



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 7, 2022 – 07:44 AM EST

PDB ID : 3GCC  
Title : SOLUTION STRUCTURE OF THE GCC-BOX BINDING DOMAIN, NMR,  
46 STRUCTURES  
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Deposited on : 1998-03-13

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

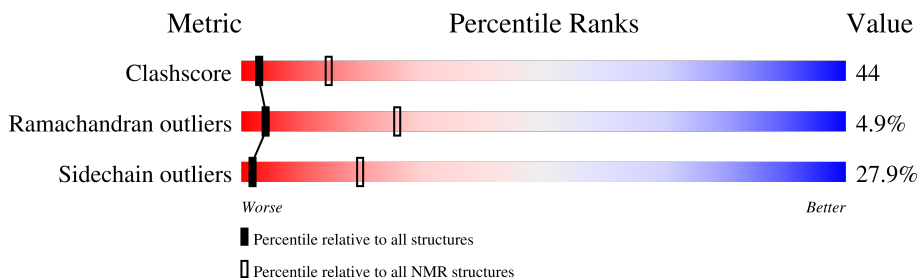
# 1 Overall quality at a glance

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	70	

## 2 Ensemble composition and analysis

This entry contains 46 models. Model 41 is the overall representative, medoid model (most similar to other models).

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:146-A:203 (58)	0.37	41

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 6 clusters and 5 single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 5, 6, 7, 9, 10, 12, 17, 18, 19, 23, 28, 29, 30, 31, 32, 35, 40, 41, 43, 44, 46
2	13, 20, 21, 34, 38
3	4, 8, 11, 39
4	25, 26, 37, 45
5	14, 33
6	27, 42
Single-model clusters	15; 16; 22; 24; 36

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

There is only 1 type of molecule in this entry. The entry contains 1024 atoms, of which 512 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called ATERF1.

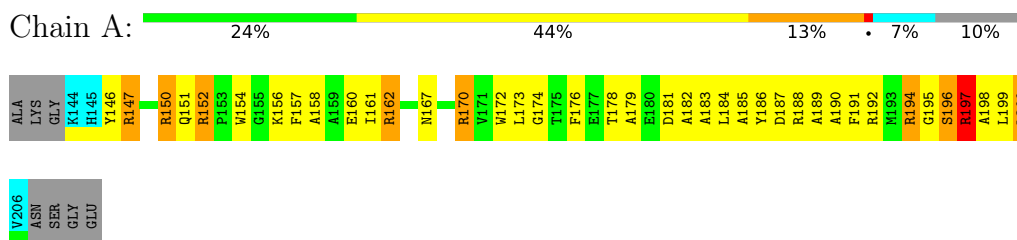
Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	63	1024	325	512	103	83	1	0

## 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: ATERF1

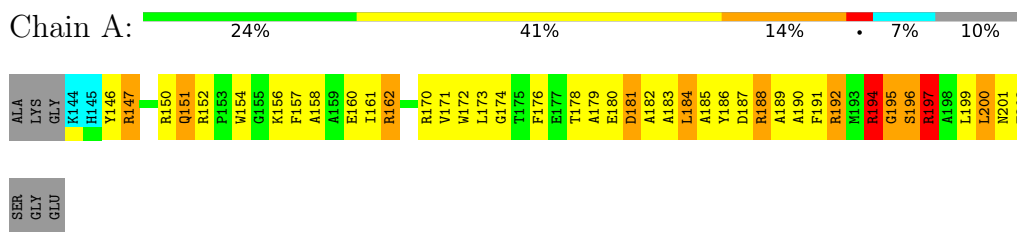


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

- Molecule 1: ATERF1



#### 4.2.2 Score per residue for model 2

- Molecule 1: ATERF1



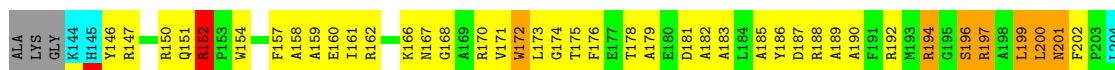


GLU

### 4.2.3 Score per residue for model 3

- Molecule 1: ATERF1

Chain A: 24% 47% 10% 7% 10%

R205  
V206  
ASN  
SER  
GLY  
GLU

### 4.2.4 Score per residue for model 4

- Molecule 1: ATERF1

Chain A: 24% 44% 13% 7% 10%



GLU

### 4.2.5 Score per residue for model 5

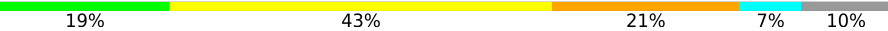
- Molecule 1: ATERF1

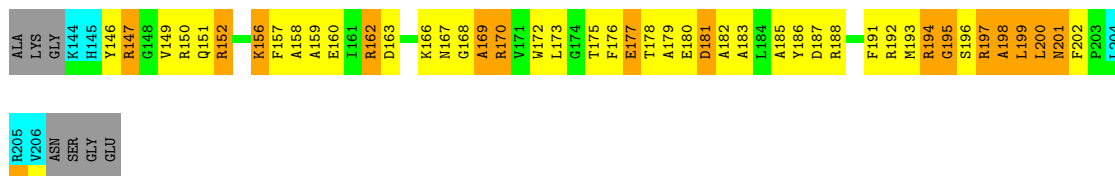
Chain A: 27% 40% 13% 7% 10%

ASN  
SER  
GLY  
GLU

### 4.2.6 Score per residue for model 6

- Molecule 1: ATERF1

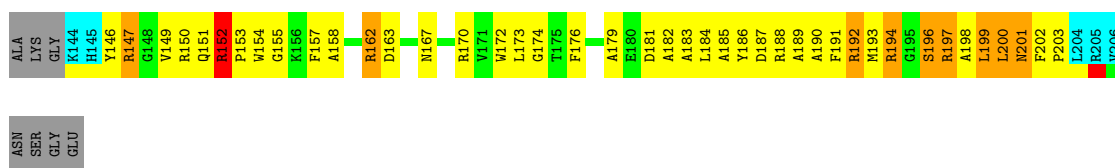
Chain A: 



#### 4.2.7 Score per residue for model 7

- Molecule 1: ATERF1

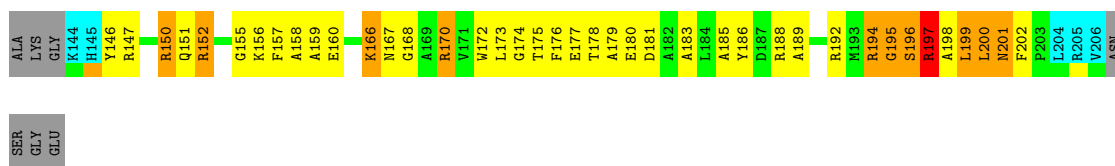
Chain A: 



#### 4.2.8 Score per residue for model 8


- Molecule 1: ATERF1

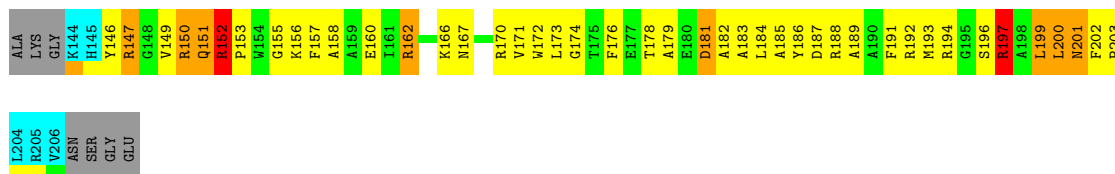
Chain A: 



#### 4.2.9 Score per residue for model 9


- Molecule 1: ATERF1

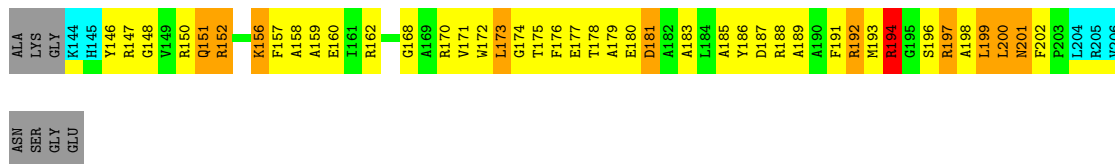
Chain A: 



### 4.2.10 Score per residue for model 10

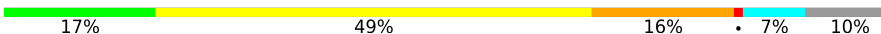
- Molecule 1: ATERF1

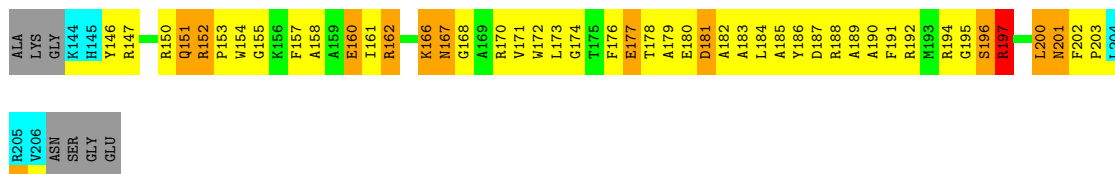
Chain A: 



### 4.2.11 Score per residue for model 11

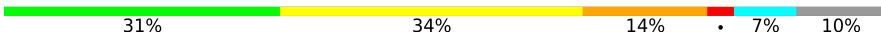
- Molecule 1: ATERF1

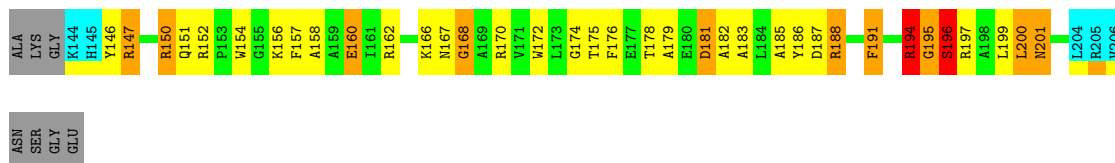
Chain A: 



### 4.2.12 Score per residue for model 12

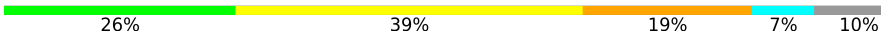
- Molecule 1: ATERF1

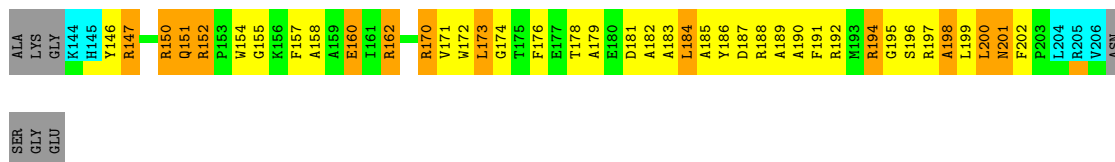
Chain A: 



### 4.2.13 Score per residue for model 13

- Molecule 1: ATERF1

Chain A: 





## 4.2.14 Score per residue for model 14

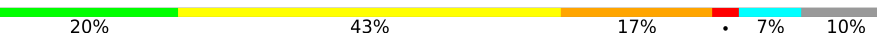
- Molecule 1: ATERF1

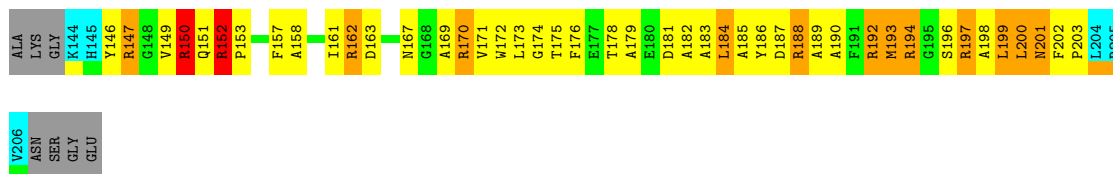
Chain A: 



## 4.2.15 Score per residue for model 15

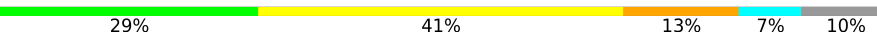
- Molecule 1: ATERF1

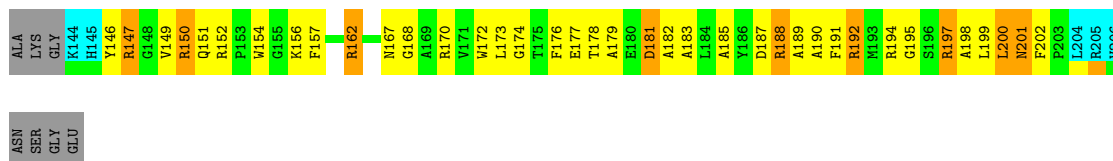
Chain A: 



## 4.2.16 Score per residue for model 16

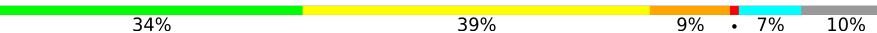
- Molecule 1: ATERF1

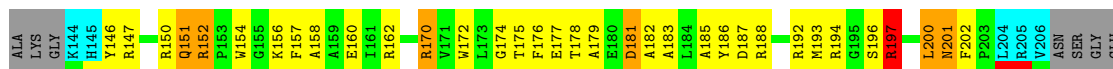
Chain A: 



## 4.2.17 Score per residue for model 17

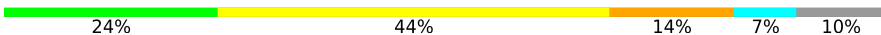
- Molecule 1: ATERF1

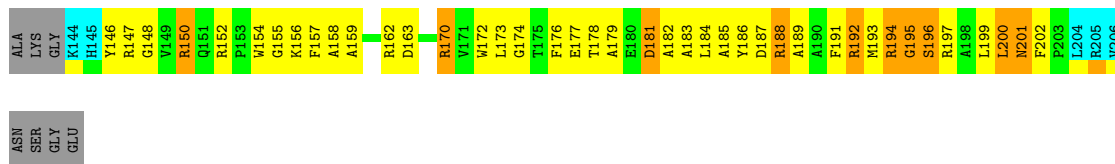
Chain A: 



### 4.2.18 Score per residue for model 18

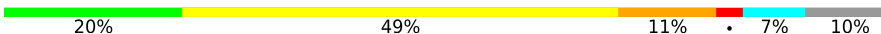
- Molecule 1: ATERF1

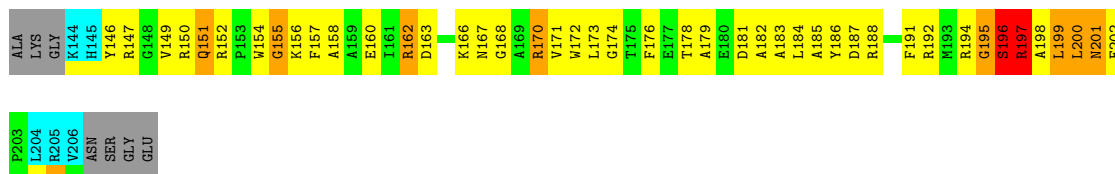
Chain A: 



### 4.2.19 Score per residue for model 19

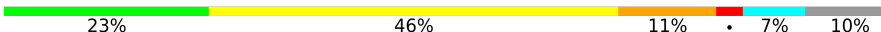
- Molecule 1: ATERF1

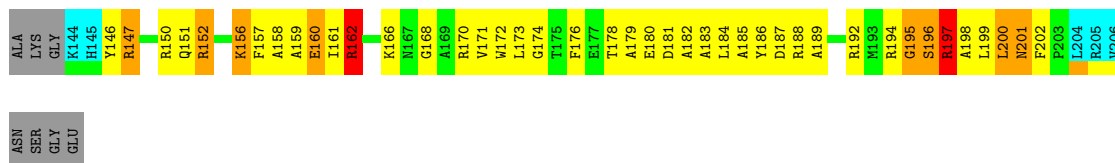
Chain A: 



### 4.2.20 Score per residue for model 20

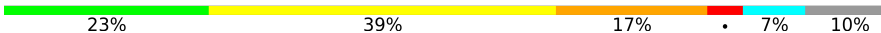
- Molecule 1: ATERF1

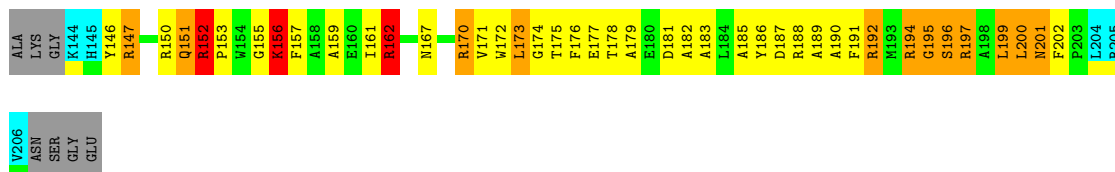
Chain A: 



### 4.2.21 Score per residue for model 21

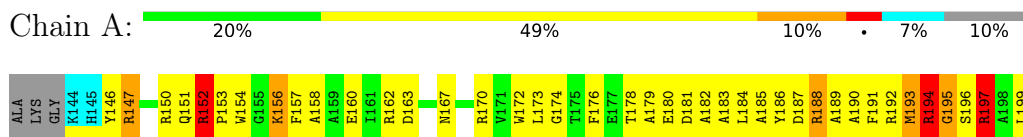
- Molecule 1: ATERF1

Chain A: 



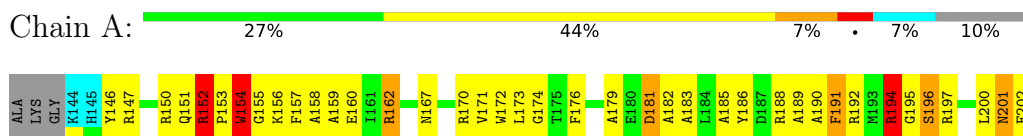
### 4.2.22 Score per residue for model 22

- Molecule 1: ATERF1



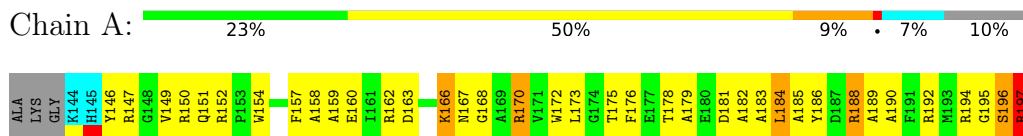
### 4.2.23 Score per residue for model 23

- Molecule 1: ATERF1



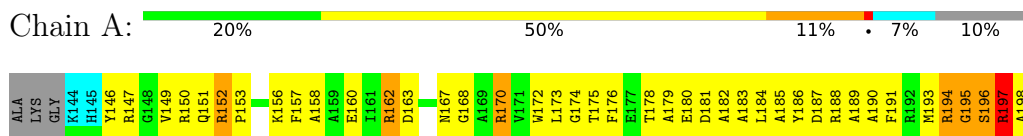
### 4.2.24 Score per residue for model 24

- Molecule 1: ATERF1



### 4.2.25 Score per residue for model 25

- Molecule 1: ATERF1





### 4.2.30 Score per residue for model 30

- Molecule 1: ATERF1

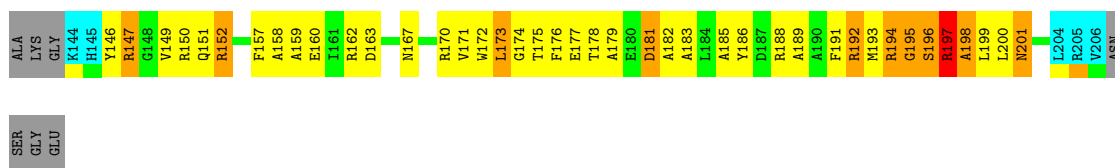
Chain A: 23% 47% 10% 7% 10%



### 4.2.31 Score per residue for model 31

- Molecule 1: ATERF1

Chain A: 24% 43% 14% 7% 10%



### 4.2.32 Score per residue for model 32

- Molecule 1: ATERF1

Chain A: 24% 43% 13% 7% 10%



### 4.2.33 Score per residue for model 33

- Molecule 1: ATERF1

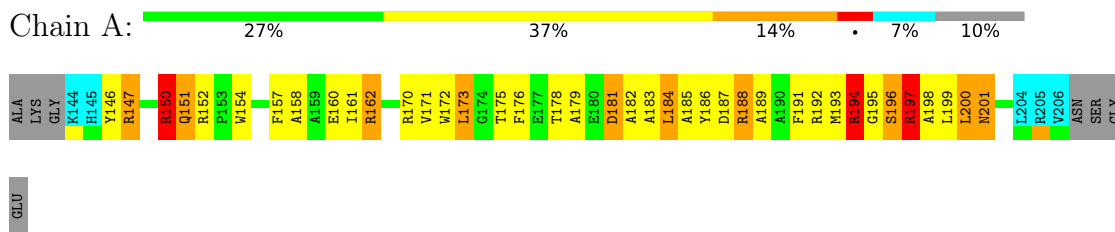
Chain A: 19% 46% 13% 6% 7% 10%





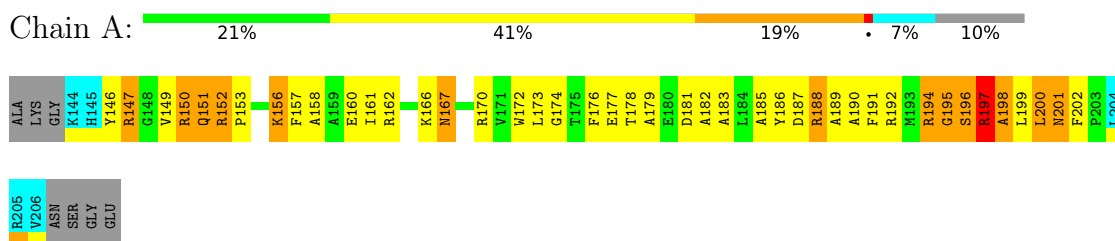
### 4.2.38 Score per residue for model 38

- Molecule 1: ATERF1



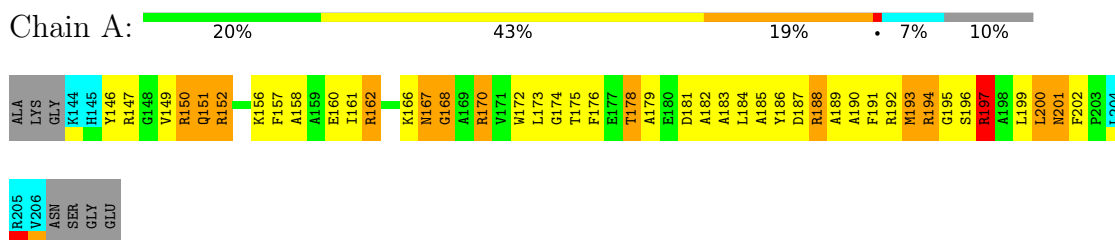
### 4.2.39 Score per residue for model 39

- Molecule 1: ATERF1



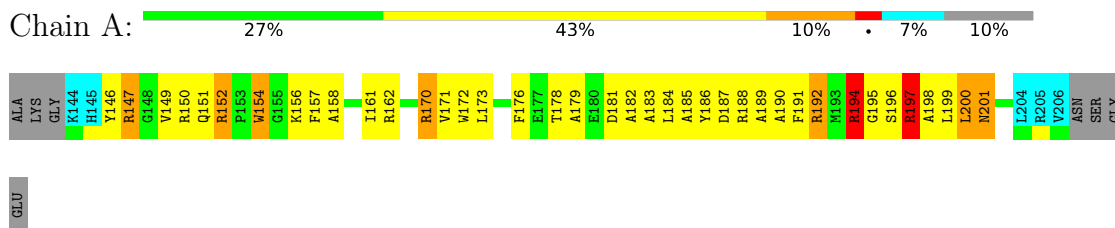
### 4.2.40 Score per residue for model 40

- Molecule 1: ATERF1



### 4.2.41 Score per residue for model 41 (medoid)

- Molecule 1: ATERF1



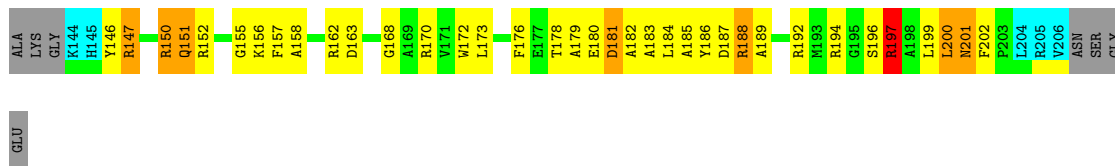




#### 4.2.46 Score per residue for model 46

- Molecule 1: ATERF1

Chain A: 



GLU

## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *SIMULATED ANNEALING PROTOCOL IN X-PLOR 3.1 WAS CARRIED OUT TO OBTAIN 46 STRUCTURES.*

Of the 46 calculated structures, 46 were deposited, based on the following criterion: *NO NOE VIOLATIONS.*

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

Software name	Classification	Version
X-PLOR	refinement	3.1
X-PLOR	structure solution	3.1

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.

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	8.6±0.6
All	All	0	397

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	170	ARG	Sidechain	46
1	A	150	ARG	Sidechain	45
1	A	197	ARG	Sidechain	45
1	A	147	ARG	Sidechain	44
1	A	152	ARG	Sidechain	44
1	A	162	ARG	Sidechain	44
1	A	194	ARG	Sidechain	44
1	A	188	ARG	Sidechain	43
1	A	192	ARG	Sidechain	42

### 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	467	459	459	41±8
All	All	21482	21114	21114	1887

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 44.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:173:LEU:HD21	1:A:189:ALA:HB2	1.06	1.27	42	28
1:A:157:PHE:CE2	1:A:179:ALA:HB2	1.03	1.88	33	40
1:A:146:TYR:CD2	1:A:183:ALA:HB2	0.92	1.99	35	46
1:A:150:ARG:HG3	1:A:158:ALA:HB3	0.90	1.44	33	1
1:A:150:ARG:CG	1:A:158:ALA:HB3	0.89	1.97	33	2
1:A:173:LEU:HD21	1:A:189:ALA:CB	0.88	1.98	25	29
1:A:173:LEU:HD11	1:A:189:ALA:CB	0.83	2.03	43	7
1:A:157:PHE:CE1	1:A:179:ALA:HB2	0.80	2.11	18	3
1:A:149:VAL:HG11	1:A:179:ALA:HA	0.78	1.54	15	8
1:A:194:ARG:O	1:A:198:ALA:HB2	0.78	1.79	39	3
1:A:176:PHE:HB2	1:A:182:ALA:HB2	0.76	1.57	15	26
1:A:184:LEU:O	1:A:184:LEU:HD13	0.75	1.80	7	9
1:A:183:ALA:HB1	1:A:201:ASN:ND2	0.75	1.95	45	40
1:A:177:GLU:HG3	1:A:178:THR:HG23	0.74	1.59	17	1
1:A:173:LEU:HD11	1:A:189:ALA:HB3	0.73	1.59	43	6
1:A:199:LEU:C	1:A:200:LEU:HD23	0.73	2.03	3	19
1:A:158:ALA:HB1	1:A:172:TRP:CZ2	0.72	2.19	46	37
1:A:149:VAL:HG13	1:A:182:ALA:HB3	0.72	1.61	36	17
1:A:199:LEU:N	1:A:199:LEU:HD12	0.71	2.00	45	2
1:A:191:PHE:CD2	1:A:200:LEU:HD11	0.71	2.21	12	1
1:A:187:ASP:HB3	1:A:200:LEU:HD13	0.70	1.63	9	19
1:A:184:LEU:HD22	1:A:202:PHE:HD2	0.69	1.48	35	6
1:A:161:ILE:HD13	1:A:193:MET:HE2	0.69	1.65	14	3
1:A:161:ILE:HD12	1:A:190:ALA:HB2	0.68	1.65	41	5
1:A:173:LEU:CD2	1:A:189:ALA:HB2	0.67	2.19	5	8
1:A:157:PHE:CD1	1:A:179:ALA:HB2	0.66	2.25	18	1
1:A:184:LEU:C	1:A:184:LEU:HD13	0.66	2.11	14	1
1:A:184:LEU:HD13	1:A:184:LEU:O	0.66	1.91	14	1
1:A:158:ALA:HB1	1:A:160:GLU:OE2	0.66	1.90	24	2
1:A:146:TYR:CD2	1:A:183:ALA:CB	0.66	2.79	35	32
1:A:199:LEU:HD13	1:A:200:LEU:N	0.65	2.06	38	2
1:A:158:ALA:CB	1:A:172:TRP:CZ2	0.64	2.81	10	35
1:A:200:LEU:HD12	1:A:203:PRO:HA	0.64	1.69	15	2
1:A:151:GLN:CB	1:A:157:PHE:CE2	0.63	2.81	45	24
1:A:171:VAL:HG12	1:A:171:VAL:O	0.63	1.93	19	17
1:A:152:ARG:CB	1:A:153:PRO:CD	0.63	2.77	33	16
1:A:184:LEU:HD22	1:A:202:PHE:CD2	0.62	2.29	35	5
1:A:149:VAL:CG1	1:A:182:ALA:HB3	0.62	2.23	36	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:176:PHE:CZ	1:A:185:ALA:CB	0.62	2.83	46	46
1:A:183:ALA:CB	1:A:202:PHE:CZ	0.62	2.82	30	6
1:A:158:ALA:CB	1:A:172:TRP:CH2	0.62	2.83	18	26
1:A:183:ALA:HB3	1:A:202:PHE:CZ	0.62	2.29	30	11
1:A:184:LEU:HD13	1:A:184:LEU:C	0.62	2.15	36	4
1:A:149:VAL:HG13	1:A:182:ALA:CB	0.61	2.24	36	6
1:A:194:ARG:HB2	1:A:198:ALA:HB2	0.61	1.71	15	1
1:A:173:LEU:HD22	1:A:185:ALA:O	0.60	1.96	21	2
1:A:156:LYS:O	1:A:157:PHE:CD1	0.60	2.54	33	15
1:A:155:GLY:O	1:A:156:LYS:CB	0.60	2.49	21	1
1:A:194:ARG:CB	1:A:198:ALA:HB2	0.59	2.27	15	3
1:A:159:ALA:C	1:A:173:LEU:HD12	0.59	2.18	20	1
1:A:174:GLY:O	1:A:176:PHE:CE1	0.59	2.56	8	20
1:A:151:GLN:HB2	1:A:157:PHE:CE2	0.58	2.33	14	9
1:A:156:LYS:O	1:A:157:PHE:CD2	0.58	2.57	18	3
1:A:191:PHE:CZ	1:A:196:SER:O	0.58	2.57	7	3
1:A:160:GLU:OE1	1:A:172:TRP:CE3	0.58	2.56	1	3
1:A:175:THR:O	1:A:176:PHE:CD1	0.58	2.56	10	3
1:A:160:GLU:OE2	1:A:172:TRP:CZ3	0.58	2.56	45	7
1:A:175:THR:O	1:A:176:PHE:CD2	0.57	2.57	3	3
1:A:151:GLN:HB3	1:A:157:PHE:CE2	0.57	2.34	5	24
1:A:157:PHE:CD2	1:A:179:ALA:HB2	0.57	2.34	3	14
1:A:191:PHE:CE1	1:A:196:SER:O	0.57	2.57	23	2
1:A:183:ALA:CB	1:A:201:ASN:ND2	0.57	2.68	45	13
1:A:152:ARG:CB	1:A:153:PRO:HD2	0.57	2.29	33	14
1:A:153:PRO:O	1:A:154:TRP:CB	0.57	2.52	11	6
1:A:200:LEU:HD23	1:A:200:LEU:N	0.57	2.15	7	12
1:A:152:ARG:O	1:A:152:ARG:CD	0.57	2.53	21	1
1:A:195:GLY:O	1:A:196:SER:CB	0.56	2.52	18	5
1:A:186:TYR:CD1	1:A:186:TYR:C	0.56	2.78	45	45
1:A:156:LYS:C	1:A:157:PHE:CD1	0.56	2.79	45	29
1:A:174:GLY:O	1:A:176:PHE:CE2	0.56	2.58	3	2
1:A:157:PHE:CD2	1:A:179:ALA:CA	0.56	2.88	45	9
1:A:151:GLN:HB2	1:A:157:PHE:CE1	0.56	2.35	15	1
1:A:151:GLN:CG	1:A:157:PHE:CE2	0.56	2.89	3	1
1:A:152:ARG:HB3	1:A:153:PRO:CD	0.56	2.31	33	3
1:A:172:TRP:HZ2	1:A:175:THR:HG22	0.56	1.61	34	5
1:A:152:ARG:N	1:A:152:ARG:CD	0.55	2.69	26	1
1:A:157:PHE:CD2	1:A:178:THR:C	0.55	2.79	16	6
1:A:191:PHE:O	1:A:195:GLY:N	0.55	2.40	11	12
1:A:160:GLU:OE2	1:A:172:TRP:CE3	0.55	2.58	40	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:157:PHE:CD1	1:A:178:THR:C	0.55	2.80	1	12
1:A:191:PHE:O	1:A:195:GLY:CA	0.55	2.55	5	10
1:A:152:ARG:CD	1:A:152:ARG:C	0.55	2.75	21	1
1:A:151:GLN:HB3	1:A:157:PHE:CD2	0.55	2.37	14	4
1:A:199:LEU:HD13	1:A:199:LEU:C	0.55	2.23	38	1
1:A:157:PHE:CE2	1:A:179:ALA:CB	0.54	2.81	17	10
1:A:197:ARG:O	1:A:198:ALA:HB2	0.54	2.02	24	5
1:A:176:PHE:CB	1:A:182:ALA:HB2	0.54	2.31	15	3
1:A:153:PRO:O	1:A:154:TRP:CG	0.54	2.61	33	1
1:A:173:LEU:CD2	1:A:189:ALA:CB	0.54	2.85	8	8
1:A:155:GLY:O	1:A:156:LYS:CG	0.54	2.55	21	2
1:A:190:ALA:O	1:A:194:ARG:CB	0.54	2.56	26	2
1:A:187:ASP:OD1	1:A:200:LEU:CB	0.54	2.56	15	14
1:A:151:GLN:CB	1:A:157:PHE:CE1	0.54	2.90	15	2
1:A:161:ILE:HD12	1:A:190:ALA:CB	0.54	2.32	41	1
1:A:157:PHE:CD2	1:A:178:THR:HA	0.53	2.38	18	2
1:A:152:ARG:CG	1:A:153:PRO:HD2	0.53	2.33	42	8
1:A:152:ARG:HG2	1:A:155:GLY:CA	0.53	2.33	21	1
1:A:161:ILE:HD11	1:A:194:ARG:NH1	0.53	2.18	2	1
1:A:178:THR:HG1	1:A:181:ASP:CG	0.53	2.07	38	7
1:A:157:PHE:CE1	1:A:178:THR:HA	0.53	2.39	14	23
1:A:166:LYS:O	1:A:167:ASN:CB	0.53	2.57	42	9
1:A:186:TYR:CE1	1:A:190:ALA:HB2	0.53	2.39	35	5
1:A:183:ALA:HB1	1:A:201:ASN:HD22	0.53	1.64	35	31
1:A:160:GLU:O	1:A:186:TYR:CE2	0.53	2.62	28	4
1:A:157:PHE:CD1	1:A:157:PHE:N	0.53	2.75	10	9
1:A:149:VAL:HG21	1:A:183:ALA:HB2	0.53	1.81	2	1
1:A:152:ARG:HG3	1:A:156:LYS:O	0.53	2.04	21	1
1:A:160:GLU:O	1:A:186:TYR:CD2	0.52	2.62	28	6
1:A:157:PHE:CD1	1:A:178:THR:HA	0.52	2.38	21	5
1:A:181:ASP:N	1:A:181:ASP:OD1	0.52	2.42	46	9
1:A:152:ARG:HB3	1:A:153:PRO:HD2	0.52	1.80	33	8
1:A:176:PHE:CD1	1:A:182:ALA:HA	0.52	2.39	33	35
1:A:159:ALA:O	1:A:173:LEU:HD12	0.52	2.05	20	1
1:A:151:GLN:HB3	1:A:157:PHE:CE1	0.52	2.40	36	1
1:A:190:ALA:O	1:A:194:ARG:CG	0.52	2.58	40	1
1:A:178:THR:HG23	1:A:181:ASP:OD2	0.52	2.05	31	6
1:A:172:TRP:CD1	1:A:174:GLY:HA2	0.52	2.40	3	10
1:A:194:ARG:O	1:A:196:SER:N	0.52	2.42	21	4
1:A:162:ARG:CG	1:A:162:ARG:O	0.52	2.58	38	2
1:A:201:ASN:C	1:A:202:PHE:CD1	0.52	2.84	15	31

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:173:LEU:CD2	1:A:185:ALA:O	0.52	2.57	11	2
1:A:154:TRP:HA	1:A:154:TRP:CE3	0.52	2.40	41	1
1:A:152:ARG:CG	1:A:156:LYS:N	0.51	2.74	21	1
1:A:172:TRP:C	1:A:172:TRP:CD1	0.51	2.83	20	23
1:A:157:PHE:CD2	1:A:179:ALA:HA	0.51	2.40	8	2
1:A:151:GLN:HG3	1:A:157:PHE:CE2	0.51	2.40	3	1
1:A:179:ALA:O	1:A:183:ALA:HB2	0.51	2.04	24	4
1:A:152:ARG:HG2	1:A:156:LYS:N	0.51	2.19	21	1
1:A:172:TRP:CD1	1:A:174:GLY:N	0.51	2.79	17	21
1:A:158:ALA:HB1	1:A:172:TRP:CH2	0.51	2.41	39	17
1:A:197:ARG:O	1:A:198:ALA:HB3	0.51	2.06	25	6
1:A:179:ALA:O	1:A:183:ALA:CB	0.51	2.59	24	4
1:A:150:ARG:CG	1:A:150:ARG:O	0.51	2.58	33	1
1:A:156:LYS:O	1:A:157:PHE:CG	0.51	2.64	16	5
1:A:158:ALA:CB	1:A:160:GLU:OE2	0.51	2.59	4	3
1:A:200:LEU:HD12	1:A:202:PHE:O	0.51	2.05	16	1
1:A:151:GLN:HA	1:A:157:PHE:CD2	0.51	2.40	21	8
1:A:199:LEU:N	1:A:199:LEU:CD1	0.51	2.73	45	1
1:A:159:ALA:HB3	1:A:176:PHE:CE1	0.51	2.40	14	6
1:A:174:GLY:O	1:A:176:PHE:CD1	0.50	2.64	36	11
1:A:157:PHE:CD2	1:A:178:THR:CA	0.50	2.95	2	2
1:A:176:PHE:CG	1:A:182:ALA:HA	0.50	2.40	15	4
1:A:161:ILE:CG2	1:A:193:MET:HE1	0.50	2.36	40	1
1:A:176:PHE:CD2	1:A:182:ALA:HA	0.50	2.41	43	3
1:A:196:SER:O	1:A:198:ALA:N	0.50	2.44	31	4
1:A:152:ARG:HB2	1:A:153:PRO:HD2	0.50	1.83	22	4
1:A:194:ARG:HD2	1:A:198:ALA:HB1	0.50	1.83	4	3
1:A:160:GLU:CD	1:A:172:TRP:CE3	0.50	2.85	26	3
1:A:184:LEU:C	1:A:184:LEU:CD1	0.50	2.79	7	7
1:A:158:ALA:HB2	1:A:172:TRP:CH2	0.50	2.42	18	4
1:A:178:THR:O	1:A:181:ASP:OD1	0.50	2.30	11	2
1:A:151:GLN:HG3	1:A:157:PHE:CZ	0.50	2.42	3	1
1:A:199:LEU:C	1:A:199:LEU:HD13	0.49	2.27	9	1
1:A:190:ALA:O	1:A:198:ALA:HB1	0.49	2.07	36	4
1:A:183:ALA:HB3	1:A:202:PHE:CE2	0.49	2.43	24	4
1:A:161:ILE:HG23	1:A:161:ILE:O	0.49	2.08	11	4
1:A:159:ALA:HB2	1:A:182:ALA:CA	0.49	2.38	14	1
1:A:183:ALA:CA	1:A:201:ASN:ND2	0.49	2.75	41	11
1:A:194:ARG:O	1:A:195:GLY:C	0.49	2.49	38	12
1:A:166:LYS:O	1:A:167:ASN:ND2	0.49	2.46	6	2
1:A:183:ALA:HB1	1:A:202:PHE:CZ	0.49	2.42	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:187:ASP:CG	1:A:200:LEU:CB	0.49	2.80	19	10
1:A:173:LEU:HD22	1:A:189:ALA:HB2	0.49	1.85	8	1
1:A:168:GLY:O	1:A:169:ALA:HB3	0.49	2.07	5	2
1:A:152:ARG:O	1:A:152:ARG:HD2	0.49	2.08	21	1
1:A:187:ASP:N	1:A:187:ASP:OD1	0.49	2.45	17	2
1:A:151:GLN:HA	1:A:157:PHE:CD1	0.49	2.42	16	1
1:A:161:ILE:CG1	1:A:162:ARG:N	0.49	2.75	45	1
1:A:154:TRP:CD1	1:A:154:TRP:O	0.48	2.66	3	1
1:A:175:THR:O	1:A:176:PHE:CG	0.48	2.66	43	6
1:A:152:ARG:HG3	1:A:153:PRO:N	0.48	2.22	14	3
1:A:194:ARG:HB3	1:A:198:ALA:HB2	0.48	1.85	13	1
1:A:151:GLN:CB	1:A:157:PHE:CD2	0.48	2.96	45	2
1:A:178:THR:OG1	1:A:181:ASP:OD1	0.48	2.30	11	4
1:A:186:TYR:CD1	1:A:186:TYR:O	0.48	2.67	45	14
1:A:191:PHE:CE1	1:A:196:SER:HA	0.48	2.44	10	3
1:A:198:ALA:O	1:A:199:LEU:O	0.48	2.30	42	4
1:A:176:PHE:CZ	1:A:185:ALA:HB2	0.48	2.44	35	4
1:A:151:GLN:HB3	1:A:157:PHE:CG	0.48	2.43	15	1
1:A:146:TYR:CD1	1:A:201:ASN:HB3	0.48	2.43	16	7
1:A:200:LEU:N	1:A:200:LEU:CD2	0.48	2.77	7	3
1:A:172:TRP:CD1	1:A:174:GLY:CA	0.48	2.97	3	6
1:A:183:ALA:HA	1:A:201:ASN:ND2	0.48	2.24	24	1
1:A:194:ARG:O	1:A:195:GLY:O	0.48	2.32	39	11
1:A:157:PHE:CD1	1:A:178:THR:CA	0.47	2.97	1	3
1:A:191:PHE:CE2	1:A:196:SER:HA	0.47	2.44	2	2
1:A:190:ALA:O	1:A:198:ALA:CB	0.47	2.61	13	5
1:A:159:ALA:HB3	1:A:176:PHE:HE1	0.47	1.69	31	5
1:A:161:ILE:HG12	1:A:162:ARG:N	0.47	2.24	27	3
1:A:159:ALA:HB2	1:A:182:ALA:HB1	0.47	1.84	24	1
1:A:191:PHE:O	1:A:195:GLY:O	0.47	2.31	23	7
1:A:195:GLY:O	1:A:196:SER:O	0.47	2.32	29	7
1:A:151:GLN:CB	1:A:157:PHE:CD1	0.47	2.98	15	1
1:A:152:ARG:CG	1:A:153:PRO:CD	0.47	2.92	42	2
1:A:161:ILE:HB	1:A:186:TYR:CE2	0.47	2.44	41	1
1:A:161:ILE:CD1	1:A:190:ALA:HA	0.47	2.40	14	16
1:A:163:ASP:O	1:A:168:GLY:O	0.47	2.32	19	3
1:A:157:PHE:CE2	1:A:178:THR:HA	0.47	2.44	15	3
1:A:187:ASP:OD1	1:A:200:LEU:HB2	0.47	2.10	43	12
1:A:196:SER:O	1:A:197:ARG:O	0.47	2.33	24	12
1:A:162:ARG:O	1:A:162:ARG:CG	0.47	2.63	35	2
1:A:163:ASP:O	1:A:168:GLY:CA	0.47	2.63	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:167:ASN:O	1:A:167:ASN:OD1	0.47	2.33	16	2
1:A:190:ALA:O	1:A:194:ARG:HB2	0.47	2.10	26	6
1:A:152:ARG:N	1:A:152:ARG:HD2	0.47	2.25	33	1
1:A:150:ARG:O	1:A:157:PHE:CD2	0.47	2.67	40	1
1:A:157:PHE:HE2	1:A:179:ALA:HB2	0.47	1.59	41	2
1:A:151:GLN:HB3	1:A:157:PHE:CD1	0.47	2.45	36	2
1:A:150:ARG:O	1:A:150:ARG:CD	0.47	2.63	33	1
1:A:177:GLU:C	1:A:178:THR:CG2	0.46	2.83	6	3
1:A:157:PHE:O	1:A:176:PHE:N	0.46	2.48	8	4
1:A:196:SER:O	1:A:197:ARG:C	0.46	2.54	15	6
1:A:172:TRP:CD1	1:A:172:TRP:C	0.46	2.88	33	12
1:A:175:THR:C	1:A:176:PHE:CD1	0.46	2.89	45	3
1:A:194:ARG:HB2	1:A:198:ALA:CB	0.46	2.39	15	1
1:A:151:GLN:HG2	1:A:152:ARG:N	0.46	2.25	17	2
1:A:173:LEU:HD21	1:A:189:ALA:HB1	0.46	1.86	40	2
1:A:153:PRO:O	1:A:154:TRP:HB2	0.46	2.10	27	4
1:A:181:ASP:OD1	1:A:181:ASP:N	0.46	2.47	12	3
1:A:191:PHE:O	1:A:195:GLY:HA2	0.46	2.11	4	9
1:A:197:ARG:O	1:A:198:ALA:O	0.46	2.34	26	2
1:A:158:ALA:O	1:A:160:GLU:OE1	0.46	2.33	39	2
1:A:178:THR:OG1	1:A:181:ASP:OD2	0.46	2.34	27	8
1:A:147:ARG:CG	1:A:147:ARG:O	0.46	2.63	21	1
1:A:152:ARG:HB3	1:A:156:LYS:O	0.46	2.11	21	1
1:A:173:LEU:HD22	1:A:189:ALA:CB	0.46	2.40	8	2
1:A:155:GLY:O	1:A:156:LYS:HB2	0.46	2.11	21	1
1:A:167:ASN:O	1:A:168:GLY:O	0.46	2.33	40	1
1:A:187:ASP:CB	1:A:200:LEU:HB3	0.46	2.41	12	2
1:A:149:VAL:HA	1:A:158:ALA:O	0.46	2.11	37	1
1:A:146:TYR:CG	1:A:183:ALA:HB2	0.45	2.44	12	2
1:A:187:ASP:OD1	1:A:200:LEU:HB3	0.45	2.11	4	10
1:A:176:PHE:CZ	1:A:185:ALA:HB3	0.45	2.47	30	6
1:A:166:LYS:HA	1:A:166:LYS:CE	0.45	2.41	40	1
1:A:198:ALA:O	1:A:199:LEU:C	0.45	2.55	19	4
1:A:159:ALA:CB	1:A:176:PHE:CE1	0.45	2.99	20	4
1:A:148:GLY:O	1:A:160:GLU:OE1	0.45	2.34	10	1
1:A:161:ILE:CG2	1:A:171:VAL:HB	0.45	2.41	38	3
1:A:180:GLU:O	1:A:181:ASP:C	0.45	2.55	11	2
1:A:150:ARG:O	1:A:157:PHE:HA	0.45	2.12	46	10
1:A:146:TYR:CD2	1:A:179:ALA:HB1	0.45	2.47	24	1
1:A:152:ARG:CB	1:A:156:LYS:O	0.45	2.65	21	1
1:A:159:ALA:HB2	1:A:182:ALA:O	0.45	2.12	21	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:175:THR:C	1:A:176:PHE:CD2	0.45	2.90	3	2
1:A:199:LEU:O	1:A:200:LEU:HD23	0.45	2.12	21	1
1:A:202:PHE:CD1	1:A:202:PHE:N	0.45	2.83	22	6
1:A:194:ARG:HD2	1:A:198:ALA:CB	0.45	2.42	37	1
1:A:158:ALA:C	1:A:160:GLU:OE2	0.45	2.55	24	1
1:A:184:LEU:O	1:A:184:LEU:CD1	0.45	2.65	24	1
1:A:163:ASP:OD2	1:A:193:MET:SD	0.44	2.75	7	4
1:A:161:ILE:HD12	1:A:190:ALA:CA	0.44	2.42	14	1
1:A:198:ALA:O	1:A:200:LEU:CD2	0.44	2.64	30	1
1:A:195:GLY:O	1:A:196:SER:HB2	0.44	2.12	39	1
1:A:187:ASP:CG	1:A:200:LEU:HB2	0.44	2.32	45	12
1:A:152:ARG:NE	1:A:156:LYS:HB2	0.44	2.27	37	1
1:A:176:PHE:CG	1:A:182:ALA:CA	0.44	3.01	15	1
1:A:157:PHE:CD2	1:A:179:ALA:N	0.44	2.85	18	2
1:A:152:ARG:NE	1:A:155:GLY:HA3	0.44	2.27	45	1
1:A:200:LEU:O	1:A:201:ASN:C	0.44	2.56	15	4
1:A:166:LYS:O	1:A:167:ASN:C	0.44	2.56	6	1
1:A:195:GLY:O	1:A:196:SER:C	0.44	2.56	12	5
1:A:171:VAL:O	1:A:171:VAL:CG1	0.44	2.64	19	1
1:A:152:ARG:C	1:A:152:ARG:HD3	0.44	2.33	21	1
1:A:156:LYS:HD2	1:A:157:PHE:N	0.44	2.26	10	1
1:A:158:ALA:HB2	1:A:172:TRP:CZ2	0.44	2.48	18	3
1:A:169:ALA:O	1:A:170:ARG:O	0.44	2.36	34	1
1:A:160:GLU:OE2	1:A:161:ILE:O	0.44	2.35	14	1
1:A:194:ARG:HD3	1:A:198:ALA:HB1	0.44	1.89	20	2
1:A:151:GLN:N	1:A:151:GLN:CD	0.44	2.71	36	2
1:A:183:ALA:CB	1:A:202:PHE:CE2	0.44	3.01	24	2
1:A:197:ARG:HG2	1:A:198:ALA:N	0.43	2.28	45	2
1:A:195:GLY:C	1:A:196:SER:OG	0.43	2.57	11	1
1:A:163:ASP:HB2	1:A:193:MET:CE	0.43	2.43	31	1
1:A:173:LEU:CD1	1:A:186:TYR:HA	0.43	2.43	8	2
1:A:177:GLU:HG2	1:A:181:ASP:OD2	0.43	2.13	11	1
1:A:146:TYR:CZ	1:A:202:PHE:CE1	0.43	3.06	22	1
1:A:150:ARG:NH2	1:A:152:ARG:NH1	0.43	2.66	33	1
1:A:169:ALA:O	1:A:170:ARG:C	0.43	2.57	34	4
1:A:150:ARG:HG3	1:A:150:ARG:O	0.43	2.13	33	1
1:A:187:ASP:CB	1:A:200:LEU:HD13	0.43	2.42	44	2
1:A:196:SER:O	1:A:197:ARG:CB	0.43	2.64	25	2
1:A:196:SER:O	1:A:197:ARG:HB3	0.43	2.14	6	1
1:A:178:THR:OG1	1:A:181:ASP:CG	0.43	2.57	31	2
1:A:171:VAL:O	1:A:171:VAL:HG12	0.43	2.14	20	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:167:ASN:O	1:A:168:GLY:C	0.43	2.57	30	4
1:A:160:GLU:O	1:A:161:ILE:HB	0.43	2.14	42	1
1:A:161:ILE:HD13	1:A:193:MET:CE	0.43	2.44	43	1
1:A:187:ASP:HB3	1:A:200:LEU:CD1	0.43	2.44	40	4
1:A:150:ARG:NH1	1:A:150:ARG:HG3	0.43	2.28	29	1
1:A:146:TYR:CD2	1:A:179:ALA:O	0.42	2.72	42	12
1:A:196:SER:O	1:A:197:ARG:HB2	0.42	2.13	25	4
1:A:157:PHE:CG	1:A:178:THR:C	0.42	2.92	45	1
1:A:187:ASP:OD2	1:A:200:LEU:HD12	0.42	2.14	21	2
1:A:159:ALA:HB3	1:A:176:PHE:HE2	0.42	1.73	3	1
1:A:159:ALA:O	1:A:173:LEU:HB2	0.42	2.14	8	7
1:A:146:TYR:HB2	1:A:149:VAL:CG2	0.42	2.44	7	1
1:A:163:ASP:OD1	1:A:163:ASP:C	0.42	2.57	15	2
1:A:163:ASP:OD2	1:A:166:LYS:CG	0.42	2.68	24	1
1:A:198:ALA:HB3	1:A:200:LEU:HD21	0.42	1.91	33	1
1:A:194:ARG:CD	1:A:198:ALA:CB	0.42	2.98	37	1
1:A:194:ARG:CD	1:A:198:ALA:HB1	0.42	2.44	37	1
1:A:187:ASP:CG	1:A:200:LEU:HB3	0.42	2.35	4	2
1:A:166:LYS:O	1:A:167:ASN:CG	0.42	2.57	6	1
1:A:167:ASN:OD1	1:A:169:ALA:HB2	0.42	2.15	33	1
1:A:201:ASN:O	1:A:202:PHE:CD1	0.42	2.73	15	1
1:A:166:LYS:O	1:A:167:ASN:HB2	0.42	2.14	19	1
1:A:146:TYR:CZ	1:A:202:PHE:CZ	0.42	3.08	22	3
1:A:152:ARG:HB2	1:A:153:PRO:CD	0.42	2.44	22	1
1:A:187:ASP:OD2	1:A:202:PHE:O	0.42	2.38	22	1
1:A:157:PHE:O	1:A:175:THR:HA	0.42	2.15	31	1
1:A:151:GLN:CG	1:A:152:ARG:N	0.42	2.83	3	1
1:A:178:THR:C	1:A:181:ASP:OD1	0.42	2.58	11	1
1:A:199:LEU:C	1:A:199:LEU:CD1	0.42	2.87	38	2
1:A:151:GLN:O	1:A:151:GLN:NE2	0.42	2.53	17	1
1:A:194:ARG:NH1	1:A:194:ARG:HG2	0.42	2.30	1	1
1:A:158:ALA:O	1:A:160:GLU:OE2	0.42	2.38	17	1
1:A:177:GLU:HG3	1:A:181:ASP:OD2	0.42	2.14	17	1
1:A:190:ALA:O	1:A:194:ARG:HG3	0.42	2.15	41	3
1:A:199:LEU:N	1:A:199:LEU:HD23	0.42	2.29	27	1
1:A:159:ALA:HB3	1:A:176:PHE:CE2	0.41	2.50	3	1
1:A:157:PHE:CD1	1:A:179:ALA:CB	0.41	3.02	18	1
1:A:166:LYS:O	1:A:167:ASN:HB3	0.41	2.15	34	2
1:A:163:ASP:CG	1:A:166:LYS:CG	0.41	2.89	44	1
1:A:151:GLN:O	1:A:151:GLN:HG3	0.41	2.15	45	1
1:A:167:ASN:OD1	1:A:167:ASN:O	0.41	2.39	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:201:ASN:C	1:A:203:PRO:HD3	0.41	2.36	7	4
1:A:147:ARG:O	1:A:147:ARG:CG	0.41	2.68	35	1
1:A:194:ARG:CB	1:A:198:ALA:CB	0.41	2.98	38	2
1:A:160:GLU:OE1	1:A:161:ILE:N	0.41	2.53	20	1
1:A:195:GLY:O	1:A:196:SER:HB3	0.41	2.16	21	2
1:A:194:ARG:NE	1:A:194:ARG:HA	0.41	2.30	35	1
1:A:157:PHE:CD2	1:A:179:ALA:CB	0.41	3.04	21	1
1:A:146:TYR:CE2	1:A:179:ALA:O	0.41	2.73	12	1
1:A:159:ALA:CB	1:A:182:ALA:O	0.41	2.68	14	1
1:A:152:ARG:CG	1:A:156:LYS:O	0.41	2.69	21	1
1:A:152:ARG:HG3	1:A:153:PRO:HD2	0.41	1.93	22	1
1:A:163:ASP:OD2	1:A:166:LYS:HG3	0.41	2.16	24	1
1:A:155:GLY:O	1:A:156:LYS:HG2	0.41	2.15	21	1
1:A:163:ASP:CG	1:A:193:MET:SD	0.41	2.99	18	1
1:A:184:LEU:CD1	1:A:184:LEU:C	0.41	2.89	24	1
1:A:201:ASN:O	1:A:203:PRO:HD3	0.41	2.15	24	1
1:A:191:PHE:CD2	1:A:195:GLY:O	0.41	2.73	27	1
1:A:150:ARG:HG2	1:A:158:ALA:HB3	0.41	1.83	33	1
1:A:161:ILE:HD12	1:A:190:ALA:HA	0.41	1.92	1	1
1:A:160:GLU:HG2	1:A:171:VAL:O	0.41	2.16	35	1
1:A:161:ILE:HG21	1:A:193:MET:CE	0.41	2.46	40	1
1:A:187:ASP:OD2	1:A:200:LEU:HB2	0.40	2.16	4	1
1:A:149:VAL:CG1	1:A:157:PHE:HB3	0.40	2.45	16	1
1:A:191:PHE:CE1	1:A:197:ARG:O	0.40	2.74	27	1
1:A:152:ARG:HG2	1:A:153:PRO:CD	0.40	2.47	36	1
1:A:200:LEU:N	1:A:200:LEU:HD23	0.40	2.31	37	1
1:A:173:LEU:HD11	1:A:189:ALA:HB2	0.40	1.89	43	1
1:A:153:PRO:O	1:A:154:TRP:CD1	0.40	2.74	33	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	58/70 (83%)	49±3 (85±5%)	6±2 (11±4%)	3±1 (5±2%)	4	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2668/3220 (83%)	2255 (85%)	283 (11%)	130 (5%)	4 26

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

Mol	Chain	Res	Type	Models (Total)
1	A	197	ARG	27
1	A	195	GLY	21
1	A	196	SER	21
1	A	155	GLY	16
1	A	168	GLY	15
1	A	198	ALA	7
1	A	199	LEU	4
1	A	154	TRP	4
1	A	148	GLY	3
1	A	169	ALA	3
1	A	170	ARG	3
1	A	167	ASN	2
1	A	172	TRP	1
1	A	156	LYS	1
1	A	152	ARG	1
1	A	161	ILE	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	42/51 (82%)	30±2 (72±5%)	12±2 (28±5%)	2 19
All	All	1932/2346 (82%)	1393 (72%)	539 (28%)	2 19

All 28 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	200	LEU	46
1	A	201	ASN	45
1	A	181	ASP	44

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Mol	Chain	Res	Type	Models (Total)
1	A	184	LEU	27
1	A	197	ARG	27
1	A	147	ARG	25
1	A	152	ARG	25
1	A	199	LEU	22
1	A	150	ARG	22
1	A	154	TRP	21
1	A	162	ARG	19
1	A	188	ARG	19
1	A	196	SER	17
1	A	170	ARG	17
1	A	192	ARG	16
1	A	160	GLU	16
1	A	177	GLU	16
1	A	167	ASN	16
1	A	151	GLN	15
1	A	173	LEU	14
1	A	194	ARG	13
1	A	193	MET	13
1	A	156	LYS	10
1	A	175	THR	10
1	A	180	GLU	8
1	A	166	LYS	8
1	A	191	PHE	5
1	A	178	THR	3

### 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