



Full wwPDB NMR Structure Validation Report ⓘ

Feb 13, 2017 – 01:18 am GMT

PDB ID : 2MSN
Title : NMR structure of a putative phosphoglycolate phosphatase (NP_346487.1) from *Streptococcus pneumoniae* TIGR4
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Deposited on : 2014-08-04

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
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	trunk28760
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

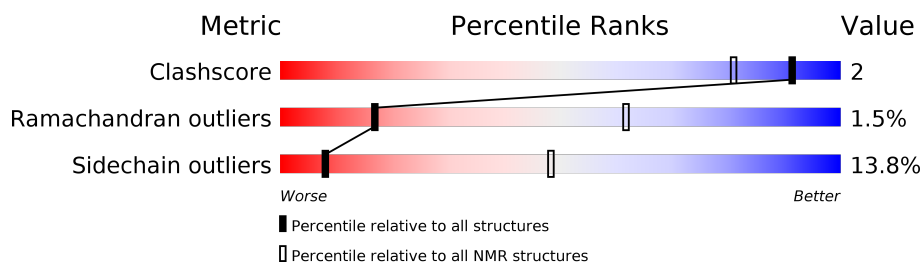
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 74%.

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	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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	208	<div> <div></div> <div>82%</div> <div>11%</div> <div>7%</div> </div>

2 Ensemble composition and analysis

This entry contains 20 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:1-A:17, A:84-A:204 (138)	0.39	1
2	A:19-A:73 (55)	0.32	18

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 4 clusters and 1 single-model cluster was found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3302 atoms, of which 1628 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Hydrolase, haloacid dehalogenase-like family.

Mol	Chain	Residues	Atoms						Trace
1	A	208	Total	C	H	N	O	S	0
			3302	1066	1628	276	330	2	

There are 2 discrepancies between the modelled and reference sequences:

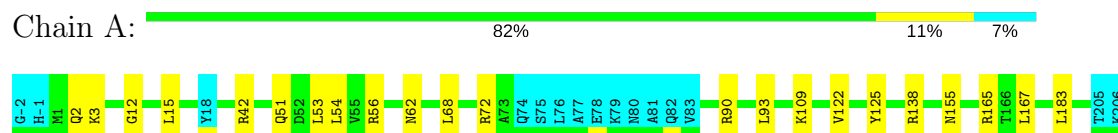
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP Q97NG6
A	-1	HIS	-	EXPRESSION TAG	UNP Q97NG6

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: Hydrolase, haloacid dehalogenase-like family

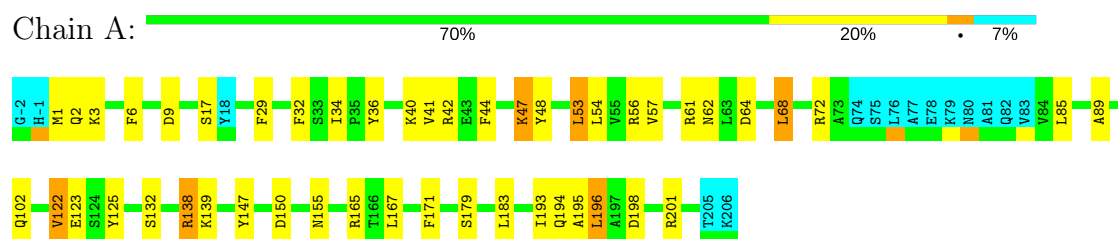


4.2 Scores per residue for each member of the ensemble

Colouring as in section [4.1](#) above.

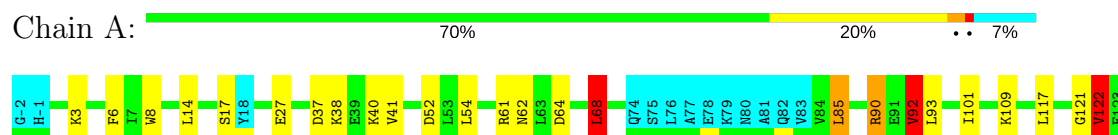
4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Hydrolase, haloacid dehalogenase-like family



4.2.2 Score per residue for model 2

- Molecule 1: Hydrolase, haloacid dehalogenase-like family

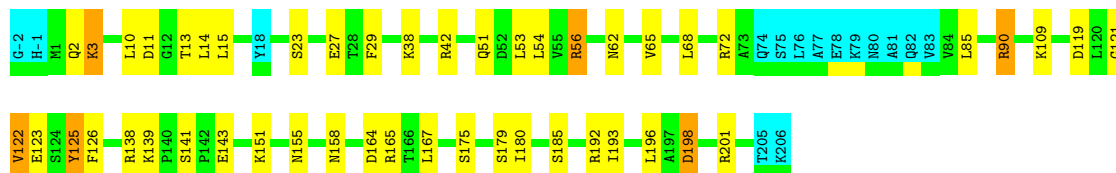




4.2.3 Score per residue for model 3

- Molecule 1: Hydrolase, haloacid dehalogenase-like family

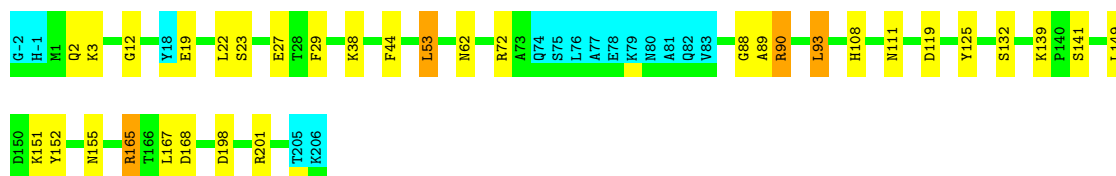
Chain A: 70% 20% 7%



4.2.4 Score per residue for model 4

- Molecule 1: Hydrolase, haloacid dehalogenase-like family

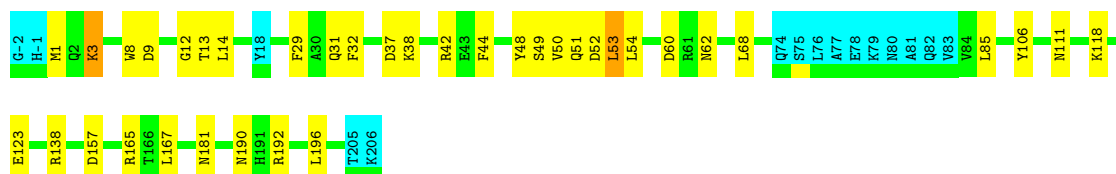
Chain A: 77% 14% 7%



4.2.5 Score per residue for model 5

- Molecule 1: Hydrolase, haloacid dehalogenase-like family

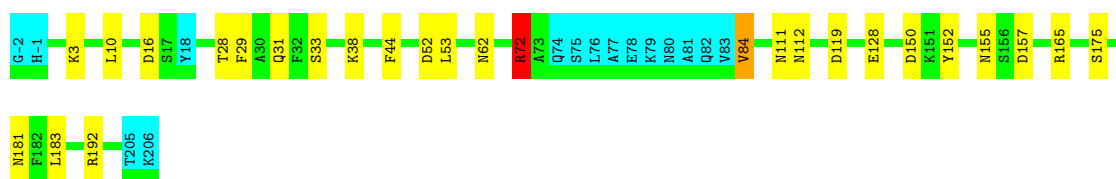
Chain A: 75% 17% 7%



4.2.6 Score per residue for model 6

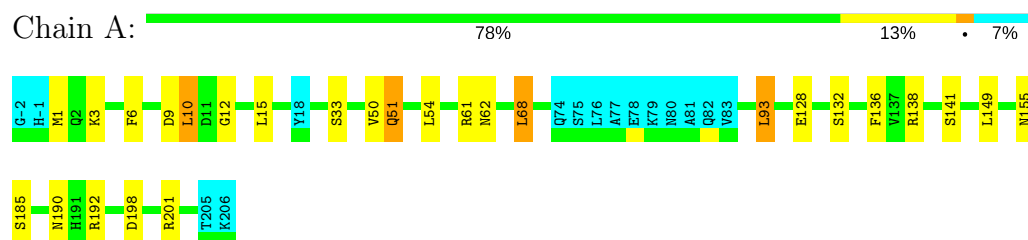
- Molecule 1: Hydrolase, haloacid dehalogenase-like family

Chain A: 80% 12% 7%



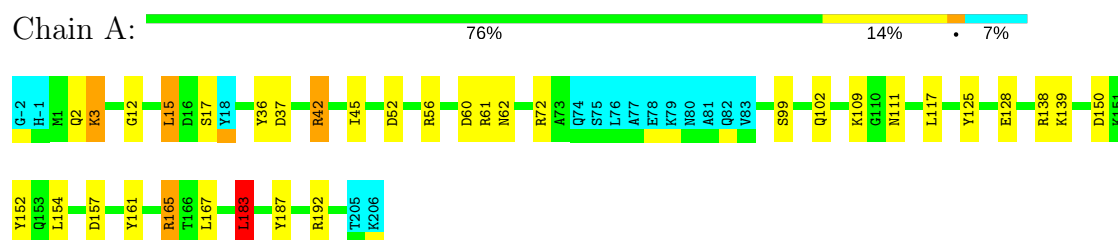
4.2.7 Score per residue for model 7

- Molecule 1: Hydrolase, haloacid dehalogenase-like family



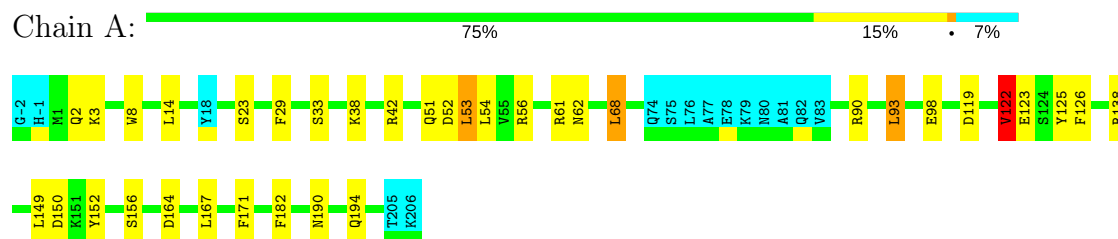
4.2.8 Score per residue for model 8

- Molecule 1: Hydrolase, haloacid dehalogenase-like family



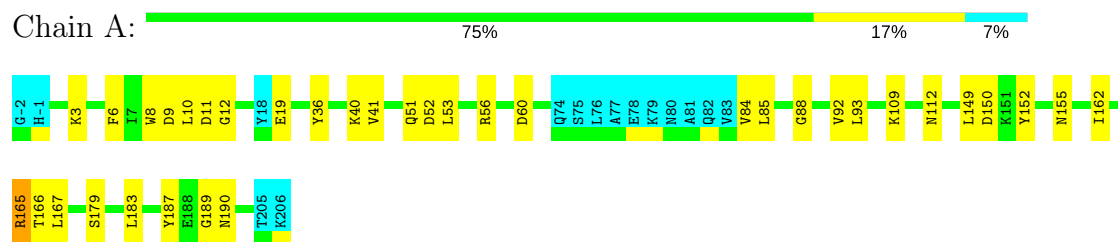
4.2.9 Score per residue for model 9

- Molecule 1: Hydrolase, haloacid dehalogenase-like family



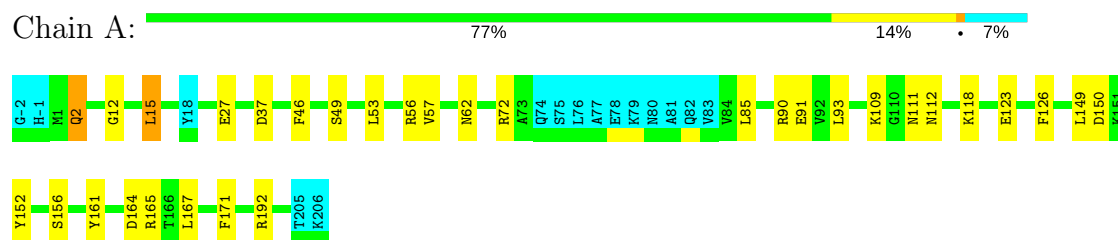
4.2.10 Score per residue for model 10

- Molecule 1: Hydrolase, haloacid dehalogenase-like family



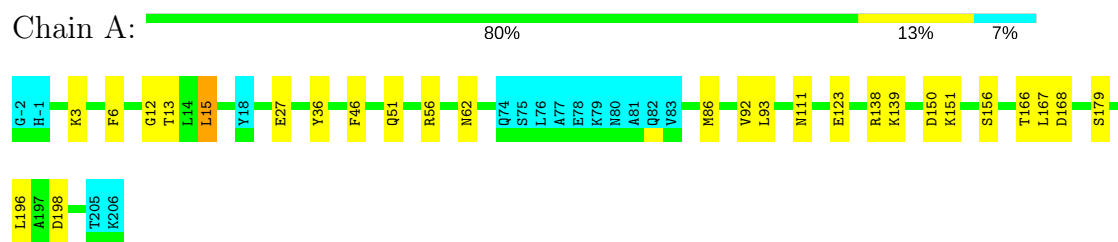
4.2.11 Score per residue for model 11

- Molecule 1: Hydrolase, haloacid dehalogenase-like family



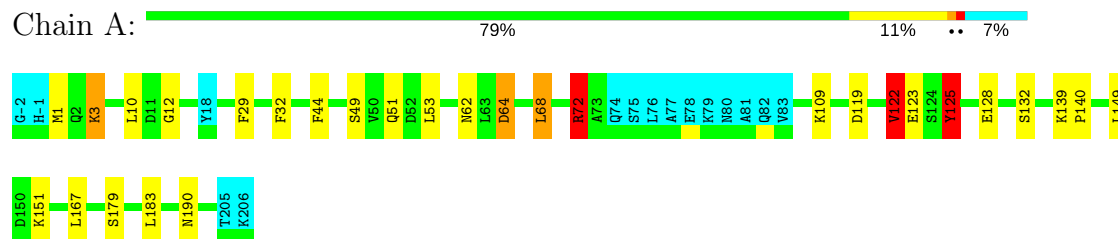
4.2.12 Score per residue for model 12

- Molecule 1: Hydrolase, haloacid dehalogenase-like family



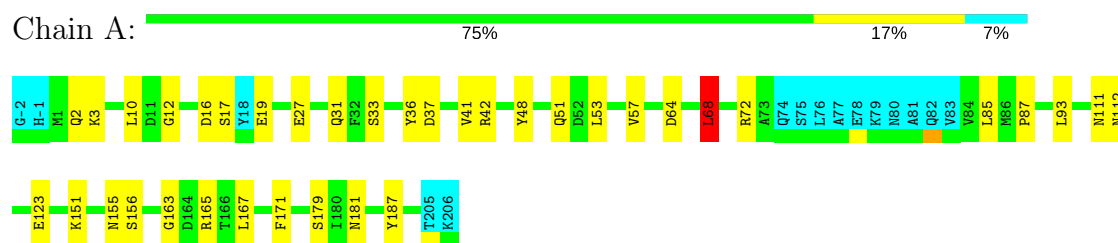
4.2.13 Score per residue for model 13

- Molecule 1: Hydrolase, haloacid dehalogenase-like family



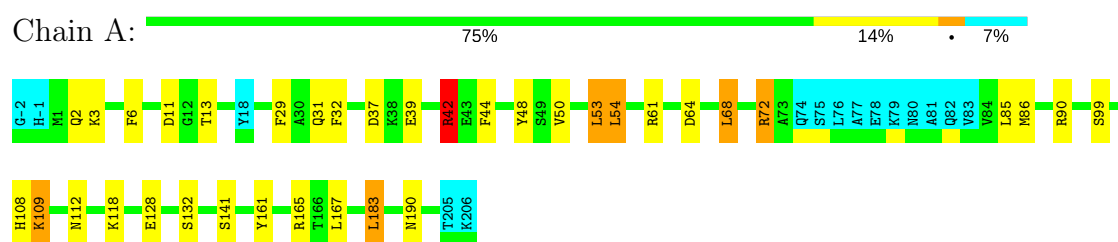
4.2.14 Score per residue for model 14

- Molecule 1: Hydrolase, haloacid dehalogenase-like family



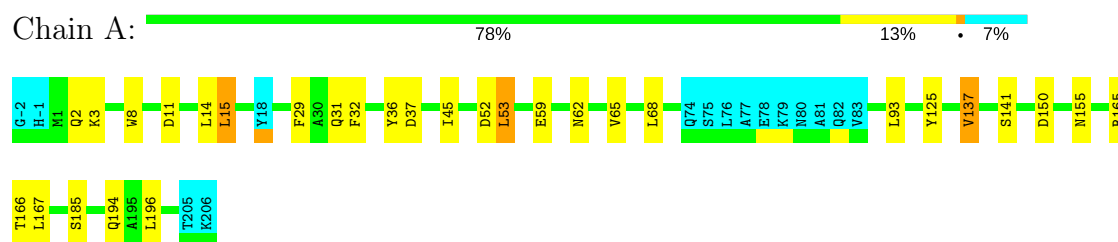
4.2.15 Score per residue for model 15

- Molecule 1: Hydrolase, haloacid dehalogenase-like family



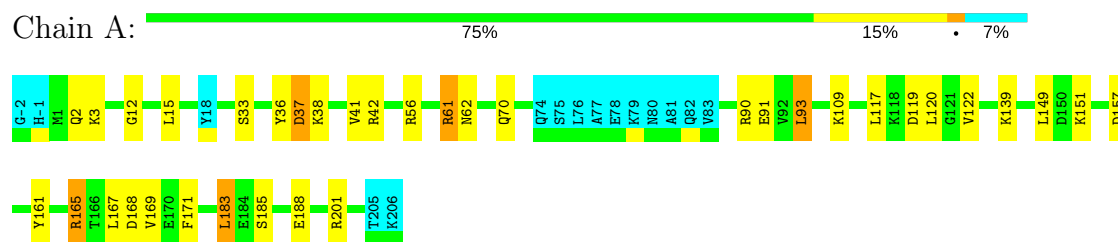
4.2.16 Score per residue for model 16

- Molecule 1: Hydrolase, haloacid dehalogenase-like family



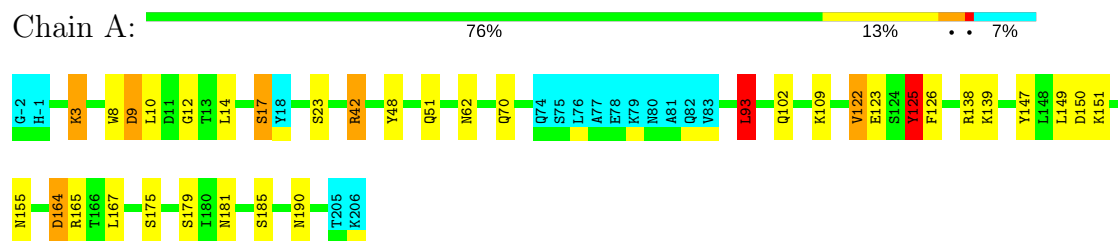
4.2.17 Score per residue for model 17

- Molecule 1: Hydrolase, haloacid dehalogenase-like family



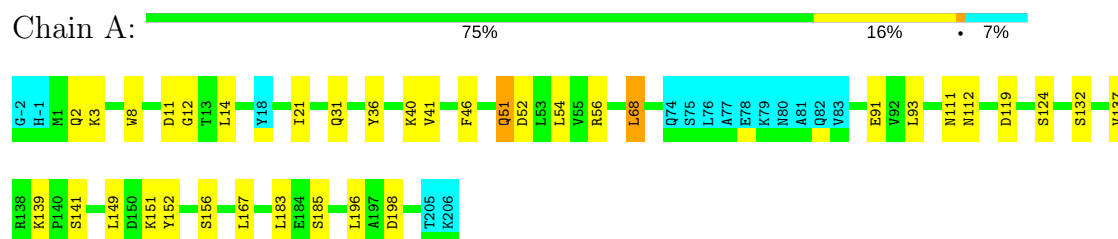
4.2.18 Score per residue for model 18

- Molecule 1: Hydrolase, haloacid dehalogenase-like family



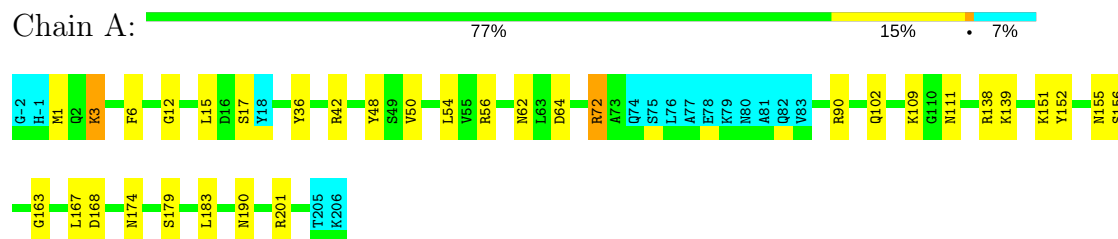
4.2.19 Score per residue for model 19

- Molecule 1: Hydrolase, haloacid dehalogenase-like family



4.2.20 Score per residue for model 20

- Molecule 1: Hydrolase, haloacid dehalogenase-like family



5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics, 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
CYANA	refinement	3.0
CYANA	structure solution	3.0
OPAL	refinement	
UNIO-ATNOS/CANDID	structure solution	

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)	2msn_cs.str
Number of chemical shift lists	1
Total number of shifts	2213
Number of shifts mapped to atoms	2213
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	74%

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

6 Model quality

6.1 Standard geometry

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	0.63±0.01	0±0/1588 (0.0±0.0%)	1.06±0.03	4±2/2153 (0.2±0.1%)
All	All	0.63	0/31760 (0.0%)	1.06	72/43060 (0.2%)

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	2.2±1.5
All	All	0	44

There are no bond-length outliers.

All unique angle 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(°)	Ideal(°)	Models	
								Worst	Total
1	A	65	VAL	CG1-CB-CG2	10.00	126.90	110.90	16	1
1	A	122	VAL	CA-CB-CG2	9.98	125.86	110.90	1	5
1	A	42	ARG	NE-CZ-NH2	-9.49	115.56	120.30	20	4
1	A	93	LEU	CB-CG-CD1	8.87	126.09	111.00	9	11
1	A	68	LEU	CB-CG-CD1	8.70	125.80	111.00	1	8
1	A	61	ARG	NE-CZ-NH2	-7.71	116.44	120.30	2	2
1	A	192	ARG	NE-CZ-NH2	-7.44	116.58	120.30	7	3
1	A	122	VAL	CG1-CB-CG2	-7.30	99.21	110.90	17	1
1	A	201	ARG	NE-CZ-NH2	-7.04	116.78	120.30	4	3
1	A	61	ARG	N-CA-CB	-6.88	98.22	110.60	1	2
1	A	138	ARG	NE-CZ-NH2	-6.76	116.92	120.30	8	1
1	A	9	ASP	CB-CG-OD1	6.74	124.37	118.30	18	2
1	A	125	TYR	CB-CG-CD2	-6.66	117.00	121.00	18	1
1	A	60	ASP	CB-CG-OD1	6.14	123.82	118.30	10	1
1	A	72	ARG	NE-CZ-NH1	6.12	123.36	120.30	13	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	42	ARG	NE-CZ-NH1	5.90	123.25	120.30	1	2
1	A	192	ARG	NE-CZ-NH1	5.81	123.20	120.30	7	2
1	A	165	ARG	NE-CZ-NH2	-5.79	117.41	120.30	11	1
1	A	61	ARG	NE-CZ-NH1	5.75	123.18	120.30	2	2
1	A	72	ARG	CD-NE-CZ	5.73	131.62	123.60	15	1
1	A	198	ASP	CB-CG-OD2	-5.65	113.22	118.30	3	2
1	A	165	ARG	CD-NE-CZ	5.55	131.38	123.60	4	1
1	A	72	ARG	NE-CZ-NH2	-5.49	117.55	120.30	4	1
1	A	6	PHE	CB-CG-CD2	-5.32	117.08	120.80	20	2
1	A	90	ARG	NE-CZ-NH2	-5.29	117.65	120.30	3	1
1	A	125	TYR	CB-CG-CD1	-5.29	117.83	121.00	16	2
1	A	154	LEU	CB-CG-CD2	-5.25	102.07	111.00	8	1
1	A	54	LEU	CB-CG-CD1	5.19	119.82	111.00	15	1
1	A	65	VAL	CA-CB-CG2	5.18	118.67	110.90	16	1
1	A	161	TYR	CB-CG-CD2	-5.09	117.94	121.00	8	1
1	A	91	GLU	CB-CA-C	5.09	120.59	110.40	17	1
1	A	183	LEU	CB-CG-CD1	5.06	119.60	111.00	8	1
1	A	92	VAL	CA-CB-CG1	5.05	118.48	110.90	2	1
1	A	165	ARG	NE-CZ-NH1	5.01	122.80	120.30	8	1

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	56	ARG	Sidechain	6
1	A	125	TYR	Sidechain	5
1	A	90	ARG	Sidechain	4
1	A	36	TYR	Sidechain	4
1	A	187	TYR	Sidechain	3
1	A	165	ARG	Sidechain	3
1	A	161	TYR	Sidechain	3
1	A	42	ARG	Sidechain	3
1	A	72	ARG	Sidechain	3
1	A	147	TYR	Sidechain	2
1	A	61	ARG	Sidechain	2
1	A	60	ASP	Peptide	1
1	A	201	ARG	Sidechain	1
1	A	106	TYR	Sidechain	1
1	A	48	TYR	Sidechain	1
1	A	139	LYS	Peptide	1

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	138	ARG	Sidechain	1

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	1557	1513	1513	6±3
All	All	31140	30260	30260	110

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 2.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:93:LEU:HD23	1:A:125:TYR:CD2	0.83	2.08	4	1
1:A:90:ARG:HD3	1:A:93:LEU:HD22	0.72	1.59	4	1
1:A:85:LEU:HD21	1:A:122:VAL:HG11	0.69	1.63	2	1
1:A:36:TYR:CE2	1:A:41:VAL:HG21	0.67	2.25	1	1
1:A:36:TYR:CE1	1:A:41:VAL:HG21	0.66	2.25	19	4
1:A:28:THR:HG21	1:A:72:ARG:NH2	0.65	2.06	6	1
1:A:22:LEU:HD13	1:A:38:LYS:HD2	0.64	1.70	4	1
1:A:54:LEU:H	1:A:54:LEU:HD12	0.63	1.54	7	3
1:A:169:VAL:HG11	1:A:185:SER:HB3	0.60	1.72	7	1
1:A:85:LEU:CD2	1:A:122:VAL:HG11	0.60	2.27	2	1
1:A:15:LEU:HD13	1:A:15:LEU:N	0.59	2.12	11	2
1:A:122:VAL:HG23	1:A:125:TYR:CD2	0.59	2.32	3	6
1:A:32:PHE:CZ	1:A:68:LEU:HD12	0.59	2.32	1	3
1:A:89:ALA:HB3	1:A:90:ARG:NH2	0.55	2.16	4	1
1:A:15:LEU:HD13	1:A:15:LEU:H	0.53	1.63	11	2
1:A:29:PHE:CZ	1:A:53:LEU:HD11	0.53	2.39	1	9
1:A:37:ASP:O	1:A:41:VAL:HG23	0.53	2.03	14	3
1:A:44:PHE:HA	1:A:47:LYS:CG	0.52	2.34	1	1
1:A:28:THR:HG21	1:A:72:ARG:HH22	0.51	1.64	6	1
1:A:32:PHE:CE1	1:A:68:LEU:HD23	0.51	2.41	5	2
1:A:85:LEU:HD13	1:A:86:MET:N	0.51	2.21	15	1
1:A:122:VAL:HG22	1:A:126:PHE:CE2	0.51	2.41	2	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:64:ASP:O	1:A:68:LEU:HD13	0.50	2.06	1	2
1:A:44:PHE:HA	1:A:47:LYS:HG3	0.50	1.83	1	1
1:A:193:ILE:HD12	1:A:195:ALA:O	0.49	2.07	2	2
1:A:8:TRP:CZ3	1:A:162:ILE:HG21	0.49	2.42	2	2
1:A:8:TRP:CE3	1:A:14:LEU:HD13	0.49	2.42	9	4
1:A:15:LEU:N	1:A:15:LEU:CD1	0.48	2.76	16	1
1:A:53:LEU:O	1:A:57:VAL:HG23	0.48	2.08	11	2
1:A:15:LEU:CD1	1:A:15:LEU:N	0.48	2.77	11	2
1:A:64:ASP:O	1:A:68:LEU:HD22	0.48	2.07	2	2
1:A:50:VAL:O	1:A:54:LEU:HD12	0.47	2.09	5	3
1:A:54:LEU:HD22	1:A:68:LEU:HB3	0.47	1.86	2	2
1:A:36:TYR:CZ	1:A:41:VAL:HG21	0.47	2.44	1	1
1:A:15:LEU:HD22	1:A:120:LEU:CD1	0.46	2.41	17	1
1:A:90:ARG:CD	1:A:93:LEU:HD22	0.46	2.36	4	1
1:A:90:ARG:HA	1:A:93:LEU:HD12	0.46	1.86	2	1
1:A:29:PHE:CZ	1:A:57:VAL:HG21	0.44	2.48	1	1
1:A:15:LEU:N	1:A:15:LEU:HD13	0.44	2.27	16	1
1:A:164:ASP:HB2	1:A:182:PHE:CD2	0.44	2.48	9	1
1:A:44:PHE:CD1	1:A:53:LEU:HB2	0.43	2.47	13	4
1:A:8:TRP:CZ3	1:A:14:LEU:HD13	0.43	2.48	5	1
1:A:34:ILE:HG21	1:A:57:VAL:HG11	0.43	1.89	1	1
1:A:183:LEU:H	1:A:183:LEU:HD12	0.43	1.72	2	1
1:A:14:LEU:C	1:A:15:LEU:HD12	0.43	2.34	3	1
1:A:16:ASP:CG	1:A:84:VAL:HG23	0.43	2.34	6	1
1:A:89:ALA:HB3	1:A:90:ARG:CZ	0.43	2.44	4	1
1:A:183:LEU:HD13	1:A:183:LEU:N	0.43	2.29	15	1
1:A:51:GLN:HA	1:A:51:GLN:HE21	0.42	1.74	19	1
1:A:12:GLY:H	1:A:15:LEU:HD11	0.42	1.74	12	2
1:A:10:LEU:HA	1:A:15:LEU:HD21	0.42	1.90	7	1
1:A:51:GLN:HA	1:A:54:LEU:HD13	0.42	1.90	7	1
1:A:93:LEU:HB3	1:A:125:TYR:CZ	0.42	2.50	18	1
1:A:137:VAL:HG23	1:A:141:SER:CB	0.42	2.45	16	1
1:A:15:LEU:N	1:A:15:LEU:HD22	0.42	2.30	8	1
1:A:169:VAL:HG11	1:A:185:SER:CB	0.41	2.45	17	1
1:A:180:ILE:HG22	1:A:193:ILE:HD13	0.41	1.91	3	1
1:A:54:LEU:HD12	1:A:54:LEU:H	0.41	1.75	20	1
1:A:183:LEU:N	1:A:183:LEU:HD13	0.41	2.31	17	2
1:A:50:VAL:HG23	1:A:51:GLN:N	0.41	2.30	5	1
1:A:6:PHE:CD1	1:A:101:ILE:HG21	0.41	2.51	2	1
1:A:89:ALA:HB2	1:A:196:LEU:HD23	0.40	1.92	1	1
1:A:8:TRP:CH2	1:A:92:VAL:HG11	0.40	2.51	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:PHE:CE1	1:A:48:TYR:HB2	0.40	2.52	5	1
1:A:54:LEU:HB2	1:A:65:VAL:HG23	0.40	1.93	3	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	193/208 (93%)	171±4 (88±2%)	20±4 (10±2%)	3±2 (1±1%)	17	62
All	All	3860/4160 (93%)	3413 (88%)	391 (10%)	56 (1%)	17	62

All 19 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	3	LYS	13
1	A	12	GLY	11
1	A	122	VAL	5
1	A	1	MET	4
1	A	139	LYS	4
1	A	138	ARG	2
1	A	121	GLY	2
1	A	88	GLY	2
1	A	163	GLY	2
1	A	2	GLN	2
1	A	17	SER	1
1	A	87	PRO	1
1	A	137	VAL	1
1	A	136	PHE	1
1	A	164	ASP	1
1	A	140	PRO	1
1	A	50	VAL	1
1	A	189	GLY	1
1	A	109	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	169/181 (93%)	146±4 (86±2%)	23±4 (14±2%)	8	48
All	All	3380/3620 (93%)	2913 (86%)	467 (14%)	8	48

All 95 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	167	LEU	19
1	A	62	ASN	16
1	A	3	LYS	12
1	A	165	ARG	12
1	A	155	ASN	11
1	A	109	LYS	10
1	A	151	LYS	10
1	A	2	GLN	10
1	A	150	ASP	10
1	A	183	LEU	10
1	A	123	GLU	9
1	A	152	TYR	9
1	A	179	SER	9
1	A	111	ASN	9
1	A	51	GLN	9
1	A	149	LEU	9
1	A	52	ASP	8
1	A	72	ARG	8
1	A	190	ASN	8
1	A	138	ARG	7
1	A	119	ASP	7
1	A	85	LEU	7
1	A	53	LEU	7
1	A	10	LEU	7
1	A	141	SER	6
1	A	38	LYS	6
1	A	37	ASP	6
1	A	27	GLU	6
1	A	112	ASN	6

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Mol	Chain	Res	Type	Models (Total)
1	A	31	GLN	6
1	A	156	SER	6
1	A	198	ASP	6
1	A	42	ARG	6
1	A	132	SER	6
1	A	196	LEU	6
1	A	128	GLU	6
1	A	168	ASP	5
1	A	171	PHE	5
1	A	11	ASP	5
1	A	15	LEU	5
1	A	68	LEU	5
1	A	185	SER	5
1	A	139	LYS	5
1	A	56	ARG	5
1	A	33	SER	5
1	A	9	ASP	4
1	A	102	GLN	4
1	A	23	SER	4
1	A	17	SER	4
1	A	93	LEU	4
1	A	90	ARG	4
1	A	48	TYR	4
1	A	13	THR	4
1	A	40	LYS	4
1	A	181	ASN	4
1	A	175	SER	4
1	A	157	ASP	4
1	A	6	PHE	4
1	A	164	ASP	3
1	A	118	LYS	3
1	A	117	LEU	3
1	A	46	PHE	3
1	A	49	SER	3
1	A	19	GLU	3
1	A	92	VAL	3
1	A	192	ARG	3
1	A	64	ASP	3
1	A	194	GLN	3
1	A	166	THR	3
1	A	124	SER	2
1	A	201	ARG	2

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Mol	Chain	Res	Type	Models (Total)
1	A	70	GLN	2
1	A	91	GLU	2
1	A	99	SER	2
1	A	108	HIS	2
1	A	143	GLU	1
1	A	137	VAL	1
1	A	158	ASN	1
1	A	1	MET	1
1	A	131	THR	1
1	A	188	GLU	1
1	A	126	PHE	1
1	A	16	ASP	1
1	A	86	MET	1
1	A	61	ARG	1
1	A	14	LEU	1
1	A	39	GLU	1
1	A	174	ASN	1
1	A	47	LYS	1
1	A	170	GLU	1
1	A	84	VAL	1
1	A	159	THR	1
1	A	98	GLU	1
1	A	59	GLU	1
1	A	60	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 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

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

7.1 Chemical shift list 1

File name: 2msn_cs.str

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	2213
Number of shifts mapped to atoms	2213
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	7

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	205	-0.09 ± 0.07	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	196	0.45 ± 0.06	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	196	0.24 ± 0.33	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 74%, i.e. 1786 atoms were assigned a chemical shift out of a possible 2401. 31 out of 31 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	554/957 (58%)	181/382 (47%)	190/386 (49%)	183/189 (97%)
Sidechain	1071/1226 (87%)	656/711 (92%)	386/460 (84%)	29/55 (53%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	161/218 (74%)	105/116 (91%)	54/98 (55%)	2/4 (50%)
Overall	1786/2401 (74%)	942/1209 (78%)	630/944 (67%)	214/248 (86%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 74%, i.e. 1917 atoms were assigned a chemical shift out of a possible 2583. 33 out of 33 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	597/1032 (58%)	196/412 (48%)	205/416 (49%)	196/204 (96%)
Sidechain	1149/1318 (87%)	705/765 (92%)	412/493 (84%)	32/60 (53%)
Aromatic	171/233 (73%)	111/124 (90%)	58/104 (56%)	2/5 (40%)
Overall	1917/2583 (74%)	1012/1301 (78%)	675/1013 (67%)	230/269 (86%)

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	162	ILE	HD12	-1.47	2.13 – -0.77	-7.4
1	A	162	ILE	HD11	-1.47	2.13 – -0.77	-7.4
1	A	162	ILE	HD13	-1.47	2.13 – -0.77	-7.4
1	A	200	SER	HB2	2.12	5.18 – 2.58	-6.8
1	A	151	LYS	HG2	-0.37	2.67 – 0.07	-6.7
1	A	173	GLN	HB2	0.59	3.30 – 0.80	-5.9
1	A	93	LEU	HB2	-0.14	3.32 – -0.08	-5.2

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:

