



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 05:44 PM BST

PDB ID : 1VYX  
Title : SOLUTION STRUCTURE OF THE KSHV K3 N-TERMINAL DOMAIN  
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Deposited on : 2004-05-07

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

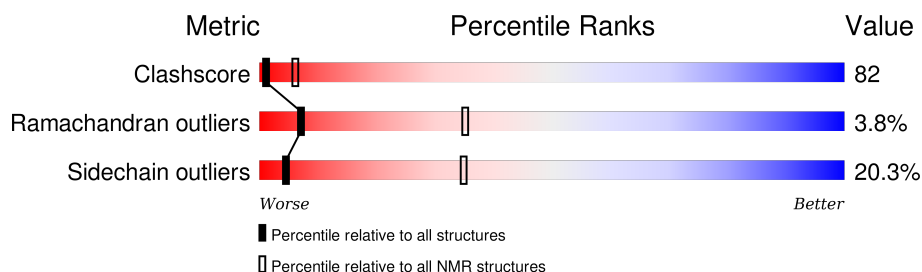
# 1 Overall quality at a glance

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	60	<div> <div>13%</div> <div>57%</div> <div>17%</div> <div>13%</div> </div>

## 2 Ensemble composition and analysis ⓘ

This entry contains 28 models. Model 1 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:6-A:57 (52)	0.26	1

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 2 single-model clusters were found.

Cluster number	Models
1	2, 3, 8, 15, 17, 18, 19, 20, 22, 24, 28
2	1, 4, 6, 10, 11, 12, 13, 16, 21, 23, 26
3	25, 27
4	9, 14
Single-model clusters	5; 7

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

There are 2 unique types of molecules in this entry. The entry contains 915 atoms, of which 441 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called ORF K3.

Mol	Chain	Residues	Atoms						Trace
1	A	60	Total	C	H	N	O	S	0
			913	285	441	85	94	8	

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

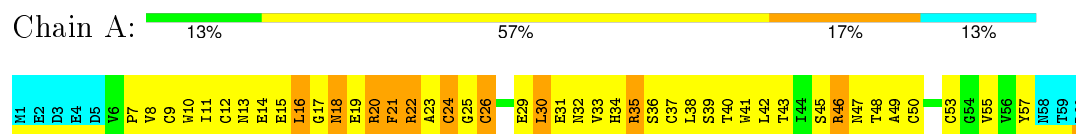
Mol	Chain	Residues	Atoms	
2	A	2	Total	Zn
			2	2

## 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: ORF K3

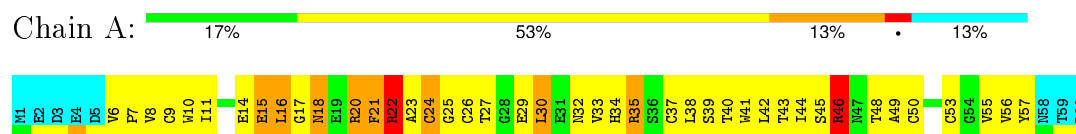


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

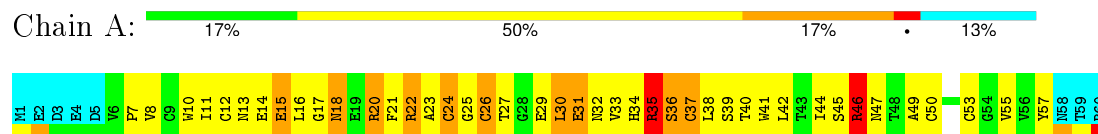
#### 4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: ORF K3



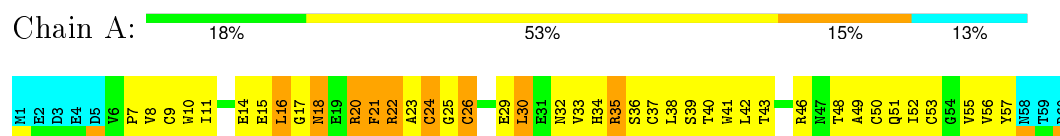
#### 4.2.2 Score per residue for model 2

- Molecule 1: ORF K3



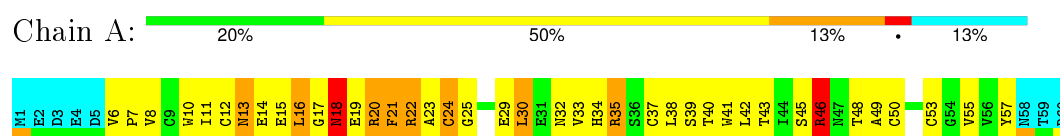
### 4.2.3 Score per residue for model 3

- Molecule 1: ORF K3



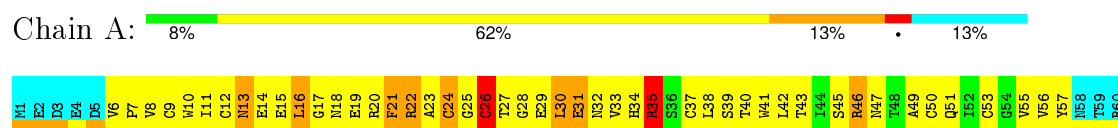
### 4.2.4 Score per residue for model 4

- Molecule 1: ORF K3



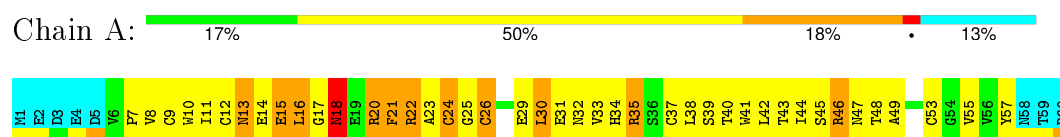
### 4.2.5 Score per residue for model 5

- Molecule 1: ORF K3



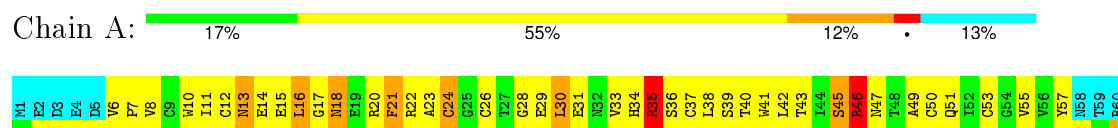
### 4.2.6 Score per residue for model 6

- Molecule 1: ORF K3



### 4.2.7 Score per residue for model 7

- Molecule 1: ORF K3



### 4.2.8 Score per residue for model 8

- Molecule 1: ORF K3

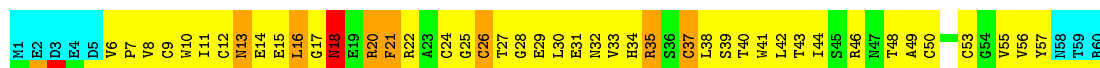
Chain A: 15% 53% 17% 13%



### 4.2.9 Score per residue for model 9

- Molecule 1: ORF K3

Chain A: 13% 60% 12% 13%



### 4.2.10 Score per residue for model 10

- Molecule 1: ORF K3

Chain A: 15% 53% 17% 13%



### 4.2.11 Score per residue for model 11

- Molecule 1: ORF K3

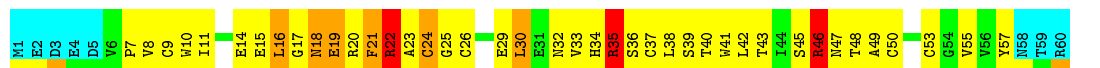
Chain A: 17% 57% 8% 5% 13%



### 4.2.12 Score per residue for model 12

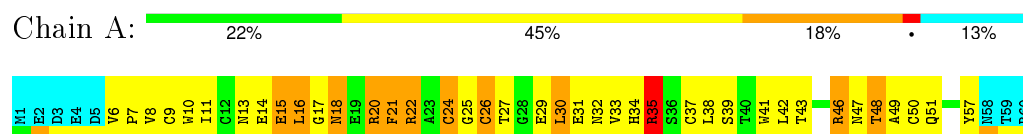
- Molecule 1: ORF K3

Chain A: 18% 53% 10% 5% 13%



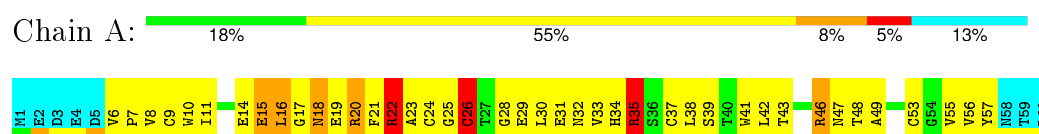
### 4.2.13 Score per residue for model 13

- Molecule 1: ORF K3



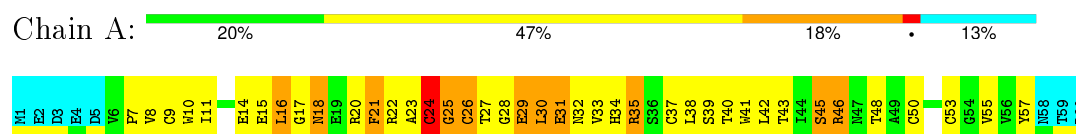
### 4.2.14 Score per residue for model 14

- Molecule 1: ORF K3



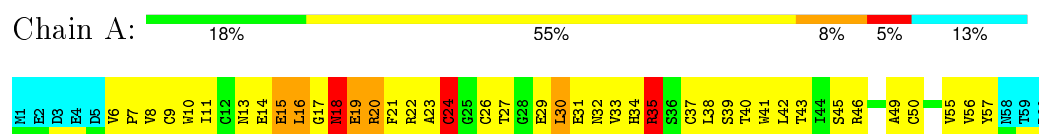
### 4.2.15 Score per residue for model 15

- Molecule 1: ORF K3



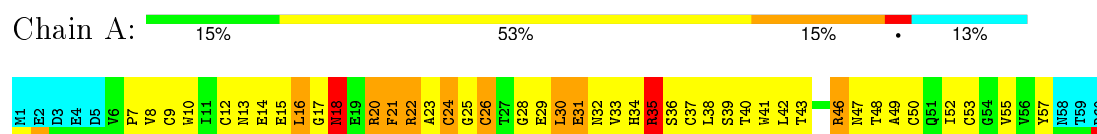
### 4.2.16 Score per residue for model 16

- Molecule 1: ORF K3



### 4.2.17 Score per residue for model 17

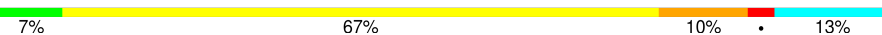
- Molecule 1: ORF K3





### 4.2.18 Score per residue for model 18

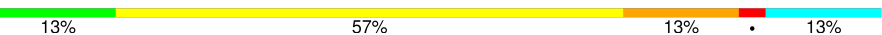
- Molecule 1: ORF K3

Chain A:  7% 67% 10% • 13%



### 4.2.19 Score per residue for model 19

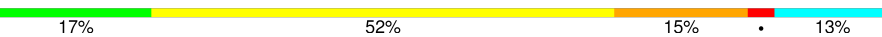
- Molecule 1: ORF K3

Chain A:  13% 57% 13% • 13%



### 4.2.20 Score per residue for model 20

- Molecule 1: ORF K3

Chain A:  17% 52% 15% • 13%



### 4.2.21 Score per residue for model 21

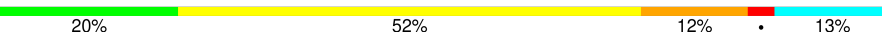
- Molecule 1: ORF K3

Chain A:  20% 52% 13% • 13%



### 4.2.22 Score per residue for model 22

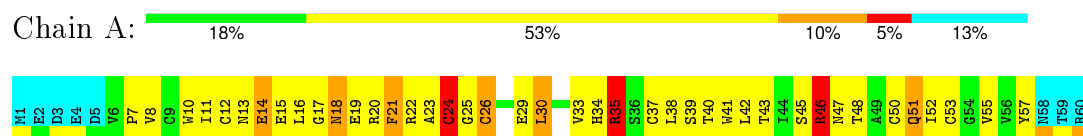
- Molecule 1: ORF K3

Chain A:  20% 52% 12% • 13%



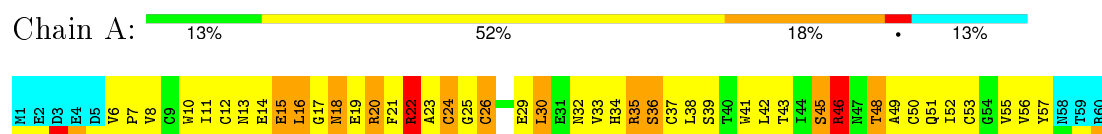
#### 4.2.23 Score per residue for model 23

- Molecule 1: ORF K3



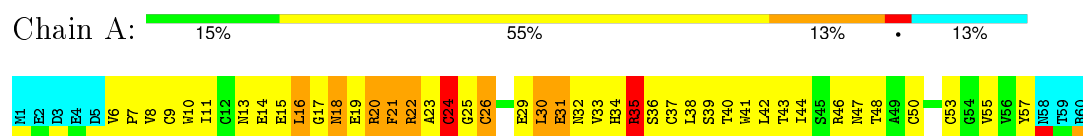
#### 4.2.24 Score per residue for model 24

- Molecule 1: ORF K3



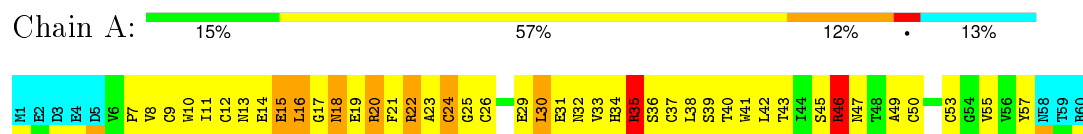
#### 4.2.25 Score per residue for model 25

- Molecule 1: ORF K3



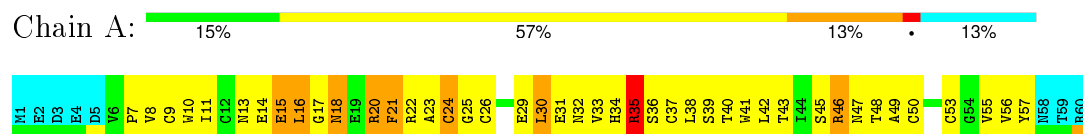
#### 4.2.26 Score per residue for model 26

- Molecule 1: ORF K3



#### 4.2.27 Score per residue for model 27

- Molecule 1: ORF K3



#### 4.2.28 Score per residue for model 28

- Molecule 1: ORF K3

Chain A: 12% 60% 13% • 13%



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *XPLOR3.8*.

Of the 30 calculated structures, 28 were deposited, based on the following criterion: *NO VIOLATIONS GREATER THAN 0.25Å, NO ANGLE VIOLATIONS*.

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

Software name	Classification	Version
X-PLOR	refinement	
XWIN-NMR	structure solution	
ANSIG	structure solution	
XPLOR3.8	structure solution	

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

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.

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	3.9±0.3
All	All	0	109

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	20	ARG	Sidechain	28
1	A	22	ARG	Sidechain	28
1	A	46	ARG	Sidechain	27
1	A	35	ARG	Sidechain	26

### 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	403	384	381	64±6
All	All	11340	10752	10668	1796

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 82.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:6:VAL:HG13	1:A:17:GLY:CA	0.99	1.88	5	4
1:A:33:VAL:HG21	1:A:38:LEU:HD22	0.94	1.38	27	21
1:A:21:PHE:CE2	1:A:38:LEU:HD23	0.92	2.00	15	28
1:A:42:LEU:HD22	1:A:57:TYR:CD2	0.88	2.04	21	21
1:A:16:LEU:HD13	1:A:16:LEU:N	0.86	1.85	24	2
1:A:21:PHE:CZ	1:A:23:ALA:HB2	0.84	2.08	23	21
1:A:26:CYS:SG	1:A:30:LEU:HD13	0.82	2.14	14	2
1:A:24:CYS:SG	1:A:30:LEU:HD12	0.81	2.14	24	16
1:A:39:SER:HA	1:A:42:LEU:HD21	0.80	1.51	10	28
1:A:6:VAL:HG13	1:A:17:GLY:HA2	0.80	1.51	5	7
1:A:16:LEU:N	1:A:16:LEU:HD23	0.78	1.94	20	13
1:A:16:LEU:HD11	1:A:32:ASN:HB3	0.78	1.55	12	15
1:A:8:VAL:HG22	1:A:15:GLU:HG3	0.77	1.57	15	15
1:A:16:LEU:H	1:A:16:LEU:HD23	0.76	1.41	23	5
1:A:40:THR:O	1:A:44:ILE:HD12	0.76	1.81	1	8
1:A:16:LEU:HD23	1:A:16:LEU:N	0.75	1.96	13	13
1:A:16:LEU:HD23	1:A:16:LEU:H	0.75	1.41	19	18
1:A:42:LEU:HD12	1:A:43:THR:N	0.73	1.99	7	25
1:A:53:CYS:SG	1:A:55:VAL:HG23	0.72	2.24	15	26
1:A:47:ASN:C	1:A:48:THR:HG23	0.72	2.05	28	10
1:A:10:TRP:NE1	1:A:30:LEU:HD22	0.72	1.99	7	15
1:A:24:CYS:CB	1:A:30:LEU:HD12	0.71	2.14	24	11
1:A:17:GLY:O	1:A:18:ASN:CB	0.71	2.38	27	25
1:A:21:PHE:CE1	1:A:23:ALA:HB2	0.71	2.19	20	19
1:A:24:CYS:HB3	1:A:30:LEU:HD12	0.70	1.64	3	10
1:A:8:VAL:HG13	1:A:14:GLU:C	0.68	2.08	3	26
1:A:8:VAL:HG13	1:A:15:GLU:N	0.68	2.04	7	21
1:A:33:VAL:CG2	1:A:38:LEU:HD22	0.67	2.20	11	11
1:A:10:TRP:CE2	1:A:30:LEU:HD22	0.66	2.26	20	24
1:A:10:TRP:CE2	1:A:30:LEU:CD2	0.65	2.79	2	16
1:A:16:LEU:H	1:A:16:LEU:HD22	0.65	1.51	24	2
1:A:10:TRP:CE2	1:A:11:ILE:CG1	0.64	2.80	15	21
1:A:50:CYS:N	1:A:57:TYR:CE1	0.64	2.66	2	13
1:A:16:LEU:N	1:A:16:LEU:CD1	0.64	2.59	5	2
1:A:9:CYS:SG	1:A:33:VAL:HG23	0.63	2.33	16	6
1:A:33:VAL:HG21	1:A:38:LEU:CD2	0.63	2.22	25	10
1:A:26:CYS:SG	1:A:52:ILE:HG21	0.62	2.34	22	2
1:A:30:LEU:HD13	1:A:30:LEU:O	0.62	1.93	13	10
1:A:21:PHE:CG	1:A:35:ARG:CG	0.61	2.82	2	5
1:A:24:CYS:HA	1:A:55:VAL:HG11	0.61	1.73	11	13
1:A:7:PRO:CB	1:A:32:ASN:ND2	0.61	2.64	26	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:TRP:CD2	1:A:30:LEU:HD22	0.60	2.32	22	6
1:A:6:VAL:HG12	1:A:15:GLU:HB2	0.60	1.73	5	1
1:A:30:LEU:O	1:A:30:LEU:HD13	0.59	1.97	7	9
1:A:9:CYS:N	1:A:16:LEU:HD22	0.59	2.12	8	10
1:A:9:CYS:N	1:A:16:LEU:CD2	0.59	2.66	3	17
1:A:36:SER:O	1:A:40:THR:HG22	0.58	1.98	17	5
1:A:11:ILE:HD11	1:A:38:LEU:HD13	0.58	1.76	27	11
1:A:48:THR:O	1:A:57:TYR:CD2	0.57	2.57	15	4
1:A:23:ALA:HA	1:A:57:TYR:HA	0.57	1.77	6	21
1:A:41:TRP:CZ2	1:A:47:ASN:ND2	0.57	2.73	25	1
1:A:38:LEU:CD1	1:A:42:LEU:HD23	0.57	2.30	20	8
1:A:48:THR:C	1:A:57:TYR:CD2	0.57	2.78	13	17
1:A:29:GLU:CG	1:A:30:LEU:N	0.56	2.68	24	18
1:A:7:PRO:O	1:A:16:LEU:HD23	0.56	1.99	19	4
1:A:21:PHE:CG	1:A:35:ARG:HG3	0.56	2.35	12	5
1:A:6:VAL:HG12	1:A:15:GLU:HG2	0.56	1.78	25	3
1:A:17:GLY:O	1:A:18:ASN:HB2	0.56	2.00	15	16
1:A:8:VAL:HG22	1:A:15:GLU:CD	0.56	2.20	1	2
1:A:16:LEU:HD11	1:A:32:ASN:CB	0.56	2.30	14	10
1:A:7:PRO:O	1:A:15:GLU:CB	0.56	2.54	5	1
1:A:49:ALA:C	1:A:57:TYR:CZ	0.55	2.79	26	13
1:A:50:CYS:N	1:A:55:VAL:O	0.55	2.40	2	17
1:A:30:LEU:O	1:A:30:LEU:CD1	0.55	2.55	7	3
1:A:16:LEU:CD2	1:A:16:LEU:N	0.55	2.66	13	9
1:A:34:HIS:HB2	1:A:37:CYS:SG	0.55	2.42	25	26
1:A:6:VAL:HG13	1:A:17:GLY:N	0.55	2.16	5	1
1:A:16:LEU:HB3	1:A:34:HIS:CD2	0.55	2.37	24	9
1:A:24:CYS:SG	1:A:25:GLY:N	0.55	2.80	17	20
1:A:14:GLU:OE1	1:A:34:HIS:CE1	0.55	2.60	10	2
1:A:24:CYS:SG	1:A:50:CYS:CB	0.55	2.95	19	4
1:A:6:VAL:HG13	1:A:7:PRO:HD2	0.54	1.79	24	1
1:A:50:CYS:SG	1:A:52:ILE:HD12	0.54	2.42	8	2
1:A:37:CYS:O	1:A:41:TRP:CB	0.54	2.55	8	26
1:A:49:ALA:N	1:A:57:TYR:CE2	0.54	2.76	27	7
1:A:16:LEU:N	1:A:16:LEU:CD2	0.54	2.69	17	15
1:A:10:TRP:CE2	1:A:11:ILE:HG12	0.54	2.38	19	16
1:A:11:ILE:HD12	1:A:38:LEU:HB2	0.54	1.78	5	4
1:A:21:PHE:HE2	1:A:38:LEU:HD23	0.54	1.60	16	16
1:A:33:VAL:HG21	1:A:38:LEU:HB2	0.54	1.80	22	7
1:A:21:PHE:CD1	1:A:21:PHE:C	0.53	2.80	13	14
1:A:10:TRP:CE2	1:A:11:ILE:HG13	0.53	2.37	15	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:GLY:O	1:A:31:GLU:CG	0.53	2.55	2	1
1:A:53:CYS:SG	1:A:55:VAL:CG2	0.53	2.96	26	22
1:A:48:THR:C	1:A:57:TYR:CE2	0.53	2.82	24	3
1:A:8:VAL:HG22	1:A:15:GLU:CG	0.53	2.32	15	7
1:A:26:CYS:SG	1:A:52:ILE:CG2	0.53	2.97	3	6
1:A:21:PHE:C	1:A:21:PHE:CD1	0.53	2.80	15	14
1:A:18:ASN:ND2	1:A:18:ASN:N	0.53	2.57	17	1
1:A:38:LEU:HD12	1:A:41:TRP:HE3	0.53	1.63	15	5
1:A:15:GLU:C	1:A:16:LEU:HD13	0.53	2.24	5	1
1:A:36:SER:OG	1:A:37:CYS:N	0.52	2.42	27	3
1:A:23:ALA:O	1:A:24:CYS:CB	0.52	2.57	22	16
1:A:7:PRO:HB3	1:A:32:ASN:ND2	0.52	2.19	12	13
1:A:10:TRP:CZ2	1:A:11:ILE:HG12	0.52	2.39	25	12
1:A:30:LEU:CD1	1:A:30:LEU:O	0.52	2.57	10	3
1:A:24:CYS:SG	1:A:30:LEU:CD1	0.52	2.98	20	6
1:A:47:ASN:O	1:A:48:THR:CB	0.52	2.57	13	11
1:A:21:PHE:CD1	1:A:35:ARG:CG	0.52	2.92	16	1
1:A:29:GLU:HG3	1:A:30:LEU:N	0.52	2.20	22	15
1:A:42:LEU:O	1:A:46:ARG:N	0.52	2.43	28	15
1:A:45:SER:O	1:A:46:ARG:CB	0.52	2.58	24	13
1:A:36:SER:O	1:A:40:THR:CG2	0.52	2.58	26	6
1:A:47:ASN:C	1:A:48:THR:CG2	0.52	2.76	28	6
1:A:8:VAL:HA	1:A:15:GLU:HA	0.52	1.81	5	3
1:A:35:ARG:O	1:A:39:SER:CB	0.52	2.58	13	3
1:A:40:THR:O	1:A:44:ILE:CD1	0.52	2.57	9	2
1:A:29:GLU:HG2	1:A:30:LEU:N	0.52	2.19	15	3
1:A:31:GLU:OE1	1:A:31:GLU:CA	0.52	2.57	17	1
1:A:10:TRP:CD1	1:A:30:LEU:HD22	0.52	2.40	19	7
1:A:34:HIS:CB	1:A:37:CYS:SG	0.51	2.98	25	7
1:A:10:TRP:CZ2	1:A:11:ILE:CG1	0.51	2.92	13	7
1:A:8:VAL:HA	1:A:15:GLU:CA	0.51	2.36	5	1
1:A:17:GLY:O	1:A:18:ASN:HB3	0.51	2.06	1	11
1:A:14:GLU:O	1:A:34:HIS:CE1	0.51	2.64	5	1
1:A:10:TRP:CH2	1:A:11:ILE:HG12	0.51	2.40	22	10
1:A:29:GLU:HG3	1:A:30:LEU:HD12	0.51	1.83	14	1
1:A:18:ASN:OD1	1:A:18:ASN:N	0.51	2.44	1	1
1:A:16:LEU:HB3	1:A:34:HIS:NE2	0.51	2.20	19	21
1:A:10:TRP:CD1	1:A:30:LEU:HA	0.51	2.42	20	8
1:A:41:TRP:CH2	1:A:47:ASN:ND2	0.50	2.79	25	2
1:A:21:PHE:CE2	1:A:38:LEU:CD2	0.50	2.91	5	14
1:A:47:ASN:O	1:A:48:THR:OG1	0.50	2.28	14	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:ASN:CG	1:A:18:ASN:O	0.50	2.49	24	6
1:A:40:THR:CG2	1:A:41:TRP:N	0.50	2.74	4	12
1:A:21:PHE:CD2	1:A:35:ARG:HA	0.50	2.42	6	25
1:A:17:GLY:O	1:A:18:ASN:ND2	0.50	2.45	6	2
1:A:21:PHE:CZ	1:A:23:ALA:CB	0.50	2.89	20	6
1:A:19:GLU:OE2	1:A:21:PHE:CB	0.50	2.59	16	1
1:A:33:VAL:CG2	1:A:38:LEU:HB2	0.50	2.36	15	26
1:A:37:CYS:HA	1:A:40:THR:CG2	0.50	2.37	7	11
1:A:10:TRP:HB3	1:A:29:GLU:CG	0.50	2.37	12	9
1:A:26:CYS:SG	1:A:30:LEU:CB	0.50	3.00	5	2
1:A:10:TRP:CD1	1:A:30:LEU:HG	0.50	2.42	14	2
1:A:24:CYS:HA	1:A:55:VAL:CG1	0.49	2.36	19	21
1:A:10:TRP:CZ2	1:A:11:ILE:HD11	0.49	2.42	10	5
1:A:8:VAL:HA	1:A:16:LEU:HD23	0.49	1.84	18	6
1:A:10:TRP:CZ3	1:A:11:ILE:HG12	0.49	2.42	9	6
1:A:21:PHE:CD1	1:A:35:ARG:HG3	0.49	2.42	16	2
1:A:21:PHE:CD2	1:A:35:ARG:HB2	0.49	2.43	5	1
1:A:19:GLU:OE2	1:A:35:ARG:N	0.49	2.46	16	1
1:A:10:TRP:CB	1:A:29:GLU:OE1	0.49	2.60	23	1
1:A:7:PRO:O	1:A:15:GLU:HA	0.49	2.06	24	6
1:A:26:CYS:N	1:A:31:GLU:OE1	0.49	2.46	17	1
1:A:10:TRP:CD2	1:A:30:LEU:CD2	0.49	2.94	24	2
1:A:21:PHE:CE2	1:A:35:ARG:HA	0.49	2.43	16	21
1:A:47:ASN:O	1:A:48:THR:HG23	0.49	2.08	28	7
1:A:9:CYS:HB2	1:A:34:HIS:ND1	0.49	2.22	15	6
1:A:23:ALA:CA	1:A:57:TYR:HA	0.49	2.38	17	2
1:A:45:SER:OG	1:A:47:ASN:ND2	0.49	2.46	2	3
1:A:25:GLY:O	1:A:26:CYS:O	0.49	2.31	11	9
1:A:10:TRP:CD1	1:A:33:VAL:HB	0.49	2.43	13	3
1:A:7:PRO:HB2	1:A:32:ASN:CB	0.48	2.38	8	21
1:A:42:LEU:O	1:A:47:ASN:N	0.48	2.42	26	2
1:A:6:VAL:HG11	1:A:15:GLU:OE2	0.48	2.08	18	1
1:A:24:CYS:SG	1:A:50:CYS:HB3	0.48	2.49	15	5
1:A:16:LEU:CB	1:A:34:HIS:NE2	0.48	2.77	11	2
1:A:12:CYS:O	1:A:13:ASN:CB	0.48	2.60	24	11
1:A:22:ARG:O	1:A:57:TYR:O	0.48	2.32	3	11
1:A:40:THR:HG23	1:A:41:TRP:N	0.48	2.23	21	9
1:A:10:TRP:CB	1:A:29:GLU:HG3	0.48	2.39	13	5
1:A:19:GLU:OE2	1:A:33:VAL:O	0.47	2.32	16	1
1:A:39:SER:O	1:A:43:THR:OG1	0.47	2.33	6	5
1:A:6:VAL:CG1	1:A:17:GLY:HA2	0.47	2.38	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:8:VAL:C	1:A:16:LEU:CD2	0.47	2.83	8	3
1:A:38:LEU:HD12	1:A:41:TRP:CE3	0.47	2.43	15	2
1:A:18:ASN:O	1:A:18:ASN:CG	0.47	2.53	15	5
1:A:10:TRP:HB3	1:A:29:GLU:CB	0.47	2.39	13	3
1:A:26:CYS:O	1:A:31:GLU:OE2	0.47	2.33	6	2
1:A:28:GLY:O	1:A:31:GLU:N	0.47	2.46	22	2
1:A:46:ARG:O	1:A:47:ASN:OD1	0.47	2.33	20	2
1:A:11:ILE:CD1	1:A:38:LEU:HB2	0.46	2.40	6	13
1:A:19:GLU:HG3	1:A:19:GLU:O	0.46	2.10	16	1
1:A:19:GLU:CG	1:A:19:GLU:O	0.46	2.62	16	1
1:A:6:VAL:CG1	1:A:17:GLY:N	0.46	2.78	5	1
1:A:25:GLY:O	1:A:26:CYS:C	0.46	2.53	18	5
1:A:10:TRP:NE1	1:A:30:LEU:HG	0.46	2.26	14	2
1:A:7:PRO:CB	1:A:32:ASN:CG	0.46	2.84	14	3
1:A:6:VAL:CG1	1:A:15:GLU:HG2	0.46	2.41	16	2
1:A:10:TRP:CG	1:A:30:LEU:HD22	0.46	2.46	24	2
1:A:21:PHE:CD2	1:A:35:ARG:HG2	0.46	2.45	12	4
1:A:17:GLY:C	1:A:18:ASN:OD1	0.46	2.54	1	1
1:A:45:SER:O	1:A:46:ARG:HB3	0.46	2.11	7	5
1:A:25:GLY:O	1:A:31:GLU:HG2	0.46	2.10	2	1
1:A:42:LEU:CD1	1:A:43:THR:N	0.46	2.78	7	2
1:A:8:VAL:HG22	1:A:15:GLU:HG2	0.46	1.87	17	1
1:A:23:ALA:O	1:A:56:VAL:O	0.46	2.34	14	1
1:A:10:TRP:CB	1:A:29:GLU:CG	0.45	2.94	13	3
1:A:18:ASN:ND2	1:A:18:ASN:O	0.45	2.49	26	1
1:A:17:GLY:C	1:A:18:ASN:ND2	0.45	2.69	18	1
1:A:33:VAL:HG11	1:A:38:LEU:CD2	0.45	2.42	19	3
1:A:8:VAL:CA	1:A:16:LEU:CD2	0.45	2.95	18	3
1:A:7:PRO:O	1:A:15:GLU:CA	0.45	2.64	5	1
1:A:38:LEU:HD12	1:A:38:LEU:C	0.45	2.30	17	5
1:A:16:LEU:HB3	1:A:34:HIS:CE1	0.45	2.46	25	1
1:A:24:CYS:HB3	1:A:30:LEU:CD1	0.45	2.40	3	1
1:A:38:LEU:C	1:A:38:LEU:HD12	0.45	2.32	22	4
1:A:49:ALA:HB1	1:A:55:VAL:O	0.45	2.10	4	3
1:A:57:TYR:CD1	1:A:57:TYR:N	0.45	2.83	9	1
1:A:27:THR:HG22	1:A:27:THR:O	0.45	2.11	9	1
1:A:6:VAL:CG1	1:A:7:PRO:HD2	0.45	2.41	21	2
1:A:9:CYS:CB	1:A:34:HIS:ND1	0.45	2.80	15	1
1:A:26:CYS:SG	1:A:30:LEU:HB3	0.45	2.52	5	2
1:A:21:PHE:CD1	1:A:35:ARG:HD2	0.45	2.47	15	2
1:A:37:CYS:HA	1:A:40:THR:HG22	0.45	1.88	4	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:GLY:CA	1:A:31:GLU:HB2	0.45	2.42	17	4
1:A:6:VAL:CG1	1:A:15:GLU:OE2	0.44	2.65	18	1
1:A:8:VAL:HA	1:A:16:LEU:CD2	0.44	2.42	18	1
1:A:10:TRP:CE2	1:A:30:LEU:HD21	0.44	2.47	2	2
1:A:8:VAL:CG1	1:A:14:GLU:C	0.44	2.81	3	3
1:A:37:CYS:O	1:A:41:TRP:HB3	0.44	2.11	12	8
1:A:29:GLU:CD	1:A:29:GLU:N	0.44	2.71	10	1
1:A:21:PHE:CD2	1:A:35:ARG:CA	0.44	3.00	6	5
1:A:18:ASN:C	1:A:18:ASN:ND2	0.44	2.69	22	1
1:A:38:LEU:CD1	1:A:41:TRP:CE3	0.44	3.00	16	2
1:A:10:TRP:CD2	1:A:11:ILE:HG12	0.44	2.48	20	4
1:A:19:GLU:C	1:A:19:GLU:OE1	0.44	2.56	16	1
1:A:10:TRP:CE3	1:A:11:ILE:HG12	0.44	2.47	14	1
1:A:47:ASN:C	1:A:48:THR:OG1	0.44	2.55	13	1
1:A:11:ILE:CD1	1:A:38:LEU:HA	0.44	2.42	4	4
1:A:28:GLY:O	1:A:29:GLU:C	0.44	2.56	19	8
1:A:42:LEU:HD12	1:A:42:LEU:C	0.44	2.33	17	1
1:A:19:GLU:OE1	1:A:34:HIS:HA	0.44	2.13	11	1
1:A:16:LEU:HD13	1:A:16:LEU:H	0.44	1.67	24	1
1:A:37:CYS:O	1:A:41:TRP:HB2	0.44	2.12	5	2
1:A:19:GLU:OE1	1:A:19:GLU:CA	0.44	2.65	12	1
1:A:26:CYS:O	1:A:31:GLU:CD	0.44	2.56	25	1
1:A:49:ALA:CB	1:A:56:VAL:HA	0.44	2.43	24	9
1:A:26:CYS:CB	1:A:30:LEU:HB3	0.44	2.43	22	2
1:A:18:ASN:OD1	1:A:18:ASN:O	0.43	2.37	21	1
1:A:7:PRO:HG2	1:A:16:LEU:CD2	0.43	2.44	24	1
1:A:38:LEU:O	1:A:42:LEU:HG	0.43	2.13	13	8
1:A:19:GLU:CD	1:A:21:PHE:CB	0.43	2.86	16	1
1:A:19:GLU:CD	1:A:21:PHE:HB3	0.43	2.34	16	1
1:A:19:GLU:OE2	1:A:21:PHE:HB3	0.43	2.13	16	1
1:A:17:GLY:O	1:A:18:ASN:CG	0.43	2.57	20	1
1:A:37:CYS:O	1:A:40:THR:HG22	0.43	2.13	16	2
1:A:21:PHE:CD2	1:A:35:ARG:CG	0.43	3.01	12	1
1:A:19:GLU:OE1	1:A:21:PHE:HB2	0.43	2.13	16	1
1:A:20:ARG:O	1:A:35:ARG:NH1	0.43	2.51	11	1
1:A:38:LEU:O	1:A:38:LEU:HD12	0.43	2.13	28	1
1:A:42:LEU:CB	1:A:47:ASN:HB2	0.43	2.43	22	1
1:A:8:VAL:HG12	1:A:14:GLU:N	0.43	2.29	26	5
1:A:38:LEU:HD12	1:A:38:LEU:O	0.43	2.13	22	2
1:A:45:SER:O	1:A:46:ARG:C	0.43	2.56	6	1
1:A:25:GLY:C	1:A:31:GLU:OE2	0.43	2.57	28	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:48:THR:O	1:A:57:TYR:CG	0.43	2.72	9	1
1:A:12:CYS:O	1:A:13:ASN:HB3	0.43	2.14	10	1
1:A:21:PHE:CG	1:A:35:ARG:HB2	0.43	2.49	6	2
1:A:7:PRO:O	1:A:15:GLU:HB2	0.42	2.14	5	1
1:A:21:PHE:CG	1:A:35:ARG:HG2	0.42	2.49	2	1
1:A:14:GLU:HA	1:A:14:GLU:OE1	0.42	2.14	15	1
1:A:28:GLY:N	1:A:31:GLU:HB3	0.42	2.30	19	1
1:A:16:LEU:N	1:A:16:LEU:HD22	0.42	2.26	24	2
1:A:34:HIS:O	1:A:38:LEU:HB3	0.42	2.15	11	1
1:A:7:PRO:HB2	1:A:32:ASN:CG	0.42	2.35	14	1
1:A:25:GLY:O	1:A:31:GLU:CD	0.42	2.58	11	1
1:A:51:GLN:HG3	1:A:52:ILE:N	0.42	2.30	23	1
1:A:33:VAL:O	1:A:33:VAL:HG13	0.42	2.15	14	1
1:A:48:THR:CA	1:A:57:TYR:CD2	0.42	3.03	13	1
1:A:27:THR:HA	1:A:31:GLU:CD	0.42	2.35	13	1
1:A:35:ARG:O	1:A:39:SER:HB3	0.42	2.14	16	2
1:A:26:CYS:HB2	1:A:30:LEU:HB3	0.42	1.91	22	1
1:A:49:ALA:HA	1:A:56:VAL:HA	0.42	1.92	27	1
1:A:33:VAL:CG2	1:A:38:LEU:CD2	0.42	2.95	25	2
1:A:27:THR:HA	1:A:31:GLU:OE2	0.42	2.14	16	1
1:A:10:TRP:HB3	1:A:29:GLU:HG3	0.42	1.92	4	4
1:A:41:TRP:O	1:A:45:SER:OG	0.42	2.38	11	1
1:A:7:PRO:HB2	1:A:32:ASN:ND2	0.42	2.30	16	1
1:A:21:PHE:CE2	1:A:35:ARG:HG2	0.41	2.50	12	1
1:A:10:TRP:HB2	1:A:29:GLU:OE2	0.41	2.15	11	1
1:A:8:VAL:HG22	1:A:15:GLU:OE1	0.41	2.15	28	1
1:A:6:VAL:CG1	1:A:15:GLU:HB2	0.41	2.44	24	1
1:A:23:ALA:CB	1:A:57:TYR:HA	0.41	2.45	17	1
1:A:35:ARG:O	1:A:39:SER:OG	0.41	2.35	10	1
1:A:14:GLU:HG2	1:A:34:HIS:CE1	0.41	2.50	22	1
1:A:30:LEU:C	1:A:32:ASN:N	0.41	2.74	9	1
1:A:23:ALA:O	1:A:24:CYS:HB2	0.41	2.16	17	4
1:A:12:CYS:SG	1:A:14:GLU:HB3	0.41	2.56	28	3
1:A:7:PRO:HB2	1:A:32:ASN:HB2	0.41	1.93	5	1
1:A:12:CYS:O	1:A:13:ASN:HB2	0.41	2.16	26	3
1:A:28:GLY:O	1:A:31:GLU:HB2	0.41	2.16	7	1
1:A:42:LEU:HD22	1:A:57:TYR:CG	0.41	2.51	7	1
1:A:45:SER:OG	1:A:47:ASN:OD1	0.41	2.38	7	1
1:A:45:SER:O	1:A:46:ARG:HB2	0.41	2.14	23	2
1:A:10:TRP:HB3	1:A:29:GLU:HB2	0.41	1.92	26	2
1:A:49:ALA:N	1:A:57:TYR:CD2	0.41	2.89	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:30:LEU:O	1:A:31:GLU:C	0.41	2.57	14	1
1:A:6:VAL:CG1	1:A:17:GLY:CA	0.41	2.99	7	1
1:A:26:CYS:HB2	1:A:30:LEU:HB2	0.41	1.93	9	1
1:A:16:LEU:HD12	1:A:19:GLU:H	0.41	1.75	25	1
1:A:17:GLY:C	1:A:18:ASN:CG	0.41	2.79	17	2
1:A:23:ALA:HB1	1:A:38:LEU:HD21	0.40	1.93	16	1
1:A:49:ALA:CA	1:A:55:VAL:O	0.40	2.70	2	1
1:A:6:VAL:HB	1:A:15:GLU:OE2	0.40	2.17	4	1
1:A:10:TRP:HB2	1:A:29:GLU:CD	0.40	2.37	6	1
1:A:10:TRP:CZ2	1:A:30:LEU:HD21	0.40	2.51	2	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	52/60 (87%)	42±2 (80±5%)	8±3 (16±5%)	2±1 (4±2%)	7	35
All	All	1456/1680 (87%)	1166 (80%)	234 (16%)	56 (4%)	7	35

All 6 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	18	ASN	28
1	A	26	CYS	19
1	A	24	CYS	4
1	A	20	ARG	3
1	A	28	GLY	1
1	A	25	GLY	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	46/54 (85%)	37±2 (80±4%)	9±2 (20±4%)	4	35
All	All	1288/1512 (85%)	1027 (80%)	261 (20%)	4	35

All 23 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	30	LEU	26
1	A	24	CYS	26
1	A	16	LEU	24
1	A	20	ARG	19
1	A	46	ARG	17
1	A	35	ARG	15
1	A	21	PHE	15
1	A	13	ASN	14
1	A	26	CYS	13
1	A	31	GLU	12
1	A	19	GLU	12
1	A	15	GLU	12
1	A	51	GLN	9
1	A	18	ASN	9
1	A	27	THR	9
1	A	22	ARG	7
1	A	45	SER	7
1	A	36	SER	7
1	A	37	CYS	3
1	A	48	THR	2
1	A	14	GLU	1
1	A	29	GLU	1
1	A	9	CYS	1

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

Of 2 ligands modelled in this entry, 2 are 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