



# Full wwPDB NMR Structure Validation Report ⓘ

Feb 10, 2022 – 10:08 AM EST

PDB ID : 1EYF  
Title : REFINED STRUCTURE OF THE DNA METHYL PHOSPHOTRIESTER REPAIR DOMAIN OF E. COLI ADA  
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Deposited on : 2000-05-06

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 : 2.26  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.26

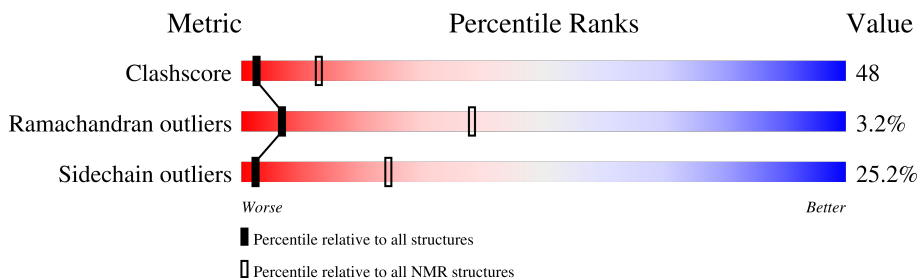
# 1 Overall quality at a glance

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	92	

## 2 Ensemble composition and analysis i

This entry contains 25 models. Model 4 is the overall representative, medoid model (most similar to other models). The authors have identified model 13 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:9-A:73 (65)	0.23	4

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 4 clusters and 5 single-model clusters were found.

Cluster number	Models
1	4, 7, 9, 12, 14, 15
2	6, 11, 13, 17, 20, 23
3	1, 2, 8, 21, 25
4	3, 16, 18
Single-model clusters	5; 10; 19; 22; 24

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

There are 2 unique types of molecules in this entry. The entry contains 1449 atoms, of which 717 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called ADA REGULATORY PROTEIN.

Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		S
1	A	92	1448	447	717	148	129	7	0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

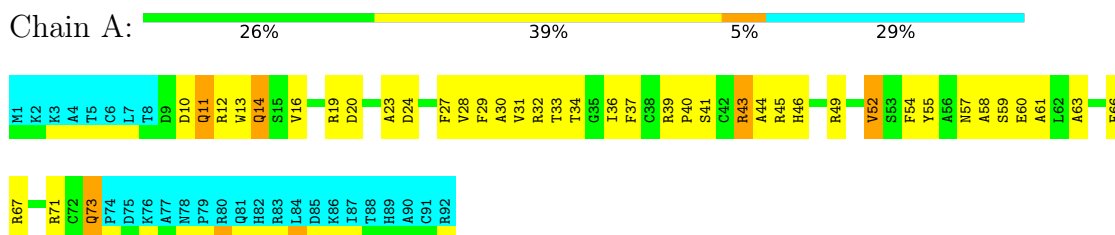
Mol	Chain	Residues	Atoms	
2	A	1	Total	Zn
			1	1

## 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: ADA REGULATORY PROTEIN

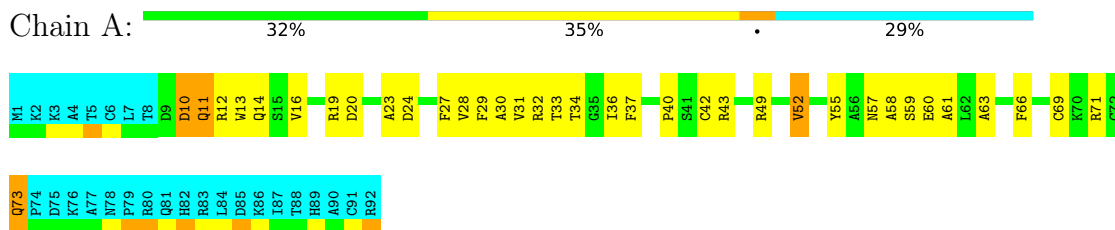


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

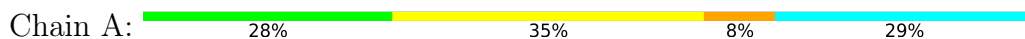
#### 4.2.1 Score per residue for model 1

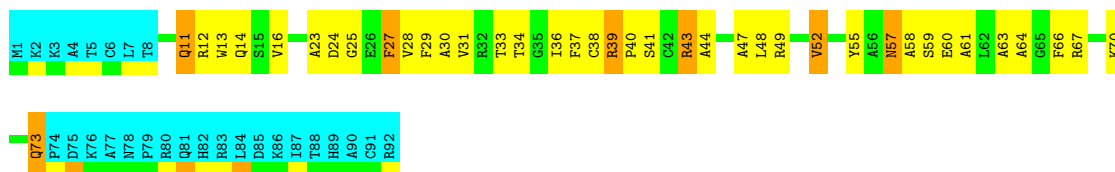
- Molecule 1: ADA REGULATORY PROTEIN



#### 4.2.2 Score per residue for model 2

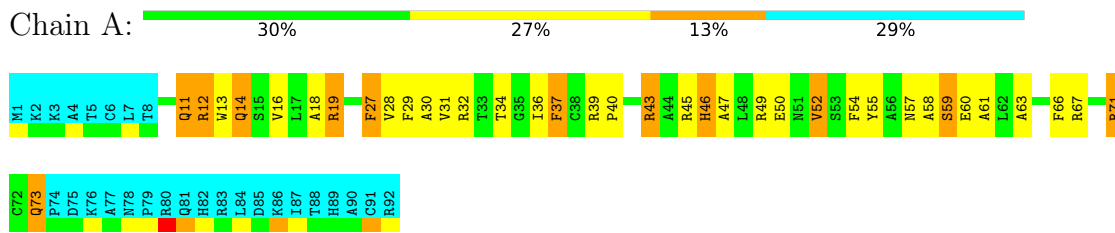
- Molecule 1: ADA REGULATORY PROTEIN





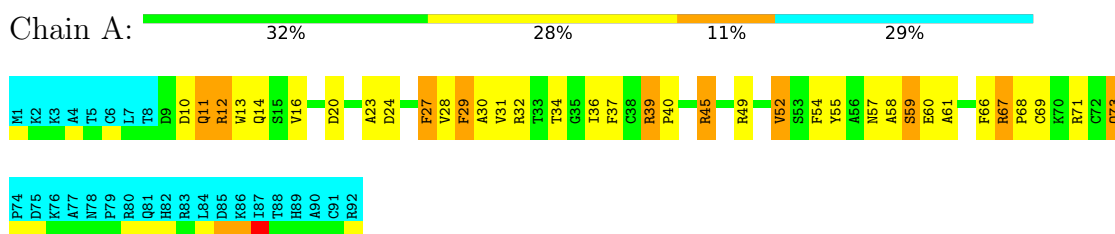
### 4.2.3 Score per residue for model 3

- Molecule 1: ADA REGULATORY PROTEIN



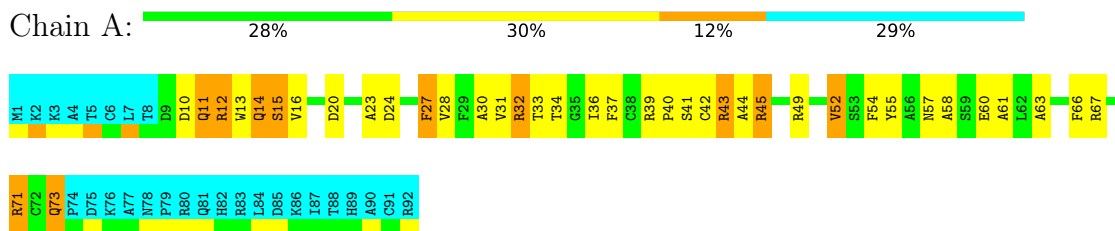
### 4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: ADA REGULATORY PROTEIN



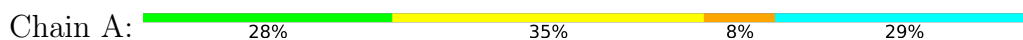
### 4.2.5 Score per residue for model 5

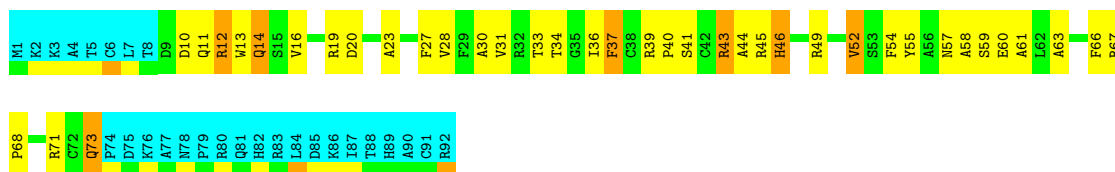
- Molecule 1: ADA REGULATORY PROTEIN



### 4.2.6 Score per residue for model 6

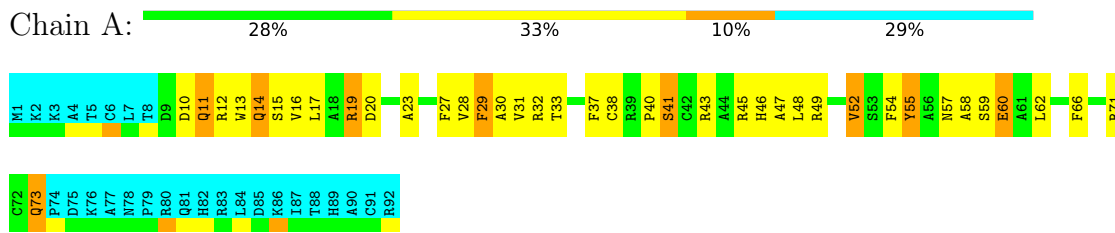
- Molecule 1: ADA REGULATORY PROTEIN





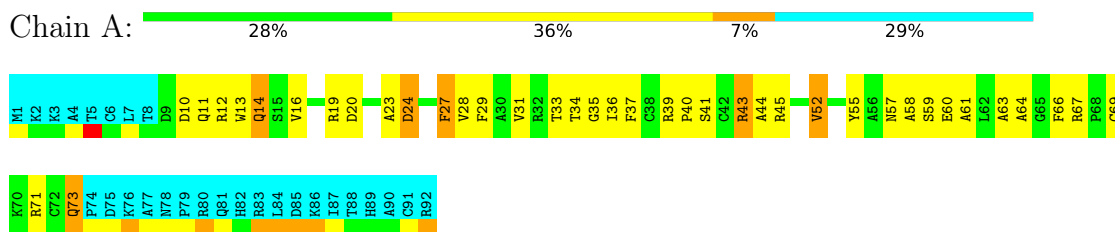
#### 4.2.7 Score per residue for model 7

- Molecule 1: ADA REGULATORY PROTEIN



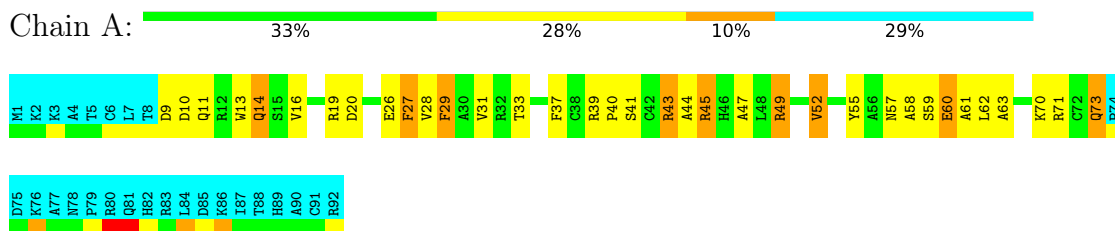
#### 4.2.8 Score per residue for model 8

- Molecule 1: ADA REGULATORY PROTEIN



#### 4.2.9 Score per residue for model 9

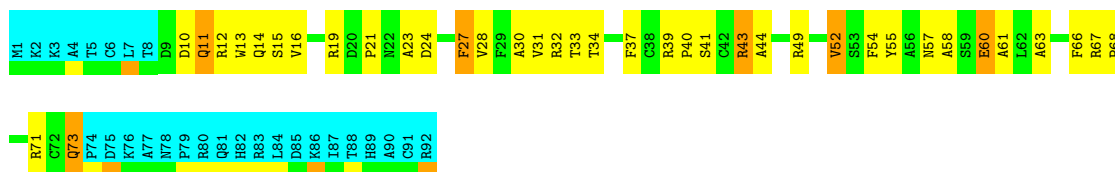
- Molecule 1: ADA REGULATORY PROTEIN



#### 4.2.10 Score per residue for model 10

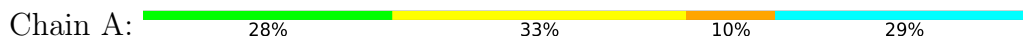
- Molecule 1: ADA REGULATORY PROTEIN





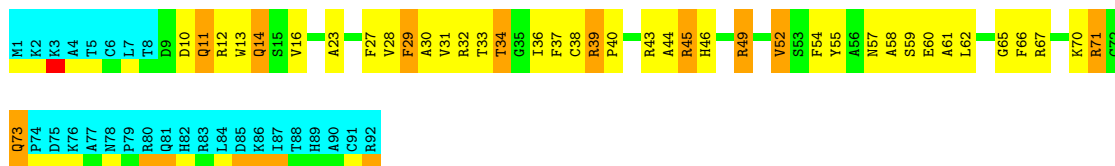
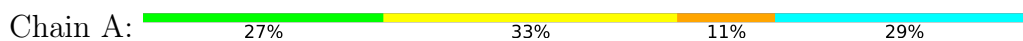
#### 4.2.11 Score per residue for model 11

- Molecule 1: ADA REGULATORY PROTEIN



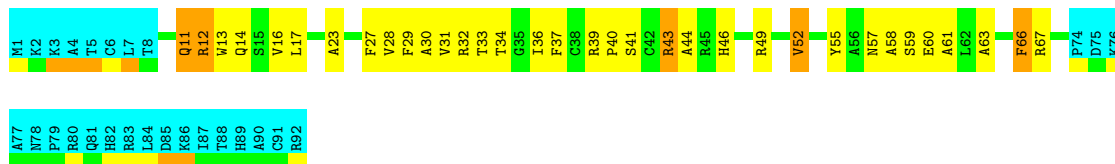
#### 4.2.12 Score per residue for model 12

- Molecule 1: ADA REGULATORY PROTEIN



#### 4.2.13 Score per residue for model 13

- Molecule 1: ADA REGULATORY PROTEIN



#### 4.2.14 Score per residue for model 14

- Molecule 1: ADA REGULATORY PROTEIN



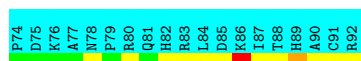
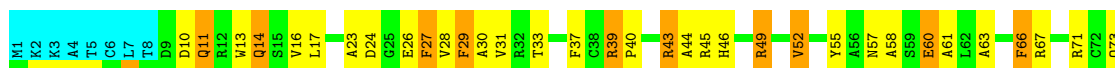




#### 4.2.15 Score per residue for model 15

- Molecule 1: ADA REGULATORY PROTEIN

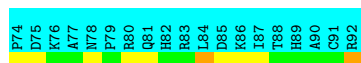
Chain A: 34% 26% 11% 29%



#### 4.2.16 Score per residue for model 16

- Molecule 1: ADA REGULATORY PROTEIN

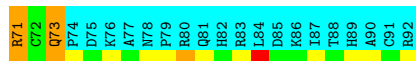
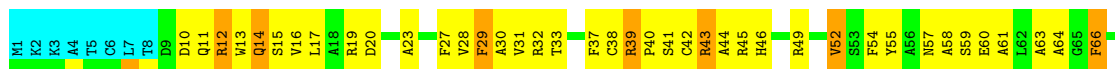
Chain A: 29% 34% 7% 29%



#### 4.2.17 Score per residue for model 17

- Molecule 1: ADA REGULATORY PROTEIN

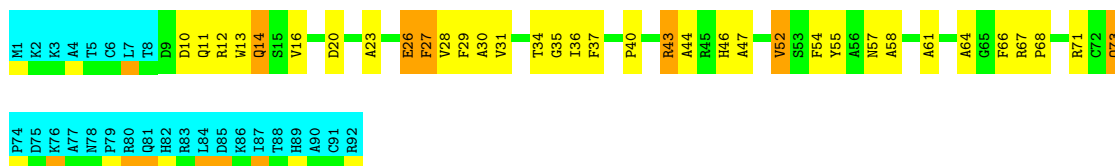
Chain A: 25% 36% 10% 29%



#### 4.2.18 Score per residue for model 18

- Molecule 1: ADA REGULATORY PROTEIN

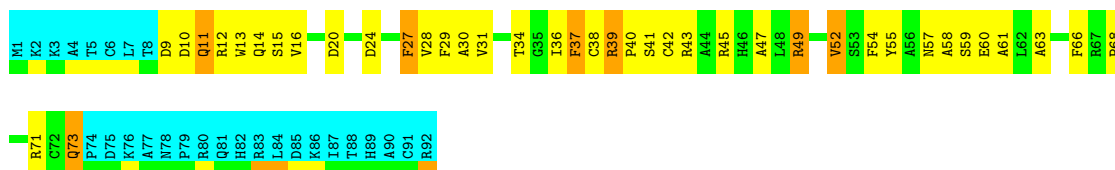
Chain A: 33% 32% 7% 29%



#### 4.2.19 Score per residue for model 19

- Molecule 1: ADA REGULATORY PROTEIN

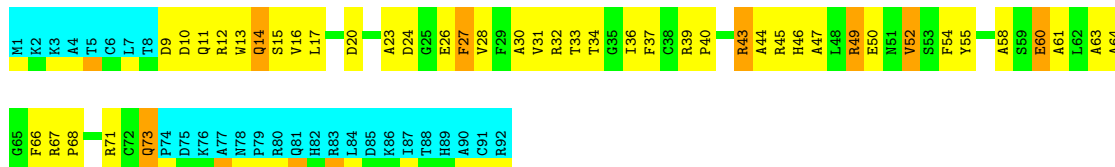
Chain A: 27% 36% 8% 29%



#### 4.2.20 Score per residue for model 20

- Molecule 1: ADA REGULATORY PROTEIN

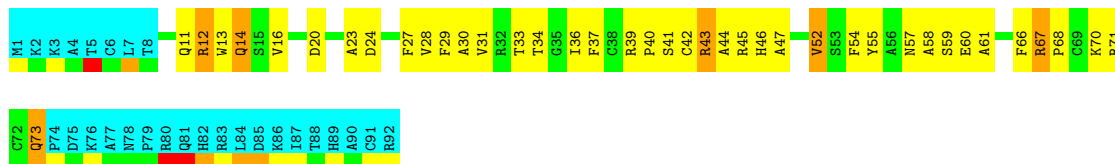
Chain A: 23% 40% 8% 29%



#### 4.2.21 Score per residue for model 21

- Molecule 1: ADA REGULATORY PROTEIN

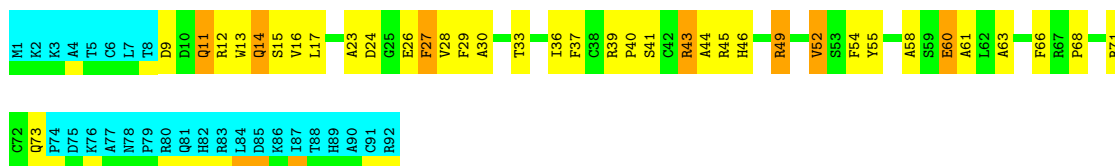
Chain A: 27% 37% 7% 29%



#### 4.2.22 Score per residue for model 22

- Molecule 1: ADA REGULATORY PROTEIN

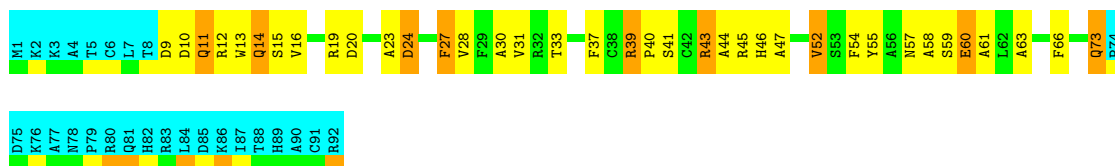
Chain A: 30% 33% 8% 29%



#### 4.2.23 Score per residue for model 23

- Molecule 1: ADA REGULATORY PROTEIN

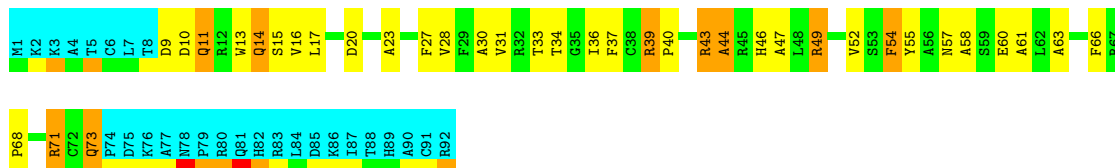
Chain A: 30% 30% 10% 29%



#### 4.2.24 Score per residue for model 24

- Molecule 1: ADA REGULATORY PROTEIN

Chain A: 30% 30% 10% 29%



#### 4.2.25 Score per residue for model 25

- Molecule 1: ADA REGULATORY PROTEIN

Chain A: 27% 36% 8% 29%



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *distance geometry*.

Of the 50 calculated structures, 25 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
DGII	structure solution	
DGII	refinement	

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

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	514	487	487	48±5
All	All	12875	12175	12175	1207

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 48.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:67:ARG:HG2	1:A:68:PRO:HD2	1.10	1.23	4	1
1:A:30:ALA:HB2	1:A:55:TYR:HE2	0.96	1.18	23	9
1:A:55:TYR:CD2	1:A:61:ALA:HB2	0.95	1.97	19	11
1:A:30:ALA:HB2	1:A:55:TYR:HE1	0.93	1.23	22	7
1:A:31:VAL:HG22	1:A:52:VAL:HG23	0.93	1.39	1	21
1:A:16:VAL:HG22	1:A:40:PRO:HB3	0.91	1.42	22	5
1:A:37:PHE:CE1	1:A:58:ALA:HB1	0.90	2.00	17	16
1:A:67:ARG:HG2	1:A:68:PRO:CD	0.89	1.95	4	1
1:A:28:VAL:HG22	1:A:55:TYR:HB2	0.88	1.46	6	25
1:A:30:ALA:HB2	1:A:55:TYR:CE2	0.88	2.03	23	12
1:A:30:ALA:HB2	1:A:55:TYR:CE1	0.86	2.05	16	7
1:A:11:GLN:HA	1:A:14:GLN:HB3	0.85	1.47	7	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:27:PHE:CE2	1:A:40:PRO:HB3	0.85	2.05	7	2
1:A:39:ARG:HG2	1:A:40:PRO:HD2	0.85	1.45	23	12
1:A:11:GLN:HA	1:A:14:GLN:HB2	0.85	1.49	23	15
1:A:31:VAL:HG12	1:A:33:THR:HG22	0.84	1.47	9	13
1:A:31:VAL:CG1	1:A:33:THR:HG22	0.84	2.01	10	13
1:A:11:GLN:NE2	1:A:14:GLN:HB3	0.83	1.88	2	1
1:A:16:VAL:HG22	1:A:40:PRO:HA	0.80	1.53	21	15
1:A:37:PHE:HD2	1:A:61:ALA:HB3	0.80	1.34	19	3
1:A:27:PHE:CE1	1:A:40:PRO:HB3	0.80	2.11	6	7
1:A:43:ARG:HG3	1:A:44:ALA:N	0.80	1.92	23	12
1:A:37:PHE:CE2	1:A:58:ALA:HB1	0.79	2.12	19	8
1:A:23:ALA:HB3	1:A:40:PRO:HG2	0.79	1.55	1	9
1:A:30:ALA:HB1	1:A:66:PHE:CE2	0.79	2.12	22	21
1:A:24:ASP:HA	1:A:39:ARG:HG2	0.79	1.53	22	3
1:A:37:PHE:HD2	1:A:61:ALA:CB	0.79	1.91	19	2
1:A:43:ARG:HG2	1:A:44:ALA:N	0.78	1.93	5	5
1:A:13:TRP:CZ3	1:A:52:VAL:HG11	0.78	2.12	11	10
1:A:13:TRP:CZ3	1:A:16:VAL:HG11	0.78	2.12	20	25
1:A:23:ALA:HB3	1:A:40:PRO:CG	0.78	2.08	5	16
1:A:11:GLN:HG2	1:A:14:GLN:HG2	0.77	1.55	7	1
1:A:34:THR:HG23	1:A:36:ILE:HG13	0.77	1.57	1	9
1:A:28:VAL:HG23	1:A:55:TYR:HD2	0.76	1.38	23	6
1:A:28:VAL:CG2	1:A:55:TYR:HD2	0.75	1.94	18	11
1:A:37:PHE:CG	1:A:61:ALA:HB1	0.74	2.16	21	7
1:A:43:ARG:HG2	1:A:71:ARG:HD3	0.74	1.57	12	2
1:A:23:ALA:HB3	1:A:40:PRO:HG3	0.74	1.60	11	12
1:A:37:PHE:HE2	1:A:58:ALA:CB	0.74	1.95	15	6
1:A:37:PHE:HE2	1:A:58:ALA:HB1	0.72	1.44	5	6
1:A:55:TYR:CE2	1:A:61:ALA:HB2	0.72	2.18	9	11
1:A:37:PHE:CD2	1:A:61:ALA:HB3	0.71	2.20	11	4
1:A:55:TYR:HD2	1:A:61:ALA:HB2	0.71	1.43	2	3
1:A:30:ALA:HB1	1:A:66:PHE:HE2	0.70	1.45	25	12
1:A:31:VAL:CG2	1:A:52:VAL:HG23	0.70	2.16	1	13
1:A:29:PHE:HD2	1:A:52:VAL:CG2	0.70	2.00	2	1
1:A:11:GLN:HG2	1:A:14:GLN:CG	0.69	2.18	7	1
1:A:14:GLN:HG3	1:A:15:SER:N	0.68	2.03	22	2
1:A:27:PHE:HE1	1:A:40:PRO:CG	0.68	2.00	15	2
1:A:39:ARG:HG2	1:A:40:PRO:CD	0.68	2.17	16	7
1:A:30:ALA:CB	1:A:55:TYR:HE1	0.67	2.01	16	7
1:A:16:VAL:HG22	1:A:40:PRO:CA	0.67	2.20	25	8
1:A:28:VAL:HG23	1:A:55:TYR:HD1	0.66	1.48	3	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:ALA:HB1	1:A:27:PHE:HE1	0.65	1.50	2	2
1:A:28:VAL:HG23	1:A:55:TYR:CD1	0.65	2.26	5	7
1:A:28:VAL:HG13	1:A:57:ASN:HA	0.63	1.70	24	12
1:A:27:PHE:CZ	1:A:40:PRO:HB3	0.63	2.27	7	5
1:A:57:ASN:OD1	1:A:59:SER:HB3	0.63	1.94	13	7
1:A:11:GLN:O	1:A:15:SER:HB2	0.63	1.92	20	3
1:A:43:ARG:HG3	1:A:44:ALA:H	0.62	1.54	8	2
1:A:37:PHE:HE1	1:A:73:GLN:CG	0.62	2.07	2	7
1:A:31:VAL:HG21	1:A:47:ALA:HB3	0.62	1.71	7	8
1:A:60:GLU:O	1:A:63:ALA:HB3	0.62	1.94	20	18
1:A:55:TYR:HE2	1:A:61:ALA:CB	0.62	2.08	9	2
1:A:57:ASN:OD1	1:A:59:SER:HB2	0.61	1.94	17	4
1:A:28:VAL:CG2	1:A:55:TYR:CD2	0.61	2.84	8	15
1:A:37:PHE:HE1	1:A:73:GLN:HG3	0.61	1.56	3	5
1:A:55:TYR:HE2	1:A:61:ALA:HB2	0.60	1.56	9	2
1:A:9:ASP:HB3	1:A:12:ARG:NH1	0.60	2.10	23	1
1:A:16:VAL:CG2	1:A:40:PRO:HB3	0.60	2.27	25	6
1:A:28:VAL:CG2	1:A:55:TYR:CD1	0.60	2.84	20	7
1:A:13:TRP:CE3	1:A:16:VAL:HG11	0.60	2.31	7	21
1:A:37:PHE:CE1	1:A:58:ALA:CB	0.60	2.85	21	14
1:A:43:ARG:HD3	1:A:71:ARG:HD3	0.60	1.72	11	1
1:A:31:VAL:CG2	1:A:47:ALA:HB3	0.60	2.26	21	6
1:A:28:VAL:HG11	1:A:58:ALA:N	0.59	2.11	12	3
1:A:37:PHE:CZ	1:A:58:ALA:HB1	0.59	2.31	17	10
1:A:28:VAL:HG23	1:A:55:TYR:CD2	0.59	2.31	25	8
1:A:43:ARG:HD3	1:A:71:ARG:HD2	0.59	1.74	5	1
1:A:55:TYR:CE2	1:A:61:ALA:CB	0.59	2.86	9	11
1:A:34:THR:HG23	1:A:36:ILE:CG1	0.58	2.28	5	7
1:A:30:ALA:CB	1:A:55:TYR:CE1	0.58	2.82	16	7
1:A:64:ALA:HB1	1:A:66:PHE:CE2	0.58	2.33	18	2
1:A:16:VAL:HG22	1:A:40:PRO:CB	0.58	2.29	25	5
1:A:37:PHE:CD2	1:A:61:ALA:CB	0.58	2.86	6	11
1:A:27:PHE:HE1	1:A:40:PRO:HG3	0.58	1.59	8	6
1:A:37:PHE:CE1	1:A:73:GLN:CG	0.58	2.87	2	8
1:A:39:ARG:HG3	1:A:40:PRO:HD2	0.58	1.75	4	4
1:A:37:PHE:CE2	1:A:58:ALA:CB	0.58	2.87	22	8
1:A:45:ARG:O	1:A:45:ARG:HG2	0.57	1.98	9	3
1:A:29:PHE:HD2	1:A:52:VAL:HG22	0.57	1.59	2	1
1:A:24:ASP:CA	1:A:39:ARG:HG2	0.57	2.28	22	1
1:A:44:ALA:HB2	1:A:71:ARG:NH2	0.57	2.15	14	1
1:A:24:ASP:HA	1:A:39:ARG:HG3	0.57	1.76	25	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:13:TRP:CE3	1:A:52:VAL:HG11	0.57	2.34	11	5
1:A:44:ALA:HB2	1:A:71:ARG:NH1	0.57	2.15	15	2
1:A:29:PHE:CD1	1:A:52:VAL:HG21	0.56	2.34	21	3
1:A:30:ALA:HB1	1:A:66:PHE:CD2	0.56	2.34	4	7
1:A:31:VAL:CG1	1:A:34:THR:HG22	0.56	2.30	10	2
1:A:37:PHE:HE2	1:A:58:ALA:CA	0.56	2.13	11	2
1:A:34:THR:HG21	1:A:36:ILE:HD12	0.56	1.77	12	1
1:A:37:PHE:HE2	1:A:58:ALA:O	0.56	1.83	19	2
1:A:64:ALA:HB3	1:A:66:PHE:CD2	0.56	2.36	8	2
1:A:13:TRP:CZ3	1:A:16:VAL:CG1	0.56	2.88	22	21
1:A:36:ILE:HG21	1:A:69:CYS:HA	0.56	1.75	8	3
1:A:30:ALA:CB	1:A:55:TYR:CE2	0.55	2.88	4	5
1:A:67:ARG:CG	1:A:68:PRO:HD2	0.55	2.16	4	1
1:A:16:VAL:HG13	1:A:29:PHE:HE2	0.55	1.60	7	1
1:A:59:SER:HA	1:A:62:LEU:HD12	0.55	1.77	7	2
1:A:11:GLN:CA	1:A:14:GLN:HB3	0.55	2.30	16	5
1:A:27:PHE:CD1	1:A:27:PHE:N	0.55	2.75	20	13
1:A:27:PHE:CE1	1:A:40:PRO:CB	0.55	2.90	10	4
1:A:27:PHE:HE1	1:A:40:PRO:CB	0.55	2.13	15	2
1:A:37:PHE:CE2	1:A:73:GLN:CG	0.55	2.89	4	2
1:A:23:ALA:HB1	1:A:27:PHE:CE1	0.55	2.34	2	4
1:A:37:PHE:CG	1:A:61:ALA:CB	0.55	2.90	21	4
1:A:37:PHE:HE1	1:A:73:GLN:HG2	0.54	1.62	17	1
1:A:16:VAL:CG1	1:A:29:PHE:HE2	0.54	2.15	7	2
1:A:55:TYR:CD2	1:A:61:ALA:CB	0.54	2.89	2	2
1:A:29:PHE:HD1	1:A:52:VAL:HG22	0.54	1.63	25	3
1:A:31:VAL:HG11	1:A:47:ALA:CB	0.54	2.33	20	1
1:A:29:PHE:CD2	1:A:52:VAL:CG2	0.54	2.88	2	1
1:A:55:TYR:CE2	1:A:61:ALA:CA	0.54	2.91	9	4
1:A:37:PHE:CD2	1:A:61:ALA:HB1	0.54	2.37	9	10
1:A:35:GLY:C	1:A:66:PHE:HD1	0.54	2.06	8	1
1:A:28:VAL:CG2	1:A:55:TYR:HD1	0.54	2.16	22	2
1:A:27:PHE:HE1	1:A:40:PRO:HB3	0.54	1.61	10	4
1:A:11:GLN:O	1:A:14:GLN:HB3	0.54	2.02	18	1
1:A:29:PHE:CD1	1:A:52:VAL:CG2	0.53	2.91	13	6
1:A:23:ALA:CB	1:A:27:PHE:HE1	0.53	2.16	2	1
1:A:64:ALA:CB	1:A:66:PHE:CE2	0.53	2.92	18	2
1:A:29:PHE:HE1	1:A:39:ARG:O	0.53	1.85	2	2
1:A:61:ALA:O	1:A:64:ALA:HB3	0.53	2.04	20	4
1:A:24:ASP:HB2	1:A:39:ARG:HG3	0.53	1.80	23	1
1:A:11:GLN:HE22	1:A:14:GLN:HB3	0.52	1.62	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:66:PHE:CD1	1:A:66:PHE:N	0.52	2.77	17	5
1:A:55:TYR:CD1	1:A:55:TYR:N	0.52	2.77	7	4
1:A:37:PHE:CE1	1:A:73:GLN:HG2	0.52	2.40	21	9
1:A:44:ALA:HB2	1:A:71:ARG:HH11	0.52	1.65	15	1
1:A:29:PHE:CD1	1:A:52:VAL:HG22	0.52	2.40	13	2
1:A:37:PHE:HE1	1:A:58:ALA:HB1	0.52	1.57	16	3
1:A:31:VAL:HG12	1:A:33:THR:CG2	0.52	2.34	6	2
1:A:43:ARG:HG2	1:A:71:ARG:HE	0.52	1.64	17	1
1:A:27:PHE:CE1	1:A:40:PRO:HG2	0.51	2.41	3	1
1:A:54:PHE:CD1	1:A:54:PHE:N	0.51	2.79	24	5
1:A:13:TRP:CE3	1:A:16:VAL:CG1	0.51	2.93	7	12
1:A:20:ASP:OD2	1:A:23:ALA:HB2	0.51	2.04	16	3
1:A:37:PHE:CE2	1:A:58:ALA:CA	0.51	2.93	11	1
1:A:68:PRO:CB	1:A:73:GLN:CG	0.51	2.89	18	1
1:A:55:TYR:HE2	1:A:61:ALA:HA	0.51	1.66	21	1
1:A:29:PHE:HD1	1:A:52:VAL:CG2	0.51	2.19	3	4
1:A:45:ARG:O	1:A:45:ARG:HG3	0.51	2.06	8	1
1:A:39:ARG:CG	1:A:40:PRO:HD2	0.51	2.36	4	9
1:A:37:PHE:HE1	1:A:73:GLN:CD	0.51	2.10	10	1
1:A:11:GLN:CA	1:A:14:GLN:HB2	0.50	2.32	3	4
1:A:55:TYR:CD1	1:A:60:GLU:CG	0.50	2.94	12	1
1:A:43:ARG:HD2	1:A:71:ARG:CZ	0.50	2.37	3	1
1:A:23:ALA:CB	1:A:40:PRO:CG	0.50	2.89	24	4
1:A:27:PHE:N	1:A:27:PHE:HD1	0.50	2.04	2	6
1:A:37:PHE:CE2	1:A:73:GLN:HG3	0.50	2.42	4	1
1:A:36:ILE:HG21	1:A:69:CYS:CA	0.50	2.37	8	2
1:A:29:PHE:CD1	1:A:29:PHE:C	0.50	2.85	9	9
1:A:34:THR:HG23	1:A:36:ILE:HB	0.50	1.84	6	6
1:A:37:PHE:CD1	1:A:73:GLN:HG2	0.50	2.41	12	3
1:A:29:PHE:O	1:A:29:PHE:HD1	0.49	1.91	7	2
1:A:37:PHE:CE1	1:A:73:GLN:HG3	0.49	2.41	2	8
1:A:9:ASP:HB2	1:A:49:ARG:NH2	0.49	2.22	11	1
1:A:39:ARG:CG	1:A:40:PRO:CD	0.49	2.91	16	2
1:A:44:ALA:HB2	1:A:71:ARG:HE	0.49	1.68	24	1
1:A:16:VAL:CG1	1:A:29:PHE:CE2	0.48	2.96	7	2
1:A:31:VAL:HG12	1:A:34:THR:HG22	0.48	1.84	19	2
1:A:23:ALA:CB	1:A:40:PRO:HG3	0.48	2.39	5	5
1:A:27:PHE:CZ	1:A:40:PRO:CG	0.48	2.97	9	2
1:A:31:VAL:HG22	1:A:52:VAL:CG2	0.48	2.27	1	1
1:A:9:ASP:CB	1:A:49:ARG:CZ	0.48	2.92	9	1
1:A:28:VAL:HG21	1:A:55:TYR:CD2	0.48	2.43	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:27:PHE:CE1	1:A:40:PRO:CG	0.48	2.97	21	3
1:A:55:TYR:OH	1:A:64:ALA:HB2	0.48	2.09	17	1
1:A:34:THR:HG23	1:A:36:ILE:N	0.48	2.23	24	5
1:A:37:PHE:CE2	1:A:73:GLN:CD	0.48	2.88	22	1
1:A:28:VAL:HG22	1:A:55:TYR:CB	0.47	2.31	9	2
1:A:31:VAL:CG2	1:A:52:VAL:CG2	0.47	2.89	1	1
1:A:43:ARG:HG2	1:A:71:ARG:CD	0.47	2.40	3	1
1:A:55:TYR:CE2	1:A:61:ALA:HA	0.47	2.45	9	9
1:A:27:PHE:CE1	1:A:40:PRO:HG3	0.47	2.42	15	7
1:A:27:PHE:CZ	1:A:40:PRO:HG3	0.47	2.44	17	2
1:A:34:THR:HG23	1:A:36:ILE:H	0.47	1.69	21	4
1:A:37:PHE:HB3	1:A:61:ALA:HB1	0.47	1.86	12	1
1:A:31:VAL:HG13	1:A:33:THR:HG22	0.47	1.86	16	2
1:A:28:VAL:CG2	1:A:55:TYR:HB2	0.47	2.33	2	14
1:A:29:PHE:CD2	1:A:52:VAL:HG21	0.47	2.45	2	2
1:A:19:ARG:HD3	1:A:41:SER:O	0.47	2.10	7	1
1:A:29:PHE:CE1	1:A:38:CYS:HB2	0.47	2.45	12	4
1:A:11:GLN:HG2	1:A:14:GLN:NE2	0.47	2.25	18	1
1:A:34:THR:HG23	1:A:36:ILE:CB	0.47	2.40	25	2
1:A:55:TYR:CD1	1:A:60:GLU:HG3	0.47	2.45	12	1
1:A:36:ILE:CG2	1:A:69:CYS:CA	0.47	2.93	1	3
1:A:64:ALA:HB1	1:A:66:PHE:HE2	0.46	1.71	8	2
1:A:43:ARG:CG	1:A:44:ALA:N	0.46	2.79	16	7
1:A:12:ARG:CB	1:A:54:PHE:CE2	0.46	2.98	25	2
1:A:35:GLY:HA2	1:A:66:PHE:HD1	0.46	1.70	18	1
1:A:67:ARG:HD3	1:A:68:PRO:HD2	0.46	1.86	21	1
1:A:28:VAL:HG13	1:A:57:ASN:CA	0.46	2.41	13	3
1:A:37:PHE:CB	1:A:61:ALA:HB1	0.46	2.41	12	2
1:A:58:ALA:HA	1:A:61:ALA:HB3	0.46	1.87	17	1
1:A:37:PHE:CE1	1:A:68:PRO:HA	0.45	2.47	19	3
1:A:68:PRO:CB	1:A:73:GLN:HG2	0.45	2.41	18	1
1:A:24:ASP:CB	1:A:39:ARG:HG2	0.45	2.40	20	1
1:A:55:TYR:HD2	1:A:60:GLU:HB3	0.45	1.71	7	2
1:A:37:PHE:C	1:A:37:PHE:CD1	0.45	2.89	3	1
1:A:9:ASP:CB	1:A:49:ARG:NH2	0.45	2.80	11	1
1:A:37:PHE:CE2	1:A:58:ALA:HA	0.45	2.46	11	1
1:A:10:ASP:O	1:A:14:GLN:N	0.45	2.50	24	3
1:A:28:VAL:HG11	1:A:57:ASN:C	0.45	2.31	12	2
1:A:29:PHE:CZ	1:A:38:CYS:HB2	0.45	2.46	19	1
1:A:64:ALA:HB3	1:A:66:PHE:HD2	0.45	1.70	8	1
1:A:44:ALA:CB	1:A:71:ARG:NH1	0.45	2.80	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:13:TRP:O	1:A:17:LEU:N	0.45	2.50	24	3
1:A:37:PHE:HE1	1:A:58:ALA:CB	0.45	2.23	16	1
1:A:45:ARG:HD3	1:A:45:ARG:C	0.44	2.32	4	1
1:A:12:ARG:HB3	1:A:54:PHE:CE2	0.44	2.48	25	4
1:A:29:PHE:HD2	1:A:52:VAL:HG21	0.44	1.69	2	1
1:A:31:VAL:CG1	1:A:33:THR:CG2	0.44	2.96	5	1
1:A:66:PHE:N	1:A:66:PHE:HD1	0.44	2.08	17	2
1:A:28:VAL:HG21	1:A:55:TYR:HD2	0.44	1.72	8	2
1:A:12:ARG:HB3	1:A:54:PHE:CZ	0.44	2.48	21	12
1:A:44:ALA:HB2	1:A:71:ARG:CZ	0.44	2.43	14	1
1:A:37:PHE:CE1	1:A:73:GLN:CD	0.44	2.90	10	1
1:A:37:PHE:H	1:A:37:PHE:HD1	0.44	1.55	11	1
1:A:68:PRO:HB3	1:A:73:GLN:CG	0.44	2.42	18	2
1:A:26:GLU:HB3	1:A:27:PHE:CD1	0.44	2.48	22	2
1:A:29:PHE:CZ	1:A:38:CYS:CB	0.44	3.01	19	1
1:A:45:ARG:HD2	1:A:45:ARG:H	0.43	1.72	16	1
1:A:11:GLN:HA	1:A:14:GLN:CB	0.43	2.43	18	5
1:A:37:PHE:CE2	1:A:73:GLN:HG2	0.43	2.49	22	1
1:A:13:TRP:CD1	1:A:17:LEU:HG	0.43	2.49	22	7
1:A:55:TYR:CD2	1:A:60:GLU:HB3	0.43	2.49	16	5
1:A:24:ASP:HB2	1:A:39:ARG:CD	0.43	2.44	8	2
1:A:44:ALA:CB	1:A:71:ARG:NH2	0.43	2.80	14	1
1:A:43:ARG:CG	1:A:71:ARG:NE	0.43	2.82	3	1
1:A:37:PHE:HE1	1:A:68:PRO:N	0.43	2.12	11	1
1:A:32:ARG:O	1:A:32:ARG:HG2	0.42	2.13	5	1
1:A:23:ALA:CB	1:A:27:PHE:CE1	0.42	3.01	11	1
1:A:55:TYR:CD2	1:A:61:ALA:N	0.42	2.87	21	1
1:A:68:PRO:CB	1:A:73:GLN:HB3	0.42	2.45	11	5
1:A:37:PHE:CE1	1:A:73:GLN:NE2	0.42	2.87	10	1
1:A:9:ASP:HB2	1:A:49:ARG:NH1	0.42	2.30	19	1
1:A:12:ARG:C	1:A:54:PHE:CE2	0.42	2.93	20	1
1:A:35:GLY:HA2	1:A:66:PHE:CD1	0.42	2.49	8	2
1:A:16:VAL:HG11	1:A:29:PHE:CE2	0.42	2.50	17	1
1:A:55:TYR:CG	1:A:60:GLU:CD	0.42	2.92	9	1
1:A:68:PRO:HB3	1:A:73:GLN:HB3	0.42	1.92	25	3
1:A:27:PHE:CE1	1:A:40:PRO:HD3	0.42	2.50	1	1
1:A:29:PHE:C	1:A:29:PHE:HD1	0.42	2.18	14	2
1:A:28:VAL:CG1	1:A:57:ASN:C	0.42	2.88	12	1
1:A:31:VAL:CG1	1:A:47:ALA:HB3	0.42	2.45	3	1
1:A:67:ARG:HG2	1:A:68:PRO:N	0.42	2.25	4	1
1:A:36:ILE:HG23	1:A:67:ARG:O	0.42	2.14	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:43:ARG:HG2	1:A:71:ARG:NE	0.42	2.30	3	1
1:A:45:ARG:HD2	1:A:46:HIS:N	0.41	2.30	3	1
1:A:65:GLY:C	1:A:66:PHE:HD1	0.41	2.19	12	1
1:A:66:PHE:N	1:A:66:PHE:CD1	0.41	2.88	12	1
1:A:16:VAL:HG21	1:A:29:PHE:HD2	0.41	1.74	14	1
1:A:11:GLN:OE1	1:A:14:GLN:HG3	0.41	2.14	2	1
1:A:37:PHE:CD1	1:A:37:PHE:N	0.41	2.87	11	1
1:A:31:VAL:HG21	1:A:47:ALA:CB	0.41	2.44	7	1
1:A:13:TRP:CD1	1:A:49:ARG:HB2	0.41	2.50	15	3
1:A:64:ALA:CB	1:A:66:PHE:CD2	0.41	3.04	8	2
1:A:12:ARG:HD3	1:A:54:PHE:CD1	0.41	2.50	20	2
1:A:36:ILE:HG22	1:A:37:PHE:N	0.41	2.30	22	1
1:A:36:ILE:CG2	1:A:69:CYS:HB2	0.41	2.45	4	3
1:A:13:TRP:CG	1:A:49:ARG:HB2	0.41	2.51	12	3
1:A:23:ALA:HB1	1:A:40:PRO:HG3	0.41	1.93	24	1
1:A:29:PHE:N	1:A:29:PHE:CD1	0.41	2.89	12	1
1:A:31:VAL:HG23	1:A:52:VAL:HG23	0.41	1.91	21	1
1:A:55:TYR:CD2	1:A:60:GLU:HG3	0.41	2.50	21	1
1:A:35:GLY:HA2	1:A:66:PHE:CE1	0.41	2.51	8	1
1:A:58:ALA:HB2	1:A:73:GLN:NE2	0.40	2.31	5	1
1:A:46:HIS:CD2	1:A:46:HIS:N	0.40	2.89	6	1
1:A:59:SER:HA	1:A:62:LEU:CG	0.40	2.46	25	1
1:A:18:ALA:C	1:A:19:ARG:CG	0.40	2.90	3	1
1:A:46:HIS:N	1:A:46:HIS:CD2	0.40	2.89	3	1
1:A:12:ARG:HB3	1:A:54:PHE:CE1	0.40	2.51	6	1
1:A:9:ASP:HB2	1:A:49:ARG:CZ	0.40	2.47	9	1
1:A:31:VAL:CG1	1:A:47:ALA:CB	0.40	2.99	20	1
1:A:29:PHE:CD2	1:A:52:VAL:HG22	0.40	2.47	2	1
1:A:24:ASP:CB	1:A:39:ARG:HD2	0.40	2.47	10	1
1:A:28:VAL:CG1	1:A:57:ASN:HA	0.40	2.45	12	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	65/92 (71%)	54±2 (83±3%)	9±2 (13±3%)	2±1 (3±2%)	7	38
All	All	1625/2300 (71%)	1356 (83%)	217 (13%)	52 (3%)	7	38

All 9 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	20	ASP	17
1	A	10	ASP	14
1	A	45	ARG	9
1	A	42	CYS	7
1	A	24	ASP	1
1	A	25	GLY	1
1	A	21	PRO	1
1	A	44	ALA	1
1	A	40	PRO	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	52/76 (68%)	39±2 (75±4%)	13±2 (25±4%)	2	24
All	All	1300/1900 (68%)	973 (75%)	327 (25%)	2	24

All 36 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	43	ARG	23
1	A	73	GLN	23
1	A	52	VAL	22
1	A	49	ARG	19
1	A	11	GLN	17
1	A	14	GLN	17
1	A	71	ARG	16
1	A	41	SER	16
1	A	67	ARG	15

*Continued on next page...*

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Mol	Chain	Res	Type	Models (Total)
1	A	27	PHE	14
1	A	46	HIS	14
1	A	19	ARG	12
1	A	32	ARG	12
1	A	39	ARG	11
1	A	45	ARG	11
1	A	12	ARG	10
1	A	60	GLU	10
1	A	24	ASP	7
1	A	29	PHE	7
1	A	15	SER	7
1	A	70	LYS	5
1	A	59	SER	5
1	A	26	GLU	5
1	A	37	PHE	4
1	A	33	THR	4
1	A	9	ASP	4
1	A	10	ASP	3
1	A	66	PHE	3
1	A	48	LEU	2
1	A	50	GLU	2
1	A	54	PHE	2
1	A	57	ASN	1
1	A	55	TYR	1
1	A	68	PRO	1
1	A	34	THR	1
1	A	62	LEU	1

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

## 7 Chemical shift validation

No chemical shift data were provided