Full wwPDB NMR Structure Validation Report (i)

Jun 22, 2024 – 03:49 PM EDT

PDB ID	:	5LVY
BMRB ID	:	34042
Title	:	Structural studies of the Aggregative Adherence Fimbriae of Enteroaggregative Escherichia coli
Authors	:	Liu, B.; Matthews, S.
Deposited on	:	2016-09-14

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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

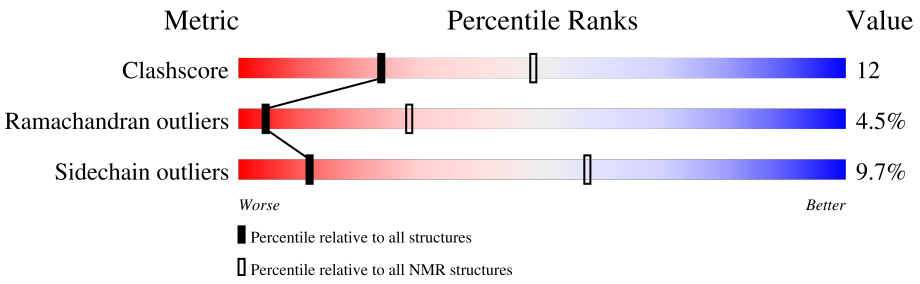
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 88%.

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	154	60% 25% • 11%

2 Ensemble composition and analysis (i)

This entry contains 10 models. Model 6 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

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:11-A:79, A:89-A:144, A:151-A:162 (137)	0.50	6

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 1 clusters. No single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2311 atoms, of which 1151 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Adhesin protein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	154	2311	732	1151	192	232	4	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	113	VAL	ALA	conflict	UNP C9K5V2
A	132	ASP	-	expression tag	UNP C9K5V2
A	133	ASN	-	expression tag	UNP C9K5V2
A	134	LYS	-	expression tag	UNP C9K5V2
A	135	GLN	-	expression tag	UNP C9K5V2
A	136	ALA	-	expression tag	UNP C9K5V2
A	137	ASN	-	expression tag	UNP C9K5V2
A	138	PRO	-	expression tag	UNP C9K5V2
A	139	THR	-	expression tag	UNP C9K5V2
A	140	PRO	-	expression tag	UNP C9K5V2
A	141	SER	-	expression tag	UNP C9K5V2
A	142	SER	-	expression tag	UNP C9K5V2
A	143	LEU	-	expression tag	UNP C9K5V2
A	144	THR	-	expression tag	UNP C9K5V2
A	145	SER	-	expression tag	UNP C9K5V2
A	146	LYS	-	expression tag	UNP C9K5V2
A	147	ALA	-	expression tag	UNP C9K5V2
A	148	ALA	-	expression tag	UNP C9K5V2
A	149	GLY	-	expression tag	UNP C9K5V2
A	150	LYS	-	expression tag	UNP C9K5V2
A	151	ASN	-	expression tag	UNP C9K5V2
A	152	ILE	-	expression tag	UNP C9K5V2
A	153	VAL	-	expression tag	UNP C9K5V2
A	154	SER	-	expression tag	UNP C9K5V2
A	155	SER	-	expression tag	UNP C9K5V2
A	156	THR	-	expression tag	UNP C9K5V2
A	157	GLY	-	expression tag	UNP C9K5V2
A	158	THR	-	expression tag	UNP C9K5V2
A	159	ILE	-	expression tag	UNP C9K5V2
A	160	THR	-	expression tag	UNP C9K5V2
A	161	ILE	-	expression tag	UNP C9K5V2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	162	SER	-	expression tag	UNP C9K5V2

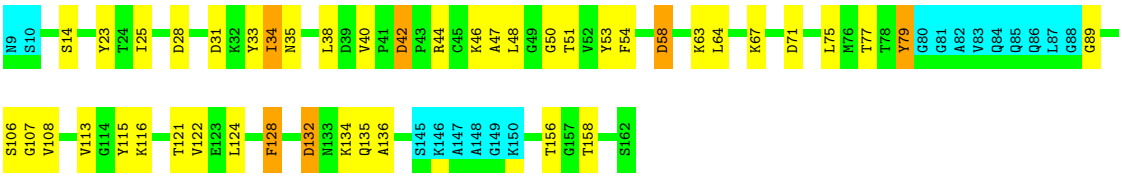
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: Adhesin protein

Chain A: 60% 25% • 11%



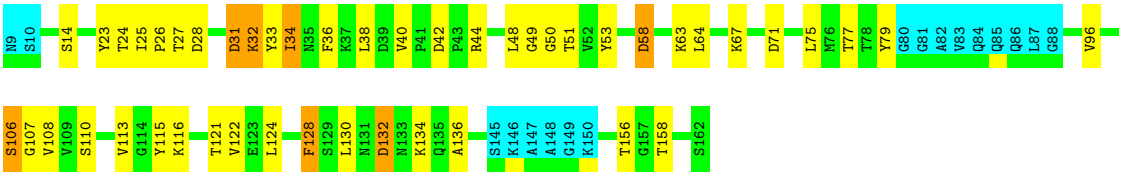
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Adhesin protein

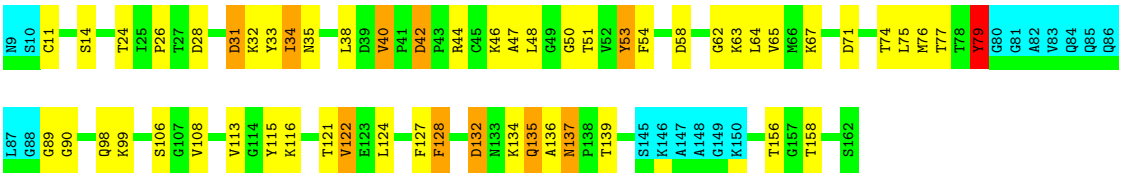
Chain A: 58% 26% 5% 11%



4.2.2 Score per residue for model 2

• Molecule 1: Adhesin protein

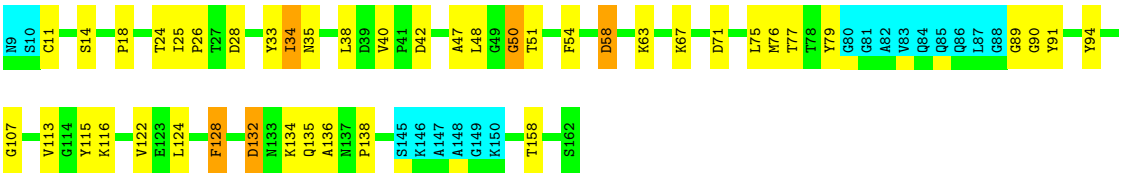
Chain A: 53% 29% 6% • 11%



4.2.3 Score per residue for model 3

- Molecule 1: Adhesin protein

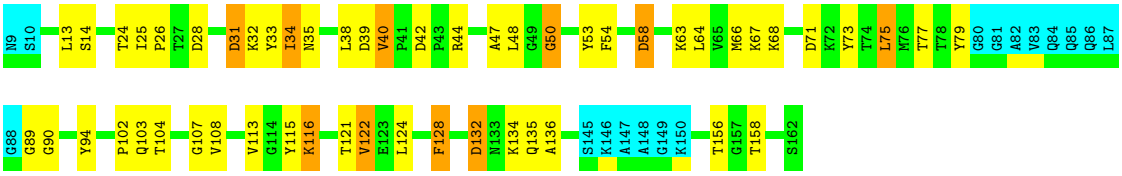
Chain A: 61% 25% • 11%



4.2.4 Score per residue for model 4

- Molecule 1: Adhesin protein

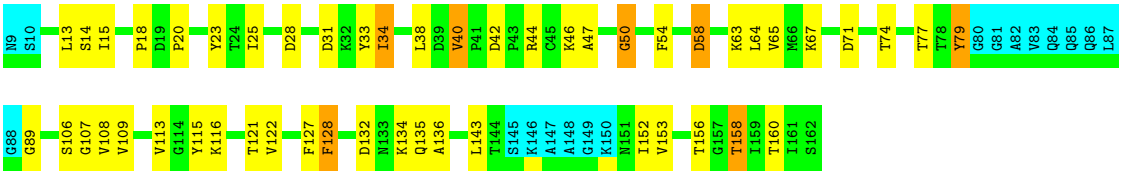
Chain A: 55% 28% 6% 11%



4.2.5 Score per residue for model 5

- Molecule 1: Adhesin protein

Chain A: 56% 28% 5% 11%



4.2.6 Score per residue for model 6 (medoid)

- Molecule 1: Adhesin protein

Chain A: 57% 27% 5% 11%

N9 S10 C11 S14 P18 V21 T22 Y23 T24 I25 D28 D31 K32 Y33 I34 N35 L38 D39 V40 P41 D42 P43 R44 A47 G50 Y53 F54 W55 G56 A57 D58 K63 L64 K67 D71 L75 M76 T77 T78 Y79 G80 G81 A82 V83 Q84 Q85 Q86

L87 G88 G89 G90 G107 V108 V109 S110 V113 G114 Y115 K116 T121 L124 F127 F128 S129 L130 N131 D132 N133 K134 Q135 A136 S142 L143 T144 S145 K146 A147 A148 G149 K150 T156 G157 T158 S162

4.2.7 Score per residue for model 7

- Molecule 1: Adhesin protein

Chain A: 58% 26% 5% 11%

N9 S10 S14 P20 Y23 T24 I25 D28 K32 Y33 I34 N35 L38 D42 P43 R44 C45 K46 A47 L48 G49 G50 T51 V52 Y53 D58 K63 L64 V65 M66 K67 D71 L75 M76 T77 T78 Y79 G80 G81 A82 V83 Q84 Q85 Q86 L87 G88 H95

S106 G107 V108 V109 V113 G114 Y115 K116 T121 V122 E123 L124 F128 D132 N133 K134 Q135 A136 N137 P138 S145 K146 A147 A148 G149 K150 T156 G157 T158 I161 S162

4.2.8 Score per residue for model 8

- Molecule 1: Adhesin protein

Chain A: 64% 22% • 11%

N9 S10 L13 S14 P18 I25 P26 T27 D28 Y33 I34 N35 L38 D39 V40 P41 D42 P43 R44 C45 K46 A47 L48 G49 G50 Y53 D58 K63 L64 K67 D71 L75 M76 T77 T78 Y79 G80 G81 A82 V83 Q84 Q85 Q86 L87 G88 S106 G107

V113 G114 Y115 K116 L124 F128 N131 D132 N133 K134 Q135 S145 K146 A147 A148 G149 K150 T158 S162

4.2.9 Score per residue for model 9

- Molecule 1: Adhesin protein

Chain A: 61% 21% 6% • 11%

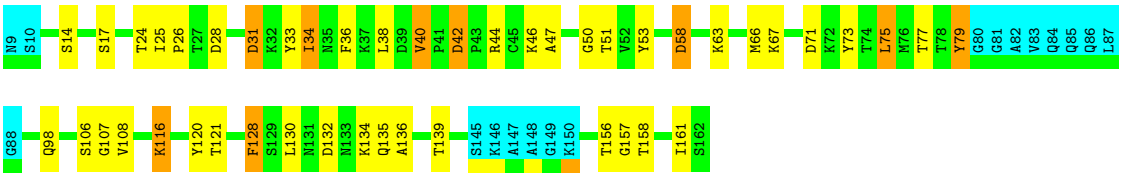
N9 S10 S14 Y23 T24 I25 D31 K32 Y33 I34 N35 L38 D39 V40 P41 D42 P43 R44 C45 K46 A47 L48 G49 G50 F54 D58 K63 L64 V65 M66 K67 D71 L75 M76 T77 T78 Y79 G80 G81 A82 V83 Q84 Q85 Q86 L87 G88 G89 Q98 S106

G107 V108 V113 G114 Y115 K116 T121 V122 F128 N131 D132 N133 K134 S145 K146 A147 A148 G149 K150 T156 G157 T158 S162

4.2.10 Score per residue for model 10

- Molecule 1: Adhesin protein

Chain A: 59% 24% 6% 11%



5 Refinement protocol and experimental data overview (i)

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

Of the 10 calculated structures, 10 were deposited, based on the following criterion: *all calculated structures submitted*.

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

Software name	Classification	Version
ARIA	structure calculation	

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	1661
Number of shifts mapped to atoms	1661
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	88%

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	0.52±0.08	3±1/1075 (0.2± 0.1%)	0.49±0.02	0±0/1462 (0.0± 0.0%)
All	All	0.53	26/10750 (0.2%)	0.49	0/14620 (0.0%)

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	79	TYR	CE1-CZ	-9.08	1.26	1.38	9	5
1	A	23	TYR	CE2-CZ	-8.48	1.27	1.38	9	1
1	A	79	TYR	CE2-CZ	8.47	1.49	1.38	9	5
1	A	53	TYR	CE2-CZ	-8.03	1.28	1.38	6	7
1	A	23	TYR	CE1-CZ	7.92	1.48	1.38	9	1
1	A	53	TYR	CE1-CZ	7.46	1.48	1.38	1	7

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	1049	1036	1035	26±4
All	All	10490	10360	10350	255

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 12.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:128:PHE:CZ	1:A:130:LEU:HG	0.71	2.19	10	2
1:A:14:SER:O	1:A:38:LEU:HA	0.70	1.87	1	10
1:A:50:GLY:HA2	1:A:128:PHE:CD2	0.62	2.30	10	9
1:A:67:LYS:HA	1:A:71:ASP:O	0.61	1.95	10	10
1:A:58:ASP:HB3	1:A:63:LYS:H	0.61	1.56	4	10
1:A:33:TYR:HA	1:A:107:GLY:O	0.60	1.96	3	9
1:A:47:ALA:O	1:A:135:GLN:HA	0.60	1.97	7	7
1:A:58:ASP:OD1	1:A:63:LYS:HG2	0.59	1.97	10	7
1:A:63:LYS:CB	1:A:77:THR:HB	0.58	2.29	10	9
1:A:42:ASP:O	1:A:46:LYS:HG3	0.57	1.98	5	3
1:A:24:THR:O	1:A:26:PRO:HD3	0.57	1.98	4	5
1:A:113:VAL:HG11	1:A:115:TYR:CE1	0.57	2.34	7	9
1:A:58:ASP:HB3	1:A:63:LYS:N	0.57	2.15	5	7
1:A:54:PHE:CZ	1:A:89:GLY:HA2	0.56	2.35	4	4
1:A:48:LEU:HG	1:A:132:ASP:H	0.54	1.63	9	7
1:A:20:PRO:CB	1:A:158:THR:HB	0.53	2.33	7	1
1:A:76:MET:O	1:A:108:VAL:HB	0.53	2.03	9	1
1:A:33:TYR:CE2	1:A:108:VAL:HG22	0.53	2.38	6	6
1:A:34:ILE:HD13	1:A:35:ASN:N	0.53	2.19	6	7
1:A:56:GLY:HA3	1:A:63:LYS:O	0.52	2.05	6	1
1:A:34:ILE:O	1:A:106:SER:HA	0.52	2.05	5	7
1:A:121:THR:CG2	1:A:156:THR:HB	0.52	2.34	4	8
1:A:25:ILE:CG2	1:A:28:ASP:HA	0.51	2.36	10	7
1:A:11:CYS:SG	1:A:42:ASP:HB2	0.51	2.46	3	2
1:A:42:ASP:OD1	1:A:44:ARG:HB3	0.51	2.05	8	2
1:A:127:PHE:CD1	1:A:152:ILE:HG13	0.50	2.41	5	1
1:A:46:LYS:HD3	1:A:98:GLN:O	0.49	2.08	10	2
1:A:64:LEU:HD21	1:A:124:LEU:HB2	0.49	1.83	6	6
1:A:46:LYS:CB	1:A:98:GLN:HA	0.48	2.38	2	1
1:A:33:TYR:CE1	1:A:108:VAL:HG22	0.48	2.43	4	1
1:A:17:SER:OG	1:A:157:GLY:HA2	0.48	2.08	10	1
1:A:63:LYS:HB3	1:A:77:THR:HB	0.48	1.84	4	8
1:A:54:PHE:CE1	1:A:89:GLY:HA2	0.48	2.43	2	5
1:A:51:THR:O	1:A:128:PHE:HA	0.48	2.09	3	5
1:A:128:PHE:CZ	1:A:130:LEU:HD23	0.48	2.43	1	1
1:A:45:CYS:O	1:A:48:LEU:HD23	0.47	2.09	8	1
1:A:65:VAL:HG22	1:A:74:THR:HA	0.47	1.84	5	2
1:A:58:ASP:HB3	1:A:64:LEU:H	0.47	1.70	4	2
1:A:128:PHE:CE2	1:A:130:LEU:HG	0.47	2.45	10	2
1:A:20:PRO:HB2	1:A:160:THR:OG1	0.47	2.10	5	1
1:A:63:LYS:HB2	1:A:77:THR:HB	0.46	1.87	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:46:LYS:HB3	1:A:46:LYS:NZ	0.46	2.26	2	1
1:A:21:VAL:HG21	1:A:33:TYR:O	0.46	2.11	6	1
1:A:64:LEU:HB2	1:A:77:THR:OG1	0.45	2.12	5	2
1:A:23:TYR:CE2	1:A:109:VAL:HG11	0.45	2.46	5	2
1:A:48:LEU:HG	1:A:132:ASP:N	0.45	2.26	9	1
1:A:40:VAL:HG21	1:A:128:PHE:CE1	0.45	2.46	10	2
1:A:33:TYR:CD1	1:A:108:VAL:HG22	0.45	2.46	4	1
1:A:23:TYR:CZ	1:A:25:ILE:HG12	0.45	2.47	6	3
1:A:23:TYR:CD1	1:A:32:LYS:HD2	0.45	2.47	1	1
1:A:11:CYS:SG	1:A:42:ASP:HB3	0.45	2.51	6	1
1:A:51:THR:HA	1:A:94:TYR:O	0.44	2.13	3	1
1:A:54:PHE:CD1	1:A:124:LEU:HD11	0.44	2.47	3	1
1:A:58:ASP:CB	1:A:63:LYS:H	0.44	2.24	4	2
1:A:131:ASN:OD1	1:A:134:LYS:HD2	0.43	2.13	9	1
1:A:48:LEU:HD11	1:A:133:ASN:N	0.43	2.28	7	1
1:A:39:ASP:O	1:A:41:PRO:HD3	0.43	2.12	9	1
1:A:66:MET:HB2	1:A:120:TYR:CB	0.43	2.44	10	1
1:A:64:LEU:HD22	1:A:122:VAL:HB	0.43	1.91	4	1
1:A:48:LEU:HD13	1:A:135:GLN:H	0.43	1.73	3	1
1:A:79:TYR:HA	1:A:106:SER:OG	0.42	2.13	2	1
1:A:20:PRO:HA	1:A:158:THR:O	0.42	2.14	7	2
1:A:51:THR:HG23	1:A:138:PRO:HD2	0.42	1.91	7	2
1:A:66:MET:HG2	1:A:75:LEU:HD21	0.42	1.90	4	2
1:A:32:LYS:C	1:A:33:TYR:HD2	0.42	2.18	7	1
1:A:33:TYR:HB3	1:A:106:SER:HB3	0.42	1.91	8	1
1:A:34:ILE:HD12	1:A:36:PHE:CE1	0.42	2.49	1	2
1:A:73:TYR:OH	1:A:116:LYS:HD2	0.42	2.15	10	2
1:A:67:LYS:HG2	1:A:121:THR:O	0.42	2.14	5	1
1:A:25:ILE:HG23	1:A:28:ASP:HA	0.42	1.92	6	1
1:A:131:ASN:OD1	1:A:134:LYS:HB2	0.42	2.15	8	1
1:A:40:VAL:O	1:A:46:LYS:HE2	0.41	2.15	2	1
1:A:32:LYS:C	1:A:33:TYR:HD1	0.41	2.19	4	1
1:A:15:ILE:HD11	1:A:153:VAL:HG23	0.41	1.93	5	1
1:A:20:PRO:HB3	1:A:158:THR:HB	0.41	1.91	7	1
1:A:27:THR:O	1:A:28:ASP:HB2	0.41	2.16	1	2
1:A:33:TYR:CD1	1:A:33:TYR:N	0.41	2.86	4	1
1:A:65:VAL:O	1:A:122:VAL:HA	0.41	2.16	2	2
1:A:33:TYR:N	1:A:33:TYR:CD2	0.41	2.89	10	1
1:A:53:TYR:HB2	1:A:127:PHE:CE1	0.41	2.50	2	2
1:A:13:LEU:HD23	1:A:40:VAL:N	0.41	2.31	4	3
1:A:66:MET:SD	1:A:161:ILE:HD11	0.41	2.56	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:49:GLY:HA2	1:A:96:VAL:O	0.40	2.16	1	1
1:A:137:ASN:HD22	1:A:137:ASN:N	0.40	2.14	2	1
1:A:46:LYS:HB2	1:A:98:GLN:HA	0.40	1.93	2	1
1:A:68:LYS:HG3	1:A:68:LYS:O	0.40	2.16	4	1
1:A:13:LEU:HD23	1:A:39:ASP:C	0.40	2.36	4	1
1:A:116:LYS:H	1:A:116:LYS:HD2	0.40	1.77	9	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	136/154 (88%)	112±2 (82±2%)	18±2 (13±1%)	6±1 (4±1%)	4 28
All	All	1360/1540 (88%)	1118 (82%)	181 (13%)	61 (4%)	4 28

All 15 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	132	ASP	9
1	A	134	LYS	9
1	A	42	ASP	8
1	A	136	ALA	8
1	A	31	ASP	5
1	A	50	GLY	5
1	A	90	GLY	4
1	A	18	PRO	4
1	A	110	SER	2
1	A	28	ASP	2
1	A	62	GLY	1
1	A	89	GLY	1
1	A	133	ASN	1
1	A	135	GLN	1
1	A	139	THR	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	120/130 (92%)	108±2 (90±2%)	12±2 (10±2%)	12	57
All	All	1200/1300 (92%)	1084 (90%)	116 (10%)	12	57

All 27 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	34	ILE	10
1	A	79	TYR	10
1	A	116	LYS	10
1	A	128	PHE	10
1	A	158	THR	10
1	A	58	ASP	9
1	A	75	LEU	9
1	A	40	VAL	8
1	A	44	ARG	7
1	A	122	VAL	7
1	A	31	ASP	6
1	A	32	LYS	2
1	A	76	MET	2
1	A	143	LEU	2
1	A	46	LYS	2
1	A	106	SER	1
1	A	99	LYS	1
1	A	135	GLN	1
1	A	137	ASN	1
1	A	139	THR	1
1	A	91	TYR	1
1	A	102	PRO	1
1	A	103	GLN	1
1	A	132	ASP	1
1	A	51	THR	1
1	A	95	HIS	1
1	A	42	ASP	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 88% for the well-defined parts and 85% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *agg3.str*

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	1661
Number of shifts mapped to atoms	1661
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	134

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	144	0.11 ± 0.09	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	127	-0.13 ± 0.20	None needed (< 0.5 ppm)
$^{13}C'$	139	0.30 ± 0.12	None needed (< 0.5 ppm)
^{15}N	129	-0.52 ± 0.42	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 88%, i.e. 1553 atoms were assigned a chemical shift out of a possible 1768. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	642/679 (95%)	264/278 (95%)	259/274 (95%)	119/127 (94%)
Sidechain	799/939 (85%)	540/612 (88%)	259/298 (87%)	0/29 (0%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	112/150 (75%)	56/70 (80%)	55/77 (71%)	1/3 (33%)
Overall	1553/1768 (88%)	860/960 (90%)	573/649 (88%)	120/159 (75%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 85%, i.e. 1660 atoms were assigned a chemical shift out of a possible 1961. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	700/768 (91%)	288/316 (91%)	283/308 (92%)	129/144 (90%)
Sidechain	848/1043 (81%)	572/679 (84%)	276/329 (84%)	0/35 (0%)
Aromatic	112/150 (75%)	56/70 (80%)	55/77 (71%)	1/3 (33%)
Overall	1660/1961 (85%)	916/1065 (86%)	614/714 (86%)	130/182 (71%)

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.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	128	PHE	CE2	89.97	124.80 – 136.72	-34.2
1	A	127	PHE	CE2	90.47	124.80 – 136.72	-33.8
1	A	53	TYR	CE2	75.75	111.68 – 124.17	-33.8
1	A	36	PHE	CE2	90.58	124.80 – 136.72	-33.7
1	A	128	PHE	CD2	91.39	125.53 – 137.61	-33.3
1	A	127	PHE	CD2	91.57	125.53 – 137.61	-33.1
1	A	54	PHE	CD2	91.66	125.53 – 137.61	-33.0
1	A	36	PHE	CD2	91.83	125.53 – 137.61	-32.9
1	A	93	TYR	CE2	76.92	111.68 – 124.17	-32.8
1	A	120	TYR	CE2	76.93	111.68 – 124.17	-32.8
1	A	33	TYR	CE2	77.38	111.68 – 124.17	-32.5
1	A	79	TYR	CE2	77.47	111.68 – 124.17	-32.4
1	A	23	TYR	CE2	77.56	111.68 – 124.17	-32.3
1	A	128	PHE	CD1	91.39	125.33 – 137.83	-32.1
1	A	15	ILE	CG2	59.91	10.93 – 24.12	32.1
1	A	105	ILE	CG2	59.80	10.93 – 24.12	32.1
1	A	73	TYR	CE2	77.92	111.68 – 124.17	-32.0
1	A	127	PHE	CD1	91.57	125.33 – 137.83	-32.0
1	A	54	PHE	CD1	91.66	125.33 – 137.83	-31.9
1	A	152	ILE	CG2	59.58	10.93 – 24.12	31.9
1	A	115	TYR	CE2	78.19	111.68 – 124.17	-31.8
1	A	36	PHE	CD1	91.83	125.33 – 137.83	-31.8

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List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	53	TYR	CE1	75.75	111.24 – 124.66	-31.4
1	A	128	PHE	CE1	89.97	124.17 – 137.29	-31.1
1	A	159	ILE	CG2	58.17	10.93 – 24.12	30.8
1	A	127	PHE	CE1	90.47	124.17 – 137.29	-30.7
1	A	161	ILE	CG2	57.92	10.93 – 24.12	30.6
1	A	36	PHE	CE1	90.58	124.17 – 137.29	-30.6
1	A	93	TYR	CE1	76.92	111.24 – 124.66	-30.6
1	A	120	TYR	CE1	76.93	111.24 – 124.66	-30.6
1	A	25	ILE	CG2	57.84	10.93 – 24.12	30.6
1	A	23	TYR	CD1	90.78	125.84 – 139.60	-30.5
1	A	33	TYR	CE1	77.38	111.24 – 124.66	-30.2
1	A	79	TYR	CE1	77.47	111.24 – 124.66	-30.2
1	A	23	TYR	CE1	77.56	111.24 – 124.66	-30.1
1	A	73	TYR	CE1	77.92	111.24 – 124.66	-29.8
1	A	115	TYR	CD1	91.67	125.84 – 139.60	-29.8
1	A	115	TYR	CE1	78.19	111.24 – 124.66	-29.6
1	A	34	ILE	CG2	56.34	10.93 – 24.12	29.4
1	A	93	TYR	CD1	92.29	125.84 – 139.60	-29.4
1	A	33	TYR	CD1	92.47	125.84 – 139.60	-29.2
1	A	94	TYR	CD1	92.97	125.84 – 139.60	-28.9
1	A	79	TYR	CD1	93.01	125.84 – 139.60	-28.9
1	A	153	VAL	CG1	60.57	14.71 – 28.29	28.8
1	A	91	TYR	CD1	93.58	125.84 – 139.60	-28.4
1	A	73	TYR	CD1	93.64	125.84 – 139.60	-28.4
1	A	53	TYR	CD1	93.72	125.84 – 139.60	-28.3
1	A	120	TYR	CD1	93.88	125.84 – 139.60	-28.2
1	A	23	TYR	CD2	90.78	125.28 – 140.14	-28.2
1	A	55	TRP	CH2	80.97	116.19 – 131.43	-28.1
1	A	55	TRP	CZ2	74.59	107.20 – 121.33	-28.1
1	A	138	PRO	CA	21.88	55.85 – 70.84	-27.7
1	A	141	SER	CB	22.21	56.28 – 71.32	-27.7
1	A	145	SER	CB	22.21	56.28 – 71.32	-27.7
1	A	115	TYR	CD2	91.67	125.28 – 140.14	-27.6
1	A	16	SER	CB	22.39	56.28 – 71.32	-27.5
1	A	102	PRO	CA	22.11	55.85 – 70.84	-27.5
1	A	17	SER	CB	22.47	56.28 – 71.32	-27.5
1	A	20	PRO	CA	22.29	55.85 – 70.84	-27.4
1	A	10	SER	CB	22.68	56.28 – 71.32	-27.4
1	A	142	SER	CB	22.73	56.28 – 71.32	-27.3
1	A	93	TYR	CD2	92.29	125.28 – 140.14	-27.2
1	A	117	PRO	CA	22.64	55.85 – 70.84	-27.2
1	A	33	TYR	CD2	92.47	125.28 – 140.14	-27.1

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List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	127	PHE	CZ	89.23	121.82 – 136.66	-27.0
1	A	94	TYR	CD2	92.97	125.28 – 140.14	-26.7
1	A	79	TYR	CD2	93.01	125.28 – 140.14	-26.7
1	A	110	SER	CB	23.76	56.28 – 71.32	-26.6
1	A	129	SER	CB	23.84	56.28 – 71.32	-26.6
1	A	140	PRO	CA	23.65	55.85 – 70.84	-26.5
1	A	14	SER	CB	24.00	56.28 – 71.32	-26.5
1	A	12	SER	CB	24.18	56.28 – 71.32	-26.4
1	A	91	TYR	CD2	93.58	125.28 – 140.14	-26.3
1	A	43	PRO	CA	23.88	55.85 – 70.84	-26.3
1	A	106	SER	CB	24.21	56.28 – 71.32	-26.3
1	A	159	ILE	CD1	56.60	5.18 – 21.60	26.3
1	A	73	TYR	CD2	93.64	125.28 – 140.14	-26.3
1	A	53	TYR	CD2	93.72	125.28 – 140.14	-26.2
1	A	162	SER	CB	24.34	56.28 – 71.32	-26.2
1	A	120	TYR	CD2	93.88	125.28 – 140.14	-26.1
1	A	26	PRO	CA	24.18	55.85 – 70.84	-26.1
1	A	97	SER	CB	24.55	56.28 – 71.32	-26.1
1	A	153	VAL	CG2	60.57	13.71 – 28.88	25.9
1	A	34	ILE	CD1	55.33	5.18 – 21.60	25.5
1	A	155	SER	CB	25.62	56.28 – 71.32	-25.4
1	A	25	ILE	CD1	54.95	5.18 – 21.60	25.3
1	A	154	SER	CB	25.77	56.28 – 71.32	-25.3
1	A	15	ILE	CD1	54.58	5.18 – 21.60	25.1
1	A	152	ILE	CD1	53.83	5.18 – 21.60	24.6
1	A	105	ILE	CD1	53.63	5.18 – 21.60	24.5
1	A	74	THR	CB	27.77	61.12 – 78.27	-24.4
1	A	59	THR	CB	27.88	61.12 – 78.27	-24.4
1	A	144	THR	CB	27.88	61.12 – 78.27	-24.4
1	A	139	THR	CB	28.26	61.12 – 78.27	-24.2
1	A	104	THR	CB	28.48	61.12 – 78.27	-24.0
1	A	147	ALA	CB	61.02	10.19 – 27.75	23.9
1	A	160	THR	CB	28.67	61.12 – 78.27	-23.9
1	A	24	THR	CB	29.00	61.12 – 78.27	-23.7
1	A	57	ALA	CB	60.55	10.19 – 27.75	23.7
1	A	100	THR	CB	29.14	61.12 – 78.27	-23.6
1	A	136	ALA	CB	60.44	10.19 – 27.75	23.6
1	A	27	THR	CB	29.22	61.12 – 78.27	-23.6
1	A	22	THR	CB	29.63	61.12 – 78.27	-23.4
1	A	161	ILE	CD1	51.73	5.18 – 21.60	23.4
1	A	125	THR	CB	29.84	61.12 – 78.27	-23.2
1	A	82	ALA	CB	59.60	10.19 – 27.75	23.1

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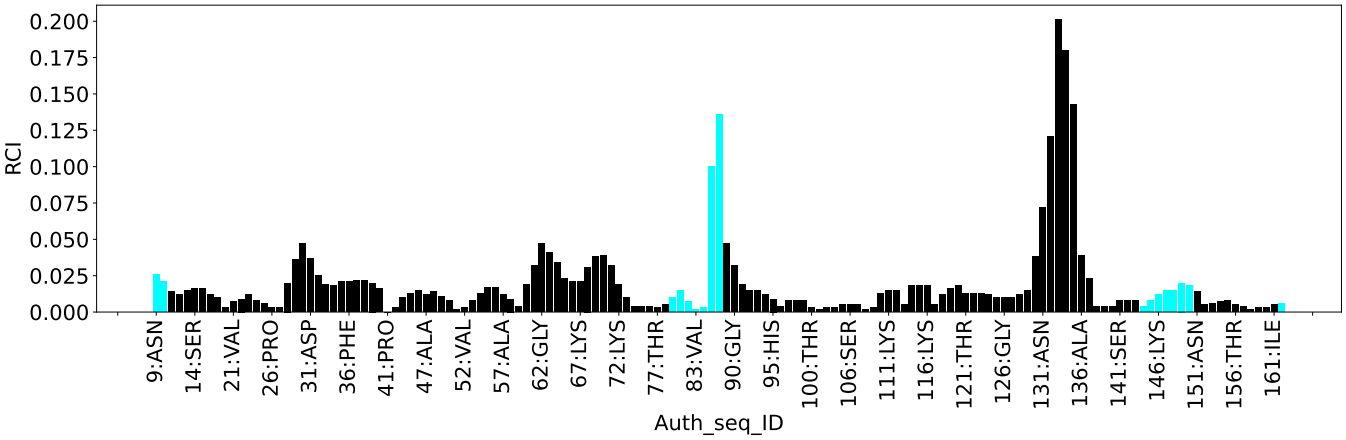
List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	148	ALA	CB	59.16	10.19 – 27.75	22.9
1	A	121	THR	CB	30.45	61.12 – 78.27	-22.9
1	A	47	ALA	CB	59.08	10.19 – 27.75	22.8
1	A	77	THR	CB	30.64	61.12 – 78.27	-22.8
1	A	78	THR	CB	30.89	61.12 – 78.27	-22.6
1	A	156	THR	CB	30.94	61.12 – 78.27	-22.6
1	A	158	THR	CB	30.97	61.12 – 78.27	-22.6
1	A	51	THR	CB	31.07	61.12 – 78.27	-22.5
1	A	55	TRP	CD1	88.08	117.34 – 135.80	-20.9
1	A	158	THR	CA	20.30	49.41 – 75.05	-16.4
1	A	77	THR	CA	20.77	49.41 – 75.05	-16.2
1	A	51	THR	CA	20.98	49.41 – 75.05	-16.1
1	A	104	THR	CA	20.98	49.41 – 75.05	-16.1
1	A	27	THR	CA	21.02	49.41 – 75.05	-16.1
1	A	160	THR	CA	21.30	49.41 – 75.05	-16.0
1	A	100	THR	CA	21.87	49.41 – 75.05	-15.7
1	A	59	THR	CA	22.28	49.41 – 75.05	-15.6
1	A	144	THR	CA	22.29	49.41 – 75.05	-15.6
1	A	74	THR	CA	22.65	49.41 – 75.05	-15.4
1	A	152	ILE	CA	20.88	48.30 – 75.08	-15.2
1	A	96	VAL	CA	20.67	48.38 – 76.73	-14.8
1	A	52	VAL	CA	20.80	48.38 – 76.73	-14.7
1	A	109	VAL	CA	20.98	48.38 – 76.73	-14.7
1	A	83	VAL	CA	21.16	48.38 – 76.73	-14.6
1	A	113	VAL	CA	21.37	48.38 – 76.73	-14.5
1	A	108	VAL	CA	21.44	48.38 – 76.73	-14.5
1	A	95	HIS	CD2	79.80	103.95 – 136.66	-12.4
1	A	125	THR	HB	2.51	2.57 – 5.77	-5.2

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.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:


RCI
0.200
0.175
0.150
0.125
0.100
0.075
0.050
0.025
0.000
9:ASN
14:SER
21:VAL
26:PRO
31:ASP
36:PHE
41:PRO
47:ALA
52:VAL
57:ALA
62:GLY
67:LYS
72:LYS
77:THR
83:VAL
90:GLY
95:HIS
100:THR
106:SER
111:LYS
116:LYS
121:THR
126:GLY
131:ASN
136:ALA
141:SER
146:LYS
151:ASN
156:THR
161:ILE
Auth_seq_ID