241:ARG:HG2	0.49	1.84	20	1
1:A:227:LEU:HD22	1:A:227:LEU:N	0.49	2.22	12	1
1:A:194:PRO:HA	1:A:268:ALA:HB2	0.48	1.85	14	3
1:A:240:PHE:HB2	1:A:253:LEU:HD22	0.48	1.85	18	1
1:A:245:TRP:NE1	1:A:252:VAL:HG21	0.48	2.24	15	2
1:A:228:LEU:HD23	1:A:284:LEU:CD1	0.48	2.39	8	1
1:A:226:VAL:HG12	1:A:242:TYR:HB3	0.48	1.83	9	1
1:A:188:PHE:CZ	1:A:274:PHE:CD2	0.48	3.02	6	2
1:A:251:TYR:N	1:A:251:TYR:CD1	0.48	2.81	3	4
1:A:245:TRP:CD1	1:A:252:VAL:CG2	0.47	2.97	2	7
1:A:226:VAL:C	1:A:227:LEU:HD22	0.47	2.29	18	2
1:A:242:TYR:CZ	1:A:251:TYR:CB	0.47	2.97	2	3
1:A:243:SER:HB3	1:A:252:VAL:HG23	0.47	1.86	20	2
1:A:228:LEU:N	1:A:228:LEU:HD12	0.46	2.25	13	1
1:A:226:VAL:C	1:A:227:LEU:HD13	0.46	2.30	9	1
1:A:243:SER:OG	1:A:252:VAL:HG23	0.46	2.11	12	1
1:A:206:PRO:CB	1:A:208:HIS:CE1	0.45	2.99	7	7
1:A:245:TRP:CG	1:A:252:VAL:CG2	0.45	2.99	9	2
1:A:190:LYS:O	1:A:271:VAL:HG23	0.45	2.11	12	1
1:A:208:HIS:NE2	1:A:209:HIS:CD2	0.45	2.84	8	1
1:A:192:VAL:HG12	1:A:270:ASP:C	0.45	2.32	2	2
1:A:244:TYR:CE1	1:A:251:TYR:CE1	0.45	3.05	11	1
1:A:227:LEU:HD13	1:A:240:PHE:O	0.44	2.13	1	1
1:A:190:LYS:O	1:A:271:VAL:HG13	0.44	2.11	18	1
1:A:210:ALA:HB1	1:A:251:TYR:CG	0.44	2.48	11	1
1:A:193:THR:O	1:A:195:SER:N	0.43	2.51	16	1
1:A:227:LEU:HD21	1:A:241:ARG:HG3	0.43	1.89	3	1
1:A:230:PHE:CE1	1:A:274:PHE:CD1	0.43	3.06	11	1
1:A:230:PHE:CZ	1:A:284:LEU:HD22	0.43	2.48	4	1
1:A:275:SER:O	1:A:284:LEU:HD23	0.43	2.13	8	1
1:A:236:LYS:CD	1:A:238:TRP:CZ2	0.43	3.01	16	1
1:A:208:HIS:CD2	1:A:209:HIS:N	0.43	2.87	18	1
1:A:210:ALA:CB	1:A:251:TYR:CG	0.43	3.01	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:196:ASP:OD1	1:A:203:LEU:HD12	0.43	2.14	18	1
1:A:203:LEU:HD23	1:A:253:LEU:HD22	0.43	1.91	1	1
1:A:205:ILE:HD11	1:A:253:LEU:HD12	0.42	1.91	17	1
1:A:203:LEU:HD22	1:A:257:TRP:CZ3	0.42	2.49	1	1
1:A:237:VAL:HG12	1:A:238:TRP:N	0.42	2.29	12	4
1:A:212:LYS:CD	1:A:213:HIS:CE1	0.42	3.02	3	1
1:A:184:ALA:HB2	1:A:285:TYR:CE1	0.42	2.49	13	1
1:A:196:ASP:OD2	1:A:204:VAL:HG23	0.42	2.13	10	1
1:A:243:SER:CB	1:A:254:THR:HG23	0.42	2.44	13	1
1:A:187:LEU:HD11	1:A:276:ARG:HD3	0.42	1.90	17	1
1:A:202:ARG:CB	1:A:254:THR:HG22	0.42	2.44	6	1
1:A:226:VAL:HG12	1:A:227:LEU:N	0.42	2.30	15	5
1:A:244:TYR:OH	1:A:251:TYR:CZ	0.42	2.72	14	4
1:A:283:GLN:C	1:A:284:LEU:HD22	0.42	2.35	14	1
1:A:206:PRO:HB2	1:A:208:HIS:CE1	0.42	2.50	2	5
1:A:244:TYR:CZ	1:A:251:TYR:CE1	0.42	3.08	17	2
1:A:210:ALA:HB3	1:A:251:TYR:CD1	0.42	2.50	3	1
1:A:208:HIS:CG	1:A:209:HIS:N	0.41	2.88	15	1
1:A:214:PHE:CZ	1:A:284:LEU:HD21	0.41	2.50	10	1
1:A:226:VAL:HG23	1:A:242:TYR:HB3	0.41	1.92	12	2
1:A:206:PRO:HB3	1:A:208:HIS:CE1	0.41	2.51	10	3
1:A:205:ILE:HD12	1:A:253:LEU:CD1	0.41	2.45	1	1
1:A:228:LEU:HD13	1:A:242:TYR:HB2	0.41	1.92	5	1
1:A:242:TYR:HH	1:A:251:TYR:HD2	0.41	1.57	16	1
1:A:230:PHE:CZ	1:A:284:LEU:HD13	0.41	2.51	9	1
1:A:227:LEU:CD2	1:A:227:LEU:N	0.41	2.84	12	1
1:A:230:PHE:CD1	1:A:230:PHE:N	0.41	2.89	13	1
1:A:187:LEU:HD11	1:A:276:ARG:CB	0.41	2.45	5	1
1:A:187:LEU:HD11	1:A:276:ARG:CG	0.41	2.46	5	1
1:A:214:PHE:CE2	1:A:228:LEU:HD21	0.41	2.51	15	1
1:A:187:LEU:HD21	1:A:276:ARG:HG2	0.41	1.91	17	1
1:A:228:LEU:HD12	1:A:228:LEU:N	0.41	2.30	18	1
1:A:202:ARG:CG	1:A:254:THR:HG22	0.41	2.45	18	1
1:A:230:PHE:CE2	1:A:274:PHE:CD1	0.41	3.09	9	1
1:A:239:ARG:O	1:A:240:PHE:CD1	0.40	2.74	20	1
1:A:202:ARG:CD	1:A:254:THR:HG22	0.40	2.46	9	1
1:A:231:GLU:OE1	1:A:285:TYR:CE2	0.40	2.74	15	1
1:A:242:TYR:CZ	1:A:251:TYR:HB3	0.40	2.52	2	1
1:A:202:ARG:NH1	1:A:204:VAL:CG2	0.40	2.85	4	1
1:A:228:LEU:N	1:A:228:LEU:CD1	0.40	2.85	13	1

## 6.3 Torsion angles

### 6.3.1 Protein backbone

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	86/130 (66%)	78±2 (91±2%)	6±1 (7±2%)	2±1 (2±1%)	13	52
All	All	1720/2600 (66%)	1565 (91%)	117 (7%)	38 (2%)	13	52

All 8 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	255	LYS	17
1	A	215	PRO	6
1	A	195	SER	4
1	A	202	ARG	3
1	A	197	VAL	2
1	A	194	PRO	2
1	A	208	HIS	2
1	A	206	PRO	2

### 6.3.2 Protein sidechains

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	77/111 (69%)	63±3 (82±4%)	14±3 (18±4%)	5	39
All	All	1540/2220 (69%)	1258 (82%)	282 (18%)	5	39

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	244	TYR	18
1	A	289	LYS	15

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Mol	Chain	Res	Type	Models (Total)
1	A	207	LYS	15
1	A	242	TYR	14
1	A	236	LYS	13
1	A	190	LYS	12
1	A	193	THR	10
1	A	255	LYS	10
1	A	262	LYS	9
1	A	290	SER	9
1	A	263	GLU	9
1	A	189	GLU	9
1	A	196	ASP	8
1	A	267	ARG	7
1	A	259	ARG	7
1	A	241	ARG	7
1	A	212	LYS	7
1	A	195	SER	6
1	A	243	SER	6
1	A	249	GLN	6
1	A	211	GLU	6
1	A	250	SER	6
1	A	270	ASP	6
1	A	239	ARG	6
1	A	275	SER	6
1	A	202	ARG	6
1	A	258	SER	5
1	A	185	GLU	5
1	A	227	LEU	5
1	A	277	SER	4
1	A	273	SER	4
1	A	284	LEU	4
1	A	265	ASN	3
1	A	276	ARG	3
1	A	234	ASN	3
1	A	231	GLU	2
1	A	232	ASP	2
1	A	252	VAL	2
1	A	245	TRP	1
1	A	228	LEU	1
1	A	283	GLN	1
1	A	203	LEU	1
1	A	226	VAL	1
1	A	197	VAL	1

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Mol	Chain	Res	Type	Models (Total)
1	A	264	LYS	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 carbohydrates in this entry.

## 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

## 6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 7 Chemical shift validation

No chemical shift data were provided