



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 09:38 PM BST

PDB ID : 2JZA
Title : Solution NMR structure of nitrite reductase [NAD(P)H] small subunit from *Erwinia carotovora*. Northeast Structural Genomics Consortium target EwR120
Authors : Sathyamoorthy, B.; Eletsky, A.; Wang, D.; Stokes, K.; Owens, L.; Xiao, R.; Liu, J.; Baran, M.C.; Swapna, G.V.T.; Acton, T.B.; Rost, B.; Montelione, G.T.; Szyperski, T.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2007-12-31

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 ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

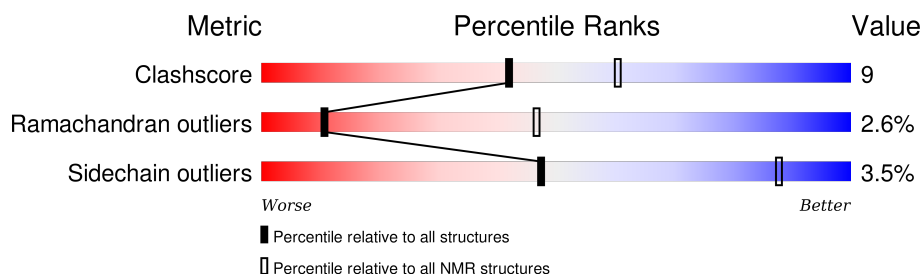
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 92%.

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	130	 72% 9% • 18%

2 Ensemble composition and analysis

This entry contains 20 models. Model 14 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:3-A:109 (107)	0.66	14

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 16 single-model clusters were found.

Cluster number	Models
1	7, 17
2	11, 14
Single-model clusters	1; 2; 3; 4; 5; 6; 8; 9; 10; 12; 13; 15; 16; 18; 19; 20

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1992 atoms, of which 972 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Nitrite reductase [NAD(P)H] small subunit.

Mol	Chain	Residues	Atoms						Trace
1	A	130	Total	C	H	N	O	S	0
			1992	638	972	179	199	4	

There are 8 discrepancies between the modelled and reference sequences:

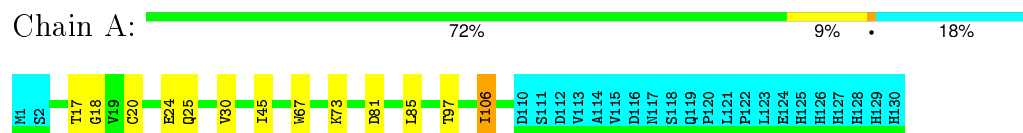
Chain	Residue	Modelled	Actual	Comment	Reference
A	123	LEU	-	EXPRESSION TAG	UNP Q6CZS1
A	124	GLU	-	EXPRESSION TAG	UNP Q6CZS1
A	125	HIS	-	EXPRESSION TAG	UNP Q6CZS1
A	126	HIS	-	EXPRESSION TAG	UNP Q6CZS1
A	127	HIS	-	EXPRESSION TAG	UNP Q6CZS1
A	128	HIS	-	EXPRESSION TAG	UNP Q6CZS1
A	129	HIS	-	EXPRESSION TAG	UNP Q6CZS1
A	130	HIS	-	EXPRESSION TAG	UNP Q6CZS1

4 Residue-property plots

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: Nitrite reductase [NAD(P)H] small subunit

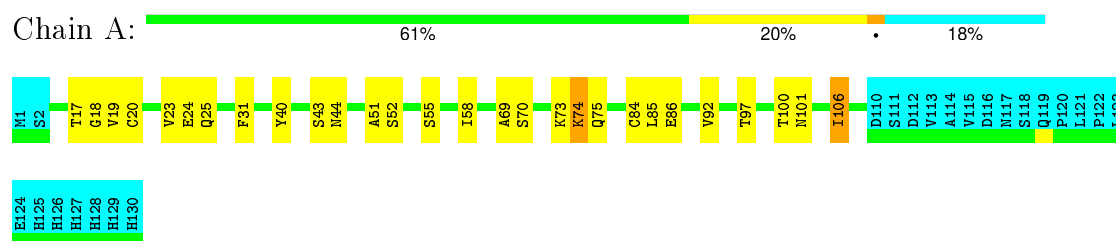


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

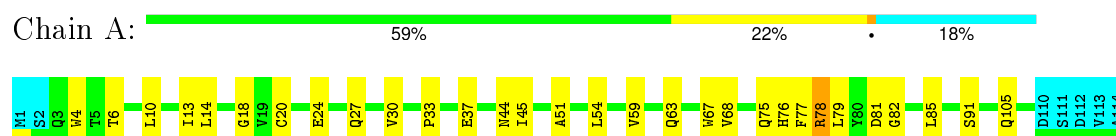
4.2.1 Score per residue for model 1

- Molecule 1: Nitrite reductase [NAD(P)H] small subunit



4.2.2 Score per residue for model 2

- Molecule 1: Nitrite reductase [NAD(P)H] small subunit



V115
D116
M117
S118
Q119
P120
L121
P122
L123
E124
H125
H126
H127
H128
H129
H130

4.2.3 Score per residue for model 3

- Molecule 1: Nitrite reductase [NAD(P)H] small subunit

Chain A: 59% 22% 18%

M1 S2 Q3 G18 V19 C20 E24 Q25 Q26 V30 F31 R32 P33 R34 N35 D36 Y40 A41 I42 I45 A51 S52 V53 G57 L66 P71 H76 F77 R78 L79 W80 D81 L85 S91 A94 V95 D96 T97 I106 S107 D110 S111 D112 V113 A114

V115
D116
M117
S118
Q119
P120
L121
P122
L123
E124
H125
H126
H127
H128
H129
H130

4.2.4 Score per residue for model 4

- Molecule 1: Nitrite reductase [NAD(P)H] small subunit

Chain A: 58% 22% 18%

M1 S2 Q3 K9 D12 G18 V19 C20 E24 Q27 V30 F31 R32 D36 E37 Q38 A41 I42 S43 N44 I45 A51 S52 G57 H62 W67 P71 R78 D81 L85 E86 V92 A93 T97 I106 D110 S111 D112 V113 A114

V115
D116
M117
S118
Q119
P120
L121
P122
L123
E124
H125
H126
H127
H128
H129
H130

4.2.5 Score per residue for model 5

- Molecule 1: Nitrite reductase [NAD(P)H] small subunit

Chain A: 57% 24% 18%

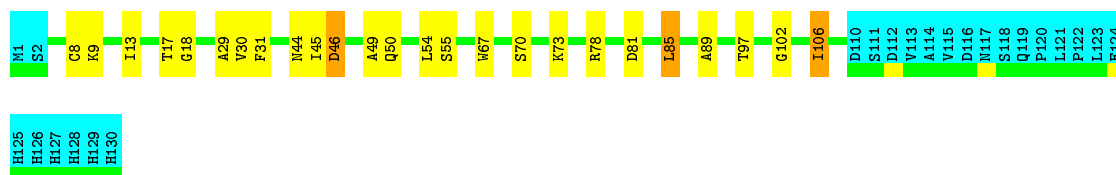
M1 S2 Q3 T6 L10 P15 G16 T17 C20 E24 Q25 Q26 Q27 T28 N35 D36 E37 A41 N44 I45 D46 S52 V53 L54 S55 W67 L72 C84 L85 E86 D87 V92 T97 Q98 V99 N103 I106 S107 I108 A109 D110 S111 D112 V113

A114
V115
D116
M117
S118
Q119
P120
L121
P122
L123
E124
H125
H126
H127
H128
H129
H130

4.2.6 Score per residue for model 6

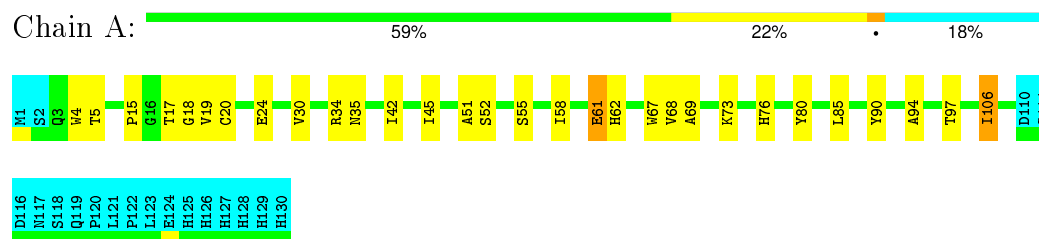
- Molecule 1: Nitrite reductase [NAD(P)H] small subunit

Chain A: 63% 17% 18%



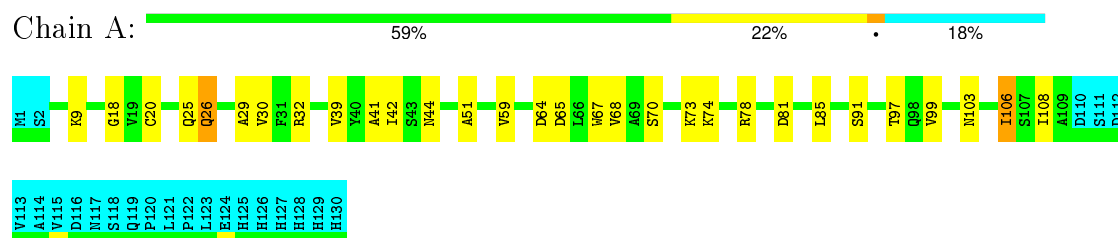
4.2.7 Score per residue for model 7

- Molecule 1: Nitrite reductase [NAD(P)H] small subunit



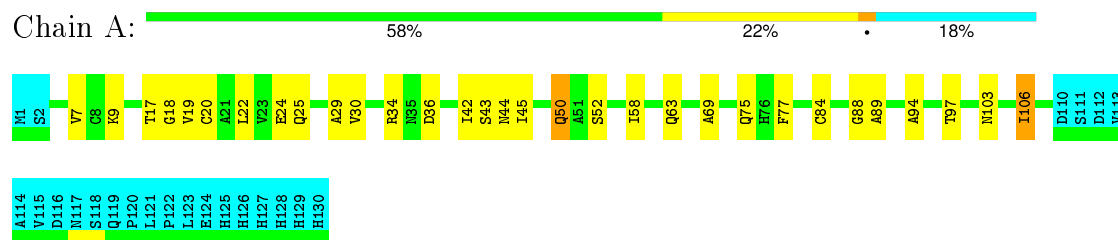
4.2.8 Score per residue for model 8

- Molecule 1: Nitrite reductase [NAD(P)H] small subunit



4.2.9 Score per residue for model 9

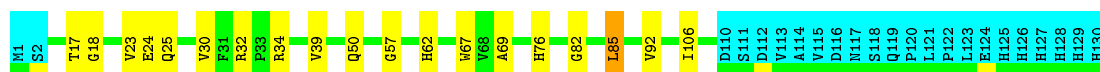
- Molecule 1: Nitrite reductase [NAD(P)H] small subunit



4.2.10 Score per residue for model 10

- Molecule 1: Nitrite reductase [NAD(P)H] small subunit

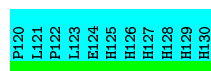
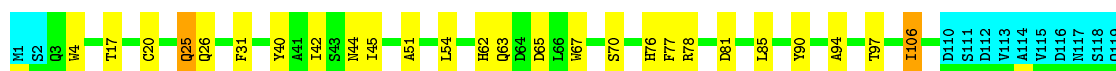
Chain A:  68% 14% 18%



4.2.11 Score per residue for model 11

- Molecule 1: Nitrite reductase [NAD(P)H] small subunit

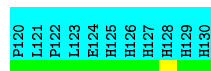
Chain A:  62% 18% 18%



4.2.12 Score per residue for model 12

- Molecule 1: Nitrite reductase [NAD(P)H] small subunit

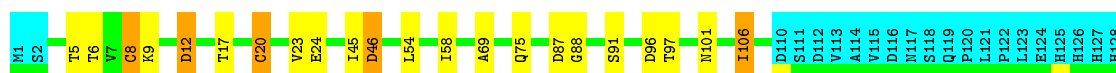
Chain A:  62% 19% 18%



4.2.13 Score per residue for model 13

- Molecule 1: Nitrite reductase [NAD(P)H] small subunit

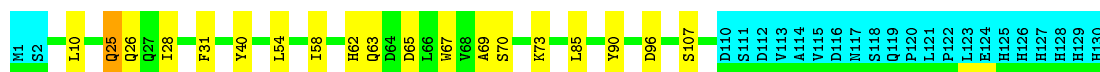
Chain A:  65% 13% 18%



4.2.14 Score per residue for model 14 (medoid)

- Molecule 1: Nitrite reductase [NAD(P)H] small subunit

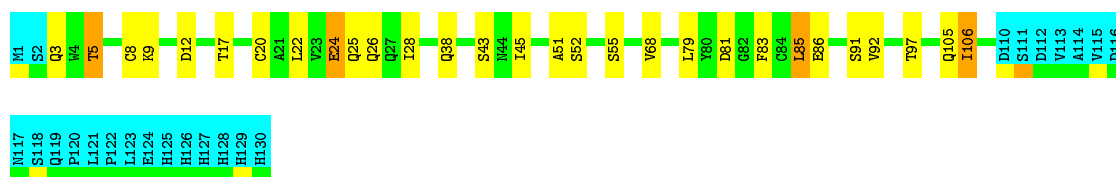
Chain A:  68% 14% 18%



4.2.15 Score per residue for model 15

- Molecule 1: Nitrite reductase [NAD(P)H] small subunit

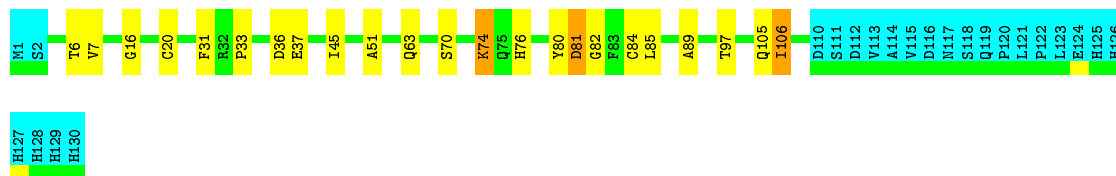
Chain A:  60% 19% 18%



4.2.16 Score per residue for model 16

- Molecule 1: Nitrite reductase [NAD(P)H] small subunit

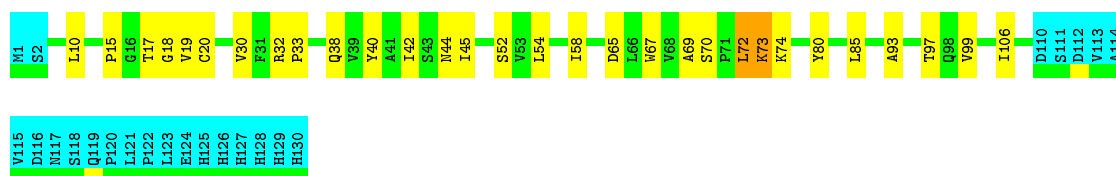
Chain A:  65% 15% 18%



4.2.17 Score per residue for model 17

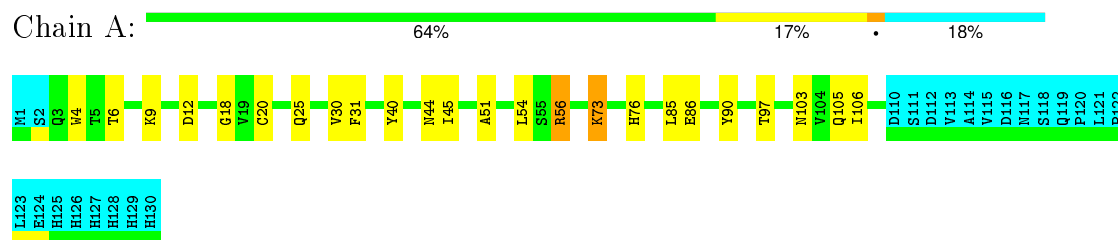
- Molecule 1: Nitrite reductase [NAD(P)H] small subunit

Chain A:  59% 22% 18%



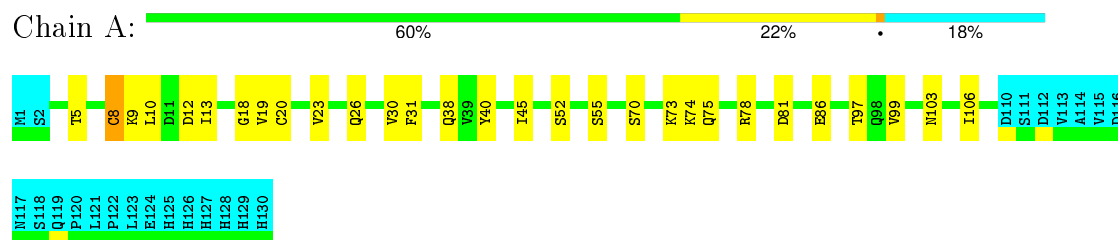
4.2.18 Score per residue for model 18

- Molecule 1: Nitrite reductase [NAD(P)H] small subunit



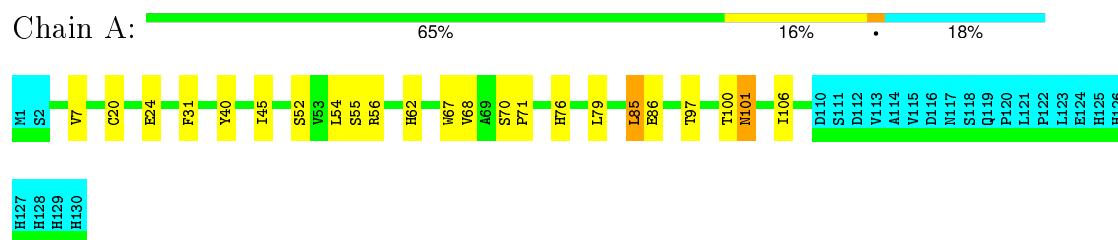
4.2.19 Score per residue for model 19

- Molecule 1: Nitrite reductase [NAD(P)H] small subunit



4.2.20 Score per residue for model 20

- Molecule 1: Nitrite reductase [NAD(P)H] small subunit



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
AutoStructure	structure solution	2.0.0
CARA	refinement	1.8.4
CNS	refinement	1.2
CYANA	structure solution	2.1

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)	BMRB entry 15611
Number of chemical shift lists	1
Total number of shifts	1505
Number of shifts mapped to atoms	1505
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	92%

No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality

6.1 Standard geometry

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

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	834	807	806	14±3
All	All	16680	16140	16120	287

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 9.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:97:THR:HG22	1:A:106:ILE:HG22	0.82	1.50	19	14
1:A:52:SER:HB2	1:A:55:SER:HB3	0.78	1.55	7	1
1:A:56:ARG:HE	1:A:56:ARG:HA	0.73	1.43	18	1
1:A:50:GLN:HA	1:A:50:GLN:HE21	0.73	1.44	9	1
1:A:8:CYS:SG	1:A:13:ILE:HG12	0.68	2.29	6	1
1:A:85:LEU:HG	1:A:86:GLU:HG3	0.68	1.66	4	2
1:A:20:CYS:SG	1:A:51:ALA:HA	0.68	2.28	7	10
1:A:46:ASP:HB2	1:A:54:LEU:HG	0.67	1.65	13	3
1:A:26:GLN:HE21	1:A:26:GLN:HA	0.67	1.47	8	1
1:A:67:TRP:HB3	1:A:76:HIS:HB3	0.67	1.64	20	3
1:A:76:HIS:O	1:A:84:CYS:HA	0.67	1.90	16	1
1:A:20:CYS:HB3	1:A:45:ILE:HD12	0.65	1.68	3	11
1:A:9:LYS:HE3	1:A:12:ASP:HB2	0.64	1.69	13	1
1:A:9:LYS:HD2	1:A:12:ASP:HB2	0.64	1.67	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:73:LYS:HD3	1:A:90:TYR:HE2	0.64	1.52	18	1
1:A:20:CYS:HB3	1:A:45:ILE:HD11	0.63	1.70	9	1
1:A:31:PHE:HZ	1:A:44:ASN:HB3	0.63	1.52	6	1
1:A:31:PHE:HB2	1:A:40:TYR:HB2	0.63	1.70	12	8
1:A:42:ILE:HG22	1:A:94:ALA:HA	0.63	1.71	3	4
1:A:19:VAL:HA	1:A:52:SER:OG	0.61	1.95	1	6
1:A:44:ASN:HB3	1:A:92:VAL:HG11	0.61	1.72	5	1
1:A:67:TRP:CZ3	1:A:85:LEU:HB2	0.61	2.30	6	5
1:A:10:LEU:HD21	1:A:37:GLU:HB3	0.61	1.73	5	1
1:A:78:ARG:HB2	1:A:81:ASP:HB3	0.60	1.73	8	2
1:A:15:PRO:HB3	1:A:35:ASN:HA	0.60	1.73	5	2
1:A:62:HIS:HB3	1:A:67:TRP:CD1	0.60	2.32	20	4
1:A:6:THR:HA	1:A:105:GLN:HG2	0.60	1.73	2	3
1:A:100:THR:HG23	1:A:101:ASN:H	0.59	1.56	1	2
1:A:41:ALA:HB3	1:A:97:THR:HG21	0.59	1.74	5	3
1:A:6:THR:HG22	1:A:8:CYS:H	0.59	1.57	13	1
1:A:77:PHE:HA	1:A:84:CYS:HA	0.58	1.75	9	1
1:A:23:VAL:HB	1:A:26:GLN:O	0.58	1.99	19	1
1:A:58:ILE:HB	1:A:69:ALA:HB3	0.58	1.75	14	6
1:A:18:GLY:HA3	1:A:30:VAL:O	0.58	1.99	9	1
1:A:70:SER:O	1:A:74:LYS:HA	0.57	1.99	17	5
1:A:78:ARG:HB3	1:A:81:ASP:HB3	0.57	1.76	19	2
1:A:55:SER:HA	1:A:68:VAL:HG21	0.57	1.74	20	1
1:A:76:HIS:HB2	1:A:85:LEU:HB2	0.56	1.74	10	1
1:A:27:GLN:HB3	1:A:45:ILE:HG13	0.56	1.77	5	1
1:A:70:SER:HB2	1:A:77:PHE:HE2	0.56	1.60	11	1
1:A:34:ARG:HB2	1:A:36:ASP:OD1	0.56	2.00	9	1
1:A:18:GLY:HA2	1:A:30:VAL:O	0.56	2.01	4	10
1:A:73:LYS:HE3	1:A:90:TYR:HE2	0.55	1.61	7	1
1:A:73:LYS:HD3	1:A:90:TYR:CE2	0.55	2.36	18	2
1:A:97:THR:HG23	1:A:106:ILE:HG22	0.54	1.78	11	2
1:A:15:PRO:HA	1:A:32:ARG:CG	0.54	2.31	12	2
1:A:29:ALA:HB2	1:A:45:ILE:HD13	0.54	1.77	6	1
1:A:44:ASN:OD1	1:A:54:LEU:HB2	0.53	2.03	2	4
1:A:54:LEU:HA	1:A:70:SER:HB3	0.53	1.79	20	2
1:A:67:TRP:HA	1:A:78:ARG:HA	0.53	1.81	2	1
1:A:32:ARG:HG2	1:A:34:ARG:O	0.52	2.04	10	1
1:A:5:THR:HG21	1:A:23:VAL:HG11	0.52	1.80	13	1
1:A:26:GLN:HB3	1:A:28:ILE:HD11	0.52	1.82	5	1
1:A:9:LYS:HB2	1:A:12:ASP:HB2	0.52	1.81	15	2
1:A:75:GLN:HG3	1:A:77:PHE:HE1	0.52	1.65	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:9:LYS:HA	1:A:103:ASN:HA	0.52	1.82	18	4
1:A:96:ASP:O	1:A:106:ILE:HA	0.52	2.05	13	1
1:A:68:VAL:HB	1:A:79:LEU:HD21	0.52	1.81	2	3
1:A:31:PHE:HZ	1:A:44:ASN:HD22	0.52	1.45	1	1
1:A:20:CYS:HB3	1:A:45:ILE:CD1	0.51	2.35	4	5
1:A:62:HIS:HB2	1:A:67:TRP:CD1	0.51	2.41	10	2
1:A:57:GLY:HA3	1:A:71:PRO:HD3	0.51	1.81	3	1
1:A:72:LEU:HB3	1:A:73:LYS:HD2	0.51	1.81	17	1
1:A:16:GLY:HA2	1:A:33:PRO:HA	0.51	1.82	16	1
1:A:43:SER:O	1:A:92:VAL:HB	0.51	2.06	15	3
1:A:29:ALA:HB3	1:A:44:ASN:HB3	0.51	1.82	9	1
1:A:82:GLY:HA2	1:A:92:VAL:HG22	0.51	1.82	10	1
1:A:9:LYS:HB2	1:A:12:ASP:H	0.51	1.64	4	1
1:A:10:LEU:HD22	1:A:99:VAL:HG11	0.50	1.82	5	2
1:A:3:GLN:O	1:A:107:SER:HA	0.50	2.07	3	2
1:A:75:GLN:HE22	1:A:89:ALA:HB3	0.50	1.65	9	1
1:A:33:PRO:HB3	1:A:59:VAL:HG21	0.50	1.83	2	1
1:A:54:LEU:HD22	1:A:70:SER:HB2	0.50	1.81	14	1
1:A:24:GLU:HG3	1:A:25:GLN:H	0.50	1.65	15	1
1:A:67:TRP:CZ3	1:A:78:ARG:HB2	0.49	2.42	4	2
1:A:52:SER:HB2	1:A:55:SER:HB2	0.49	1.84	15	3
1:A:96:ASP:HB3	1:A:107:SER:HB3	0.49	1.83	3	1
1:A:65:ASP:HB2	1:A:67:TRP:HE1	0.49	1.68	12	1
1:A:68:VAL:O	1:A:76:HIS:HA	0.48	2.07	7	1
1:A:70:SER:OG	1:A:73:LYS:HB2	0.48	2.09	12	1
1:A:25:GLN:HE21	1:A:25:GLN:HA	0.48	1.69	14	1
1:A:78:ARG:HD3	1:A:81:ASP:HB3	0.48	1.85	11	1
1:A:17:THR:HG22	1:A:18:GLY:H	0.47	1.69	7	4
1:A:33:PRO:HG2	1:A:38:GLN:HE22	0.47	1.70	17	1
1:A:78:ARG:HD3	1:A:81:ASP:CB	0.47	2.39	4	3
1:A:20:CYS:HB2	1:A:27:GLN:HB3	0.47	1.87	4	2
1:A:53:VAL:HG21	1:A:72:LEU:HD12	0.47	1.87	5	1
1:A:65:ASP:HB3	1:A:67:TRP:HE1	0.47	1.70	17	2
1:A:65:ASP:HB3	1:A:67:TRP:NE1	0.47	2.24	17	2
1:A:4:TRP:HA	1:A:106:ILE:O	0.47	2.10	7	1
1:A:99:VAL:HA	1:A:103:ASN:O	0.47	2.10	8	1
1:A:31:PHE:HB3	1:A:33:PRO:HD3	0.47	1.87	16	1
1:A:70:SER:HB2	1:A:77:PHE:CE2	0.46	2.45	11	1
1:A:27:GLN:O	1:A:45:ILE:HD11	0.46	2.11	2	1
1:A:97:THR:HG23	1:A:106:ILE:HG12	0.46	1.87	20	1
1:A:96:ASP:HB2	1:A:107:SER:HB3	0.46	1.86	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:8:CYS:SG	1:A:9:LYS:N	0.46	2.88	6	2
1:A:56:ARG:NE	1:A:56:ARG:HA	0.46	2.20	18	1
1:A:76:HIS:HB2	1:A:85:LEU:HB3	0.46	1.87	3	2
1:A:14:LEU:HD12	1:A:14:LEU:H	0.46	1.69	2	1
1:A:31:PHE:CE1	1:A:55:SER:HB3	0.46	2.45	6	1
1:A:66:LEU:HB3	1:A:79:LEU:HD12	0.46	1.86	3	1
1:A:10:LEU:HD12	1:A:99:VAL:HG21	0.46	1.87	17	1
1:A:97:THR:HG22	1:A:106:ILE:CG2	0.46	2.41	18	1
1:A:69:ALA:HA	1:A:75:GLN:O	0.46	2.11	12	1
1:A:84:CYS:HB2	1:A:87:ASP:O	0.46	2.11	5	1
1:A:70:SER:HB3	1:A:73:LYS:O	0.46	2.10	6	1
1:A:78:ARG:HD3	1:A:81:ASP:HB2	0.46	1.88	4	1
1:A:25:GLN:NE2	1:A:26:GLN:H	0.45	2.10	11	1
1:A:50:GLN:HA	1:A:50:GLN:NE2	0.45	2.21	9	1
1:A:20:CYS:HA	1:A:29:ALA:HA	0.45	1.86	8	1
1:A:57:GLY:CA	1:A:71:PRO:HD3	0.45	2.41	4	1
1:A:23:VAL:HG11	1:A:106:ILE:HD11	0.45	1.89	10	2
1:A:75:GLN:OE1	1:A:87:ASP:HB3	0.45	2.12	13	1
1:A:106:ILE:H	1:A:106:ILE:HD13	0.44	1.71	13	2
1:A:42:ILE:HB	1:A:93:ALA:O	0.44	2.13	17	2
1:A:36:ASP:CG	1:A:37:GLU:H	0.44	2.16	4	2
1:A:75:GLN:HG3	1:A:86:GLU:HB2	0.44	1.90	19	1
1:A:108:ILE:O	1:A:108:ILE:HD12	0.44	2.12	5	2
1:A:42:ILE:HG13	1:A:44:ASN:HB2	0.44	1.90	8	1
1:A:75:GLN:HB3	1:A:84:CYS:HB3	0.44	1.89	1	1
1:A:5:THR:HG21	1:A:23:VAL:HG13	0.43	1.90	19	1
1:A:78:ARG:CB	1:A:81:ASP:HB3	0.43	2.43	19	1
1:A:34:ARG:HA	1:A:34:ARG:NE	0.43	2.28	7	1
1:A:32:ARG:HD3	1:A:39:VAL:HG12	0.43	1.89	12	1
1:A:32:ARG:N	1:A:33:PRO:HD3	0.43	2.27	12	2
1:A:65:ASP:HB2	1:A:67:TRP:NE1	0.43	2.28	14	1
1:A:81:ASP:OD2	1:A:83:PHE:HB2	0.43	2.13	15	1
1:A:24:GLU:O	1:A:25:GLN:HB2	0.43	2.14	10	1
1:A:73:LYS:N	1:A:73:LYS:HD2	0.42	2.29	17	1
1:A:84:CYS:HB2	1:A:88:GLY:HA2	0.42	1.91	9	1
1:A:32:ARG:HG3	1:A:39:VAL:HG12	0.42	1.91	10	2
1:A:10:LEU:HD12	1:A:13:ILE:HB	0.42	1.90	2	1
1:A:76:HIS:H	1:A:87:ASP:CG	0.42	2.18	12	1
1:A:10:LEU:HD23	1:A:10:LEU:O	0.42	2.14	14	1
1:A:31:PHE:CE2	1:A:55:SER:HA	0.42	2.50	19	1
1:A:49:ALA:O	1:A:50:GLN:HB2	0.42	2.14	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:9:LYS:HB2	1:A:12:ASP:CB	0.42	2.44	18	1
1:A:59:VAL:HG22	1:A:68:VAL:HG23	0.42	1.92	8	1
1:A:77:PHE:O	1:A:78:ARG:HB3	0.42	2.14	2	1
1:A:53:VAL:O	1:A:71:PRO:HD2	0.42	2.15	3	1
1:A:45:ILE:N	1:A:45:ILE:HD12	0.41	2.30	7	1
1:A:6:THR:HG23	1:A:103:ASN:HB3	0.41	1.92	5	1
1:A:10:LEU:HD21	1:A:37:GLU:HA	0.41	1.91	2	1
1:A:67:TRP:CZ3	1:A:85:LEU:HA	0.41	2.50	20	1
1:A:7:VAL:CG2	1:A:106:ILE:HD12	0.41	2.45	16	1
1:A:57:GLY:HA3	1:A:69:ALA:O	0.41	2.15	10	1
1:A:31:PHE:CE2	1:A:55:SER:HB3	0.41	2.51	20	1
1:A:32:ARG:HE	1:A:36:ASP:HA	0.41	1.76	12	1
1:A:5:THR:O	1:A:105:GLN:HA	0.41	2.16	15	1
1:A:86:GLU:CD	1:A:86:GLU:H	0.40	2.20	5	1
1:A:28:ILE:HD12	1:A:106:ILE:HG13	0.40	1.93	15	1
1:A:56:ARG:HD3	1:A:71:PRO:HG3	0.40	1.94	20	1
1:A:61:GLU:H	1:A:61:GLU:CD	0.40	2.19	7	1
1:A:44:ASN:HA	1:A:92:VAL:HG11	0.40	1.92	4	1
1:A:8:CYS:SG	1:A:13:ILE:HD11	0.40	2.56	19	1
1:A:26:GLN:HG3	1:A:28:ILE:HD11	0.40	1.93	14	1
1:A:106:ILE:HD13	1:A:106:ILE:H	0.40	1.76	15	1
1:A:52:SER:HB3	1:A:55:SER:OG	0.40	2.16	5	1
1:A:45:ILE:HD12	1:A:45:ILE:N	0.40	2.32	16	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	107/130 (82%)	90±3 (84±2%)	15±2 (14±1%)	3±2 (3±2%)	11	47
All	All	2140/2600 (82%)	1792 (84%)	292 (14%)	56 (3%)	11	47

All 21 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	24	GLU	10
1	A	85	LEU	10
1	A	63	GLN	5
1	A	91	SER	4
1	A	80	TYR	3
1	A	46	ASP	3
1	A	7	VAL	2
1	A	8	CYS	2
1	A	89	ALA	2
1	A	82	GLY	2
1	A	101	ASN	2
1	A	81	ASP	2
1	A	64	ASP	1
1	A	45	ILE	1
1	A	88	GLY	1
1	A	102	GLY	1
1	A	78	ARG	1
1	A	18	GLY	1
1	A	36	ASP	1
1	A	35	ASN	1
1	A	74	LYS	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	90/112 (80%)	87±1 (96±1%)	3±1 (4±1%)	47	88
All	All	1800/2240 (80%)	1737 (96%)	63 (4%)	47	88

All 28 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	106	ILE	13
1	A	17	THR	7
1	A	25	GLN	5
1	A	73	LYS	5
1	A	86	GLU	3

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Mol	Chain	Res	Type	Models (Total)
1	A	38	GLN	3
1	A	5	THR	2
1	A	3	GLN	2
1	A	81	ASP	2
1	A	26	GLN	2
1	A	50	GLN	2
1	A	100	THR	1
1	A	80	TYR	1
1	A	91	SER	1
1	A	90	TYR	1
1	A	22	LEU	1
1	A	101	ASN	1
1	A	32	ARG	1
1	A	20	CYS	1
1	A	12	ASP	1
1	A	63	GLN	1
1	A	74	LYS	1
1	A	40	TYR	1
1	A	43	SER	1
1	A	24	GLU	1
1	A	72	LEU	1
1	A	56	ARG	1
1	A	61	GLU	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers [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

The completeness of assignment taking into account all chemical shift lists is 92% for the well-defined parts and 86% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 15611

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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	1505
Number of shifts mapped to atoms	1505
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	123	-0.06 ± 0.16	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	117	0.47 ± 0.14	None needed (< 0.5 ppm)
$^{13}\text{C}'$	114	0.12 ± 0.12	None needed (< 0.5 ppm)
^{15}N	115	0.84 ± 0.37	Should be applied

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 92%, i.e. 1177 atoms were assigned a chemical shift out of a possible 1280. 19 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	517/527 (98%)	208/210 (99%)	208/214 (97%)	101/103 (98%)
Sidechain	581/645 (90%)	356/373 (95%)	207/243 (85%)	18/29 (62%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	79/108 (73%)	46/56 (82%)	27/46 (59%)	6/6 (100%)
Overall	1177/1280 (92%)	610/639 (95%)	442/503 (88%)	125/138 (91%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 86%, i.e. 1334 atoms were assigned a chemical shift out of a possible 1560. 21 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	589/638 (92%)	237/254 (93%)	237/260 (91%)	115/124 (93%)
Sidechain	666/766 (87%)	409/445 (92%)	237/290 (82%)	20/31 (65%)
Aromatic	79/156 (51%)	46/80 (58%)	27/58 (47%)	6/18 (33%)
Overall	1334/1560 (86%)	692/779 (89%)	501/608 (82%)	141/173 (82%)

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	107	SER	HB3	2.05	5.25 – 2.45	-6.4
1	A	98	GLN	HG2	0.86	3.67 – 0.97	-5.4

7.1.5 Random Coil Index (RCI) plots ⓘ

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:

