



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 03:44 PM BST

PDB ID : 1NIL  
Title : A COMPARISON OF NMR SOLUTION STRUCTURES OF THE RECEPTOR BINDING DOMAINS OF PSEUDOMONAS AERUGINOSA PILI STRAINS PAO, KB7, AND PAK: IMPLICATIONS FOR RECEPTOR BINDING AND SYNTHETIC VACCINE DESIGN  
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Deposited on : 1995-10-05

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

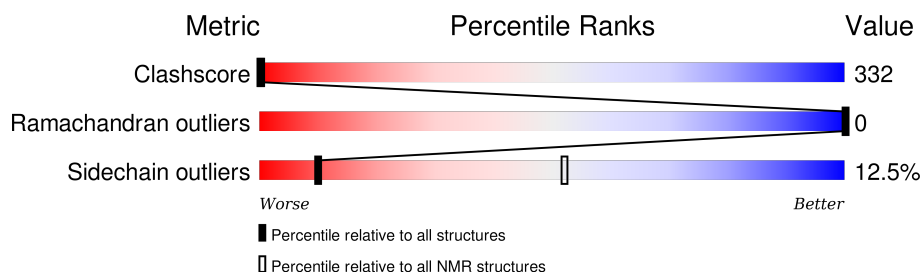
# 1 Overall quality at a glance

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	18	

## 2 Ensemble composition and analysis ⓘ

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

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

There is only 1 type of molecule in this entry. The entry contains 263 atoms, of which 128 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PAK PILIN, TRANS.

Mol	Chain	Residues	Atoms						Trace
1	A	18	Total	C	H	N	O	S	0
			263	81	128	22	30	2	

## 4 Residue-property plots

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: PAK PILIN, TRANS

Chain A: 



## 5 Refinement protocol and experimental data overview

Of the ? calculated structures, 1 were deposited, based on the following criterion: ?.

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

Software name	Classification	Version
PEPFLEX II	refinement	

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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ACE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	19.14	80/134 (59.7%)	17.31	44/176 (25.0%)
All	All	19.14	80/134 (59.7%)	17.31	44/176 (25.0%)

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	1	0
All	All	1	0

All bond outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	131	SER	CB-OG	-89.99	0.25	1.42
1	A	143	SER	CB-OG	-68.75	0.52	1.42
1	A	137	PHE	CG-CD1	-46.89	0.68	1.38
1	A	135	GLU	CD-OE1	-45.62	0.75	1.25
1	A	137	PHE	CG-CD2	-44.13	0.72	1.38
1	A	135	GLU	CD-OE2	-43.20	0.78	1.25
1	A	132	ASP	CG-OD1	-39.98	0.33	1.25
1	A	132	ASP	CG-OD2	-37.39	0.39	1.25
1	A	133	GLN	CD-NE2	-37.07	0.40	1.32
1	A	133	GLN	CD-OE1	-36.98	0.42	1.24
1	A	137	PHE	CE2-CZ	-36.96	0.67	1.37
1	A	144	LYS	C-O	-36.32	0.54	1.23
1	A	144	LYS	C-OXT	-35.98	0.55	1.23
1	A	137	PHE	CE1-CZ	-34.79	0.71	1.37
1	A	144	LYS	CE-NZ	-32.83	0.67	1.49
1	A	130	THR	CB-OG1	-31.88	0.79	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	132	ASP	CB-CG	-31.52	0.85	1.51
1	A	134	ASP	CG-OD1	-30.66	0.54	1.25
1	A	134	ASP	CG-OD2	-29.34	0.57	1.25
1	A	140	LYS	CE-NZ	-28.68	0.77	1.49
1	A	136	GLN	CD-NE2	-28.06	0.62	1.32
1	A	136	GLN	CD-OE1	-28.04	0.62	1.24
1	A	131	SER	CA-CB	-24.16	1.16	1.52
1	A	133	GLN	CG-CD	-22.76	0.98	1.51
1	A	133	GLN	CA-CB	-21.32	1.07	1.53
1	A	136	GLN	CB-CG	-20.96	0.95	1.52
1	A	144	LYS	CG-CD	-20.57	0.82	1.52
1	A	128	LYS	CD-CE	-19.53	1.02	1.51
1	A	144	LYS	CB-CG	-19.13	1.00	1.52
1	A	144	LYS	CD-CE	-19.11	1.03	1.51
1	A	144	LYS	CA-CB	-18.45	1.13	1.53
1	A	128	LYS	CE-NZ	-18.25	1.03	1.49
1	A	128	LYS	CB-CG	-18.17	1.03	1.52
1	A	130	THR	CB-CG2	-18.03	0.92	1.52
1	A	128	LYS	N-CA	-17.33	1.11	1.46
1	A	133	GLN	CB-CG	-16.45	1.08	1.52
1	A	140	LYS	CB-CG	-16.07	1.09	1.52
1	A	144	LYS	CA-C	-15.09	1.13	1.52
1	A	132	ASP	C-O	-15.07	0.94	1.23
1	A	131	SER	C-O	-13.64	0.97	1.23
1	A	143	SER	CA-CB	-13.50	1.32	1.52
1	A	127	ACE	C-N	-13.21	1.03	1.34
1	A	128	LYS	C-O	-12.98	0.98	1.23
1	A	131	SER	C-N	-12.89	1.04	1.34
1	A	140	LYS	CD-CE	-12.41	1.20	1.51
1	A	143	SER	C-O	-12.03	1.00	1.23
1	A	129	CYS	N-CA	-11.94	1.22	1.46
1	A	129	CYS	CB-SG	-11.73	1.62	1.82
1	A	128	LYS	CA-CB	-11.64	1.28	1.53
1	A	128	LYS	C-N	-11.22	1.08	1.34
1	A	136	GLN	CG-CD	-11.21	1.25	1.51
1	A	144	LYS	N-CA	-10.59	1.25	1.46
1	A	128	LYS	CG-CD	-10.58	1.16	1.52
1	A	143	SER	C-N	-10.38	1.10	1.34
1	A	128	LYS	CA-C	-10.22	1.26	1.52
1	A	130	THR	C-O	-9.67	1.04	1.23
1	A	133	GLN	N-CA	-9.24	1.27	1.46
1	A	135	GLU	CG-CD	-9.19	1.38	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	134	ASP	CB-CG	-9.14	1.32	1.51
1	A	132	ASP	CA-CB	-9.07	1.33	1.53
1	A	142	CYS	CB-SG	-8.97	1.67	1.82
1	A	130	THR	CA-CB	-8.44	1.31	1.53
1	A	143	SER	CA-C	-8.34	1.31	1.52
1	A	129	CYS	CA-CB	-8.29	1.35	1.53
1	A	132	ASP	CA-C	-8.20	1.31	1.52
1	A	129	CYS	C-O	-8.13	1.07	1.23
1	A	131	SER	N-CA	-7.94	1.30	1.46
1	A	142	CYS	C-N	-7.41	1.17	1.34
1	A	129	CYS	C-N	-7.04	1.17	1.34
1	A	130	THR	CA-C	-6.80	1.35	1.52
1	A	132	ASP	N-CA	-6.63	1.33	1.46
1	A	142	CYS	C-O	-5.76	1.12	1.23
1	A	132	ASP	C-N	-5.68	1.21	1.34
1	A	130	THR	C-N	-5.65	1.21	1.34
1	A	140	LYS	CG-CD	-5.63	1.33	1.52
1	A	143	SER	N-CA	-5.53	1.35	1.46
1	A	133	GLN	C-O	-5.41	1.13	1.23
1	A	142	CYS	CA-CB	-5.27	1.42	1.53
1	A	134	ASP	N-CA	-5.07	1.36	1.46
1	A	134	ASP	CA-CB	-5.07	1.42	1.53

All angle outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	137	PHE	CD1-CG-CD2	-84.26	8.76	118.30
1	A	137	PHE	CB-CG-CD1	76.69	174.48	120.80
1	A	137	PHE	CB-CG-CD2	74.83	173.18	120.80
1	A	137	PHE	CE1-CZ-CE2	-61.71	8.92	120.00
1	A	137	PHE	CG-CD2-CE2	50.14	175.95	120.80
1	A	137	PHE	CG-CD1-CE1	49.52	175.28	120.80
1	A	134	ASP	CB-CG-OD1	47.41	160.97	118.30
1	A	132	ASP	CB-CG-OD1	47.39	160.95	118.30
1	A	137	PHE	CD1-CE1-CZ	46.33	175.69	120.10
1	A	132	ASP	CB-CG-OD2	46.13	159.81	118.30
1	A	137	PHE	CZ-CE2-CD2	46.07	175.39	120.10
1	A	133	GLN	OE1-CD-NE2	-44.54	19.45	121.90
1	A	132	ASP	OD1-CG-OD2	-44.25	39.23	123.30
1	A	134	ASP	CB-CG-OD2	43.46	157.42	118.30
1	A	134	ASP	OD1-CG-OD2	-42.99	41.62	123.30
1	A	135	GLU	OE1-CD-OE2	-28.57	89.02	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	133	GLN	CG-CD-OE1	24.84	171.28	121.60
1	A	136	GLN	OE1-CD-NE2	-23.41	68.07	121.90
1	A	128	LYS	CD-CE-NZ	22.73	163.98	111.70
1	A	133	GLN	CG-CD-NE2	21.90	169.25	116.70
1	A	143	SER	CA-CB-OG	19.59	164.10	111.20
1	A	131	SER	CA-CB-OG	17.00	157.09	111.20
1	A	144	LYS	CA-CB-CG	16.62	149.96	113.40
1	A	144	LYS	CA-C-O	14.35	150.22	120.10
1	A	128	LYS	CG-CD-CE	13.88	153.53	111.90
1	A	132	ASP	CA-CB-CG	13.73	143.60	113.40
1	A	128	LYS	CB-CG-CD	13.47	146.62	111.60
1	A	144	LYS	CB-CG-CD	13.24	146.02	111.60
1	A	136	GLN	CG-CD-OE1	13.12	147.83	121.60
1	A	128	LYS	CA-CB-CG	13.00	142.00	113.40
1	A	136	GLN	CA-CB-CG	12.96	141.90	113.40
1	A	136	GLN	CB-CG-CD	12.81	144.91	111.60
1	A	144	LYS	CG-CD-CE	11.51	146.43	111.90
1	A	144	LYS	CD-CE-NZ	11.50	138.16	111.70
1	A	136	GLN	CG-CD-NE2	11.42	144.10	116.70
1	A	135	GLU	CG-CD-OE1	11.07	140.45	118.30
1	A	140	LYS	CD-CE-NZ	8.62	131.52	111.70
1	A	130	THR	CA-CB-CG2	8.22	123.91	112.40
1	A	130	THR	OG1-CB-CG2	-7.80	92.05	110.00
1	A	131	SER	O-C-N	-6.31	112.61	122.70
1	A	135	GLU	CG-CD-OE2	6.12	130.53	118.30
1	A	140	LYS	CB-CG-CD	6.03	127.28	111.60
1	A	140	LYS	CA-CB-CG	5.38	125.25	113.40
1	A	132	ASP	N-CA-C	-5.10	97.23	111.00

All chiral outliers are listed below.

Mol	Chain	Res	Type	Atoms
1	A	130	THR	CB

There are no planarity outliers.

## 6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	135	128	121	85
All	All	135	128	121	85

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 332.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:144:LYS:CE	1:A:144:LYS:CG	1.56	1.77
1:A:144:LYS:CD	1:A:144:LYS:CB	1.54	1.75
1:A:136:GLN:CG	1:A:136:GLN:NE2	1.44	1.79
1:A:137:PHE:CE1	1:A:137:PHE:CG	1.43	2.05
1:A:140:LYS:NZ	1:A:140:LYS:CD	1.43	1.80
1:A:137:PHE:CD2	1:A:137:PHE:CZ	1.42	2.04
1:A:130:THR:CG2	1:A:130:THR:CA	1.38	1.98
1:A:137:PHE:CD1	1:A:137:PHE:CZ	1.35	2.08
1:A:137:PHE:CE2	1:A:137:PHE:CG	1.34	2.09
1:A:136:GLN:CG	1:A:136:GLN:OE1	1.29	1.80
1:A:130:THR:OG1	1:A:130:THR:CA	1.27	1.82
1:A:143:SER:CA	1:A:143:SER:OG	1.26	1.83
1:A:134:ASP:CB	1:A:134:ASP:OD1	1.25	1.84
1:A:137:PHE:CB	1:A:137:PHE:CD1	1.24	2.20
1:A:134:ASP:CB	1:A:134:ASP:OD2	1.21	1.86
1:A:132:ASP:CG	1:A:132:ASP:CA	1.21	2.08
1:A:135:GLU:OE2	1:A:135:GLU:CG	1.10	1.97
1:A:135:GLU:OE1	1:A:135:GLU:CG	1.07	2.01
1:A:130:THR:HB	1:A:130:THR:CG2	1.02	1.60
1:A:130:THR:CB	1:A:130:THR:HG22	1.01	1.55
1:A:141:GLY:HA2	1:A:144:LYS:HD2	1.01	1.32
1:A:140:LYS:NZ	1:A:140:LYS:HE3	0.98	1.38
1:A:130:THR:CB	1:A:130:THR:HG23	0.98	1.55
1:A:133:GLN:O	1:A:133:GLN:HG2	0.96	1.56
1:A:132:ASP:HB2	1:A:132:ASP:CG	0.96	1.40
1:A:140:LYS:NZ	1:A:140:LYS:HE2	0.96	1.38
1:A:132:ASP:HB3	1:A:132:ASP:CG	0.96	1.40
1:A:130:THR:HG21	1:A:130:THR:CB	0.96	1.55
1:A:132:ASP:CG	1:A:132:ASP:CB	0.95	0.85
1:A:130:THR:CG2	1:A:130:THR:CB	0.92	0.92
1:A:140:LYS:CE	1:A:140:LYS:NZ	0.92	0.77
1:A:143:SER:HB3	1:A:143:SER:OG	0.91	1.14
1:A:143:SER:HB2	1:A:143:SER:OG	0.89	1.14
1:A:144:LYS:CD	1:A:144:LYS:HB2	0.86	2.00
1:A:130:THR:OG1	1:A:130:THR:CB	0.84	0.79

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:130:THR:HB	1:A:130:THR:OG1	0.84	1.54
1:A:144:LYS:CG	1:A:144:LYS:HD3	0.84	1.37
1:A:136:GLN:OE1	1:A:136:GLN:NE2	0.84	0.69
1:A:144:LYS:CD	1:A:144:LYS:HB3	0.84	1.99
1:A:144:LYS:HE2	1:A:144:LYS:CG	0.83	2.02
1:A:141:GLY:HA2	1:A:144:LYS:CE	0.83	2.02
1:A:144:LYS:CG	1:A:144:LYS:HD2	0.83	1.37
1:A:144:LYS:HG3	1:A:144:LYS:CD	0.83	1.37
1:A:144:LYS:HG2	1:A:144:LYS:CD	0.82	1.38
1:A:137:PHE:HZ	1:A:137:PHE:CE2	0.82	1.60
1:A:137:PHE:CB	1:A:137:PHE:CD2	0.82	2.24
1:A:130:THR:CG2	1:A:130:THR:N	0.80	2.44
1:A:136:GLN:OE1	1:A:136:GLN:CD	0.79	0.62
1:A:143:SER:CB	1:A:143:SER:OG	0.78	0.52
1:A:144:LYS:CG	1:A:144:LYS:CD	0.77	0.82
1:A:141:GLY:HA2	1:A:144:LYS:CD	0.77	2.08
1:A:130:THR:HG1	1:A:130:THR:CA	0.76	1.75
1:A:134:ASP:OD2	1:A:134:ASP:CG	0.73	0.57
1:A:141:GLY:CA	1:A:144:LYS:HD2	0.73	2.13
1:A:135:GLU:OE2	1:A:135:GLU:CD	0.71	0.78
1:A:129:CYS:CB	1:A:142:CYS:SG	0.70	2.66
1:A:135:GLU:OE1	1:A:135:GLU:CD	0.70	0.75
1:A:134:ASP:CG	1:A:134:ASP:OD1	0.69	0.54
1:A:136:GLN:CD	1:A:136:GLN:HE22	0.68	1.29
1:A:136:GLN:CD	1:A:136:GLN:HE21	0.67	1.29
1:A:137:PHE:CE2	1:A:137:PHE:CZ	0.64	0.67
1:A:140:LYS:CE	1:A:140:LYS:HZ2	0.64	1.36
1:A:140:LYS:CE	1:A:140:LYS:HZ3	0.64	1.36
1:A:140:LYS:CE	1:A:140:LYS:HZ1	0.63	1.36
1:A:136:GLN:CD	1:A:136:GLN:NE2	0.63	0.62
1:A:130:THR:C	1:A:130:THR:OG1	0.63	2.33
1:A:141:GLY:HA2	1:A:144:LYS:NZ	0.62	2.06
1:A:130:THR:C	1:A:130:THR:HG1	0.61	1.99
1:A:137:PHE:CE1	1:A:137:PHE:CZ	0.61	0.71
1:A:130:THR:CB	1:A:130:THR:HG1	0.60	1.33
1:A:132:ASP:CG	1:A:132:ASP:HA	0.56	2.16
1:A:137:PHE:CG	1:A:137:PHE:CD2	0.55	0.72
1:A:141:GLY:HA2	1:A:144:LYS:HE3	0.55	1.76
1:A:130:THR:HG23	1:A:130:THR:N	0.54	2.12
1:A:144:LYS:CG	1:A:144:LYS:HE3	0.54	2.14
1:A:137:PHE:CG	1:A:137:PHE:CD1	0.53	0.68
1:A:136:GLN:HG3	1:A:136:GLN:NE2	0.48	2.03

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:144:LYS:HB3	1:A:144:LYS:HD3	0.47	1.72
1:A:144:LYS:HB2	1:A:144:LYS:HD2	0.45	1.73
1:A:137:PHE:CG	1:A:137:PHE:HD2	0.44	1.20
1:A:137:PHE:HE1	1:A:137:PHE:CZ	0.44	1.19
1:A:143:SER:CB	1:A:143:SER:HG	0.43	1.13
1:A:137:PHE:CG	1:A:137:PHE:HD1	0.42	1.17
1:A:144:LYS:HE2	1:A:144:LYS:HG2	0.42	1.78
1:A:137:PHE:HE2	1:A:137:PHE:CZ	0.41	1.17

## 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	16/18 (89%)	12 (75%)	4 (25%)	0 (0%)	100	100
All	All	16/18 (89%)	12 (75%)	4 (25%)	0 (0%)	100	100

There are no Ramachandran outliers.

### 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	16/16 (100%)	14 (88%)	2 (12%)	10	52
All	All	16/16 (100%)	14 (88%)	2 (12%)	10	52

All 2 residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	131	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	132	ASP

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 6.7 Other polymers [i](#)

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

## 7 Chemical shift validation

No chemical shift data were provided