



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 27, 2016 – 05:04 AM BST

PDB ID : 2RO3  
Title : RDC-refined Solution Structure of the N-terminal DNA Recognition Domain  
of the Bacillus subtilis Transition-state Regulator Abh  
Authors : Sullivan, D.M.; Bobay, B.G.; Douglas, K.J.; Thompson, R.J.; Rance, M.;  
Strauch, M.A.; Cavanagh, J.  
Deposited on : 2008-03-08

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.

---

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

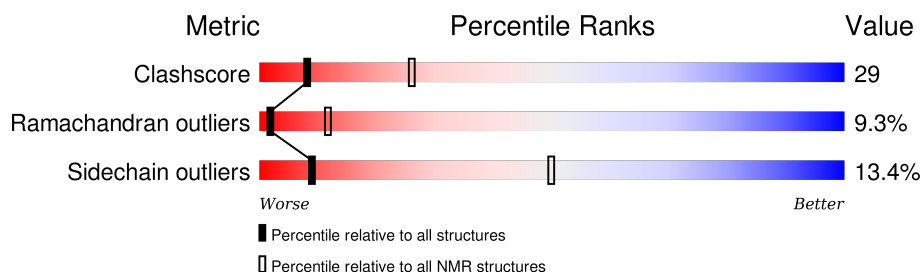
# 1 Overall quality at a glance

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	54	
1	B	54	

## 2 Ensemble composition and analysis ⓘ

This entry contains 10 models. Model 2 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:4-A:48, B:4-B:48 (90)	0.16	2

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 2 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 5, 6, 7, 8, 9
2	4, 10

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

There is only 1 type of molecule in this entry. The entry contains 1808 atoms, of which 946 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Putative transition state regulator abh.

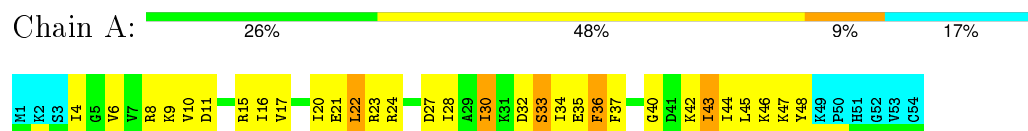
Mol	Chain	Residues	Atoms						Trace
1	A	54	Total	C	H	N	O	S	0
			904	279	473	75	74	3	
1	B	54	Total	C	H	N	O	S	0
			904	279	473	75	74	3	

## 4 Residue-property plots [i](#)

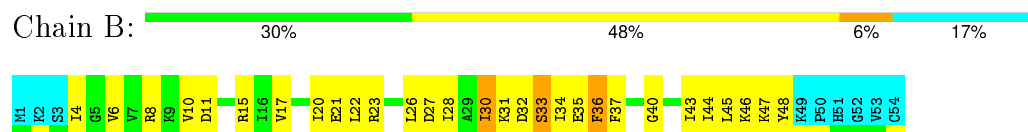
### 4.1 Average score per residue in the NMR ensemble

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: Putative transition state regulator abh



- Molecule 1: Putative transition state regulator abh

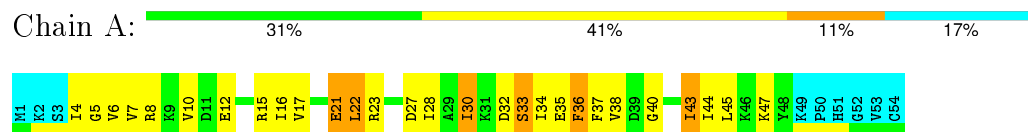


### 4.2 Scores per residue for each member of the ensemble

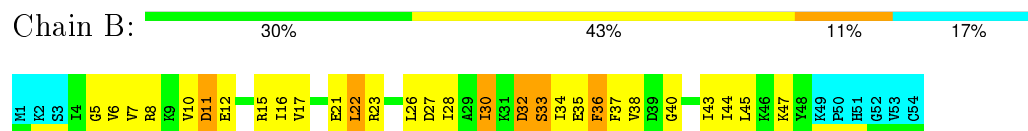
Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

- Molecule 1: Putative transition state regulator abh

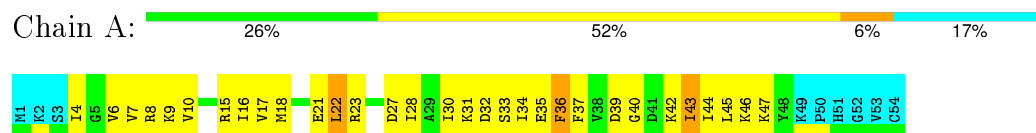


- Molecule 1: Putative transition state regulator abh

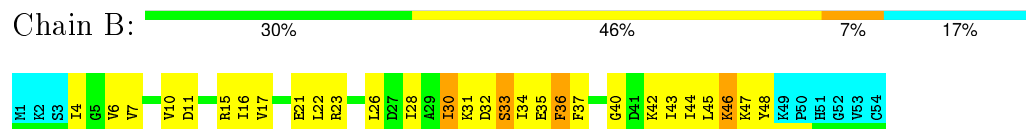


### 4.2.2 Score per residue for model 2 (medoid)

- Molecule 1: Putative transition state regulator abh

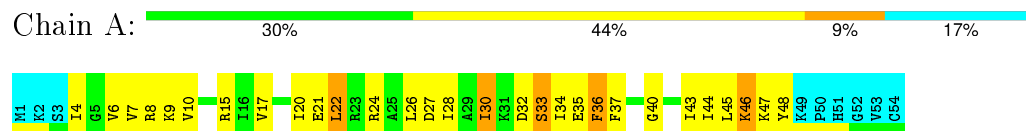


- Molecule 1: Putative transition state regulator abh

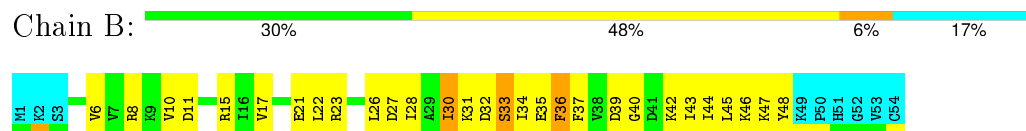


### 4.2.3 Score per residue for model 3

- Molecule 1: Putative transition state regulator abh

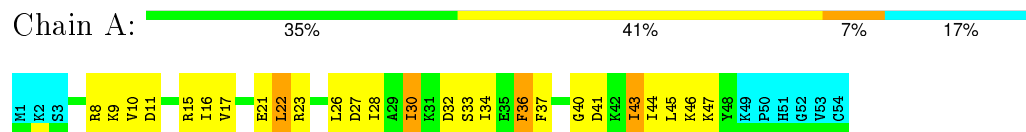


- Molecule 1: Putative transition state regulator abh

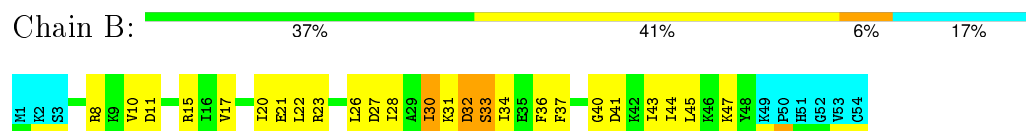


### 4.2.4 Score per residue for model 4

- Molecule 1: Putative transition state regulator abh

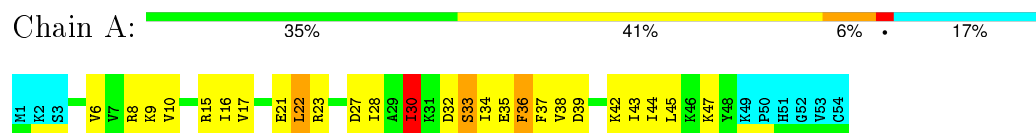


- Molecule 1: Putative transition state regulator abh

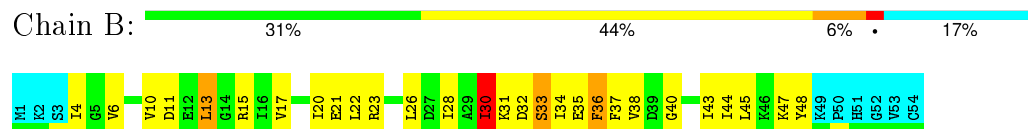


### 4.2.5 Score per residue for model 5

- Molecule 1: Putative transition state regulator abh

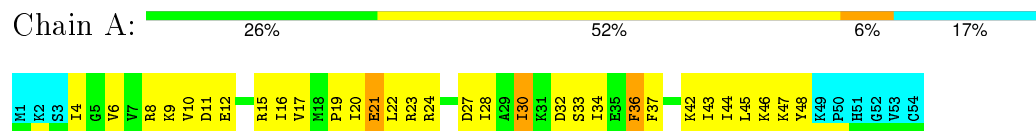


- Molecule 1: Putative transition state regulator abh

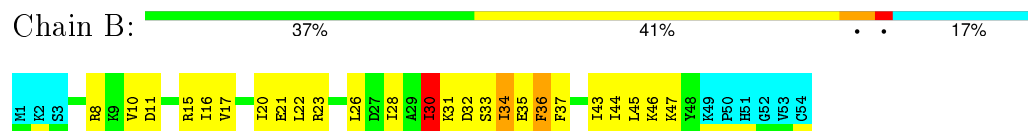


### 4.2.6 Score per residue for model 6

- Molecule 1: Putative transition state regulator abh

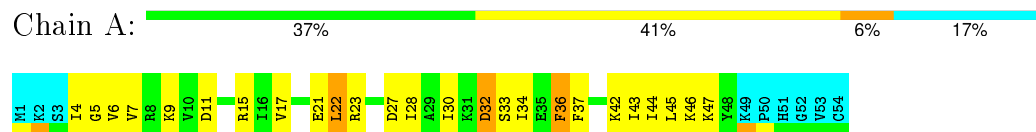


- Molecule 1: Putative transition state regulator abh

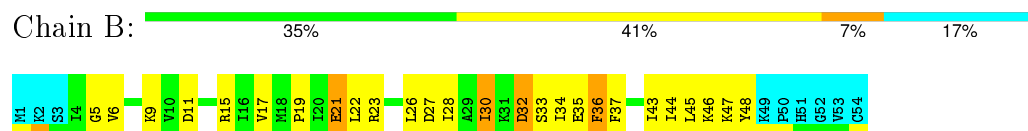


### 4.2.7 Score per residue for model 7

- Molecule 1: Putative transition state regulator abh

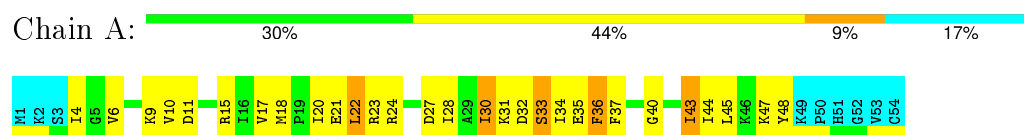


- Molecule 1: Putative transition state regulator abh

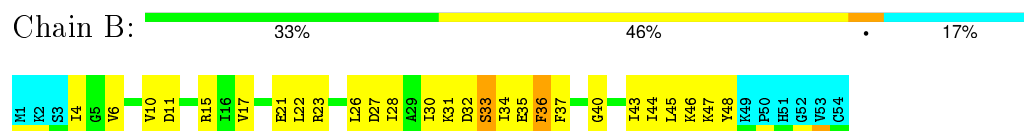


### 4.2.8 Score per residue for model 8

- Molecule 1: Putative transition state regulator abh

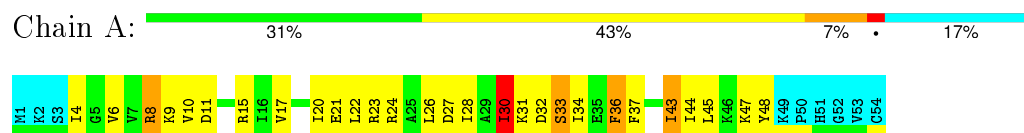


- Molecule 1: Putative transition state regulator abh

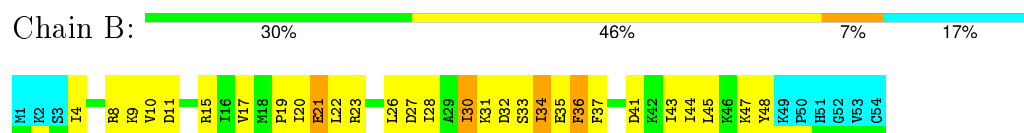


### 4.2.9 Score per residue for model 9

- Molecule 1: Putative transition state regulator abh

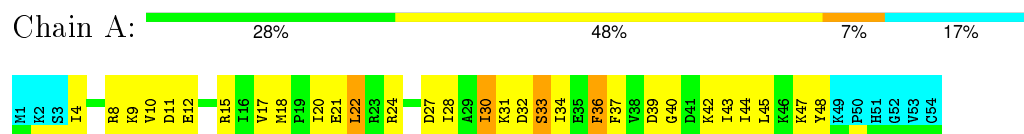


- Molecule 1: Putative transition state regulator abh

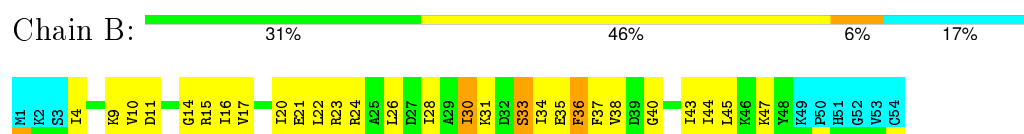


### 4.2.10 Score per residue for model 10

- Molecule 1: Putative transition state regulator abh



- Molecule 1: Putative transition state regulator abh



## 5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *DGSA-distance geometry simulated annealing*.

Of the 10 calculated structures, 10 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
ARIA	structure solution	1.2
ARIA	refinement	1.2

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 [i](#)

### 6.1 Standard geometry [i](#)

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	364	399	399	31±5
1	B	364	399	399	30±3
All	All	7280	7980	7980	437

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 29.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:45:LEU:HB2	1:B:43:ILE:HB	0.98	1.35	4	10
1:A:43:ILE:HB	1:B:45:LEU:HB2	0.83	1.48	3	10
1:B:20:ILE:HA	1:B:23:ARG:HD3	0.78	1.55	6	4
1:B:23:ARG:HA	1:B:28:ILE:HB	0.74	1.57	1	10
1:A:34:ILE:HD11	1:B:16:ILE:HG21	0.74	1.56	10	1
1:A:37:PHE:HB3	1:A:44:ILE:HB	0.74	1.59	8	10
1:B:37:PHE:HB3	1:B:44:ILE:HB	0.70	1.64	3	10
1:A:10:VAL:HG23	1:B:34:ILE:HD11	0.68	1.65	8	9
1:A:34:ILE:HD11	1:B:10:VAL:HG23	0.66	1.64	9	7
1:A:17:VAL:HB	1:B:15:ARG:HG2	0.66	1.66	7	7
1:A:28:ILE:HG13	1:A:32:ASP:HB3	0.66	1.65	2	8
1:A:36:PHE:HD1	1:A:45:LEU:HG	0.66	1.50	3	9
1:A:20:ILE:HG13	1:A:24:ARG:HD2	0.66	1.66	3	3

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:34:ILE:HG21	1:A:45:LEU:HD23	0.66	1.68	9	9
1:A:39:ASP:HB3	1:A:42:LYS:HE3	0.63	1.70	10	1
1:B:13:LEU:HD12	1:B:13:LEU:H	0.63	1.53	5	1
1:A:28:ILE:HG23	1:A:32:ASP:OD1	0.63	1.93	1	1
1:A:22:LEU:HD12	1:B:43:ILE:HG13	0.63	1.70	7	7
1:A:32:ASP:O	1:B:9:LYS:HE3	0.63	1.94	9	1
1:B:34:ILE:HG21	1:B:45:LEU:HD23	0.62	1.69	9	9
1:A:47:LYS:HD3	1:A:48:TYR:N	0.62	2.09	8	5
1:A:9:LYS:HB3	1:B:31:LYS:HB3	0.60	1.74	8	7
1:A:8:ARG:HD3	1:B:36:PHE:CZ	0.59	2.32	10	6
1:A:36:PHE:CD1	1:A:45:LEU:HG	0.59	2.31	3	8
1:A:23:ARG:HA	1:A:28:ILE:HB	0.59	1.73	1	8
1:A:17:VAL:HA	1:B:15:ARG:HA	0.59	1.74	10	10
1:B:33:SER:O	1:B:47:LYS:HG2	0.59	1.96	7	2
1:A:4:ILE:HB	1:A:6:VAL:HG22	0.58	1.75	8	4
1:A:45:LEU:HD13	1:B:45:LEU:HD13	0.57	1.76	3	6
1:B:19:PRO:HB2	1:B:21:GLU:HG3	0.57	1.75	7	1
1:A:36:PHE:HA	1:A:44:ILE:O	0.57	2.00	8	10
1:A:17:VAL:CB	1:B:15:ARG:HG2	0.57	2.30	6	5
1:A:9:LYS:HE3	1:B:32:ASP:O	0.57	1.99	9	1
1:A:6:VAL:O	1:B:35:GLU:HA	0.56	2.00	2	8
1:A:32:ASP:OD2	1:A:47:LYS:HG3	0.56	2.00	2	1
1:A:15:ARG:HA	1:B:17:VAL:HA	0.56	1.75	6	10
1:B:47:LYS:HD3	1:B:48:TYR:N	0.56	2.16	2	5
1:A:10:VAL:HG23	1:B:34:ILE:CD1	0.55	2.31	4	2
1:B:26:LEU:HB2	1:B:28:ILE:CD1	0.55	2.32	8	10
1:A:36:PHE:CZ	1:B:8:ARG:HD3	0.55	2.37	4	4
1:B:28:ILE:HG23	1:B:32:ASP:OD1	0.55	2.01	1	1
1:B:23:ARG:CA	1:B:28:ILE:HB	0.55	2.31	4	7
1:A:34:ILE:CD1	1:B:10:VAL:HG23	0.54	2.33	4	1
1:A:33:SER:O	1:A:47:LYS:HG2	0.53	2.02	10	3
1:A:35:GLU:HB3	1:A:46:LYS:HE3	0.53	1.79	3	1
1:A:37:PHE:CD1	1:A:44:ILE:HD12	0.53	2.38	8	4
1:A:8:ARG:HD2	1:B:36:PHE:CZ	0.53	2.38	9	1
1:B:33:SER:O	1:B:47:LYS:HA	0.53	2.04	10	7
1:A:35:GLU:HB3	1:A:46:LYS:CE	0.52	2.34	3	1
1:B:36:PHE:HA	1:B:44:ILE:O	0.52	2.04	8	9
1:A:34:ILE:HD13	1:B:16:ILE:HG21	0.52	1.82	1	1
1:B:28:ILE:HA	1:B:32:ASP:CG	0.52	2.26	4	2
1:A:35:GLU:HA	1:B:6:VAL:O	0.52	2.05	2	4
1:A:10:VAL:HB	1:B:31:LYS:HA	0.51	1.80	9	4

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:26:LEU:HB2	1:B:28:ILE:HD13	0.51	1.82	9	8
1:B:39:ASP:HB3	1:B:42:LYS:HE3	0.51	1.80	3	1
1:B:19:PRO:HB2	1:B:21:GLU:HG2	0.51	1.83	9	1
1:A:42:LYS:HG2	1:A:43:ILE:N	0.51	2.19	5	4
1:A:23:ARG:HD2	1:A:28:ILE:HG22	0.51	1.83	6	2
1:A:8:ARG:HD3	1:B:36:PHE:HZ	0.51	1.65	10	1
1:A:28:ILE:HA	1:A:32:ASP:CB	0.50	2.37	2	5
1:A:4:ILE:HG23	1:A:21:GLU:HG3	0.50	1.82	6	1
1:A:33:SER:O	1:A:47:LYS:HA	0.50	2.07	3	6
1:B:36:PHE:HD1	1:B:45:LEU:HG	0.50	1.67	3	2
1:A:28:ILE:HA	1:A:32:ASP:HB2	0.49	1.83	2	4
1:B:28:ILE:HA	1:B:32:ASP:HB2	0.48	1.85	7	6
1:A:9:LYS:HA	1:B:32:ASP:O	0.48	2.08	7	1
1:A:26:LEU:HA	1:B:41:ASP:OD1	0.48	2.07	4	1
1:A:15:ARG:HG2	1:B:17:VAL:HB	0.48	1.85	6	2
1:B:10:VAL:CG1	1:B:14:GLY:HA2	0.48	2.38	10	1
1:A:28:ILE:HG13	1:A:32:ASP:CB	0.48	2.39	3	7
1:A:43:ILE:O	1:B:44:ILE:HA	0.48	2.09	10	5
1:A:16:ILE:HG21	1:B:34:ILE:HD13	0.47	1.85	1	4
1:B:20:ILE:HA	1:B:23:ARG:HE	0.47	1.69	10	1
1:A:28:ILE:HA	1:A:32:ASP:CG	0.47	2.30	5	3
1:A:7:VAL:HA	1:B:34:ILE:O	0.47	2.10	2	4
1:A:36:PHE:HB2	1:B:4:ILE:HD12	0.47	1.86	5	4
1:A:32:ASP:O	1:B:9:LYS:HA	0.46	2.09	7	1
1:B:36:PHE:CD1	1:B:45:LEU:HG	0.46	2.45	3	1
1:A:47:LYS:HD3	1:A:48:TYR:H	0.46	1.69	8	1
1:A:10:VAL:CG2	1:B:34:ILE:HD11	0.45	2.42	9	1
1:A:43:ILE:HD11	1:B:22:LEU:HB2	0.45	1.88	1	1
1:B:28:ILE:HG23	1:B:32:ASP:CG	0.45	2.32	1	1
1:A:41:ASP:OD1	1:B:26:LEU:HA	0.45	2.11	4	1
1:A:43:ILE:CD1	1:B:22:LEU:HB2	0.45	2.41	1	1
1:A:15:ARG:HG2	1:B:17:VAL:HG23	0.45	1.87	9	1
1:A:45:LEU:CB	1:B:43:ILE:HB	0.45	2.27	8	2
1:B:26:LEU:HB3	1:B:47:LYS:HB2	0.45	1.88	7	2
1:A:8:ARG:HD2	1:B:36:PHE:HZ	0.45	1.69	9	1
1:B:28:ILE:N	1:B:28:ILE:HD12	0.44	2.27	7	1
1:B:42:LYS:HG2	1:B:43:ILE:N	0.44	2.27	2	1
1:A:10:VAL:HA	1:A:16:ILE:HG22	0.44	1.89	4	1
1:B:28:ILE:HA	1:B:32:ASP:CB	0.44	2.41	7	7
1:A:18:MET:HB3	1:A:22:LEU:HD13	0.44	1.89	8	2
1:A:31:LYS:HE2	1:B:9:LYS:HB3	0.44	1.89	10	1

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:LYS:HA	1:B:10:VAL:HB	0.44	1.89	2	2
1:B:34:ILE:CG2	1:B:45:LEU:HD23	0.44	2.43	6	2
1:A:20:ILE:HG13	1:A:24:ARG:CD	0.44	2.42	9	4
1:A:30:ILE:HG23	1:A:31:LYS:HG3	0.43	1.89	9	2
1:A:8:ARG:O	1:B:34:ILE:HD12	0.43	2.13	9	2
1:B:33:SER:HB3	1:B:48:TYR:HB2	0.43	1.90	7	1
1:B:23:ARG:HG2	1:B:28:ILE:CG2	0.43	2.44	6	2
1:A:12:GLU:HG2	1:B:30:ILE:HD11	0.43	1.89	6	1
1:A:8:ARG:HE	1:A:8:ARG:HA	0.43	1.73	9	1
1:A:21:GLU:HG2	1:A:21:GLU:H	0.43	1.35	1	1
1:A:36:PHE:CE2	1:B:8:ARG:HD3	0.42	2.50	6	2
1:A:23:ARG:CB	1:A:28:ILE:HB	0.42	2.44	6	2
1:A:20:ILE:O	1:A:24:ARG:HG3	0.42	2.13	3	1
1:A:34:ILE:O	1:B:7:VAL:HA	0.42	2.14	2	2
1:B:10:VAL:HG13	1:B:14:GLY:HA2	0.42	1.91	10	1
1:A:44:ILE:HA	1:B:43:ILE:O	0.42	2.14	1	2
1:A:39:ASP:HB3	1:A:42:LYS:HD2	0.42	1.91	5	2
1:A:10:VAL:HG21	1:B:28:ILE:HG21	0.42	1.90	8	1
1:A:26:LEU:HB2	1:A:28:ILE:CD1	0.42	2.45	9	2
1:A:17:VAL:CG2	1:B:15:ARG:HG2	0.41	2.45	6	1
1:A:30:ILE:O	1:B:10:VAL:HB	0.41	2.14	5	1
1:B:10:VAL:HA	1:B:16:ILE:HG22	0.41	1.91	6	2
1:A:4:ILE:HG12	1:B:38:VAL:HG12	0.41	1.92	1	1
1:A:19:PRO:HB2	1:A:21:GLU:HG2	0.41	1.92	6	1
1:A:6:VAL:HG23	1:B:36:PHE:CD2	0.41	2.50	7	1
1:B:30:ILE:HG23	1:B:31:LYS:HG3	0.41	1.92	5	1
1:A:22:LEU:HB2	1:B:43:ILE:HD11	0.41	1.92	5	1
1:A:39:ASP:CB	1:A:42:LYS:HE3	0.41	2.44	10	1
1:A:15:ARG:HG2	1:B:17:VAL:CG2	0.41	2.46	9	1
1:B:28:ILE:CD1	1:B:28:ILE:N	0.41	2.84	8	1
1:B:20:ILE:HG13	1:B:24:ARG:HD2	0.41	1.91	10	1
1:A:42:LYS:HG3	1:B:44:ILE:HG23	0.40	1.93	7	1
1:A:28:ILE:HG13	1:A:32:ASP:CG	0.40	2.37	1	1
1:A:36:PHE:CD2	1:B:6:VAL:HG23	0.40	2.52	7	1
1:B:4:ILE:HB	1:B:6:VAL:HG22	0.40	1.94	8	1

## 6.3 Torsion angles

### 6.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	45/54 (83%)	35±1 (79±2%)	6±1 (12±3%)	4±1 (9±2%)	<b>2</b>	<b>12</b>
1	B	45/54 (83%)	36±1 (80±1%)	5±1 (10±2%)	4±1 (10±2%)	<b>2</b>	<b>11</b>
All	All	900/1080 (83%)	715 (79%)	101 (11%)	84 (9%)	<b>2</b>	<b>12</b>

All 14 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	B	11	ASP	10
1	A	27	ASP	10
1	A	33	SER	9
1	B	30	ILE	9
1	B	33	SER	9
1	A	30	ILE	7
1	B	40	GLY	7
1	B	27	ASP	6
1	A	11	ASP	6
1	A	40	GLY	6
1	A	12	GLU	2
1	A	32	ASP	1
1	B	12	GLU	1
1	B	32	ASP	1

### 6.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	40/48 (83%)	35±1 (86±3%)	6±1 (14±3%)	<b>8</b>	49
1	B	40/48 (83%)	35±1 (87±2%)	5±1 (13±2%)	<b>9</b>	51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	800/960 (83%)	693 (87%)	107 (13%)	<b>9</b> 50

All 21 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	ILE	10
1	B	36	PHE	10
1	B	21	GLU	10
1	A	36	PHE	10
1	A	21	GLU	10
1	B	30	ILE	10
1	B	22	LEU	10
1	A	22	LEU	10
1	A	43	ILE	5
1	A	46	LYS	4
1	B	46	LYS	4
1	B	34	ILE	2
1	A	8	ARG	2
1	A	4	ILE	2
1	B	32	ASP	2
1	A	18	MET	1
1	B	11	ASP	1
1	B	41	ASP	1
1	A	47	LYS	1
1	B	13	LEU	1
1	B	8	ARG	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 ⓘ

There are no carbohydrates in this entry.

## 6.6 Ligand geometry

There are no ligands in this entry.

## 6.7 Other polymers

There are no such molecules in this entry.

## 6.8 Polymer linkage issues

There are no chain breaks in this entry.

## 7 Chemical shift validation

No chemical shift data were provided