



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 09:11 PM BST

PDB ID : 2HM8
Title : Solution Structure of the C-terminal MA-3 domain of Pdcd4
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Deposited on : 2006-07-11

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 ⓘ 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

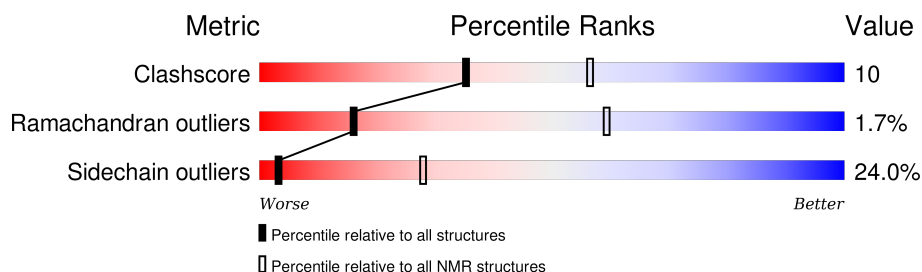
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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	136	

2 Ensemble composition and analysis

This entry contains 49 models. Model 33 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:327-A:415, A:421-A:449 (118)	0.40	33

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 8 clusters and 5 single-model clusters were found.

Cluster number	Models
1	3, 4, 6, 7, 18, 19, 29, 35, 40, 45, 48
2	1, 10, 14, 22, 27, 32, 33, 34, 37, 43
3	2, 5, 16, 21, 25, 30, 39, 42
4	11, 17, 20, 26, 49
5	13, 28, 31
6	9, 24, 38
7	12, 15
8	8, 36
Single-model clusters	23; 41; 44; 46; 47

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2197 atoms, of which 1111 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Pdcd4 C-terminal MA-3 domain.

Mol	Chain	Residues	Atoms						Trace
1	A	136	Total	C	H	N	O	S	0
			2197	694	1111	177	208	7	

There are 5 discrepancies between the modelled and reference sequences:

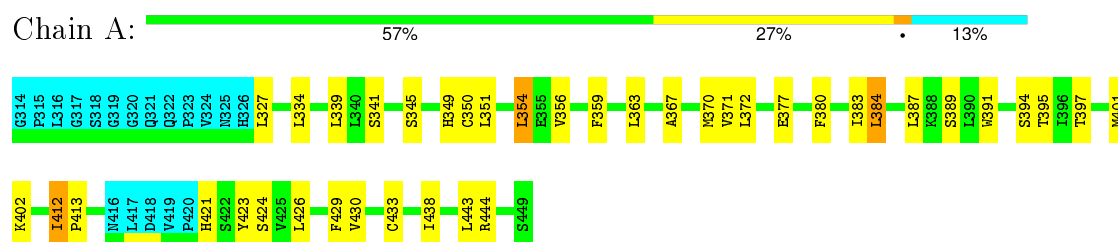
Chain	Residue	Modelled	Actual	Comment	Reference
A	314	GLY	-	INSERTION	UNP Q61823
A	315	PRO	-	INSERTION	UNP Q61823
A	316	LEU	-	INSERTION	UNP Q61823
A	317	GLY	-	INSERTION	UNP Q61823
A	318	SER	-	INSERTION	UNP Q61823

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: Pdcd4 C-terminal MA-3 domain

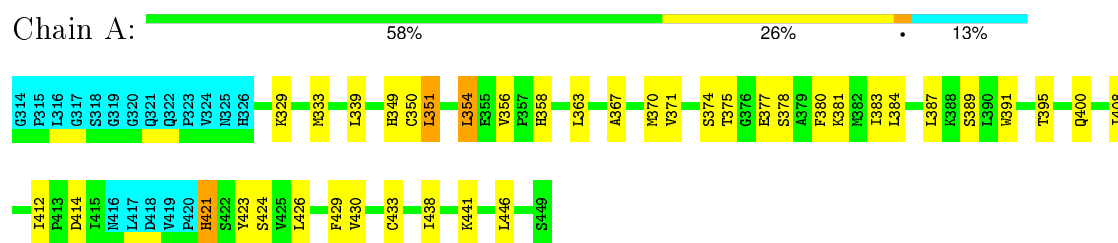


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

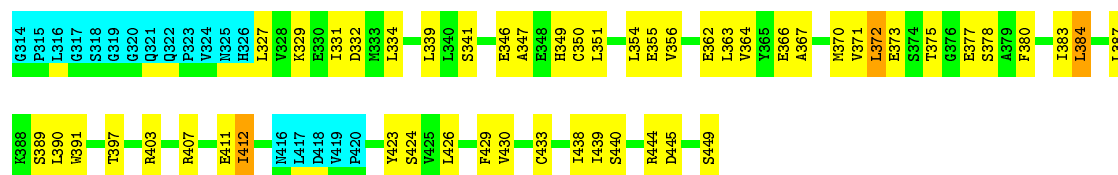
- Molecule 1: Pdcd4 C-terminal MA-3 domain



4.2.2 Score per residue for model 2

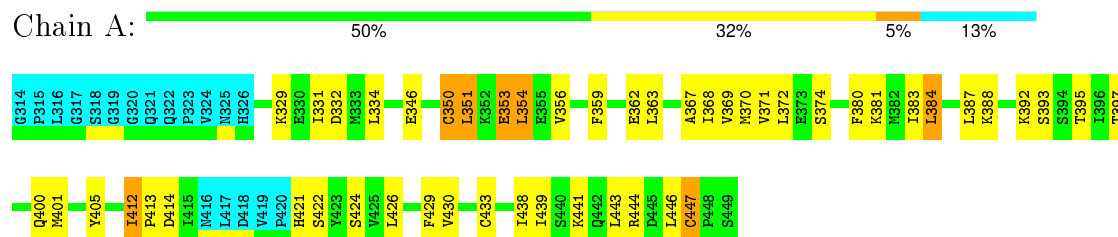
- Molecule 1: Pdcd4 C-terminal MA-3 domain





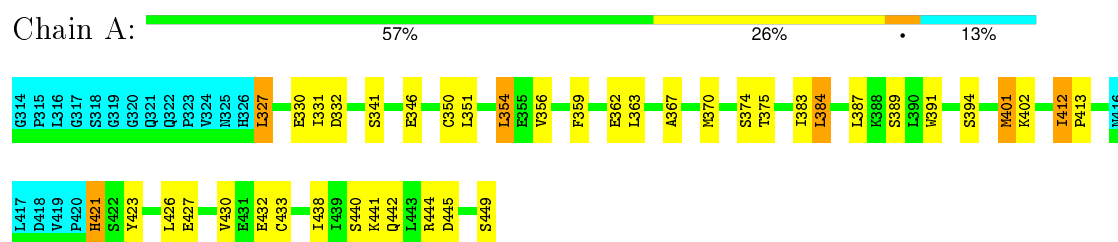
4.2.3 Score per residue for model 3

- Molecule 1: Pdcd4 C-terminal MA-3 domain



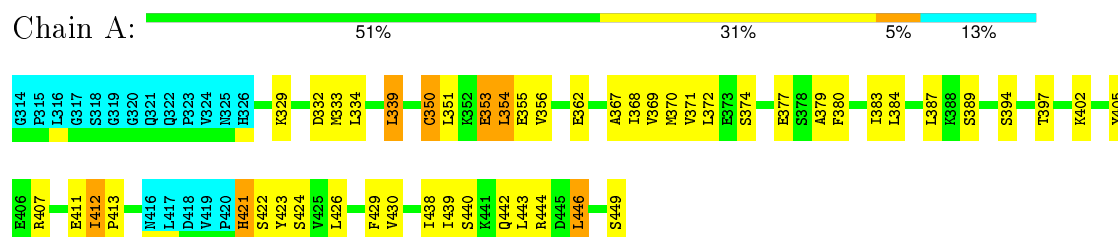
4.2.4 Score per residue for model 4

- Molecule 1: Pdcd4 C-terminal MA-3 domain



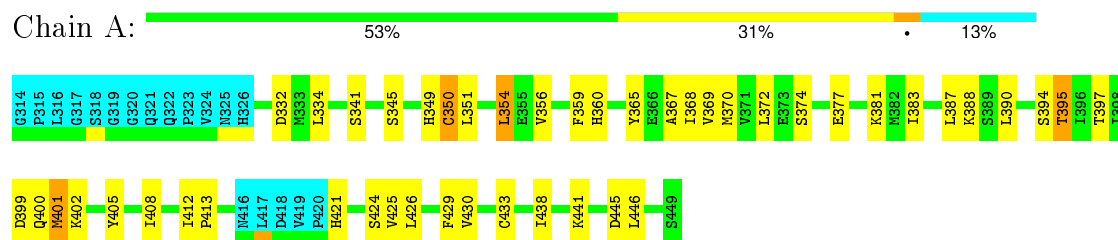
4.2.5 Score per residue for model 5

- Molecule 1: Pdcd4 C-terminal MA-3 domain



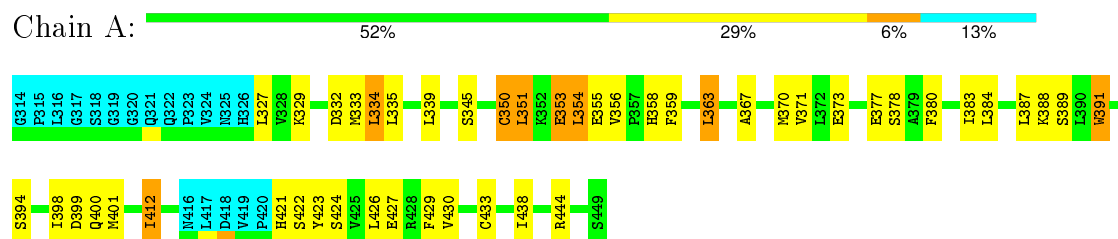
4.2.6 Score per residue for model 6

- Molecule 1: Pdcd4 C-terminal MA-3 domain



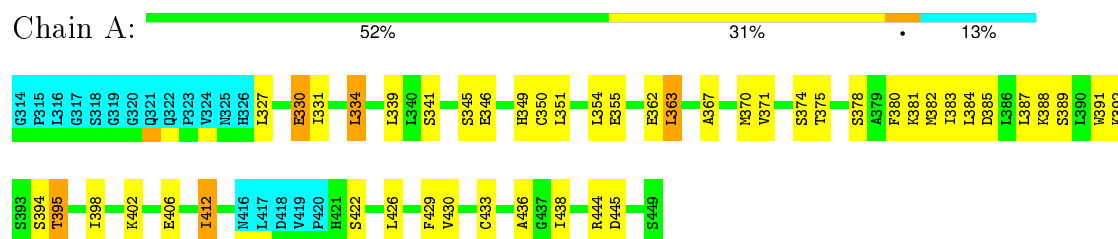
4.2.7 Score per residue for model 7

- Molecule 1: Pdcd4 C-terminal MA-3 domain



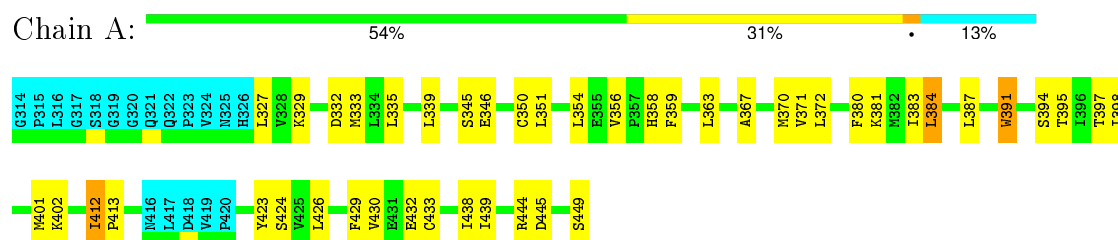
4.2.8 Score per residue for model 8

- Molecule 1: Pdcd4 C-terminal MA-3 domain



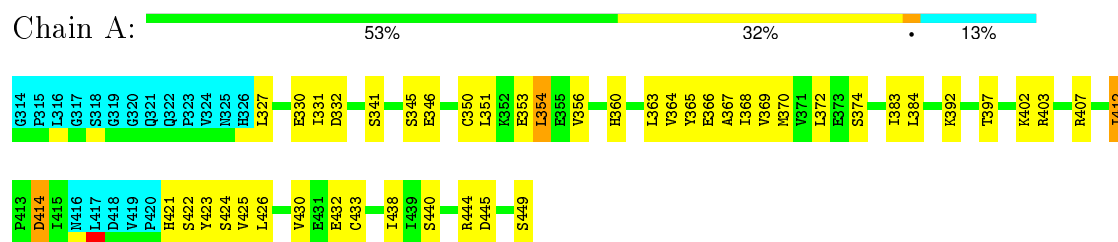
4.2.9 Score per residue for model 9

- Molecule 1: Pdcd4 C-terminal MA-3 domain



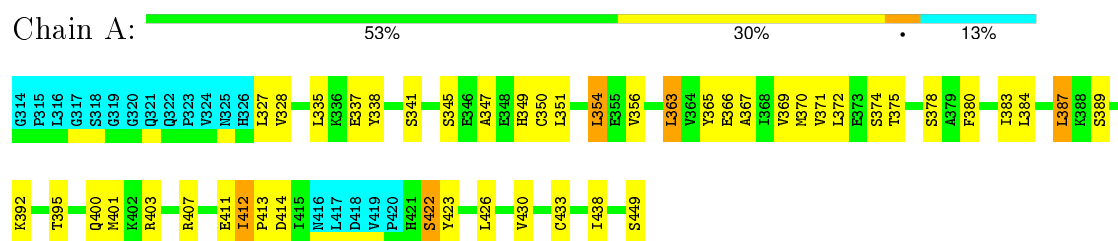
4.2.10 Score per residue for model 10

- Molecule 1: Pdcd4 C-terminal MA-3 domain



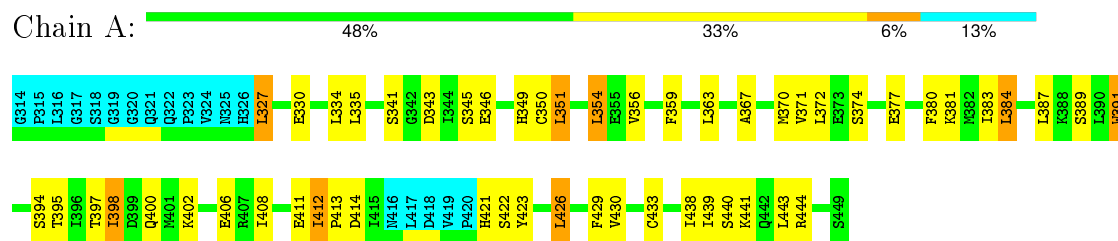
4.2.11 Score per residue for model 11

- Molecule 1: Pdcd4 C-terminal MA-3 domain



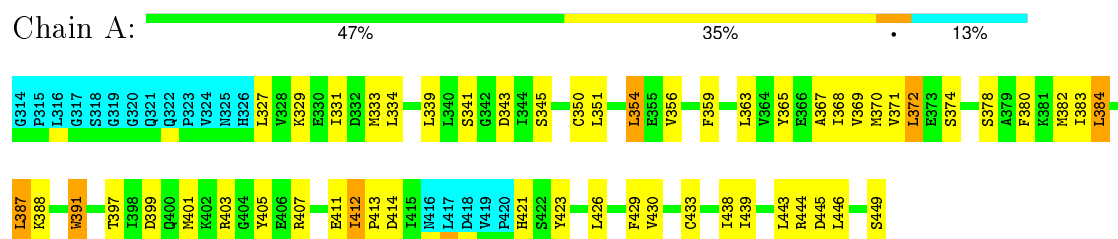
4.2.12 Score per residue for model 12

- Molecule 1: Pdcd4 C-terminal MA-3 domain



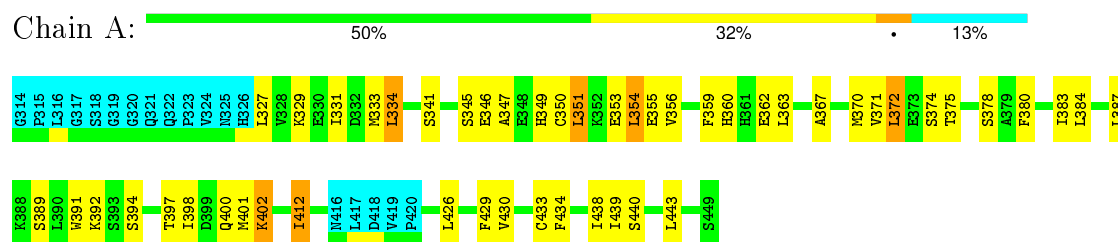
4.2.13 Score per residue for model 13

- Molecule 1: Pdcd4 C-terminal MA-3 domain



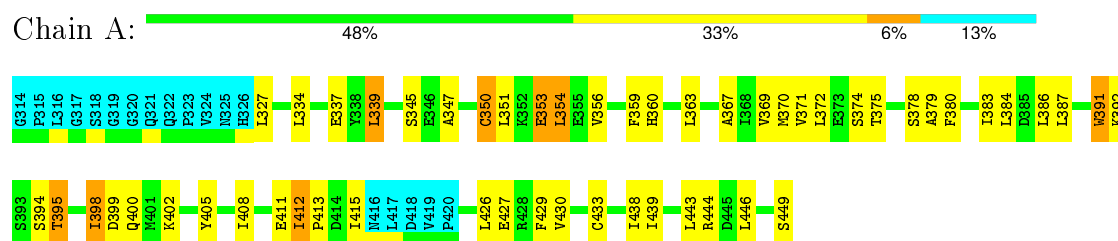
4.2.14 Score per residue for model 14

- Molecule 1: Pdcd4 C-terminal MA-3 domain



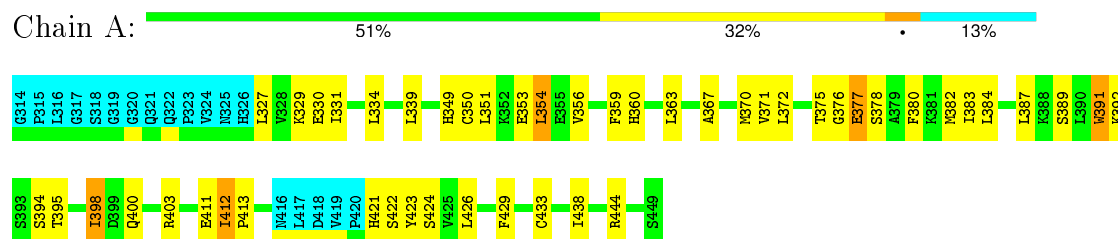
4.2.15 Score per residue for model 15

- Molecule 1: Pdcd4 C-terminal MA-3 domain



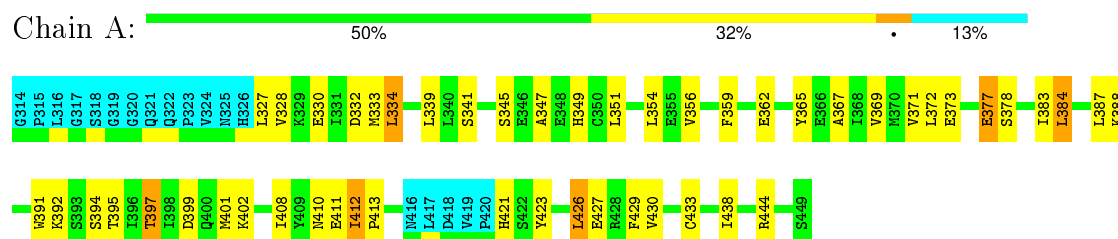
4.2.16 Score per residue for model 16

- Molecule 1: Pdcd4 C-terminal MA-3 domain



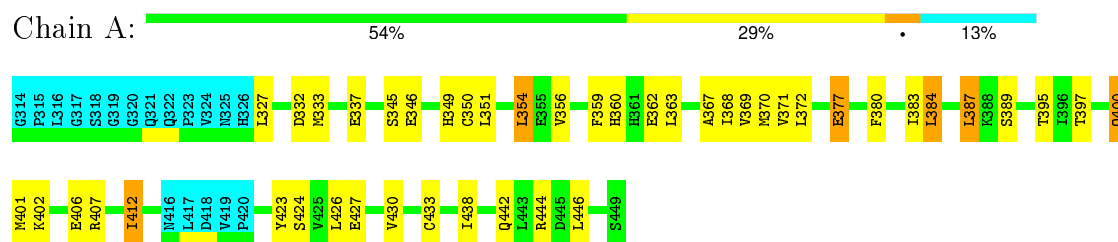
4.2.17 Score per residue for model 17

- Molecule 1: Pdcd4 C-terminal MA-3 domain



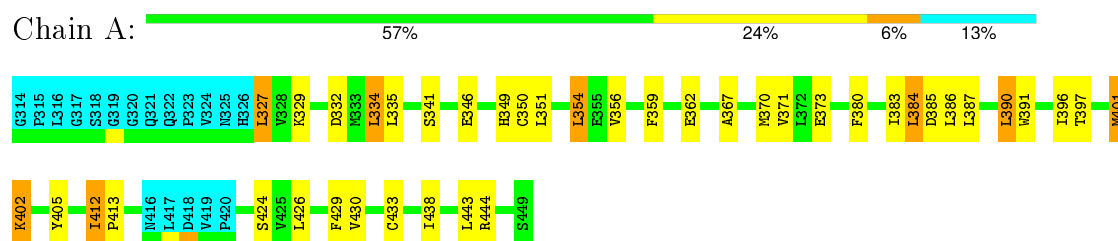
4.2.18 Score per residue for model 18

- Molecule 1: Pdcd4 C-terminal MA-3 domain



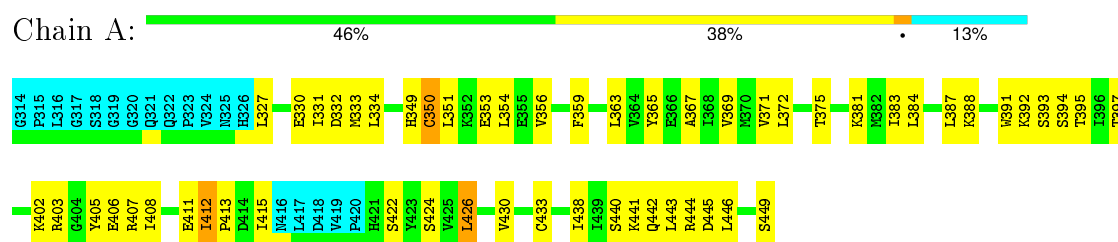
4.2.19 Score per residue for model 19

- Molecule 1: Pdcd4 C-terminal MA-3 domain



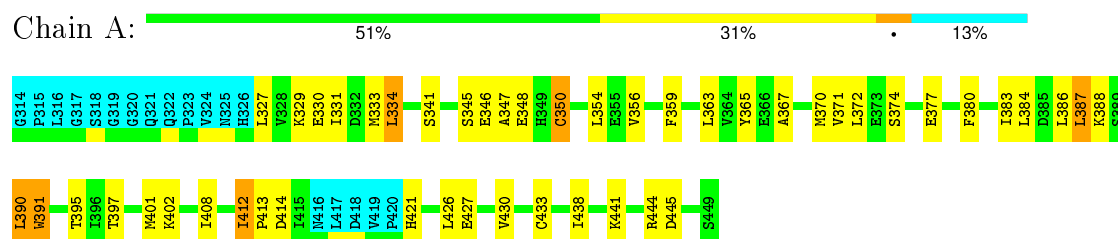
4.2.20 Score per residue for model 20

- Molecule 1: Pdcd4 C-terminal MA-3 domain



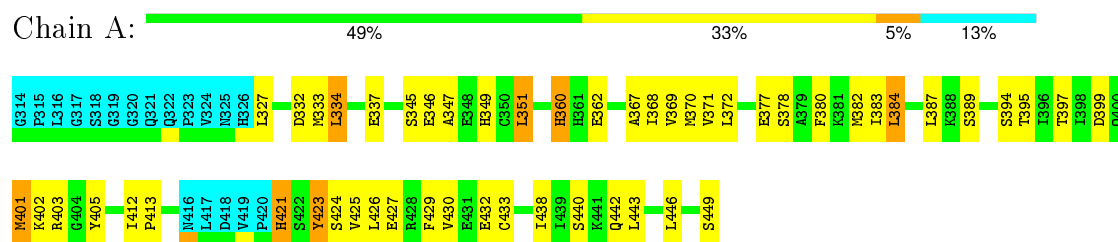
4.2.21 Score per residue for model 21

- Molecule 1: Pdcd4 C-terminal MA-3 domain



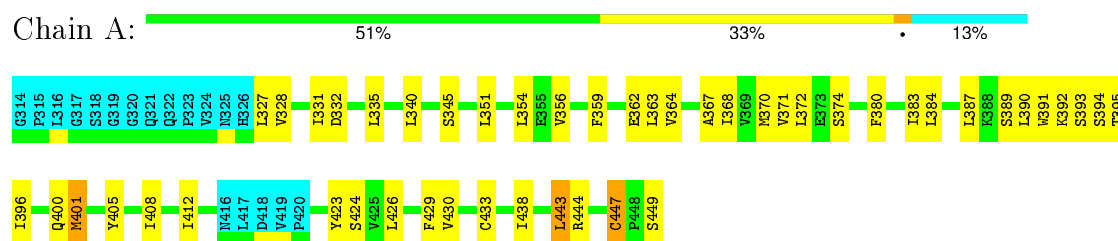
4.2.22 Score per residue for model 22

- Molecule 1: Pdcd4 C-terminal MA-3 domain



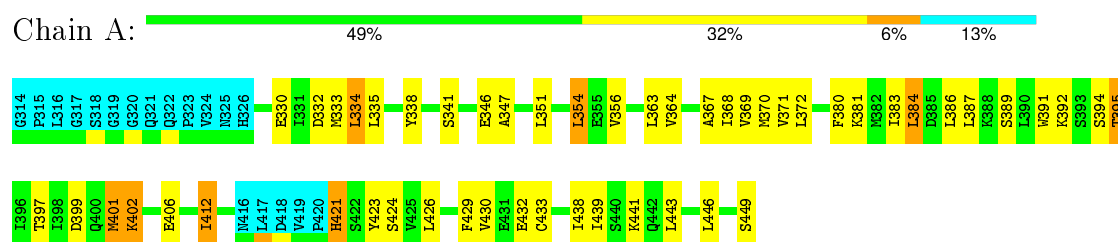
4.2.23 Score per residue for model 23

- Molecule 1: Pdcd4 C-terminal MA-3 domain



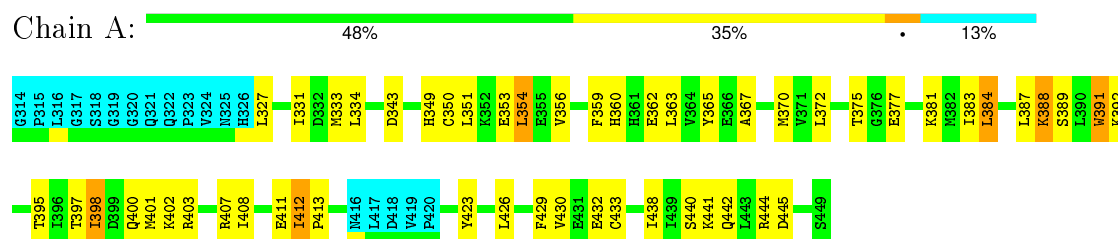
4.2.24 Score per residue for model 24

- Molecule 1: Pdcd4 C-terminal MA-3 domain



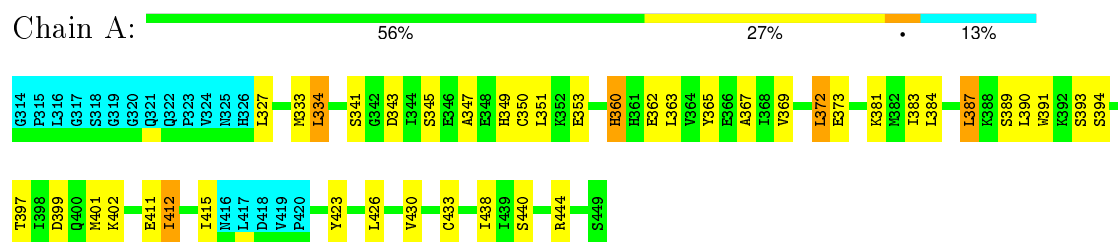
4.2.25 Score per residue for model 25

- Molecule 1: Pdcd4 C-terminal MA-3 domain



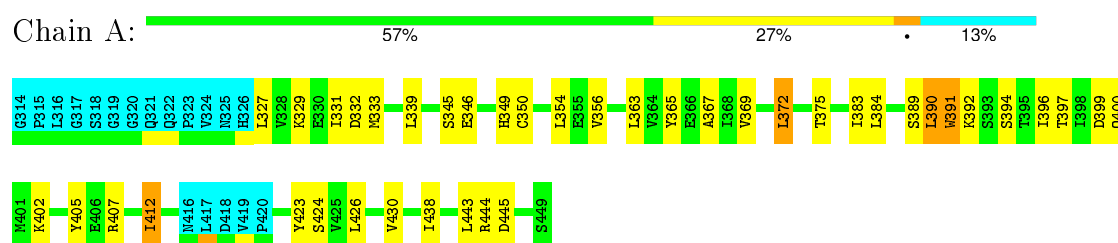
4.2.26 Score per residue for model 26

- Molecule 1: Pdcd4 C-terminal MA-3 domain



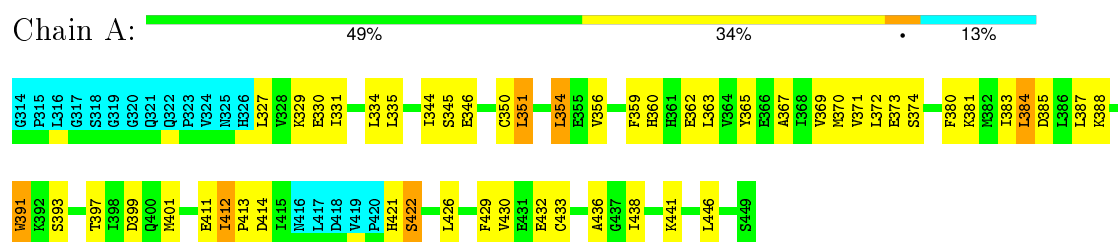
4.2.27 Score per residue for model 27

- Molecule 1: Pdcd4 C-terminal MA-3 domain



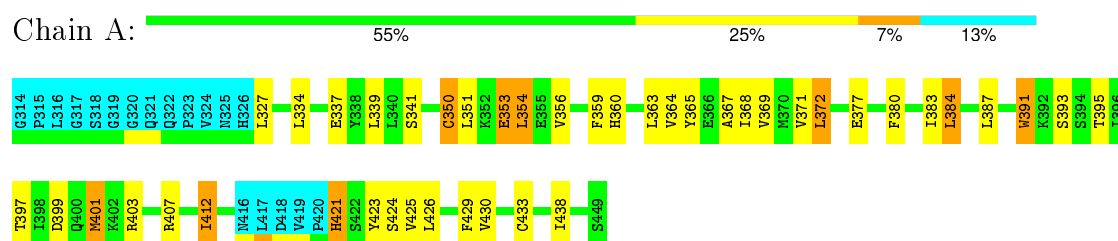
4.2.28 Score per residue for model 28

- Molecule 1: Pdcd4 C-terminal MA-3 domain



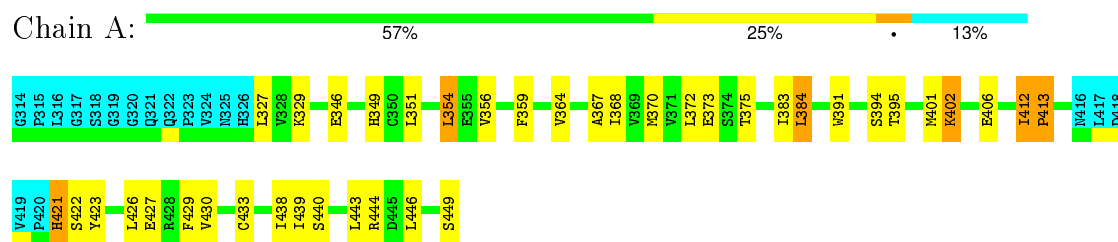
4.2.29 Score per residue for model 29

- Molecule 1: Pdcd4 C-terminal MA-3 domain



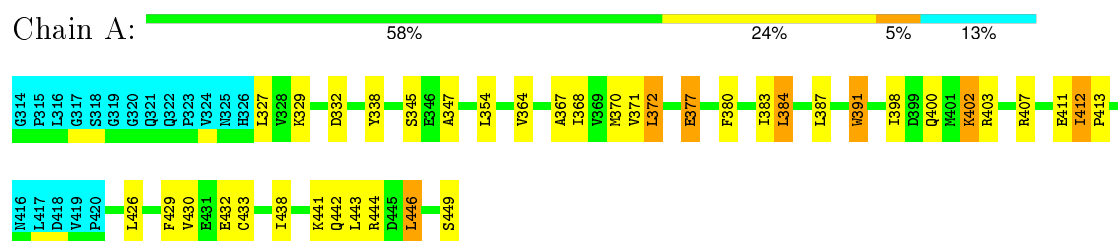
4.2.30 Score per residue for model 30

- Molecule 1: Pdcd4 C-terminal MA-3 domain



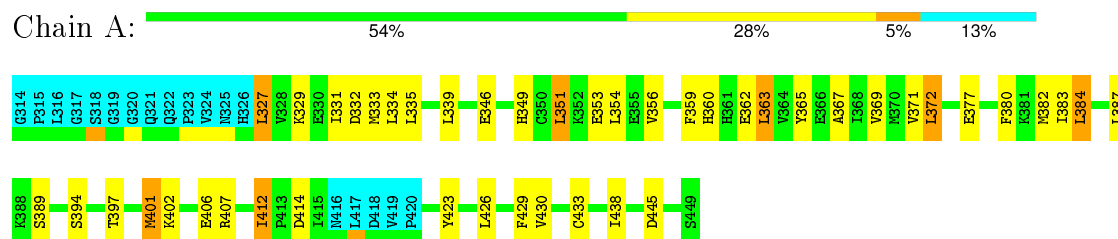
4.2.31 Score per residue for model 31

- Molecule 1: Pdcd4 C-terminal MA-3 domain



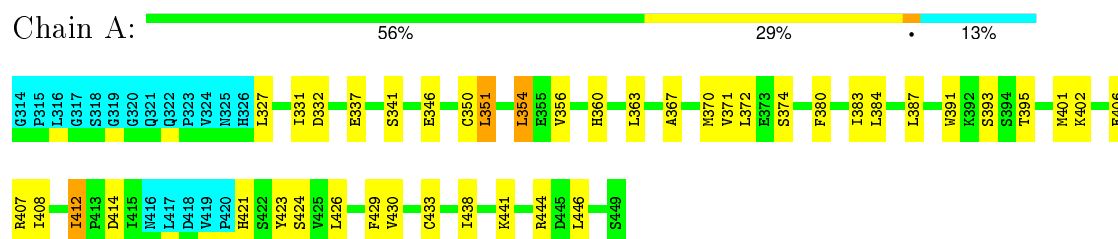
4.2.32 Score per residue for model 32

- Molecule 1: Pdcd4 C-terminal MA-3 domain



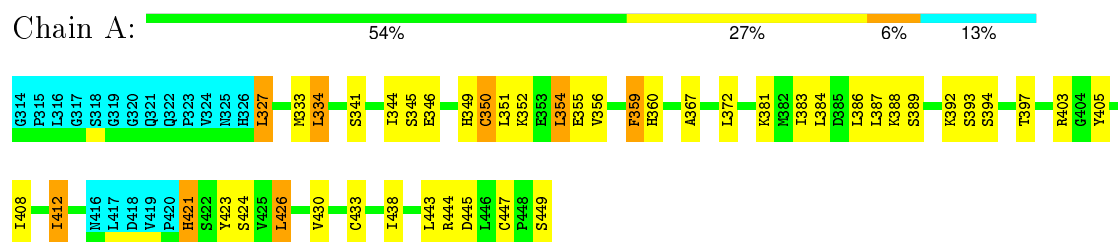
4.2.33 Score per residue for model 33 (medoid)

- Molecule 1: Pdcd4 C-terminal MA-3 domain



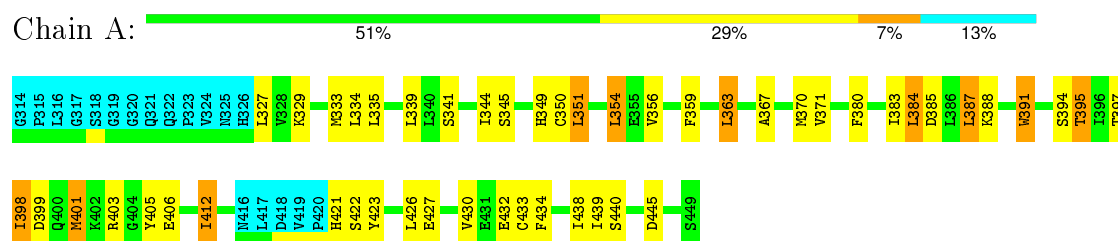
4.2.34 Score per residue for model 34

- Molecule 1: Pdcd4 C-terminal MA-3 domain



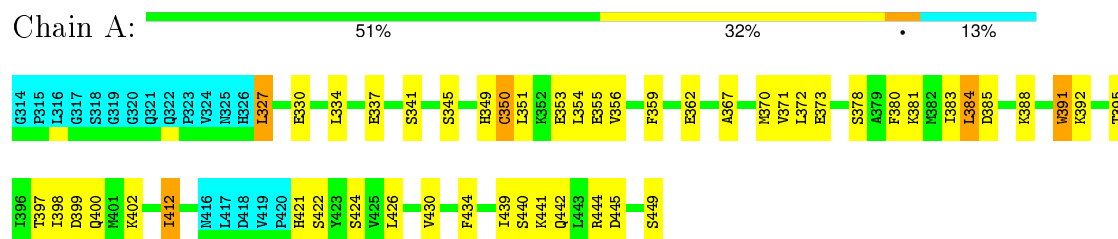
4.2.35 Score per residue for model 35

- Molecule 1: Pdcd4 C-terminal MA-3 domain



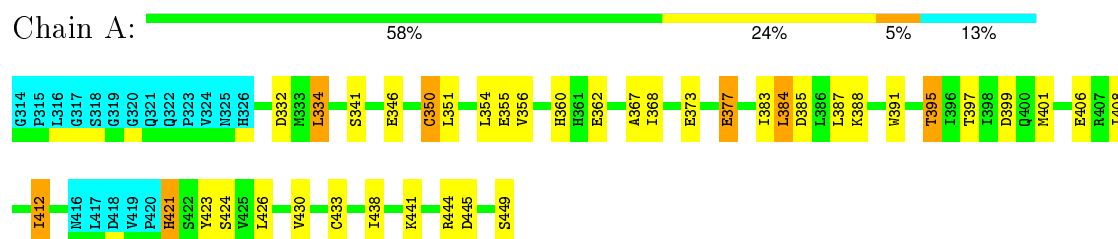
4.2.36 Score per residue for model 36

- Molecule 1: Pdcd4 C-terminal MA-3 domain



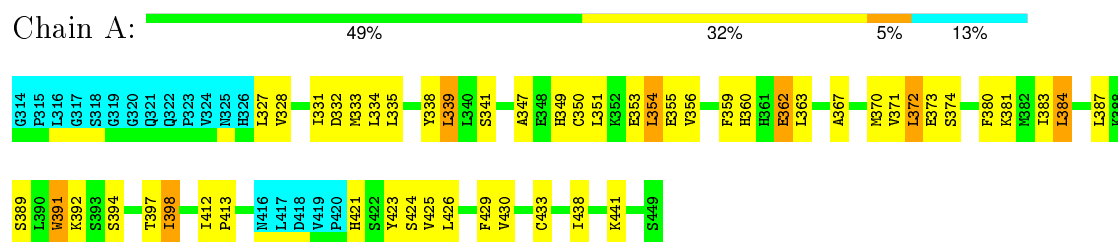
4.2.37 Score per residue for model 37

- Molecule 1: Pdcd4 C-terminal MA-3 domain



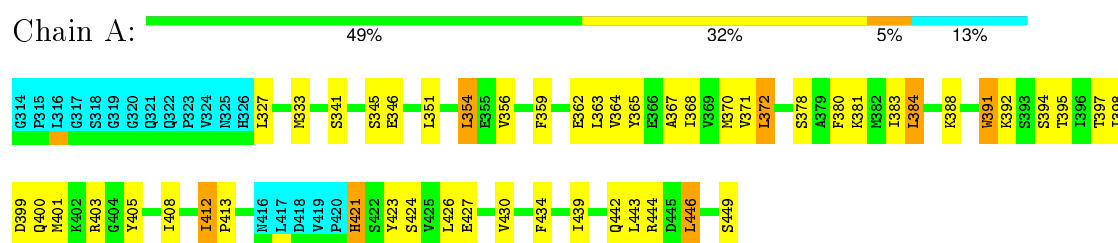
4.2.38 Score per residue for model 38

- Molecule 1: Pdcd4 C-terminal MA-3 domain



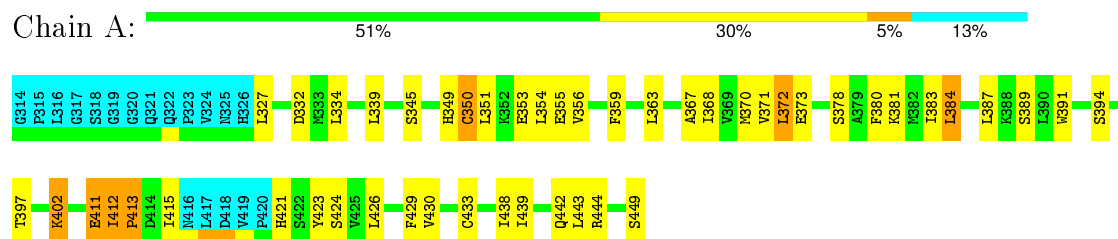
4.2.39 Score per residue for model 39

- Molecule 1: Pdcd4 C-terminal MA-3 domain



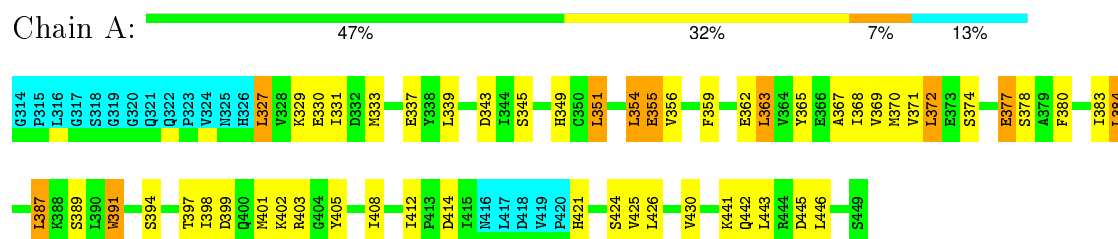
4.2.40 Score per residue for model 40

- Molecule 1: Pdcd4 C-terminal MA-3 domain



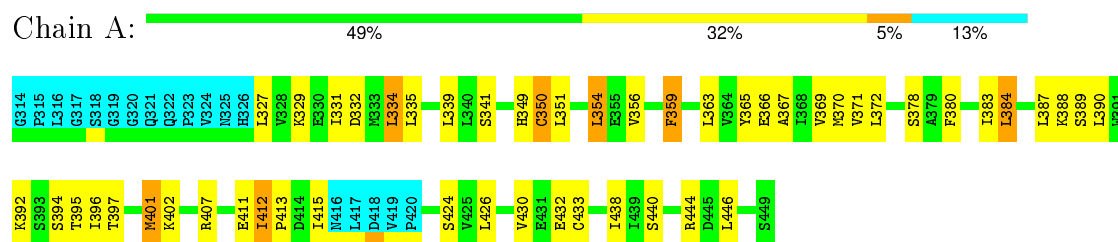
4.2.41 Score per residue for model 41

- Molecule 1: Pdcd4 C-terminal MA-3 domain



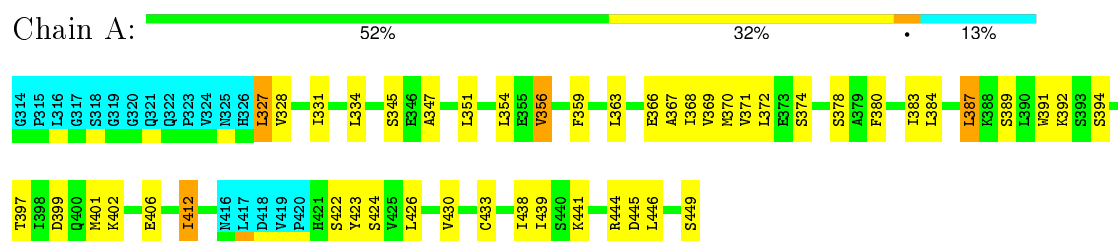
4.2.42 Score per residue for model 42

- Molecule 1: Pdcd4 C-terminal MA-3 domain



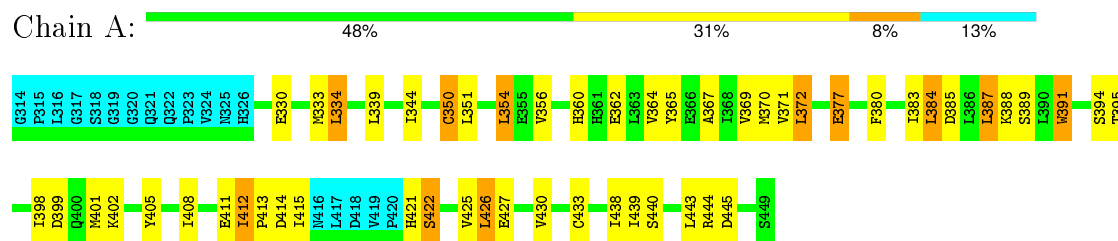
4.2.43 Score per residue for model 43

- Molecule 1: Pdcd4 C-terminal MA-3 domain



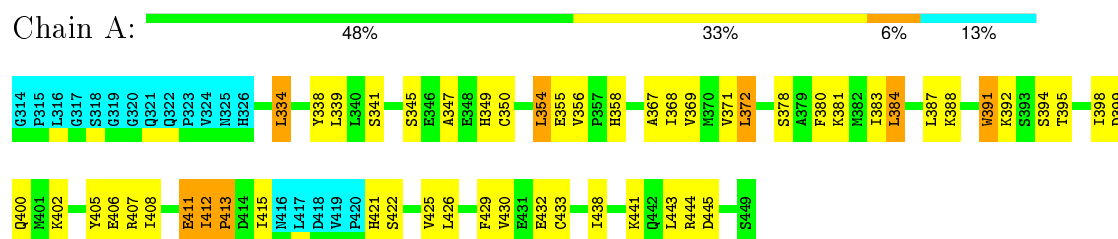
4.2.44 Score per residue for model 44

- Molecule 1: Pdcd4 C-terminal MA-3 domain



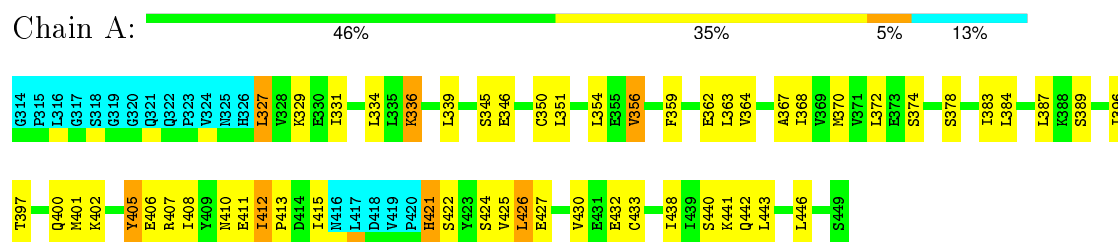
4.2.45 Score per residue for model 45

- Molecule 1: Pdcd4 C-terminal MA-3 domain



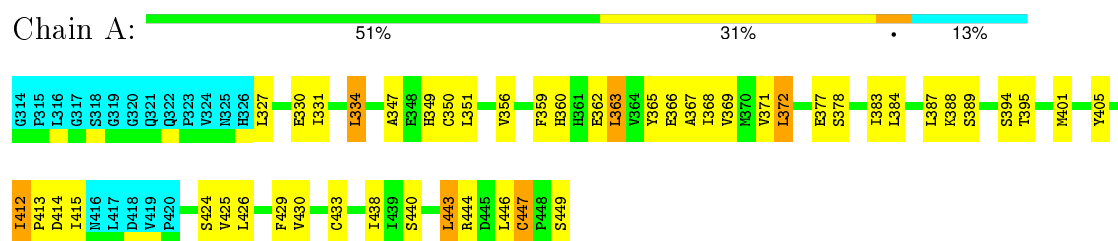
4.2.46 Score per residue for model 46

- Molecule 1: Pdcd4 C-terminal MA-3 domain



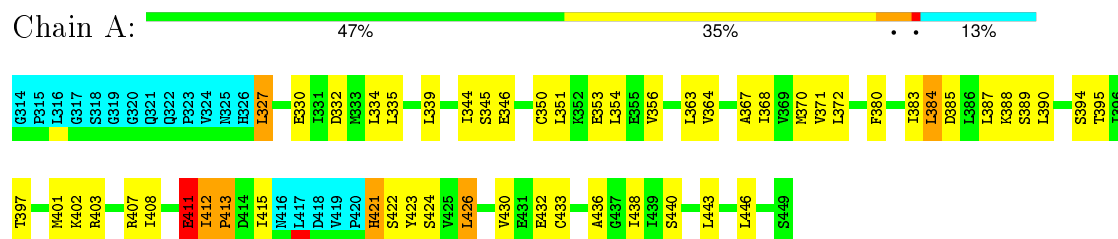
4.2.47 Score per residue for model 47

- Molecule 1: Pdcd4 C-terminal MA-3 domain



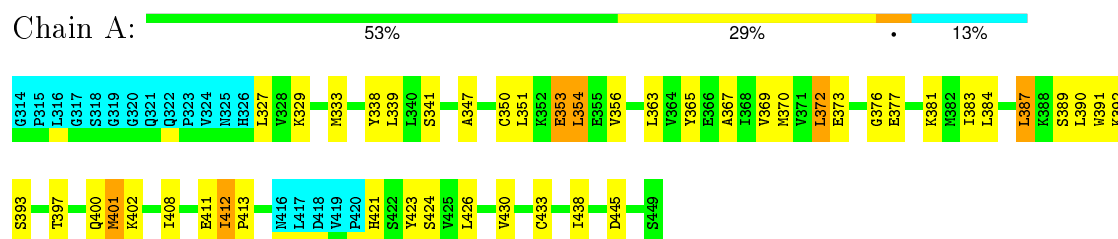
4.2.48 Score per residue for model 48

- Molecule 1: Pdcd4 C-terminal MA-3 domain



4.2.49 Score per residue for model 49

- Molecule 1: Pdcd4 C-terminal MA-3 domain



5 Refinement protocol and experimental data overview ⓘ

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

Of the 100 calculated structures, 49 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	structure solution	2.1
cyana	refinement	2.1

No chemical shift data was provided. 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	961	992	966	20±5
All	All	47089	48608	47334	982

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 10.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:331:ILE:HG23	1:A:363:LEU:HD12	0.80	1.53	25	10
1:A:351:LEU:HD12	1:A:363:LEU:HD13	0.78	1.55	43	4
1:A:367:ALA:HB1	1:A:383:ILE:HG23	0.78	1.55	25	49
1:A:351:LEU:HD13	1:A:363:LEU:HD13	0.72	1.62	23	6
1:A:364:VAL:HG12	1:A:368:ILE:HD11	0.72	1.61	23	7
1:A:327:LEU:HD11	1:A:354:LEU:HD13	0.71	1.60	12	2
1:A:368:ILE:HG22	1:A:372:LEU:HD12	0.70	1.61	40	2
1:A:327:LEU:HD21	1:A:356:VAL:HG21	0.70	1.62	46	3
1:A:408:ILE:HG21	1:A:426:LEU:HD13	0.69	1.63	23	3
1:A:351:LEU:HD23	1:A:395:THR:HG22	0.67	1.67	35	5
1:A:367:ALA:HB1	1:A:383:ILE:HD12	0.65	1.68	16	9
1:A:439:ILE:HG22	1:A:443:LEU:HD13	0.65	1.68	12	1
1:A:351:LEU:HD23	1:A:395:THR:CG2	0.64	2.23	24	12
1:A:327:LEU:HD22	1:A:359:PHE:CD2	0.64	2.27	46	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:334:LEU:HD13	1:A:363:LEU:HD12	0.64	1.68	38	1
1:A:371:VAL:HG21	1:A:380:PHE:HA	0.63	1.70	12	33
1:A:351:LEU:HD23	1:A:395:THR:HG21	0.63	1.70	30	8
1:A:367:ALA:O	1:A:383:ILE:HG21	0.63	1.94	46	4
1:A:408:ILE:CG2	1:A:426:LEU:HD11	0.63	2.23	46	9
1:A:426:LEU:O	1:A:430:VAL:HG23	0.63	1.94	30	48
1:A:351:LEU:HD11	1:A:360:HIS:CD2	0.62	2.29	14	7
1:A:408:ILE:HG21	1:A:426:LEU:HD11	0.62	1.69	46	7
1:A:354:LEU:HD12	1:A:356:VAL:HG12	0.62	1.70	35	15
1:A:339:LEU:HD21	1:A:379:ALA:HB2	0.62	1.71	5	2
1:A:334:LEU:HD13	1:A:350:CYS:HB2	0.62	1.70	40	10
1:A:372:LEU:HD23	1:A:415:ILE:HG21	0.62	1.72	42	2
1:A:335:LEU:HD21	1:A:367:ALA:HB2	0.62	1.70	38	8
1:A:387:LEU:HD13	1:A:401:MET:HE3	0.62	1.72	35	12
1:A:334:LEU:HD21	1:A:347:ALA:O	0.62	1.95	24	9
1:A:439:ILE:HB	1:A:443:LEU:HD12	0.62	1.72	3	1
1:A:331:ILE:HG23	1:A:363:LEU:CD2	0.62	2.25	33	5
1:A:334:LEU:HD13	1:A:350:CYS:CB	0.61	2.25	5	10
1:A:405:TYR:CD2	1:A:443:LEU:HD21	0.61	2.31	20	7
1:A:354:LEU:HD13	1:A:356:VAL:HG12	0.61	1.73	17	2
1:A:330:GLU:HG2	1:A:354:LEU:HD21	0.61	1.72	4	2
1:A:391:TRP:CE3	1:A:438:ILE:HG22	0.61	2.30	13	7
1:A:351:LEU:HD22	1:A:395:THR:CG2	0.61	2.26	6	3
1:A:351:LEU:HD12	1:A:395:THR:HG21	0.60	1.72	22	1
1:A:412:ILE:O	1:A:412:ILE:HG23	0.60	1.96	22	17
1:A:380:PHE:CE1	1:A:384:LEU:HD12	0.60	2.32	44	9
1:A:331:ILE:HD13	1:A:362:GLU:HB3	0.60	1.73	38	1
1:A:402:LYS:CD	1:A:443:LEU:HD13	0.60	2.27	5	2
1:A:368:ILE:HG22	1:A:372:LEU:HD13	0.60	1.74	45	4
1:A:401:MET:CE	1:A:438:ILE:HD12	0.60	2.26	32	1
1:A:412:ILE:HA	1:A:415:ILE:HD12	0.59	1.74	45	3
1:A:368:ILE:HG22	1:A:372:LEU:CD1	0.59	2.27	3	6
1:A:372:LEU:HD11	1:A:426:LEU:HB2	0.59	1.74	38	9
1:A:353:GLU:HG2	1:A:354:LEU:HD23	0.59	1.74	16	5
1:A:367:ALA:HB1	1:A:383:ILE:CG2	0.59	2.28	46	12
1:A:353:GLU:HG3	1:A:354:LEU:HD23	0.58	1.73	7	6
1:A:384:LEU:HD11	1:A:432:GLU:HB3	0.58	1.74	28	7
1:A:364:VAL:HG12	1:A:368:ILE:CD1	0.58	2.27	23	4
1:A:438:ILE:HG13	1:A:439:ILE:HG23	0.58	1.76	2	8
1:A:331:ILE:HG12	1:A:363:LEU:HD12	0.58	1.74	14	4
1:A:384:LEU:HD12	1:A:429:PHE:CD1	0.58	2.34	3	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:387:LEU:HA	1:A:390:LEU:HD12	0.58	1.75	26	4
1:A:368:ILE:HG22	1:A:372:LEU:HD11	0.58	1.76	3	6
1:A:405:TYR:CB	1:A:443:LEU:HD21	0.58	2.28	46	2
1:A:351:LEU:HD21	1:A:360:HIS:CE1	0.58	2.34	15	5
1:A:351:LEU:HD22	1:A:395:THR:HG22	0.57	1.75	6	1
1:A:365:TYR:CZ	1:A:369:VAL:HG11	0.57	2.34	13	6
1:A:338:TYR:HB2	1:A:347:ALA:HB2	0.57	1.76	11	5
1:A:331:ILE:HG23	1:A:363:LEU:HD23	0.57	1.76	28	5
1:A:405:TYR:CE1	1:A:430:VAL:HG22	0.57	2.34	19	3
1:A:388:LYS:HG3	1:A:438:ILE:HD13	0.57	1.75	25	4
1:A:351:LEU:CD1	1:A:363:LEU:HD13	0.57	2.30	12	6
1:A:334:LEU:HD21	1:A:350:CYS:HB2	0.57	1.77	37	4
1:A:331:ILE:HD13	1:A:362:GLU:CD	0.57	2.18	23	1
1:A:415:ILE:HG22	1:A:422:SER:HB3	0.57	1.75	45	1
1:A:384:LEU:HD11	1:A:432:GLU:CB	0.56	2.30	45	11
1:A:334:LEU:HD22	1:A:350:CYS:HB3	0.56	1.77	6	3
1:A:371:VAL:HG21	1:A:380:PHE:CA	0.56	2.31	15	22
1:A:387:LEU:HD13	1:A:401:MET:CE	0.56	2.31	18	22
1:A:331:ILE:HD13	1:A:362:GLU:HG2	0.56	1.77	41	1
1:A:339:LEU:HD21	1:A:379:ALA:CB	0.55	2.31	5	1
1:A:372:LEU:HD13	1:A:425:VAL:CG1	0.55	2.31	44	1
1:A:356:VAL:O	1:A:356:VAL:HG22	0.55	2.02	38	8
1:A:405:TYR:CG	1:A:443:LEU:HD21	0.55	2.37	44	6
1:A:339:LEU:HD11	1:A:383:ILE:HD11	0.54	1.79	46	1
1:A:430:VAL:HG21	1:A:447:CYS:SG	0.54	2.43	47	4
1:A:354:LEU:HD12	1:A:356:VAL:HG23	0.54	1.80	43	3
1:A:405:TYR:CD1	1:A:443:LEU:HD21	0.54	2.37	44	1
1:A:351:LEU:O	1:A:351:LEU:HD23	0.54	2.02	26	3
1:A:402:LYS:HA	1:A:443:LEU:HD11	0.54	1.79	14	4
1:A:344:ILE:HG21	1:A:389:SER:CB	0.54	2.33	34	1
1:A:402:LYS:HA	1:A:443:LEU:HD21	0.54	1.79	48	1
1:A:354:LEU:O	1:A:354:LEU:HD23	0.53	2.03	33	1
1:A:372:LEU:HD12	1:A:415:ILE:CG2	0.53	2.32	44	2
1:A:327:LEU:HD21	1:A:356:VAL:CG2	0.53	2.32	36	1
1:A:336:LYS:HA	1:A:339:LEU:HD12	0.53	1.80	46	1
1:A:340:LEU:HD12	1:A:340:LEU:C	0.53	2.24	23	1
1:A:372:LEU:HD11	1:A:426:LEU:HG	0.53	1.79	48	3
1:A:433:CYS:SG	1:A:438:ILE:HD11	0.53	2.44	14	40
1:A:388:LYS:CG	1:A:438:ILE:HD13	0.53	2.34	6	5
1:A:356:VAL:HG22	1:A:356:VAL:O	0.53	2.04	41	1
1:A:402:LYS:HD2	1:A:443:LEU:HD13	0.52	1.80	44	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:372:LEU:HD23	1:A:422:SER:HB2	0.52	1.79	46	1
1:A:387:LEU:HD12	1:A:388:LYS:N	0.52	2.20	47	5
1:A:354:LEU:HD23	1:A:354:LEU:O	0.52	2.04	44	1
1:A:364:VAL:HG21	1:A:401:MET:HA	0.52	1.82	46	2
1:A:408:ILE:HG21	1:A:426:LEU:CD1	0.52	2.33	23	3
1:A:334:LEU:HD11	1:A:350:CYS:HB3	0.51	1.82	34	4
1:A:384:LEU:HD22	1:A:388:LYS:HE3	0.51	1.82	48	2
1:A:369:VAL:HA	1:A:372:LEU:HD12	0.51	1.82	18	7
1:A:334:LEU:HD13	1:A:363:LEU:CD1	0.51	2.34	38	1
1:A:356:VAL:O	1:A:356:VAL:HG13	0.51	2.06	33	15
1:A:387:LEU:HD13	1:A:401:MET:HE2	0.51	1.82	48	3
1:A:368:ILE:CG2	1:A:372:LEU:HD13	0.51	2.36	45	1
1:A:335:LEU:O	1:A:339:LEU:HD12	0.51	2.06	32	4
1:A:372:LEU:HD11	1:A:426:LEU:HA	0.50	1.82	15	9
1:A:331:ILE:HD12	1:A:359:PHE:CE2	0.50	2.41	46	2
1:A:388:LYS:NZ	1:A:436:ALA:HB2	0.50	2.21	48	3
1:A:355:GLU:O	1:A:356:VAL:C	0.50	2.50	41	3
1:A:386:LEU:HD13	1:A:387:LEU:N	0.50	2.22	15	2
1:A:442:GLN:O	1:A:446:LEU:HD13	0.50	2.07	22	3
1:A:434:PHE:HB2	1:A:439:ILE:HD11	0.50	1.84	39	2
1:A:412:ILE:N	1:A:413:PRO:CD	0.49	2.74	38	7
1:A:356:VAL:HG13	1:A:356:VAL:O	0.49	2.07	47	21
1:A:328:VAL:HG13	1:A:362:GLU:OE1	0.49	2.06	17	1
1:A:384:LEU:HD22	1:A:388:LYS:CE	0.49	2.36	42	4
1:A:351:LEU:HD13	1:A:363:LEU:HD22	0.49	1.84	41	1
1:A:327:LEU:HD11	1:A:356:VAL:HG21	0.49	1.84	48	1
1:A:353:GLU:CG	1:A:354:LEU:HD23	0.49	2.37	14	3
1:A:433:CYS:HB2	1:A:438:ILE:HD11	0.49	1.83	32	3
1:A:384:LEU:HD12	1:A:384:LEU:C	0.49	2.27	37	2
1:A:387:LEU:HB2	1:A:401:MET:HE3	0.49	1.83	19	1
1:A:331:ILE:HD13	1:A:362:GLU:OE1	0.49	2.07	23	1
1:A:372:LEU:HD21	1:A:426:LEU:HD12	0.49	1.84	25	2
1:A:405:TYR:HB2	1:A:443:LEU:HD21	0.49	1.83	15	2
1:A:390:LEU:HB2	1:A:396:ILE:HD12	0.49	1.84	27	4
1:A:335:LEU:HD13	1:A:370:MET:HG3	0.49	1.84	23	1
1:A:365:TYR:CE1	1:A:408:ILE:HD13	0.49	2.43	20	6
1:A:354:LEU:HD13	1:A:354:LEU:H	0.49	1.68	24	1
1:A:351:LEU:O	1:A:351:LEU:HD13	0.49	2.06	22	1
1:A:415:ILE:HG22	1:A:422:SER:CB	0.49	2.38	45	1
1:A:365:TYR:CZ	1:A:369:VAL:HG21	0.48	2.42	49	10
1:A:402:LYS:HD3	1:A:443:LEU:HD13	0.48	1.84	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:372:LEU:HD11	1:A:426:LEU:CA	0.48	2.38	15	2
1:A:415:ILE:HG22	1:A:422:SER:HB2	0.48	1.85	44	1
1:A:351:LEU:HD11	1:A:360:HIS:CE1	0.48	2.44	22	1
1:A:331:ILE:HG23	1:A:363:LEU:HD22	0.47	1.84	33	1
1:A:351:LEU:HD13	1:A:390:LEU:HD23	0.47	1.87	6	1
1:A:354:LEU:HD21	1:A:360:HIS:NE2	0.47	2.24	33	2
1:A:421:HIS:O	1:A:425:VAL:HG23	0.47	2.09	10	3
1:A:412:ILE:HG23	1:A:412:ILE:O	0.47	2.10	21	8
1:A:387:LEU:HD21	1:A:429:PHE:CZ	0.47	2.45	8	22
1:A:351:LEU:HD12	1:A:363:LEU:CD1	0.47	2.36	43	1
1:A:368:ILE:CG2	1:A:372:LEU:HD12	0.47	2.37	40	1
1:A:405:TYR:CB	1:A:443:LEU:HD11	0.46	2.40	23	2
1:A:443:LEU:HA	1:A:446:LEU:HD12	0.46	1.87	13	1
1:A:354:LEU:HD12	1:A:354:LEU:O	0.46	2.10	20	1
1:A:331:ILE:HG23	1:A:363:LEU:CD1	0.46	2.40	46	2
1:A:335:LEU:HD22	1:A:383:ILE:CD1	0.46	2.39	28	1
1:A:402:LYS:HG3	1:A:443:LEU:HD13	0.46	1.87	40	1
1:A:344:ILE:HD11	1:A:385:ASP:CG	0.46	2.31	44	1
1:A:344:ILE:HD11	1:A:385:ASP:OD1	0.46	2.11	35	2
1:A:368:ILE:HG21	1:A:408:ILE:HG13	0.46	1.87	37	2
1:A:386:LEU:O	1:A:390:LEU:HD22	0.46	2.10	19	2
1:A:372:LEU:HD22	1:A:408:ILE:HD12	0.46	1.85	34	1
1:A:338:TYR:CD2	1:A:386:LEU:HD22	0.46	2.45	24	1
1:A:384:LEU:HD12	1:A:429:PHE:CD2	0.46	2.44	32	1
1:A:372:LEU:HD21	1:A:426:LEU:CD1	0.46	2.40	25	3
1:A:351:LEU:HD12	1:A:395:THR:CG2	0.46	2.41	22	1
1:A:372:LEU:HA	1:A:425:VAL:HG21	0.46	1.87	45	4
1:A:327:LEU:HD21	1:A:356:VAL:HG11	0.46	1.86	4	1
1:A:328:VAL:HA	1:A:331:ILE:HD12	0.46	1.87	38	1
1:A:372:LEU:CD2	1:A:408:ILE:HD12	0.46	2.41	34	1
1:A:360:HIS:H	1:A:400:GLN:NE2	0.45	2.09	18	1
1:A:371:VAL:HG23	1:A:383:ILE:HG13	0.45	1.88	28	5
1:A:331:ILE:CG2	1:A:363:LEU:HD12	0.45	2.40	46	1
1:A:391:TRP:CZ2	1:A:398:ILE:HD12	0.45	2.46	16	12
1:A:411:GLU:O	1:A:412:ILE:C	0.45	2.55	45	20
1:A:415:ILE:HG22	1:A:422:SER:OG	0.45	2.12	20	1
1:A:339:LEU:HD23	1:A:382:MET:SD	0.45	2.50	8	3
1:A:354:LEU:CD2	1:A:354:LEU:C	0.45	2.85	24	1
1:A:339:LEU:HD13	1:A:382:MET:SD	0.45	2.50	13	1
1:A:369:VAL:HG23	1:A:408:ILE:HD11	0.45	1.89	45	1
1:A:334:LEU:HD23	1:A:363:LEU:HD11	0.45	1.89	32	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:330:GLU:OE2	1:A:334:LEU:HD12	0.45	2.12	8	1
1:A:331:ILE:HG21	1:A:363:LEU:HA	0.45	1.88	46	1
1:A:442:GLN:O	1:A:446:LEU:HD12	0.45	2.11	39	1
1:A:334:LEU:HD11	1:A:347:ALA:HA	0.44	1.88	2	2
1:A:351:LEU:CD1	1:A:363:LEU:HD22	0.44	2.42	41	1
1:A:386:LEU:C	1:A:386:LEU:HD13	0.44	2.33	15	1
1:A:372:LEU:HD21	1:A:426:LEU:HD13	0.44	1.89	10	1
1:A:360:HIS:O	1:A:364:VAL:HG23	0.44	2.12	29	1
1:A:433:CYS:HB3	1:A:438:ILE:HD11	0.44	1.89	37	1
1:A:439:ILE:HG22	1:A:443:LEU:HD23	0.44	1.88	13	1
1:A:327:LEU:CD1	1:A:356:VAL:HG11	0.44	2.42	36	2
1:A:398:ILE:HD11	1:A:439:ILE:HA	0.44	1.88	44	1
1:A:330:GLU:CD	1:A:354:LEU:HD21	0.44	2.33	16	1
1:A:350:CYS:O	1:A:354:LEU:HD23	0.44	2.13	21	1
1:A:351:LEU:CD1	1:A:390:LEU:HD23	0.44	2.43	6	1
1:A:354:LEU:HD13	1:A:356:VAL:CG1	0.44	2.42	20	1
1:A:386:LEU:HD13	1:A:386:LEU:C	0.43	2.33	34	1
1:A:372:LEU:HA	1:A:425:VAL:HG11	0.43	1.90	6	3
1:A:363:LEU:CD2	1:A:396:ILE:HD11	0.43	2.43	46	1
1:A:363:LEU:HD23	1:A:364:VAL:N	0.43	2.28	2	2
1:A:384:LEU:C	1:A:384:LEU:HD12	0.43	2.33	39	1
1:A:442:GLN:O	1:A:446:LEU:HD23	0.43	2.13	31	2
1:A:401:MET:SD	1:A:438:ILE:HD12	0.43	2.54	24	1
1:A:344:ILE:HD11	1:A:385:ASP:OD2	0.43	2.14	28	1
1:A:334:LEU:CD2	1:A:347:ALA:HB1	0.43	2.43	43	1
1:A:372:LEU:HD21	1:A:426:LEU:HG	0.42	1.89	12	2
1:A:360:HIS:N	1:A:360:HIS:CD2	0.42	2.87	47	1
1:A:391:TRP:CH2	1:A:398:ILE:HD12	0.42	2.50	36	2
1:A:405:TYR:CB	1:A:443:LEU:HD22	0.42	2.44	3	1
1:A:363:LEU:HD13	1:A:363:LEU:C	0.42	2.34	49	6
1:A:386:LEU:O	1:A:386:LEU:HD22	0.42	2.14	15	1
1:A:351:LEU:HD11	1:A:363:LEU:HD13	0.42	1.90	1	1
1:A:351:LEU:O	1:A:354:LEU:HD23	0.42	2.14	33	1
1:A:434:PHE:N	1:A:439:ILE:HD11	0.42	2.30	14	2
1:A:401:MET:HG2	1:A:439:ILE:HG22	0.42	1.91	24	1
1:A:384:LEU:HD22	1:A:388:LYS:HD2	0.42	1.91	44	1
1:A:354:LEU:N	1:A:354:LEU:HD13	0.41	2.30	24	1
1:A:381:LYS:HA	1:A:384:LEU:HD23	0.41	1.92	36	2
1:A:351:LEU:HD22	1:A:363:LEU:HD13	0.41	1.90	9	1
1:A:363:LEU:C	1:A:363:LEU:HD13	0.41	2.35	39	2
1:A:380:PHE:CZ	1:A:384:LEU:HD12	0.41	2.50	45	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:327:LEU:CD2	1:A:356:VAL:HG21	0.41	2.44	32	1
1:A:334:LEU:HD21	1:A:347:ALA:C	0.41	2.36	43	1
1:A:401:MET:HE1	1:A:438:ILE:HD12	0.41	1.92	47	1
1:A:384:LEU:HD22	1:A:388:LYS:CD	0.41	2.46	44	1
1:A:372:LEU:HD23	1:A:415:ILE:CG2	0.41	2.45	46	1
1:A:368:ILE:HG22	1:A:372:LEU:HD23	0.41	1.92	13	1
1:A:386:LEU:HD22	1:A:386:LEU:O	0.41	2.14	34	1
1:A:426:LEU:HD23	1:A:430:VAL:HG23	0.41	1.92	46	2
1:A:402:LYS:HE3	1:A:443:LEU:HD22	0.41	1.92	40	1
1:A:412:ILE:O	1:A:412:ILE:CG1	0.41	2.68	2	1
1:A:384:LEU:HG	1:A:385:ASP:N	0.41	2.31	37	2
1:A:384:LEU:HD23	1:A:388:LYS:CD	0.41	2.46	13	1
1:A:367:ALA:CB	1:A:383:ILE:HD12	0.41	2.44	16	1
1:A:327:LEU:HD11	1:A:354:LEU:HD12	0.41	1.93	41	1
1:A:425:VAL:HG13	1:A:426:LEU:N	0.41	2.31	41	1
1:A:387:LEU:HD13	1:A:401:MET:HE1	0.41	1.92	25	1
1:A:372:LEU:HD21	1:A:426:LEU:HB2	0.40	1.94	31	1
1:A:390:LEU:H	1:A:390:LEU:HD22	0.40	1.77	27	1
1:A:372:LEU:HD12	1:A:415:ILE:HG21	0.40	1.94	44	1
1:A:369:VAL:CG1	1:A:415:ILE:HD11	0.40	2.46	15	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	117/136 (86%)	108±2 (92±2%)	7±2 (6±2%)	2±1 (2±1%)	16	59
All	All	5733/6664 (86%)	5270 (92%)	363 (6%)	100 (2%)	16	59

All 9 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	359	PHE	29
1	A	413	PRO	25

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Mol	Chain	Res	Type	Models (Total)
1	A	374	SER	17
1	A	421	HIS	13
1	A	377	GLU	11
1	A	376	GLY	2
1	A	397	THR	1
1	A	411	GLU	1
1	A	354	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	110/124 (89%)	84±3 (76±3%)	26±3 (24±3%)	3	28
All	All	5390/6076 (89%)	4097 (76%)	1293 (24%)	3	28

All 79 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	412	ILE	47
1	A	384	LEU	46
1	A	327	LEU	41
1	A	354	LEU	41
1	A	370	MET	38
1	A	391	TRP	36
1	A	397	THR	35
1	A	350	CYS	35
1	A	444	ARG	34
1	A	423	TYR	32
1	A	424	SER	31
1	A	394	SER	31
1	A	402	LYS	30
1	A	345	SER	29
1	A	389	SER	28
1	A	349	HIS	27
1	A	421	HIS	27
1	A	341	SER	25

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Mol	Chain	Res	Type	Models (Total)
1	A	351	LEU	25
1	A	332	ASP	24
1	A	346	GLU	23
1	A	333	MET	23
1	A	445	ASP	21
1	A	392	LYS	21
1	A	449	SER	21
1	A	329	LYS	21
1	A	334	LEU	21
1	A	362	GLU	20
1	A	378	SER	20
1	A	400	GLN	19
1	A	441	LYS	19
1	A	399	ASP	19
1	A	395	THR	18
1	A	440	SER	18
1	A	372	LEU	17
1	A	446	LEU	17
1	A	407	ARG	17
1	A	401	MET	16
1	A	377	GLU	16
1	A	339	LEU	16
1	A	381	LYS	16
1	A	422	SER	15
1	A	403	ARG	15
1	A	406	GLU	13
1	A	373	GLU	12
1	A	353	GLU	12
1	A	427	GLU	12
1	A	375	THR	12
1	A	330	GLU	12
1	A	414	ASP	11
1	A	387	LEU	11
1	A	355	GLU	10
1	A	393	SER	9
1	A	363	LEU	9
1	A	398	ILE	9
1	A	337	GLU	8
1	A	426	LEU	7
1	A	442	GLN	6
1	A	366	GLU	6
1	A	343	ASP	5

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Mol	Chain	Res	Type	Models (Total)
1	A	358	HIS	4
1	A	388	LYS	4
1	A	447	CYS	3
1	A	374	SER	3
1	A	411	GLU	3
1	A	390	LEU	3
1	A	385	ASP	2
1	A	443	LEU	2
1	A	356	VAL	2
1	A	410	ASN	2
1	A	360	HIS	2
1	A	432	GLU	1
1	A	405	TYR	1
1	A	352	LYS	1
1	A	382	MET	1
1	A	336	LYS	1
1	A	348	GLU	1
1	A	359	PHE	1
1	A	425	VAL	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 ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided