



Full wwPDB NMR Structure Validation Report ⓘ

Feb 1, 2021 – 10:37 AM EST

PDB ID : 6VRJ
Title : Solution structure of Pseudomonas aeruginosa IF3 C-terminal domain
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Deposited on : 2020-02-07

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/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:

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	:	2.16
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

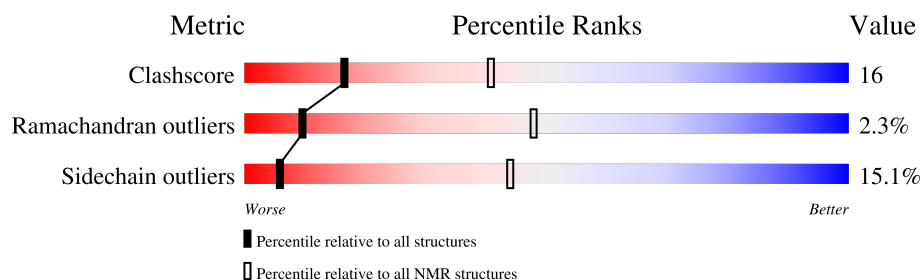
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 76%.

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 ≥ 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	97	<div> <div></div> <div>45%</div> <div>36%</div> <div>5%</div> <div>13%</div> </div>

2 Ensemble composition and analysis

This entry contains 10 models. Model 5 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:96-A:179 (84)	0.56	5

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 and 5 single-model clusters were found.

Cluster number	Models
1	4, 5, 8
2	6, 9
Single-model clusters	1; 2; 3; 7; 10

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1626 atoms, of which 836 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Translation initiation factor IF-3.

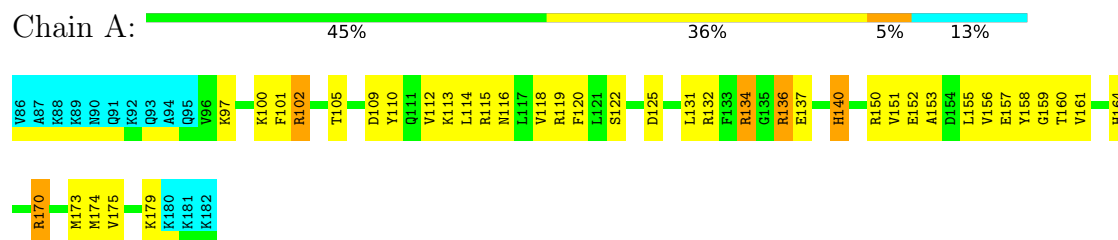
Mol	Chain	Residues	Atoms						Trace
1	A	97	Total	C	H	N	O	S	0
			1626	497	836	148	141	4	

4 Residue-property plots

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: Translation initiation factor IF-3

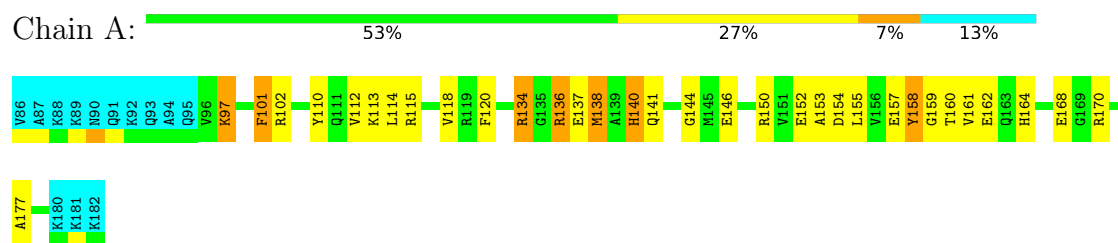


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

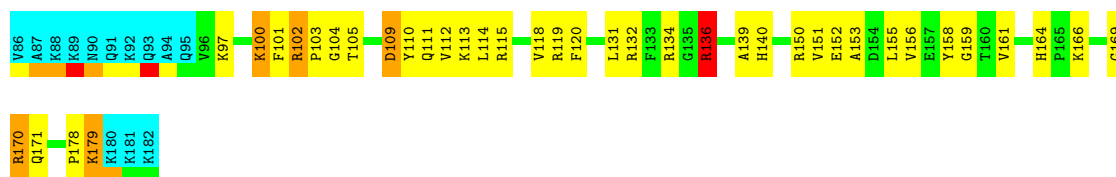
- Molecule 1: Translation initiation factor IF-3



4.2.2 Score per residue for model 2

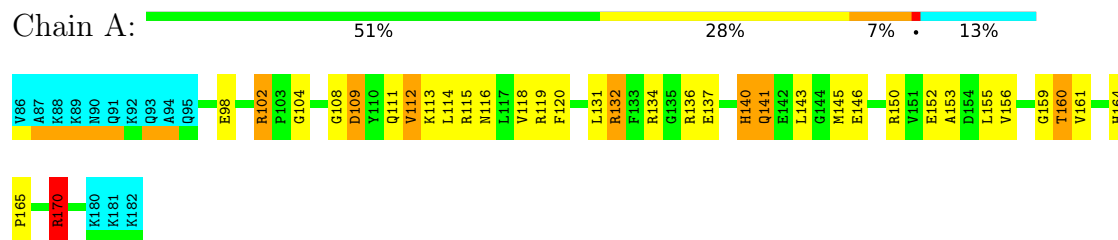
- Molecule 1: Translation initiation factor IF-3





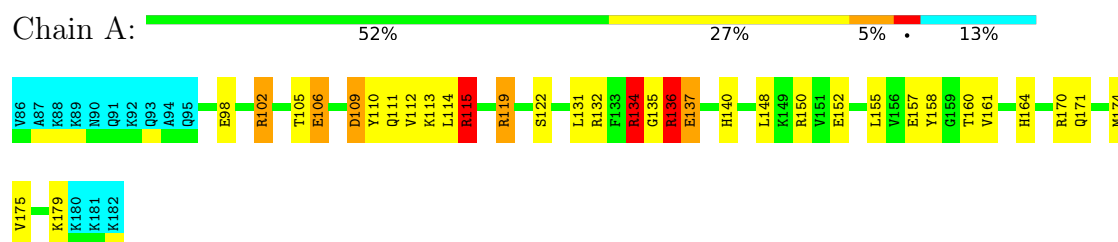
4.2.3 Score per residue for model 3

- Molecule 1: Translation initiation factor IF-3



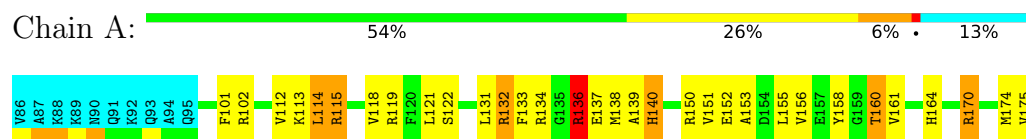
4.2.4 Score per residue for model 4

- Molecule 1: Translation initiation factor IF-3



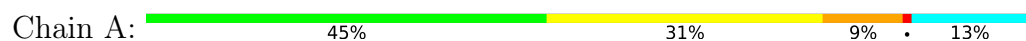
4.2.5 Score per residue for model 5 (medoid)

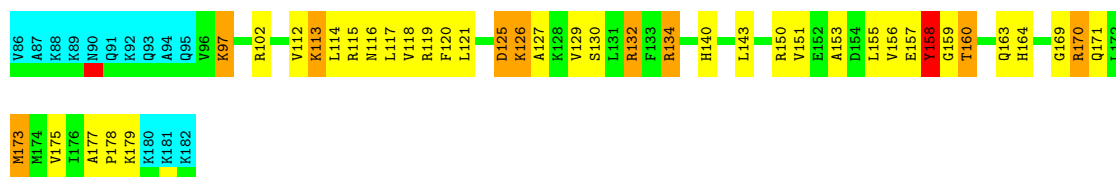
- Molecule 1: Translation initiation factor IF-3



4.2.6 Score per residue for model 6

- Molecule 1: Translation initiation factor IF-3

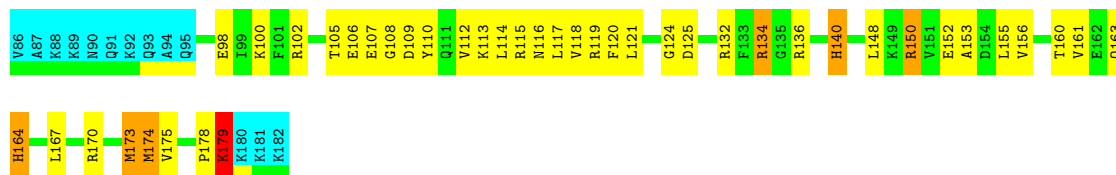




4.2.7 Score per residue for model 7

- Molecule 1: Translation initiation factor IF-3

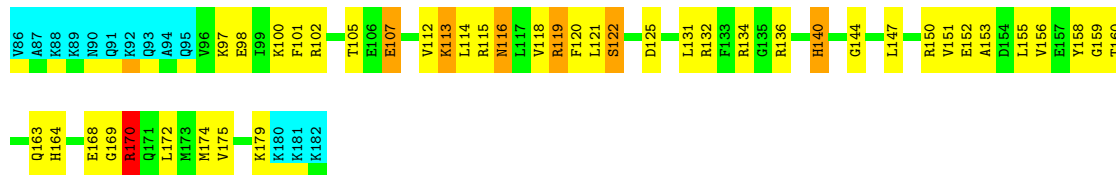
Chain A: 43% 36% 6% 13%



4.2.8 Score per residue for model 8

- Molecule 1: Translation initiation factor IF-3

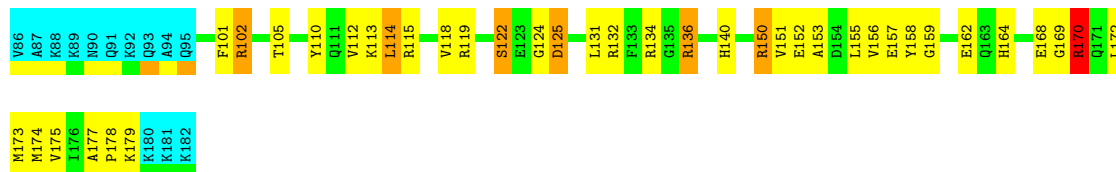
Chain A: 42% 37% 6% 13%



4.2.9 Score per residue for model 9

- Molecule 1: Translation initiation factor IF-3

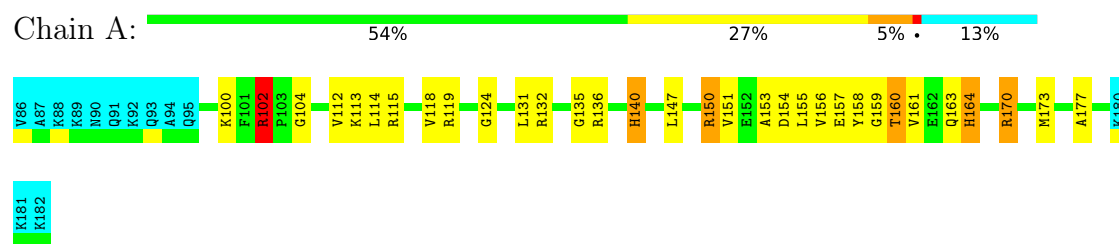
Chain A: 46% 33% 6% 13%



4.2.10 Score per residue for model 10

- Molecule 1: Translation initiation factor IF-3

Chain A:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 50 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
X-PLOR NIH	structure calculation	
X-PLOR NIH	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1025
Number of shifts mapped to atoms	1025
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	76%

6 Model quality i

6.1 Standard geometry i

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	1.09±0.00	2±0/693 (0.3± 0.0%)	1.17±0.00	0±0/925 (0.0± 0.0%)
All	All	1.09	20/6930 (0.3%)	1.17	0/9250 (0.0%)

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	0.0±0.0	7.3±0.8
All	All	0	73

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	164	HIS	CG-ND1	-6.17	1.25	1.38	10	10
1	A	140	HIS	CG-ND1	-6.16	1.25	1.38	3	10

There are no bond-angle outliers.

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	170	ARG	Sidechain	10
1	A	115	ARG	Sidechain	10
1	A	150	ARG	Sidechain	10
1	A	119	ARG	Sidechain	9
1	A	132	ARG	Sidechain	9
1	A	102	ARG	Sidechain	9

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	136	ARG	Sidechain	8
1	A	134	ARG	Sidechain	8

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	683	709	709	22±5
All	All	6830	7090	7090	219

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 16.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:153:ALA:O	1:A:156:VAL:HG22	0.79	1.77	9	6
1:A:110:TYR:CZ	1:A:114:LEU:HD11	0.76	2.15	7	2
1:A:147:LEU:O	1:A:151:VAL:HG23	0.74	1.81	10	1
1:A:152:GLU:O	1:A:156:VAL:HG13	0.74	1.82	8	2
1:A:114:LEU:O	1:A:118:VAL:HG23	0.71	1.85	1	8
1:A:136:ARG:N	1:A:136:ARG:NE	0.71	2.38	2	1
1:A:100:LYS:H	1:A:100:LYS:CD	0.71	1.98	2	1
1:A:116:ASN:HD22	1:A:116:ASN:N	0.67	1.87	8	1
1:A:173:MET:C	1:A:173:MET:SD	0.63	2.77	6	1
1:A:177:ALA:HB1	1:A:178:PRO:HD2	0.62	1.72	9	2
1:A:109:ASP:OD2	1:A:109:ASP:N	0.61	2.33	4	3
1:A:174:MET:SD	1:A:175:VAL:N	0.61	2.73	9	2
1:A:164:HIS:H	1:A:164:HIS:CD2	0.61	2.12	7	1
1:A:136:ARG:HE	1:A:136:ARG:H	0.60	1.37	2	1
1:A:112:VAL:HG23	1:A:113:LYS:N	0.60	2.11	9	9
1:A:121:LEU:CD1	1:A:155:LEU:HD22	0.59	2.26	8	3
1:A:110:TYR:CE1	1:A:114:LEU:HD11	0.59	2.32	7	1
1:A:136:ARG:H	1:A:136:ARG:NE	0.58	1.95	2	1
1:A:174:MET:CG	1:A:175:VAL:N	0.58	2.66	4	2
1:A:107:GLU:CD	1:A:107:GLU:H	0.58	2.02	8	1
1:A:160:THR:HG23	1:A:177:ALA:HB3	0.57	1.76	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:100:LYS:CD	1:A:100:LYS:N	0.56	2.68	2	1
1:A:97:LYS:CD	1:A:120:PHE:CZ	0.56	2.88	8	1
1:A:151:VAL:HG23	1:A:152:GLU:N	0.56	2.15	9	2
1:A:111:GLN:CG	1:A:115:ARG:HH11	0.56	2.14	4	1
1:A:110:TYR:CE1	1:A:114:LEU:HD13	0.55	2.37	2	1
1:A:101:PHE:CE2	1:A:105:THR:OG1	0.55	2.52	9	1
1:A:179:LYS:CD	1:A:179:LYS:C	0.55	2.76	7	1
1:A:134:ARG:CG	1:A:134:ARG:HH11	0.54	2.16	4	1
1:A:169:GLY:C	1:A:171:GLN:H	0.54	2.06	6	2
1:A:136:ARG:N	1:A:136:ARG:CD	0.54	2.71	2	1
1:A:121:LEU:HD11	1:A:155:LEU:HD22	0.54	1.80	8	1
1:A:102:ARG:O	1:A:104:GLY:N	0.54	2.41	2	3
1:A:153:ALA:C	1:A:155:LEU:N	0.54	2.61	9	7
1:A:153:ALA:O	1:A:155:LEU:N	0.54	2.41	9	3
1:A:155:LEU:O	1:A:159:GLY:N	0.53	2.41	9	7
1:A:137:GLU:CD	1:A:137:GLU:N	0.53	2.61	3	1
1:A:136:ARG:HB3	1:A:139:ALA:HB3	0.53	1.80	2	2
1:A:120:PHE:O	1:A:124:GLY:N	0.53	2.42	7	1
1:A:135:GLY:O	1:A:137:GLU:N	0.53	2.42	4	1
1:A:97:LYS:CB	1:A:120:PHE:CE2	0.53	2.92	2	1
1:A:112:VAL:CG2	1:A:113:LYS:N	0.52	2.72	3	8
1:A:161:VAL:O	1:A:161:VAL:HG13	0.52	2.05	5	2
1:A:169:GLY:O	1:A:171:GLN:N	0.52	2.43	6	1
1:A:116:ASN:N	1:A:116:ASN:ND2	0.52	2.57	8	1
1:A:137:GLU:O	1:A:141:GLN:N	0.51	2.41	3	2
1:A:155:LEU:O	1:A:158:TYR:N	0.51	2.42	2	7
1:A:102:ARG:C	1:A:104:GLY:H	0.51	2.09	2	3
1:A:151:VAL:HG23	1:A:152:GLU:H	0.51	1.64	9	1
1:A:173:MET:O	1:A:173:MET:SD	0.51	2.69	6	1
1:A:110:TYR:O	1:A:110:TYR:CD1	0.51	2.63	7	1
1:A:102:ARG:C	1:A:104:GLY:N	0.50	2.65	3	3
1:A:106:GLU:H	1:A:106:GLU:CD	0.50	2.10	4	1
1:A:100:LYS:O	1:A:113:LYS:NZ	0.50	2.42	8	1
1:A:168:GLU:O	1:A:170:ARG:N	0.50	2.44	8	2
1:A:107:GLU:CG	1:A:108:GLY:N	0.50	2.74	7	1
1:A:169:GLY:C	1:A:171:GLN:N	0.50	2.65	6	2
1:A:170:ARG:N	1:A:170:ARG:CD	0.50	2.74	3	1
1:A:171:GLN:N	1:A:171:GLN:OE1	0.49	2.45	4	1
1:A:107:GLU:C	1:A:107:GLU:CD	0.49	2.71	7	1
1:A:161:VAL:HG13	1:A:161:VAL:O	0.49	2.08	4	4
1:A:125:ASP:OD1	1:A:125:ASP:C	0.49	2.51	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:125:ASP:CG	1:A:126:LYS:H	0.49	2.10	6	1
1:A:120:PHE:N	1:A:120:PHE:CD1	0.48	2.79	1	1
1:A:125:ASP:OD2	1:A:125:ASP:N	0.48	2.43	9	1
1:A:100:LYS:H	1:A:100:LYS:HD2	0.48	1.68	2	1
1:A:179:LYS:CB	1:A:179:LYS:NZ	0.48	2.77	2	1
1:A:152:GLU:O	1:A:156:VAL:HG23	0.48	2.08	5	1
1:A:159:GLY:C	1:A:160:THR:OG1	0.48	2.52	6	1
1:A:140:HIS:O	1:A:144:GLY:N	0.48	2.43	8	2
1:A:117:LEU:HD21	1:A:129:VAL:HG22	0.48	1.85	6	1
1:A:107:GLU:CD	1:A:108:GLY:N	0.48	2.67	7	1
1:A:97:LYS:HD2	1:A:120:PHE:CZ	0.47	2.44	8	1
1:A:152:GLU:OE2	1:A:152:GLU:C	0.47	2.53	1	1
1:A:97:LYS:HZ3	1:A:97:LYS:CB	0.47	2.20	1	1
1:A:116:ASN:O	1:A:120:PHE:CD1	0.47	2.67	3	1
1:A:97:LYS:HD3	1:A:120:PHE:CZ	0.47	2.45	8	1
1:A:155:LEU:C	1:A:157:GLU:N	0.47	2.65	10	5
1:A:162:GLU:HB2	1:A:177:ALA:HB2	0.47	1.86	9	2
1:A:110:TYR:CE1	1:A:114:LEU:CD1	0.47	2.98	7	1
1:A:118:VAL:O	1:A:121:LEU:N	0.46	2.48	7	1
1:A:108:GLY:O	1:A:112:VAL:HG13	0.46	2.10	3	1
1:A:105:THR:OG1	1:A:106:GLU:N	0.46	2.48	7	1
1:A:157:GLU:O	1:A:158:TYR:CG	0.46	2.68	4	1
1:A:170:ARG:N	1:A:170:ARG:HD3	0.46	2.26	3	1
1:A:137:GLU:H	1:A:137:GLU:CD	0.45	2.14	3	1
1:A:155:LEU:O	1:A:157:GLU:N	0.45	2.50	10	1
1:A:161:VAL:O	1:A:161:VAL:CG1	0.45	2.64	1	1
1:A:100:LYS:H	1:A:100:LYS:HD3	0.45	1.71	2	1
1:A:116:ASN:O	1:A:120:PHE:CD2	0.45	2.69	7	2
1:A:98:GLU:CG	1:A:98:GLU:O	0.44	2.65	8	1
1:A:97:LYS:HB3	1:A:120:PHE:CE2	0.44	2.47	2	1
1:A:140:HIS:CD2	1:A:140:HIS:N	0.44	2.85	10	3
1:A:153:ALA:C	1:A:155:LEU:H	0.44	2.14	9	1
1:A:114:LEU:O	1:A:118:VAL:CG2	0.44	2.66	2	2
1:A:160:THR:OG1	1:A:161:VAL:N	0.44	2.51	3	3
1:A:174:MET:HG2	1:A:175:VAL:N	0.44	2.28	4	2
1:A:101:PHE:CD2	1:A:102:ARG:N	0.44	2.85	5	1
1:A:110:TYR:CE2	1:A:114:LEU:HD12	0.44	2.48	9	1
1:A:152:GLU:O	1:A:156:VAL:N	0.44	2.49	2	1
1:A:121:LEU:CD1	1:A:155:LEU:CD2	0.43	2.96	8	1
1:A:97:LYS:HB2	1:A:120:PHE:CE2	0.43	2.48	2	1
1:A:173:MET:SD	1:A:175:VAL:HG23	0.43	2.54	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:122:SER:C	1:A:124:GLY:N	0.42	2.71	9	1
1:A:97:LYS:NZ	1:A:97:LYS:CB	0.42	2.81	1	1
1:A:133:PHE:CE2	1:A:140:HIS:HB3	0.42	2.49	5	1
1:A:148:LEU:O	1:A:152:GLU:CB	0.42	2.67	7	2
1:A:97:LYS:HG2	1:A:120:PHE:CE1	0.42	2.49	6	1
1:A:161:VAL:CG1	1:A:161:VAL:O	0.42	2.68	5	1
1:A:174:MET:SD	1:A:175:VAL:O	0.42	2.77	9	1
1:A:101:PHE:CZ	1:A:113:LYS:HB3	0.42	2.50	1	1
1:A:110:TYR:CZ	1:A:114:LEU:CD1	0.42	3.02	1	1
1:A:97:LYS:CG	1:A:98:GLU:N	0.42	2.82	8	1
1:A:157:GLU:O	1:A:158:TYR:CD2	0.42	2.72	4	1
1:A:136:ARG:O	1:A:140:HIS:CG	0.42	2.73	10	1
1:A:119:ARG:O	1:A:122:SER:CB	0.42	2.68	8	1
1:A:110:TYR:OH	1:A:154:ASP:OD2	0.41	2.37	1	1
1:A:97:LYS:HZ3	1:A:97:LYS:HB2	0.41	1.73	1	1
1:A:105:THR:HG23	1:A:106:GLU:N	0.41	2.30	7	1
1:A:122:SER:O	1:A:124:GLY:N	0.41	2.53	9	1
1:A:168:GLU:C	1:A:168:GLU:CD	0.41	2.75	1	1
1:A:138:MET:N	1:A:138:MET:SD	0.41	2.94	1	1
1:A:148:LEU:O	1:A:152:GLU:N	0.41	2.44	7	1
1:A:173:MET:HG3	1:A:174:MET:N	0.41	2.30	7	1
1:A:179:LYS:HB2	1:A:179:LYS:NZ	0.40	2.31	2	1
1:A:163:GLN:HE21	1:A:175:VAL:HG21	0.40	1.76	7	1
1:A:118:VAL:O	1:A:119:ARG:C	0.40	2.60	8	1
1:A:137:GLU:O	1:A:141:GLN:CB	0.40	2.70	3	1
1:A:151:VAL:CG2	1:A:152:GLU:N	0.40	2.83	9	1
1:A:162:GLU:CG	1:A:162:GLU:O	0.40	2.70	9	1
1:A:126:LYS:HG2	1:A:127:ALA:N	0.40	2.31	6	1
1:A:113:LYS:NZ	1:A:117:LEU:CD1	0.40	2.84	7	1
1:A:100:LYS:N	1:A:100:LYS:HD2	0.40	2.29	2	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	84/97 (87%)	75±3 (89±3%)	7±2 (9±3%)	2±2 (2±2%)	9	48
All	All	840/970 (87%)	747 (89%)	74 (9%)	19 (2%)	9	48

All 12 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	179	LYS	5
1	A	169	GLY	2
1	A	105	THR	2
1	A	170	ARG	2
1	A	103	PRO	1
1	A	125	ASP	1
1	A	134	ARG	1
1	A	135	GLY	1
1	A	106	GLU	1
1	A	124	GLY	1
1	A	136	ARG	1
1	A	158	TYR	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	73/84 (87%)	62±2 (85±2%)	11±2 (15±2%)	6	44
All	All	730/840 (87%)	620 (85%)	110 (15%)	6	44

All 45 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	160	THR	8
1	A	131	LEU	7
1	A	170	ARG	6
1	A	134	ARG	5
1	A	136	ARG	5
1	A	173	MET	4

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Mol	Chain	Res	Type	Models (Total)
1	A	109	ASP	4
1	A	122	SER	4
1	A	101	PHE	3
1	A	114	LEU	3
1	A	98	GLU	3
1	A	132	ARG	3
1	A	158	TYR	3
1	A	102	ARG	3
1	A	100	LYS	3
1	A	150	ARG	3
1	A	163	GLN	3
1	A	151	VAL	3
1	A	115	ARG	2
1	A	97	LYS	2
1	A	143	LEU	2
1	A	179	LYS	2
1	A	111	GLN	2
1	A	138	MET	2
1	A	172	LEU	2
1	A	146	GLU	2
1	A	137	GLU	2
1	A	113	LYS	2
1	A	165	PRO	1
1	A	125	ASP	1
1	A	112	VAL	1
1	A	119	ARG	1
1	A	167	LEU	1
1	A	164	HIS	1
1	A	105	THR	1
1	A	116	ASN	1
1	A	107	GLU	1
1	A	174	MET	1
1	A	147	LEU	1
1	A	154	ASP	1
1	A	141	GLN	1
1	A	130	SER	1
1	A	126	LYS	1
1	A	145	MET	1
1	A	166	LYS	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](#)

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 i

The completeness of assignment taking into account all chemical shift lists is 76% for the well-defined parts and 74% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *paif3cshifts.nmrstar3.1*

7.1.1 Bookkeeping i

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1025
Number of shifts mapped to atoms	1025
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing i

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	95	-0.14 ± 0.08	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	89	0.22 ± 0.06	None needed (< 0.5 ppm)
$^{13}\text{C}'$	89	-0.17 ± 0.13	None needed (< 0.5 ppm)
^{15}N	90	-0.70 ± 0.45	None needed (imprecise)

7.1.3 Completeness of resonance assignments i

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 76%, i.e. 850 atoms were assigned a chemical shift out of a possible 1113. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	400/414 (97%)	160/165 (97%)	161/168 (96%)	79/81 (98%)
Sidechain	428/642 (67%)	264/378 (70%)	164/227 (72%)	0/37 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	22/57 (39%)	22/31 (71%)	0/24 (0%)	0/2 (0%)
Overall	850/1113 (76%)	446/574 (78%)	325/419 (78%)	79/120 (66%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 74%, i.e. 958 atoms were assigned a chemical shift out of a possible 1303. 0 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	455/479 (95%)	181/191 (95%)	184/194 (95%)	90/94 (96%)
Sidechain	481/767 (63%)	291/453 (64%)	190/267 (71%)	0/47 (0%)
Aromatic	22/57 (39%)	22/31 (71%)	0/24 (0%)	0/2 (0%)
Overall	958/1303 (74%)	494/675 (73%)	374/485 (77%)	90/143 (63%)

7.1.4 Statistically unusual chemical shifts [i](#)

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	130	SER	C	184.42	183.48 – 165.88	5.5

7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:

