



Full wwPDB NMR Structure Validation Report ⓘ

Apr 27, 2016 – 01:17 AM BST

PDB ID : 2LD5
Title : Solution NMR-derived complex structure of Hoxa13 DNA binding domain bound to DNA
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Deposited on : 2011-05-14

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
<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

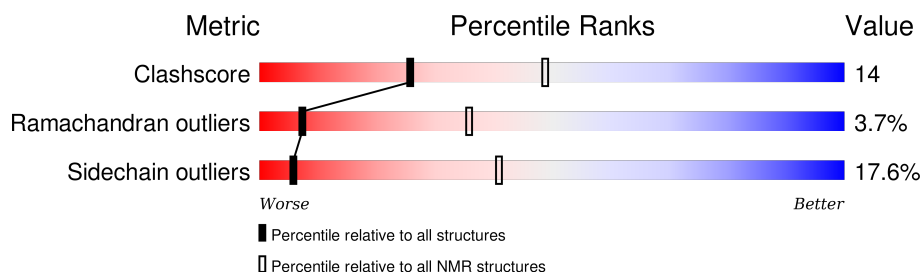
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 27%.

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	67	 60% 36% •
2	B	11	 100%
3	C	11	 100%

2 Ensemble composition and analysis

This entry contains 10 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:10-A:73 (64)	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, 5, 8, 9, 10
2	4, 6, 7

3 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1452 atoms, of which 430 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Homeobox protein Hox-A13.

Mol	Chain	Residues	Atoms					Trace
1	A	67	Total	C	H	N	O	0
			751	360	177	114	100	

- Molecule 2 is a DNA chain called DNA (5'-D(*CP*AP*AP*AP*TP*AP*AP*AP*AP*TP*C)-3').

Mol	Chain	Residues	Atoms						Trace
2	B	11	Total	C	H	N	O	P	0
			346	108	124	45	59	10	

- Molecule 3 is a DNA chain called DNA (5'-D(P*GP*AP*TP*TP*TP*TP*AP*TP*TP*TP*G)-3').

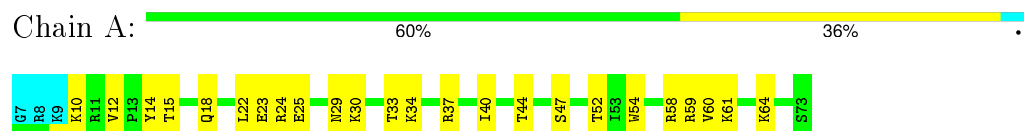
Mol	Chain	Residues	Atoms						Trace
3	C	11	Total	C	H	N	O	P	0
			355	110	129	34	71	11	

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: Homeobox protein Hox-A13



- Molecule 2: DNA (5'-D(*CP*AP*AP*AP*TP*AP*AP*AP*AP*TP*C)-3')



- Molecule 3: DNA (5'-D(P*GP*AP*TP*TP*TP*TP*AP*TP*TP*TP*G)-3')

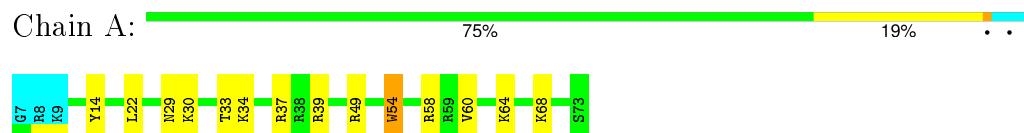


4.2 Scores per residue for each member of the ensemble

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

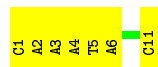
4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Homeobox protein Hox-A13



- Molecule 2: DNA (5'-D(*CP*AP*AP*AP*TP*AP*AP*AP*AP*TP*C)-3')

Chain B:  36% 64%



- Molecule 3: DNA (5'-D(P*GP*AP*TP*TP*TP*TP*AP*TP*TP*TP*G)-3')

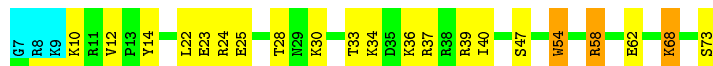
Chain C:  27% 73%



4.2.2 Score per residue for model 2

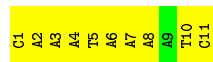
- Molecule 1: Homeobox protein Hox-A13

Chain A:  64% 27% . .



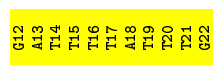
- Molecule 2: DNA (5'-D(*CP*AP*AP*AP*TP*AP*AP*AP*AP*TP*C)-3')

Chain B:  9% 91%



- Molecule 3: DNA (5'-D(P*GP*AP*TP*TP*TP*TP*AP*TP*TP*TP*G)-3')

Chain C:  100%



4.2.3 Score per residue for model 3

- Molecule 1: Homeobox protein Hox-A13

Chain A:  64% 31% .

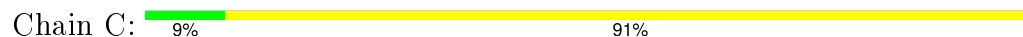


- Molecule 2: DNA (5'-D(*CP*AP*AP*AP*TP*AP*AP*AP*AP*TP*C)-3')

Chain B:  18% 82%

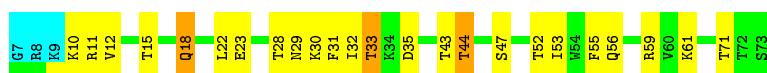


- Molecule 3: DNA (5'-D(P*GP*AP*TP*TP*TP*TP*AP*TP*TP*TP*G)-3')

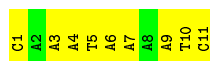


4.2.4 Score per residue for model 4

- Molecule 1: Homeobox protein Hox-A13



- Molecule 2: DNA (5'-D(*CP*AP*AP*AP*TP*AP*AP*AP*TP*C)-3')



- Molecule 3: DNA (5'-D(P*GP*AP*TP*TP*TP*TP*AP*TP*TP*TP*G)-3')

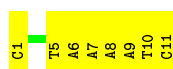


4.2.5 Score per residue for model 5

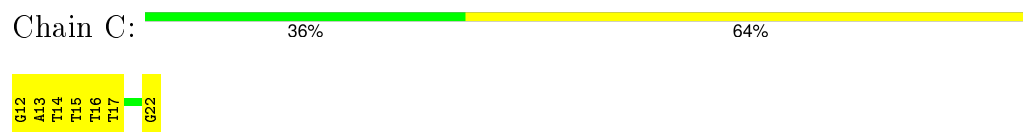
- Molecule 1: Homeobox protein Hox-A13



- Molecule 2: DNA (5'-D(*CP*AP*AP*AP*TP*AP*AP*AP*TP*C)-3')

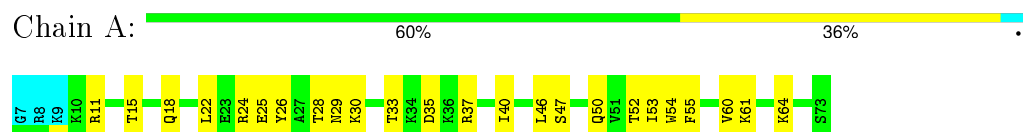


- Molecule 3: DNA (5'-D(P*GP*AP*TP*TP*TP*TP*AP*TP*TP*TP*G)-3')



4.2.6 Score per residue for model 6

- Molecule 1: Homeobox protein Hox-A13



- Molecule 2: DNA (5'-D(*CP*AP*AP*AP*TP*AP*AP*AP*AP*TP*C)-3')

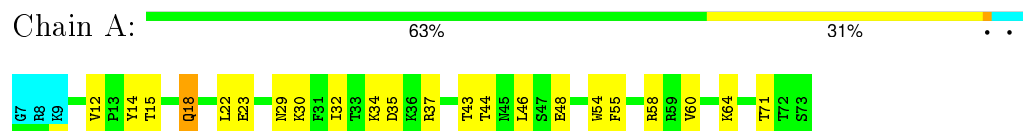


- Molecule 3: DNA (5'-D(P*GP*AP*TP*TP*TP*TP*AP*TP*TP*TP*G)-3')



4.2.7 Score per residue for model 7

- Molecule 1: Homeobox protein Hox-A13



- Molecule 2: DNA (5'-D(*CP*AP*AP*AP*TP*AP*AP*AP*AP*TP*C)-3')



- Molecule 3: DNA (5'-D(P*GP*AP*TP*TP*TP*TP*AP*TP*TP*TP*G)-3')



G12
A13
T14
T15
T16
T17
A18
T19
T20
T21
G22

4.2.8 Score per residue for model 8

- Molecule 1: Homeobox protein Hox-A13

Chain A:  63% 31%

G7 R8 K9 K10 T15 Q18 L22 E23 R24 K30 F31 K36 T44 M45 L46 S47 T52 I53 M54 F55 R58 R59 Y60 K61 K64 T71 T72 S73

- Molecule 2: DNA (5'-D(*CP*AP*AP*AP*TP*AP*AP*AP*AP*TP*C)-3')

Chain B:  100%

G1 A2 A3 A4 T5 A6 A7 A8 A9 T10 C11

- Molecule 3: DNA (5'-D(P*GP*AP*TP*TP*TP*TP*AP*TP*TP*TP*G)-3')

Chain C:  9% 91%

G12
A13
T14
T15
T16
T17
A18
T19
T20
T21
G22

4.2.9 Score per residue for model 9

- Molecule 1: Homeobox protein Hox-A13

Chain A:  66% 27%

G7 R8 K9 K10 R11 Y14 T15 L22 E23 R24 E25 K30 K34 R37 I40 E48 V51 W54 M57 R58 R59 Y60 K61 K64 K70 S73

- Molecule 2: DNA (5'-D(*CP*AP*AP*AP*TP*AP*AP*AP*AP*TP*C)-3')

Chain B:  27% 73%

G1 A2 A3 A4 T5 A6 A7 A8 A9 T10 C11

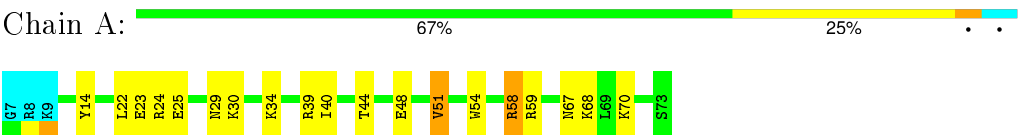
- Molecule 3: DNA (5'-D(P*GP*AP*TP*TP*TP*TP*AP*TP*TP*TP*G)-3')

Chain C:  27% 73%

G12
A13
T14
T15
T16
T17
A18
G22

4.2.10 Score per residue for model 10

- Molecule 1: Homeobox protein Hox-A13



- Molecule 2: DNA (5'-D(*CP*AP*AP*AP*TP*AP*AP*AP*AP*TP*C)-3')



- Molecule 3: DNA (5'-D(P*GP*AP*TP*TP*TP*TP*AP*TP*TP*TP*G)-3')



5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CNS	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)	2ld5_cs.str
Number of chemical shift lists	1
Total number of shifts	423
Number of shifts mapped to atoms	398
Number of unparsed shifts	0
Number of shifts with mapping errors	25
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	27%

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	550	164	596	8±2
2	B	222	124	125	10±2
3	C	226	129	129	15±4
All	All	9980	4170	8500	250

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 14.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:53:ILE:HG23	3:C:19:DT:H71	0.87	1.44	3	2
2:B:3:DA:H1'	2:B:4:DA:H5'	0.79	1.54	10	3
2:B:4:DA:H2''	2:B:5:DT:H71	0.78	1.56	3	3
2:B:11:DC:O2	3:C:12:DG:N2	0.77	2.17	4	10
2:B:1:DC:O2	3:C:22:DG:N2	0.77	2.18	4	10
1:A:64:LYS:NZ	3:C:15:DT:H3'	0.70	2.01	8	6
3:C:15:DT:H2''	3:C:16:DT:C5	0.69	2.23	9	8
2:B:1:DC:H2''	2:B:2:DA:C8	0.68	2.23	1	4
1:A:53:ILE:HA	3:C:19:DT:C7	0.67	2.20	4	1
2:B:5:DT:H2''	2:B:6:DA:C8	0.66	2.25	10	8
3:C:13:DA:H2''	3:C:14:DT:C6	0.66	2.26	2	5
1:A:53:ILE:HG12	3:C:19:DT:H71	0.65	1.67	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:15:DT:H2"	3:C:16:DT:C6	0.64	2.28	4	6
3:C:12:DG:H2"	3:C:13:DA:C8	0.64	2.28	10	10
3:C:17:DT:H2"	3:C:18:DA:C8	0.64	2.27	2	4
3:C:21:DT:H2"	3:C:22:DG:C8	0.63	2.28	4	5
1:A:14:TYR:HB2	3:C:17:DT:H5"	0.61	1.72	7	1
1:A:54:TRP:CZ2	3:C:17:DT:H5"	0.60	2.31	2	2
2:B:9:DA:H2"	2:B:10:DT:H71	0.60	1.74	8	2
1:A:64:LYS:HZ1	3:C:15:DT:H3'	0.60	1.56	1	1
3:C:13:DA:H2"	3:C:14:DT:C5	0.59	2.33	2	2
1:A:68:LYS:NZ	3:C:14:DT:H3'	0.58	2.14	1	3
1:A:23:GLU:HG2	1:A:58:ARG:HD2	0.58	1.75	2	1
2:B:3:DA:H2'	2:B:3:DA:OP2	0.57	2.00	10	2
1:A:18:GLN:HB2	1:A:44:THR:HG21	0.57	1.77	7	2
1:A:53:ILE:HG23	3:C:19:DT:C7	0.56	2.25	3	3
3:C:20:DT:H2"	3:C:21:DT:C6	0.56	2.34	3	2
1:A:10:LYS:HG3	3:C:14:DT:O2	0.56	2.01	8	2
2:B:10:DT:H2"	2:B:11:DC:C6	0.56	2.36	3	3
1:A:34:LYS:HA	1:A:37:ARG:HG2	0.56	1.76	7	3
2:B:2:DA:H2"	2:B:3:DA:C8	0.55	2.37	2	4
2:B:7:DA:H2"	2:B:8:DA:C8	0.55	2.36	8	8
3:C:22:DG:OP2	3:C:22:DG:H8	0.55	1.85	10	1
1:A:10:LYS:HD3	3:C:15:DT:H5'	0.55	1.79	9	1
3:C:18:DA:H2"	3:C:19:DT:C6	0.55	2.37	2	2
1:A:14:TYR:CD1	3:C:17:DT:H5"	0.55	2.37	9	2
3:C:19:DT:H2"	3:C:20:DT:C7	0.55	2.32	8	3
1:A:61:LYS:NZ	3:C:16:DT:H3'	0.54	2.18	3	5
1:A:25:GLU:HG3	1:A:40:ILE:HD11	0.53	1.80	9	5
2:B:3:DA:H2"	2:B:4:DA:C8	0.53	2.38	8	5
3:C:18:DA:H2"	3:C:19:DT:C5	0.53	2.39	2	2
3:C:14:DT:H2"	3:C:15:DT:C6	0.52	2.39	7	2
3:C:14:DT:H2"	3:C:15:DT:C7	0.52	2.34	3	2
2:B:4:DA:H2"	2:B:5:DT:C5	0.52	2.40	1	4
1:A:32:ILE:HB	1:A:36:LYS:HB2	0.51	1.82	3	2
1:A:67:ASN:HA	1:A:70:LYS:HE2	0.51	1.82	10	1
3:C:12:DG:OP1	3:C:12:DG:H8	0.51	1.89	3	1
2:B:9:DA:H2"	2:B:10:DT:C7	0.51	2.36	8	3
3:C:16:DT:H2"	3:C:17:DT:C7	0.51	2.35	3	2
3:C:14:DT:H2"	3:C:15:DT:C5	0.51	2.41	3	6
1:A:34:LYS:O	1:A:37:ARG:HG2	0.50	2.06	9	1
1:A:12:VAL:HG13	2:B:10:DT:H5"	0.50	1.83	2	1
1:A:12:VAL:HG22	2:B:10:DT:H5'	0.50	1.81	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:9:DA:H2"	2:B:10:DT:H72	0.50	1.83	5	2
1:A:54:TRP:HZ2	3:C:17:DT:H5"	0.50	1.66	2	1
2:B:4:DA:H8	2:B:4:DA:OP2	0.50	1.89	4	1
1:A:60:VAL:HG21	2:B:5:DT:H71	0.50	1.83	7	2
1:A:64:LYS:HZ2	3:C:15:DT:H3'	0.50	1.67	8	1
1:A:12:VAL:HG13	2:B:10:DT:H4'	0.50	1.84	5	2
2:B:10:DT:H2"	2:B:11:DC:H6	0.49	1.67	6	3
2:B:6:DA:H2"	2:B:7:DA:C8	0.49	2.43	4	3
3:C:19:DT:H2"	3:C:20:DT:H71	0.49	1.83	8	2
1:A:11:ARG:HA	2:B:10:DT:H4'	0.49	1.85	9	1
2:B:4:DA:C2'	2:B:5:DT:H71	0.48	2.36	3	1
3:C:16:DT:H2"	3:C:17:DT:H72	0.48	1.85	7	2
1:A:59:ARG:HD3	2:B:3:DA:OP2	0.47	2.09	3	2
3:C:20:DT:H2"	3:C:21:DT:C5	0.47	2.44	3	3
1:A:60:VAL:HG21	2:B:5:DT:H73	0.47	1.86	1	1
3:C:12:DG:H8	3:C:12:DG:OP2	0.47	1.92	9	1
3:C:14:DT:H2"	3:C:15:DT:H71	0.47	1.86	3	2
2:B:8:DA:H2"	2:B:9:DA:C8	0.47	2.45	5	2
3:C:19:DT:H1'	3:C:20:DT:H5'	0.47	1.87	2	1
1:A:11:ARG:HD2	3:C:16:DT:O2	0.47	2.10	6	1
1:A:54:TRP:HA	1:A:57:ASN:HB2	0.47	1.87	9	1
2:B:4:DA:H2"	2:B:5:DT:H72	0.45	1.89	2	1
1:A:56:GLN:O	1:A:59:ARG:HG2	0.45	2.12	4	1
3:C:19:DT:H2"	3:C:20:DT:C5	0.45	2.46	3	3
1:A:64:LYS:HZ3	3:C:15:DT:H3'	0.45	1.66	8	1
2:B:3:DA:C1'	2:B:4:DA:H5'	0.45	2.35	10	1
3:C:18:DA:H2"	3:C:19:DT:C7	0.45	2.42	10	2
1:A:14:TYR:CE1	3:C:17:DT:H5"	0.45	2.46	9	1
1:A:18:GLN:HA	1:A:44:THR:HG21	0.45	1.87	8	1
1:A:53:ILE:HA	3:C:19:DT:H73	0.44	1.89	4	1
1:A:57:ASN:O	1:A:60:VAL:HG12	0.44	2.13	5	1
1:A:48:GLU:O	1:A:51:VAL:HG12	0.44	2.12	9	2
1:A:10:LYS:HA	2:B:11:DC:H5"	0.44	1.90	9	1
2:B:3:DA:OP2	2:B:3:DA:H2'	0.43	2.13	3	2
3:C:18:DA:H2"	3:C:19:DT:H5'	0.43	1.90	4	1
1:A:53:ILE:HG23	3:C:19:DT:H73	0.43	1.90	8	1
3:C:20:DT:H2"	3:C:21:DT:C7	0.42	2.44	7	1
3:C:16:DT:OP2	3:C:16:DT:H2'	0.42	2.15	9	1
3:C:18:DA:H1'	3:C:19:DT:H5'	0.42	1.91	8	2
3:C:16:DT:C2'	3:C:17:DT:H72	0.42	2.45	7	1
1:A:46:LEU:HG	1:A:50:GLN:HB2	0.42	1.90	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:33:THR:HB	1:A:35:ASP:OD1	0.42	2.13	4	1
3:C:19:DT:H2''	3:C:20:DT:C6	0.42	2.50	7	1
1:A:10:LYS:HD3	3:C:15:DT:C5'	0.42	2.44	9	1
1:A:23:GLU:HG2	1:A:58:ARG:HH11	0.42	1.75	10	1
3:C:16:DT:C6	3:C:17:DT:H72	0.41	2.51	6	1
3:C:15:DT:H2''	3:C:16:DT:C7	0.41	2.45	10	1
1:A:32:ILE:HB	1:A:36:LYS:CB	0.41	2.45	3	1
1:A:10:LYS:O	2:B:10:DT:H4'	0.41	2.15	2	1
2:B:9:DA:C2'	2:B:10:DT:H72	0.41	2.46	4	1
1:A:44:THR:HB	1:A:46:LEU:CD2	0.40	2.46	7	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	63/67 (94%)	56±1 (88±1%)	5±1 (8±1%)	2±1 (4±1%)	7	36
All	All	630/670 (94%)	555 (88%)	52 (8%)	23 (4%)	7	36

All 6 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	30	LYS	10
1	A	29	ASN	6
1	A	14	TYR	4
1	A	71	THR	1
1	A	45	ASN	1
1	A	10	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	62/64 (97%)	51±3 (82±4%)	11±3 (18±4%)	6	41
All	All	620/640 (97%)	511 (82%)	109 (18%)	6	41

All 36 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	54	TRP	9
1	A	22	LEU	9
1	A	58	ARG	8
1	A	15	THR	7
1	A	33	THR	6
1	A	24	ARG	5
1	A	52	THR	5
1	A	47	SER	5
1	A	28	THR	4
1	A	55	PHE	4
1	A	43	THR	4
1	A	23	GLU	3
1	A	44	THR	3
1	A	39	ARG	3
1	A	71	THR	3
1	A	18	GLN	3
1	A	73	SER	3
1	A	31	PHE	2
1	A	51	VAL	2
1	A	36	LYS	2
1	A	32	ILE	2
1	A	59	ARG	2
1	A	35	ASP	2
1	A	11	ARG	1
1	A	19	LEU	1
1	A	62	GLU	1
1	A	69	LEU	1
1	A	37	ARG	1
1	A	14	TYR	1
1	A	49	ARG	1
1	A	70	LYS	1
1	A	68	LYS	1
1	A	60	VAL	1
1	A	34	LYS	1

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Mol	Chain	Res	Type	Models (Total)
1	A	48	GLU	1
1	A	26	TYR	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 27% for the well-defined parts and 28% for the entire structure.

7.1 Chemical shift list 1

File name: 2ld5_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	423
Number of shifts mapped to atoms	398
Number of unparsed shifts	0
Number of shifts with mapping errors	25
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- Residue not found in structure. All 25 occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	4	MET	N	121.938	0.033	1
A	3	HIS	C	174.771	0.0	1
A	5	LEU	H	8.3	0.003	1
A	6	GLU	HB3	1.997	0.0	2
A	5	LEU	HA	4.329	0.0	1
A	4	MET	C	175.951	0.0	1
A	6	GLU	N	121.823	0.161	1
A	4	MET	H	8.341	0.003	1
A	6	GLU	HB2	2.275	0.0	2
A	4	MET	CB	32.67	0.231	1
A	6	GLU	CA	56.832	0.11	1
A	6	GLU	C	176.841	0.0	1
A	3	HIS	HB2	3.156	0.0	2
A	5	LEU	CA	55.453	0.159	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	3	HIS	CB	29.79	0.0	1
A	6	GLU	HA	4.274	0.0	1
A	5	LEU	HB2	1.595	0.0	2
A	4	MET	CA	55.919	0.131	1
A	6	GLU	H	8.306	0.004	1
A	3	HIS	HA	4.68	0.0	1
A	5	LEU	N	123.735	0.031	1
A	5	LEU	C	177.221	0.0	1
A	6	GLU	CB	30.142	0.279	1
A	5	LEU	CB	42.083	0.256	1
A	3	HIS	CA	55.866	0.037	1

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	71	-0.71 ± 0.32	Should be applied
$^{13}\text{C}_\beta$	70	0.37 ± 0.08	None needed (< 0.5 ppm)
$^{13}\text{C}'$	69	-0.59 ± 0.27	Should be applied
^{15}N	69	0.06 ± 0.29	None needed (< 0.5 ppm)

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 27%, i.e. 368 atoms were assigned a chemical shift out of a possible 1343. 0 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	276/318 (87%)	87/127 (69%)	126/128 (98%)	63/63 (100%)
Sidechain	87/555 (16%)	21/327 (6%)	66/186 (35%)	0/42 (0%)
Aromatic	5/46 (11%)	4/24 (17%)	0/21 (0%)	1/1 (100%)
Overall	368/1343 (27%)	112/726 (15%)	192/487 (39%)	64/130 (49%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 28%, i.e. 386 atoms were assigned a chemical shift out of a possible 1389. 0 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	290/333 (87%)	92/133 (69%)	132/134 (99%)	66/66 (100%)
Sidechain	91/586 (16%)	23/346 (7%)	68/194 (35%)	0/46 (0%)
Aromatic	5/46 (11%)	4/24 (17%)	0/21 (0%)	1/1 (100%)
Overall	386/1389 (28%)	119/751 (16%)	200/501 (40%)	67/137 (49%)

7.1.4 Statistically unusual chemical shifts [i](#)

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

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	58	ARG	HB2	-0.54	3.15 – 0.45	-8.7
1	A	22	LEU	HB2	-1.01	3.32 – -0.08	-7.7

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:

