Full wwPDB NMR Structure Validation Report (i)

Apr 27, 2016 – 12:50 AM BST

PDB ID	:	2LAE
Title	:	NMR solution structure of the C-terminal domain of the E. coli lipoprotein BamC
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Deposited on	:	2011-03-11

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
http://wwpdb.org/validation/2016/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) 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 (i)

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

The overall completeness of chemical shifts assignment is 81%.

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.
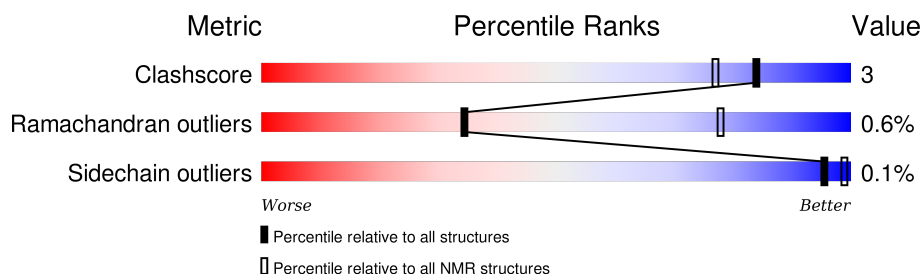
Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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 >=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	246	44% · · 52%

2 Ensemble composition and analysis (i)

This entry contains 9 models. Model 1 is the overall representative, medoid model (most similar to other models).

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:229-A:344 (116)	0.37	1

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters. No single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1756 atoms, of which 867 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Lipoprotein 34.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	118	1756	554	867	153	179	3	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	345	PRO	-	EXPRESSION TAG	UNP P0A903
A	346	GLY	-	EXPRESSION TAG	UNP P0A903

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: Lipoprotein 34

4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Lipoprotein 34

4.2.2 Score per residue for model 2

• Molecule 1: Lipoprotein 34
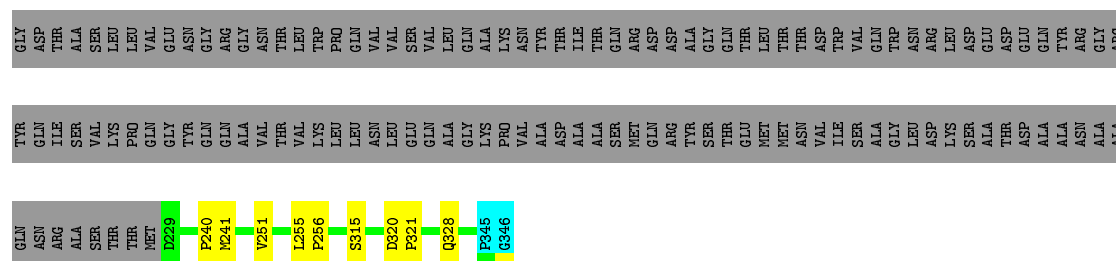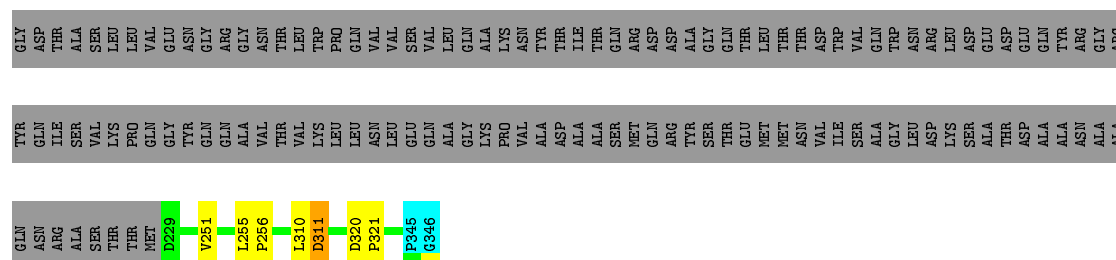
Chain A:

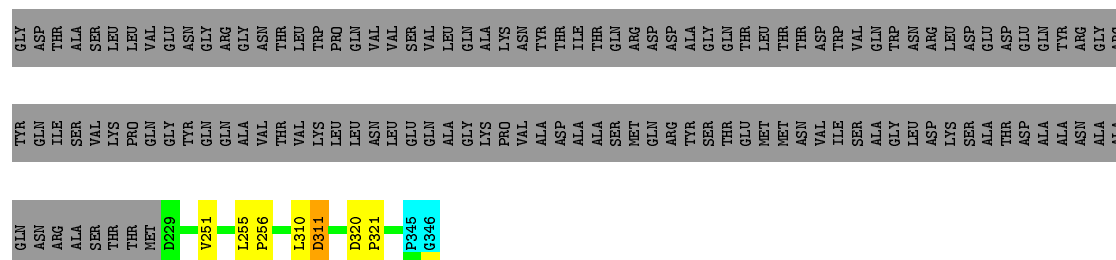### 4.2.3 Score per residue for model 3

• Molecule 1: Lipoprotein 34

Chain A:

4.2.4 Score per residue for model 4

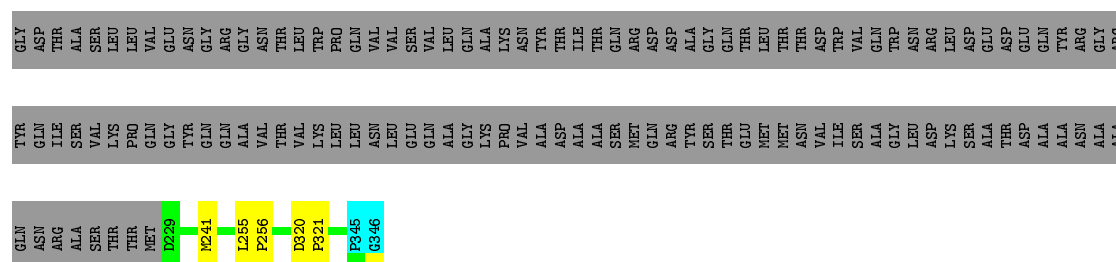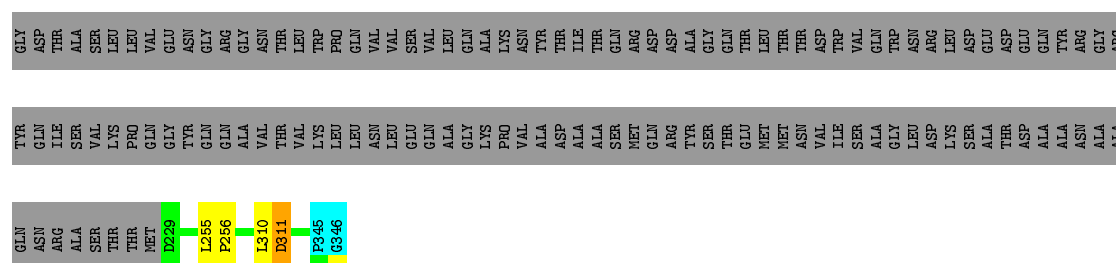• Molecule 1: Lipoprotein 34

Chain A:

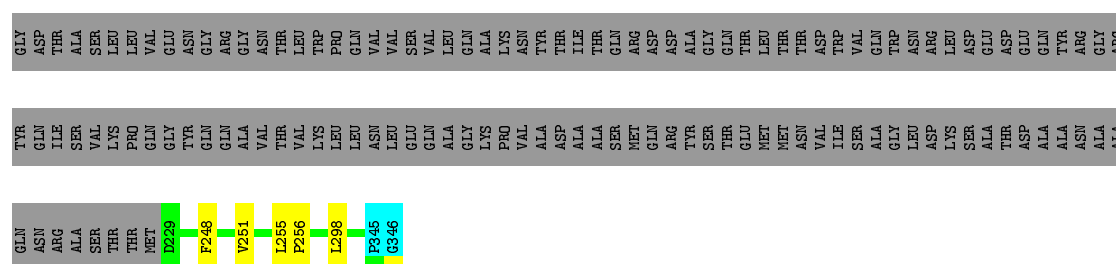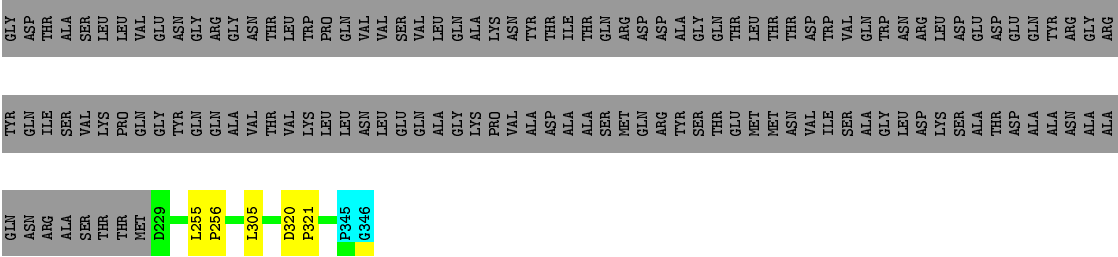### 4.2.5 Score per residue for model 5

• Molecule 1: Lipoprotein 34

Chain A:　45%　..　52%

GLY ASP THR ALA SER LEU LEU VAL GLU ASN GLY ARG GLY ASN THR LEU TRP PRO GLN VAL VAL SER VAL LEU GLN ALA LYS ASN TYR THR ILE THR GLN ARG ASP ASP ALA GLN THR LEU THR ASP TRP VAL GLN TRP ASN ARG LEU ASP GLU ASP GLN ARG GLY ARG

TYR GLN ILE VAL LYS PRO GLN GLY TYR GLN GLN ALA VAL THR VAL LYS LEU LEU ASN LEU GLU GLN ALA GLY LYS PRO VAL ALA ASP ALA ALA SER MET GLN ARG TYR SER THR GLU MET MET ASN VAL ILE SER ALA GLY LEU ASP LYS SER ALA THR ASP ALA ALA ASN ALA ALA

GLN ASN ARG ALA SER THR THR MET D229 M241 L255 P256 D320 P321 P345 G346

4.2.6 Score per residue for model 6

- Molecule 1: Lipoprotein 34

Chain A:　46%　..　52%

GLY ASP THR ALA SER LEU LEU VAL GLU ASN GLY ARG GLY ASN THR LEU TRP PRO GLN VAL VAL SER VAL LEU GLN ALA LYS ASN TYR THR ILE THR GLN ARG ASP ASP ALA GLN THR LEU THR ASP TRP VAL GLN TRP ASN ARG LEU ASP GLU ASP GLN ARG GLY ARG

TYR GLN ILE VAL LYS PRO GLN GLY TYR GLN GLN ALA VAL THR VAL LYS LEU LEU ASN LEU GLU GLN ALA GLY LYS PRO VAL ALA ASP ALA ALA SER MET GLN ARG TYR SER THR GLU MET MET ASN VAL ILE SER ALA GLY LEU ASP LYS SER ALA THR ASP ALA ALA ASN ALA ALA

GLN ASN ARG ALA SER THR THR MET D229 L255 P256 L310 D311 P345 G346

4.2.7 Score per residue for model 7

- Molecule 1: Lipoprotein 34

Chain A:　45%　..　52%

GLY ASP THR ALA SER LEU LEU VAL GLU ASN GLY ARG GLY ASN THR LEU TRP PRO GLN VAL VAL SER VAL LEU GLN ALA LYS ASN TYR THR ILE THR GLN ARG ASP ASP ALA GLY GLN THR LEU THR ASP TRP VAL GLN TRP ASN ARG LEU ASP GLU ASP GLN ARG GLY ARG

TYR GLN ILE VAL LYS PRO GLN GLY TYR GLN GLN ALA VAL THR VAL LYS LEU LEU ASN LEU GLU GLN ALA GLY LYS PRO VAL ALA ASP ALA ALA SER MET GLN ARG TYR SER THR GLU MET MET ASN VAL ILE SER ALA GLY LEU ASP LYS SER ALA THR ASP ALA ALA ASN ALA ALA

GLN ASN ARG ALA SER THR THR MET D229 F248 V251 L255 P256 L298 P345 G346

4.2.8 Score per residue for model 8

- Molecule 1: Lipoprotein 34

Chain A:　45%　..　52%

4.2.9 Score per residue for model 9

- Molecule 1: Lipoprotein 34

Chain A:

45% .. 52%
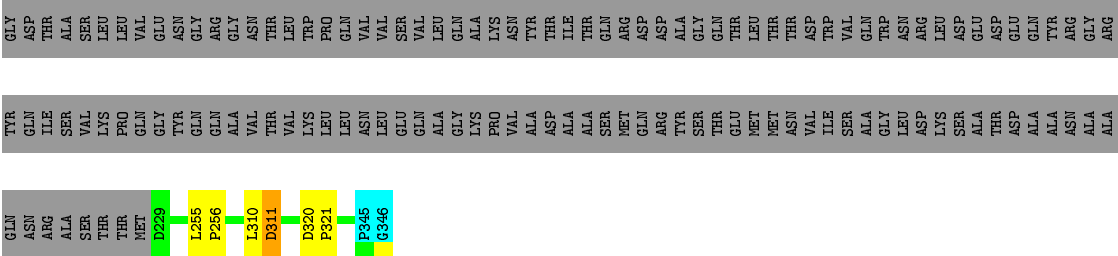
5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *molecular dynamics*.

Of the 100 calculated structures, 9 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
CS-NOE-RDC Rosetta	structure solution	
CS-NOE-RDC Rosetta	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)	2lae_cs.str
Number of chemical shift lists	1
Total number of shifts	2539
Number of shifts mapped to atoms	2368
Number of unparsed shifts	171
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	81%

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	877	857	856	5±1
All	All	7893	7713	7704	45

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 3.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Models Total
1:A:310:LEU:O	1:A:311:ASP:CB	0.70	2.39	9	5
1:A:310:LEU:O	1:A:311:ASP:HB3	0.56	2.01	9	5
1:A:255:LEU:N	1:A:256:PRO:CD	0.55	2.69	4	9
1:A:320:ASP:HB2	1:A:321:PRO:CD	0.51	2.36	5	7
1:A:255:LEU:N	1:A:256:PRO:HD2	0.51	2.20	7	1
1:A:305:LEU:C	1:A:305:LEU:HD13	0.49	2.28	8	1
1:A:255:LEU:HB3	1:A:256:PRO:HD3	0.46	1.88	5	1
1:A:251:VAL:O	1:A:255:LEU:N	0.45	2.49	1	5
1:A:248:PHE:O	1:A:248:PHE:CD1	0.44	2.70	7	1
1:A:320:ASP:OD1	1:A:320:ASP:C	0.43	2.57	4	2
1:A:248:PHE:C	1:A:248:PHE:CD1	0.41	2.91	7	1
1:A:264:MET:SD	1:A:278:VAL:HG21	0.41	2.55	1	1
1:A:320:ASP:HB2	1:A:321:PRO:HD2	0.41	1.91	9	3
1:A:241:MET:SD	1:A:315:SER:OG	0.41	2.77	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:320:ASP:C	1:A:320:ASP:OD1	0.41	2.59	5	1
1:A:240:PRO:HG3	1:A:328:GLN:HG3	0.40	1.93	2	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	115/246 (47%)	113±1 (98±1%)	2±1 (1±1%)	1±0 (1±0%)	34	78
All	All	1035/2214 (47%)	1015 (98%)	14 (1%)	6 (1%)	34	78

All 2 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	311	ASP	5
1	A	298	LEU	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	96/202 (48%)	96±0 (100±0%)	0±0 (0±0%)	95	99
All	All	864/1818 (48%)	863 (100%)	1 (0%)	95	99

All 1 unique residues with a non-rotameric sidechain are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	241	MET	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 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 (i)

The completeness of assignment taking into account all chemical shift lists is 81% for the well-defined parts and 81% for the entire structure.

7.1 Chemical shift list 1

File name: 2lae_cs.str

Chemical shift list name: *assigned_ chem_ shift_ list_ 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	2539
Number of shifts mapped to atoms	2368
Number of unparsed shifts	171
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	8

The following errors were found when reading this chemical shift list.

- Chemical shift uncertainty (if set) must be a number. The only occurence is reported below.

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1703	A	262	VAL	C	141.060	*****	1

- Entity instance (chain) must be specified. All 170 occurences are reported below.

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	?	98	GLY	HA2	3.849	0.004	2
2	?	98	GLY	C	169.711	0.006	1
3	?	98	GLY	CA	43.470	0.051	1
4	?	99	ALA	H	8.594	0.007	1
5	?	99	ALA	HA	4.515	0.004	1
6	?	99	ALA	QB	1.411	0.006	1
7	?	99	ALA	QB	1.411	0.006	1
8	?	99	ALA	QB	1.411	0.006	1
9	?	99	ALA	C	176.999	0.029	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
10	?	99	ALA	CA	52.237	0.019	1
11	?	99	ALA	CB	20.311	0.025	1
12	?	99	ALA	N	124.243	0.038	1
13	?	100	MET	H	8.443	0.003	1
14	?	100	MET	HA	4.456	0.009	1
15	?	100	MET	HB2	2.053	0.003	2
16	?	100	MET	HG2	2.607	0.000	2
17	?	100	MET	C	176.382	0.003	1
18	?	100	MET	CA	55.943	0.045	1
19	?	100	MET	CB	33.133	0.037	1
20	?	100	MET	CG	32.165	0.000	1
21	?	100	MET	N	120.185	0.014	1
22	?	101	GLY	H	8.482	0.004	1
1197	?	213	ALA	H	8.110	0.004	1
1198	?	213	ALA	HA	4.341	0.004	1
1199	?	213	ALA	QB	1.488	0.008	1
1200	?	213	ALA	QB	1.488	0.008	1
1201	?	213	ALA	QB	1.488	0.008	1
1202	?	213	ALA	C	178.973	0.008	1
1203	?	213	ALA	CA	53.609	0.041	1
1204	?	213	ALA	CB	19.002	0.064	1
1205	?	213	ALA	N	125.141	0.037	1
1206	?	214	THR	H	8.070	0.006	1
1207	?	214	THR	HA	4.227	0.016	1
1208	?	214	THR	QG2	1.234	0.000	1
1209	?	214	THR	QG2	1.234	0.000	1
1210	?	214	THR	QG2	1.234	0.000	1
1211	?	214	THR	C	175.190	0.018	1
1212	?	214	THR	CA	63.369	0.044	1
1213	?	214	THR	CB	69.468	0.034	1
1214	?	214	THR	CG2	21.730	0.000	1
1215	?	214	THR	N	113.519	0.022	1
1216	?	215	ASP	H	8.338	0.004	1
1217	?	215	ASP	HA	4.545	0.003	1
1218	?	215	ASP	HB2	2.697	0.005	2
1219	?	215	ASP	C	177.347	0.021	1
1220	?	215	ASP	CA	55.419	0.043	1
1221	?	215	ASP	CB	40.855	0.031	1
1222	?	215	ASP	N	122.820	0.018	1
1223	?	216	ALA	H	8.141	0.004	1
1224	?	216	ALA	HA	4.218	0.003	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1225	?	216	ALA	QB	1.435	0.008	1
1226	?	216	ALA	QB	1.435	0.008	1
1227	?	216	ALA	QB	1.435	0.008	1
1228	?	216	ALA	C	178.837	0.005	1
1229	?	216	ALA	CA	53.715	0.089	1
1230	?	216	ALA	CB	18.789	0.059	1
1231	?	216	ALA	N	123.953	0.025	1
1232	?	217	ALA	H	8.126	0.004	1
1233	?	217	ALA	HA	4.232	0.008	1
1234	?	217	ALA	QB	1.437	0.008	1
1235	?	217	ALA	QB	1.437	0.008	1
1236	?	217	ALA	QB	1.437	0.008	1
1237	?	217	ALA	C	178.723	0.007	1
1238	?	217	ALA	CA	53.698	0.010	1
1239	?	217	ALA	CB	18.666	0.005	1
1240	?	217	ALA	N	121.836	0.033	1
1241	?	218	ASN	H	8.134	0.003	1
1242	?	218	ASN	HA	4.633	0.005	1
1243	?	218	ASN	HB2	2.826	0.011	2
1244	?	218	ASN	C	175.925	0.005	1
1245	?	218	ASN	CA	53.891	0.040	1
1246	?	218	ASN	CB	38.737	0.042	1
1247	?	218	ASN	N	116.897	0.019	1
1248	?	219	ALA	H	8.026	0.004	1
1249	?	219	ALA	HA	4.250	0.007	1
1250	?	219	ALA	QB	1.439	0.007	1
1251	?	219	ALA	QB	1.439	0.007	1
1252	?	219	ALA	QB	1.439	0.007	1
1253	?	219	ALA	C	178.350	0.002	1
1254	?	219	ALA	CA	53.543	0.049	1
1255	?	219	ALA	CB	18.891	0.015	1
1256	?	219	ALA	N	123.635	0.017	1
1257	?	220	ALA	H	8.079	0.004	1
1258	?	220	ALA	HA	4.236	0.010	1
1259	?	220	ALA	QB	1.435	0.006	1
1260	?	220	ALA	QB	1.435	0.006	1
1261	?	220	ALA	QB	1.435	0.006	1
1262	?	220	ALA	C	178.476	0.000	1
1263	?	220	ALA	CA	53.343	0.042	1
1264	?	220	ALA	CB	18.831	0.035	1
1265	?	220	ALA	N	121.592	0.016	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1266	?	221	GLN	H	8.078	0.004	1
1267	?	221	GLN	HA	4.261	0.004	1
1268	?	221	GLN	HB2	2.120	0.008	2
1269	?	221	GLN	HB3	2.030	0.002	2
1270	?	221	GLN	HG2	2.406	0.000	2
1271	?	221	GLN	C	176.228	0.023	1
1272	?	221	GLN	CA	56.451	0.024	1
1273	?	221	GLN	CB	29.152	0.028	1
1274	?	221	GLN	CG	33.858	0.000	1
1275	?	221	GLN	N	117.995	0.021	1
1276	?	222	ASN	H	8.235	0.003	1
1277	?	222	ASN	HA	4.693	0.006	1
1278	?	222	ASN	HB2	2.873	0.000	2
1279	?	222	ASN	HB3	2.781	0.000	2
1280	?	222	ASN	C	175.442	0.017	1
1281	?	222	ASN	CA	53.628	0.075	1
1282	?	222	ASN	CB	38.801	0.017	1
1283	?	222	ASN	N	118.899	0.029	1
1284	?	223	ARG	H	8.162	0.020	1
1285	?	223	ARG	HA	4.333	0.007	1
1286	?	223	ARG	HB2	1.790	0.012	2
1287	?	223	ARG	HB3	1.885	0.014	2
1288	?	223	ARG	HG2	1.675	0.000	2
1289	?	223	ARG	HD2	3.216	0.000	1
1290	?	223	ARG	C	176.209	0.009	1
1291	?	223	ARG	CA	56.452	0.040	1
1292	?	223	ARG	CB	30.775	0.020	1
1293	?	223	ARG	CG	27.200	0.000	1
1294	?	223	ARG	CD	43.445	0.000	1
1295	?	223	ARG	N	121.244	0.139	1
1296	?	224	ALA	H	8.257	0.003	1
1297	?	224	ALA	HA	4.368	0.012	1
1298	?	224	ALA	QB	1.430	0.004	1
1299	?	224	ALA	QB	1.430	0.004	1
1300	?	224	ALA	QB	1.430	0.004	1
1301	?	224	ALA	C	177.855	0.005	1
1302	?	224	ALA	CA	52.710	0.018	1
1303	?	224	ALA	CB	19.266	0.033	1
1304	?	224	ALA	N	124.514	0.028	1
1305	?	225	SER	H	8.255	0.004	1
1306	?	225	SER	HA	4.521	0.007	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1307	?	225	SER	HB2	3.925	0.007	2
1308	?	225	SER	C	174.910	0.009	1
1309	?	225	SER	CA	58.459	0.059	1
1310	?	225	SER	CB	63.913	0.053	1
1311	?	225	SER	N	114.761	0.025	1
1312	?	226	THR	H	8.189	0.009	1
1313	?	226	THR	HA	4.479	0.008	1
1314	?	226	THR	HB	4.338	0.007	1
1315	?	226	THR	QG2	1.238	0.000	1
1316	?	226	THR	QG2	1.238	0.000	1
1317	?	226	THR	QG2	1.238	0.000	1
1318	?	226	THR	C	174.609	0.021	1
1319	?	226	THR	CA	61.744	0.047	1
1320	?	226	THR	CB	69.663	0.050	1
1321	?	226	THR	CG2	21.774	0.000	1
1322	?	226	THR	N	115.542	0.075	1
1323	?	227	THR	H	8.060	0.008	1
1324	?	227	THR	HA	4.344	0.002	1
1325	?	227	THR	HB	4.183	0.000	1
1326	?	227	THR	QG2	1.224	0.000	1
1327	?	227	THR	QG2	1.224	0.000	1
1328	?	227	THR	QG2	1.224	0.000	1
1329	?	227	THR	C	174.379	0.020	1
1330	?	227	THR	CA	62.086	0.035	1
1331	?	227	THR	CB	69.869	0.028	1
1332	?	227	THR	CG2	21.929	0.000	1
1333	?	227	THR	N	116.815	0.030	1
1334	?	228	MET	H	8.166	0.004	1
1335	?	228	MET	HA	4.368	0.012	1
1336	?	228	MET	HB2	1.592	0.009	2
1337	?	228	MET	HB3	1.708	0.018	2
1338	?	228	MET	HG2	2.235	0.000	2
1339	?	228	MET	C	174.118	0.003	1
1340	?	228	MET	CA	54.977	0.078	1
1341	?	228	MET	CB	33.409	0.075	1
1342	?	228	MET	CG	32.105	0.000	1
1343	?	228	MET	N	121.746	0.064	1
1344	?	229	ASP	H	8.020	0.011	1

7.1.2   Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_\alpha$	229	-0.20 ± 0.14	None needed (< 0.5 ppm)
$^{13}C_\beta$	208	0.02 ± 0.10	None needed (< 0.5 ppm)
$^{13}C'$	226	-0.13 ± 0.06	None needed (< 0.5 ppm)
^{15}N	220	0.30 ± 0.32	None needed (< 0.5 ppm)

7.1.3   Completeness of resonance assignments ⓘ

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 81%, i.e. 1092 atoms were assigned a chemical shift out of a possible 1348. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	564/568 (99%)	225/226 (100%)	229/232 (99%)	110/110 (100%)
Sidechain	524/697 (75%)	319/406 (79%)	205/260 (79%)	0/31 (0%)
Aromatic	4/83 (5%)	2/44 (5%)	0/36 (0%)	2/3 (67%)
Overall	1092/1348 (81%)	546/676 (81%)	434/528 (82%)	112/144 (78%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 81%, i.e. 1104 atoms were assigned a chemical shift out of a possible 1365. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	569/576 (99%)	227/229 (99%)	231/236 (98%)	111/111 (100%)
Sidechain	531/706 (75%)	323/412 (78%)	208/263 (79%)	0/31 (0%)
Aromatic	4/83 (5%)	2/44 (5%)	0/36 (0%)	2/3 (67%)
Overall	1104/1365 (81%)	552/685 (81%)	439/535 (82%)	113/145 (78%)

7.1.4   Statistically unusual chemical shifts ⓘ

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	245	ARG	HB3	4.16	$3.17 - 0.37$	8.5
1	A	295	ASP	HA	2.49	$6.15 - 3.05$	-6.8
1	A	345	PRO	HG2	3.90	$3.48 - 0.38$	6.3

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Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	139	GLN	HA	1.57	6.41 − 2.11	-6.3
1	A	283	LEU	HB3	-0.49	3.34 − -0.26	-5.6
1	A	345	PRO	HG3	3.71	3.56 − 0.26	5.5
1	A	271	ARG	HG2	0.10	2.92 − 0.22	-5.5
1	A	200	GLU	HB3	0.84	3.10 − 0.90	-5.3

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: