



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 09:07 PM BST

PDB ID : 2HQO
Title : Structure of a Atypical Orphan Response Regulator Protein Revealed a New Phosphorylation-Independent Regulatory Mechanism
Authors : Hong, E.; Lee, W.
Deposited on : 2006-07-19

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

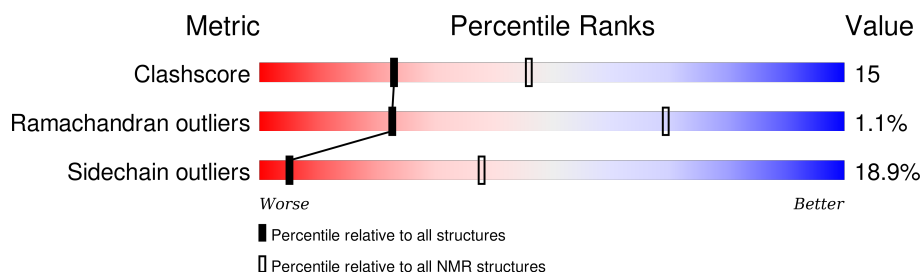
1 Overall quality at a glance

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	123	
1	B	123	

2 Ensemble composition and analysis

This entry contains 20 models. Model 2 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:2-A:113, B:302-B:413 (224)	0.21	2

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 2 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3762 atoms, of which 1882 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Putative TRANSCRIPTIONAL REGULATOR.

Mol	Chain	Residues	Atoms						Trace
1	A	119	Total	C	H	N	O	S	0
			1881	592	941	160	184	4	
1	B	119	Total	C	H	N	O	S	0
			1881	592	941	160	184	4	

There are 8 discrepancies between the modelled and reference sequences:

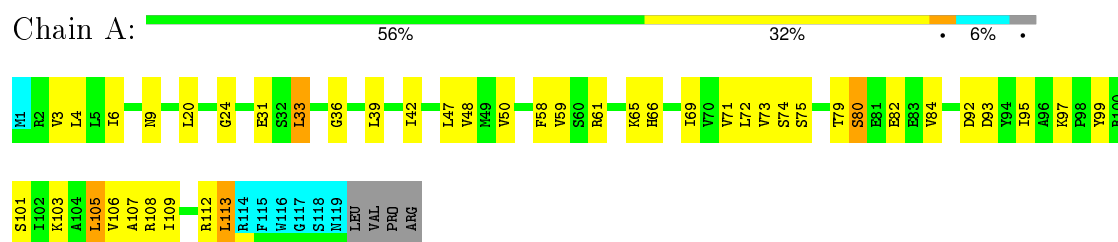
Chain	Residue	Modelled	Actual	Comment	Reference
A	120	LEU	-	CLONING ARTIFACT	UNP Q9ZM42
A	121	VAL	-	CLONING ARTIFACT	UNP Q9ZM42
A	122	PRO	-	CLONING ARTIFACT	UNP Q9ZM42
A	123	ARG	-	CLONING ARTIFACT	UNP Q9ZM42
B	420	LEU	-	CLONING ARTIFACT	UNP Q9ZM42
B	421	VAL	-	CLONING ARTIFACT	UNP Q9ZM42
B	422	PRO	-	CLONING ARTIFACT	UNP Q9ZM42
B	423	ARG	-	CLONING ARTIFACT	UNP Q9ZM42

4 Residue-property plots

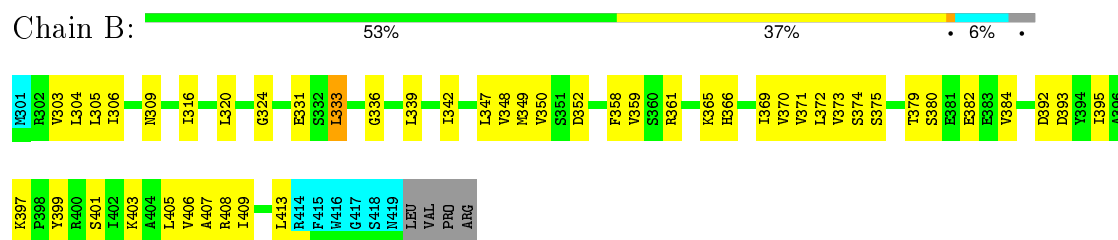
4.1 Average score per residue in the NMR ensemble

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: Putative TRANSCRIPTIONAL REGULATOR



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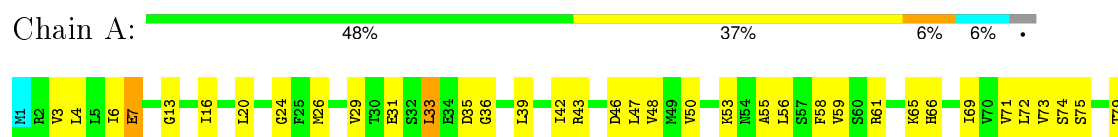


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

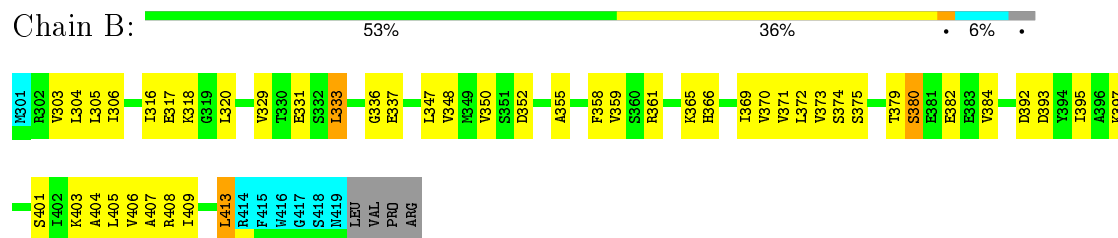
4.2.1 Score per residue for model 1

• Molecule 1: Putative TRANSCRIPTIONAL REGULATOR



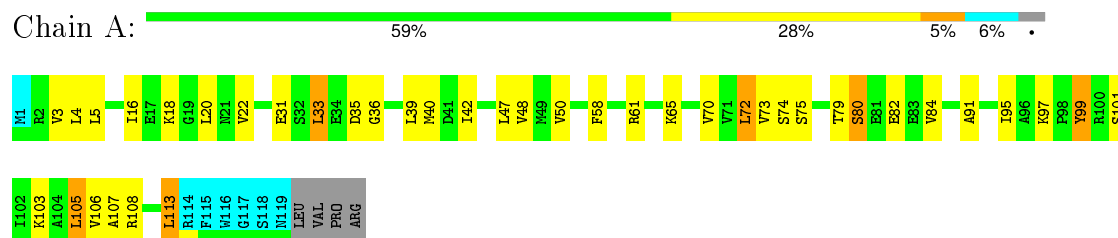


- Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

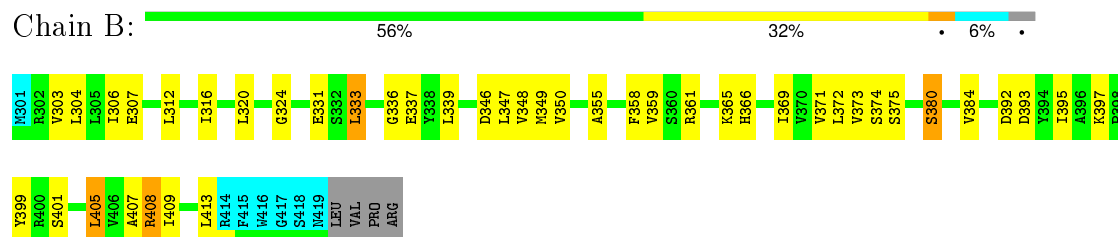


4.2.2 Score per residue for model 2 (medoid)

- Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

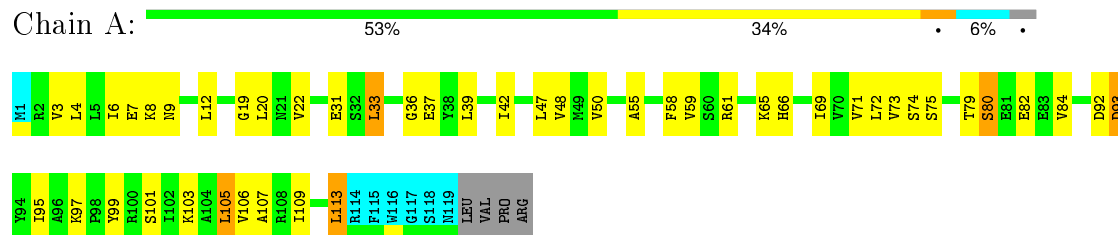


- Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

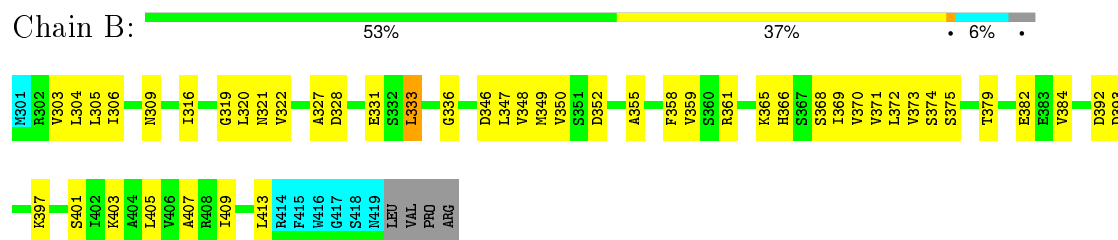


4.2.3 Score per residue for model 3

- Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

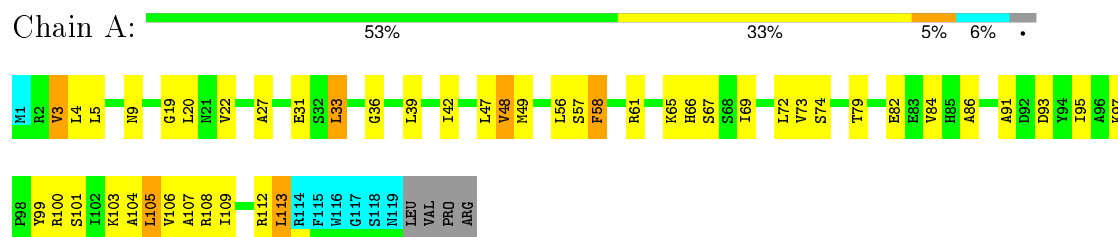


- Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

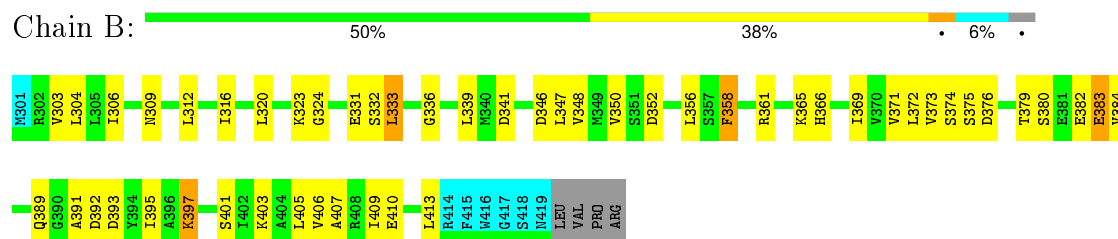


4.2.4 Score per residue for model 4

- Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

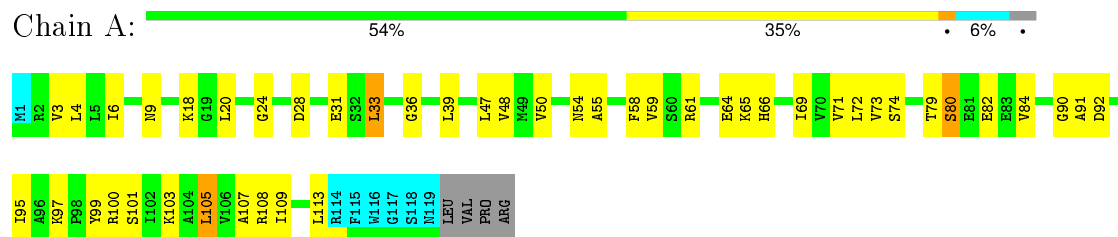


- Molecule 1: Putative TRANSCRIPTIONAL REGULATOR



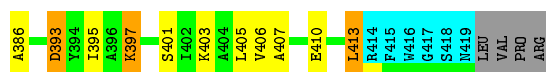
4.2.5 Score per residue for model 5

- Molecule 1: Putative TRANSCRIPTIONAL REGULATOR



- Molecule 1: Putative TRANSCRIPTIONAL REGULATOR





4.2.6 Score per residue for model 6

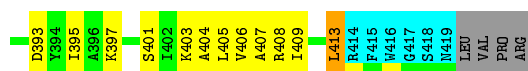
- Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

Chain A: 54% 33% 6% .



- Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

Chain B: 50% 39% 6% .



4.2.7 Score per residue for model 7

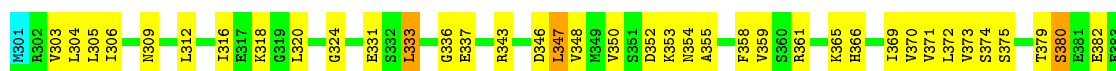
- Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

Chain A: 56% 33% 6% .



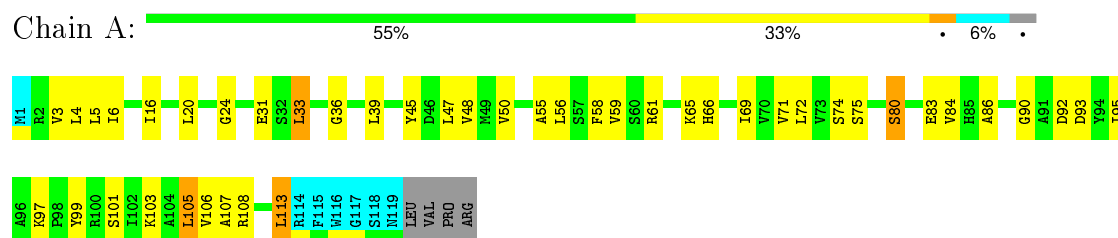
- Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

Chain B: 50% 37% 6% .

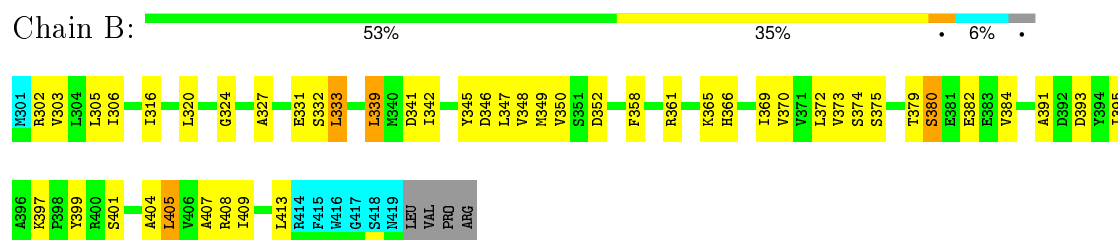


4.2.8 Score per residue for model 8

- Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

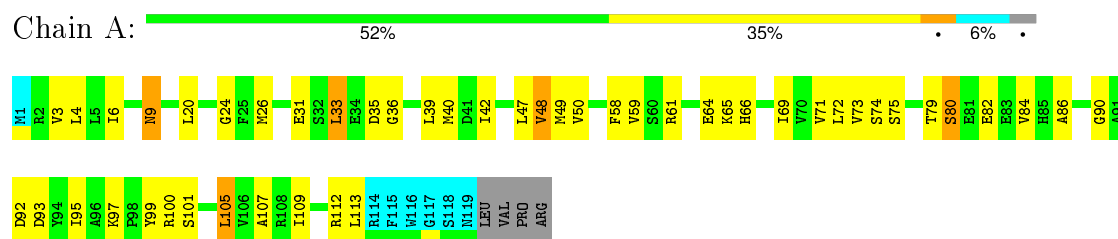


- Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

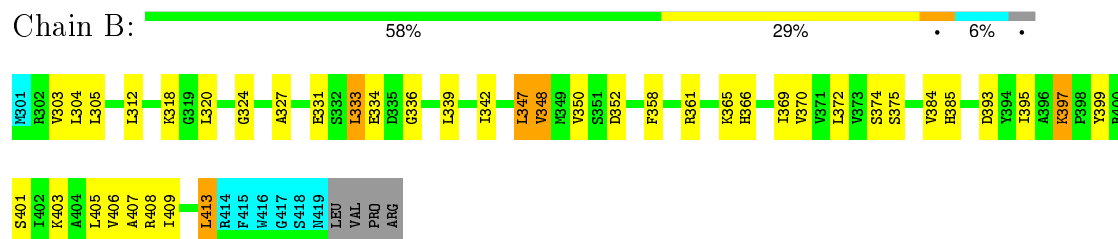


4.2.9 Score per residue for model 9

- Molecule 1: Putative TRANSCRIPTIONAL REGULATOR



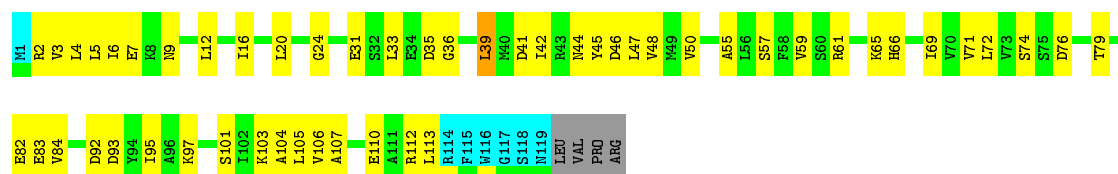
- Molecule 1: Putative TRANSCRIPTIONAL REGULATOR



4.2.10 Score per residue for model 10

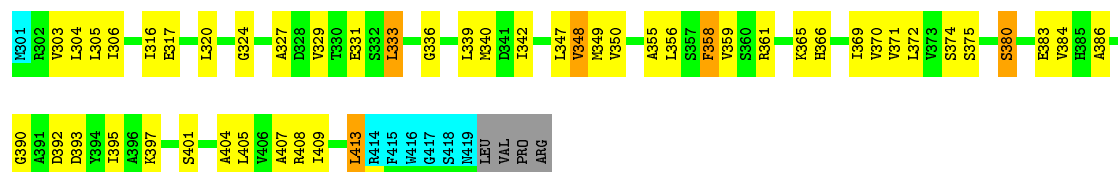
- Molecule 1: Putative TRANSCRIPTIONAL REGULATOR





• Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

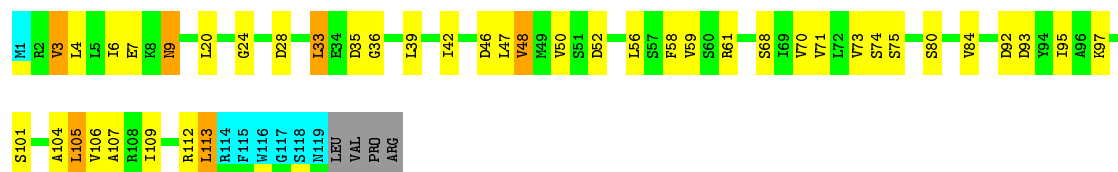
Chain B: 51% 36% 6%



4.2.11 Score per residue for model 11

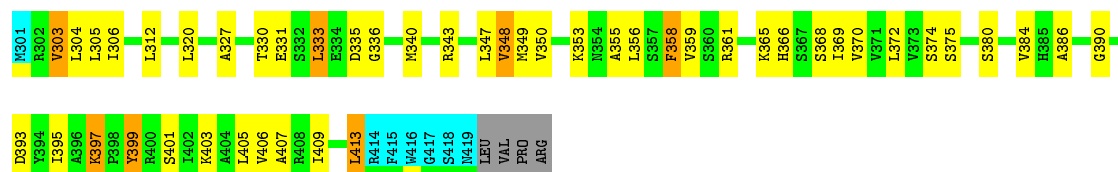
• Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

Chain A: 57% 29% 5% 6%



• Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

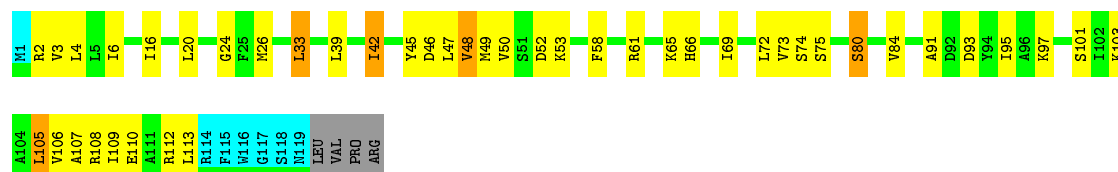
Chain B: 53% 33% 6% 6%



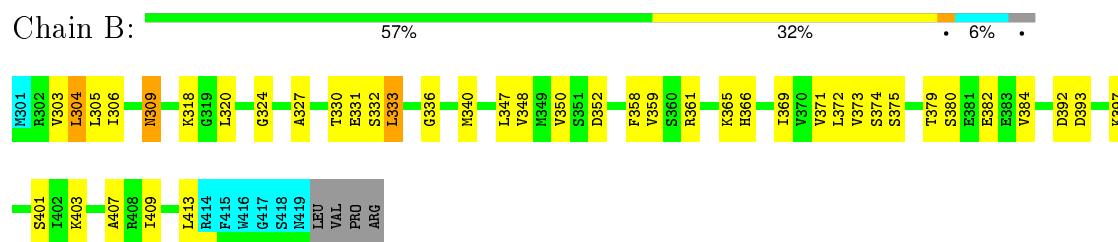
4.2.12 Score per residue for model 12

• Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

Chain A: 55% 32% 6%

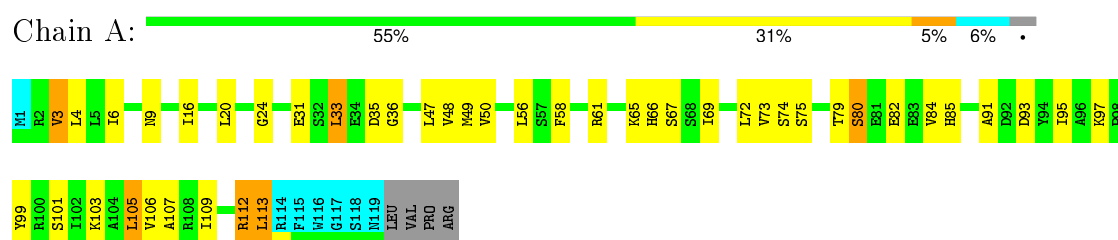


- Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

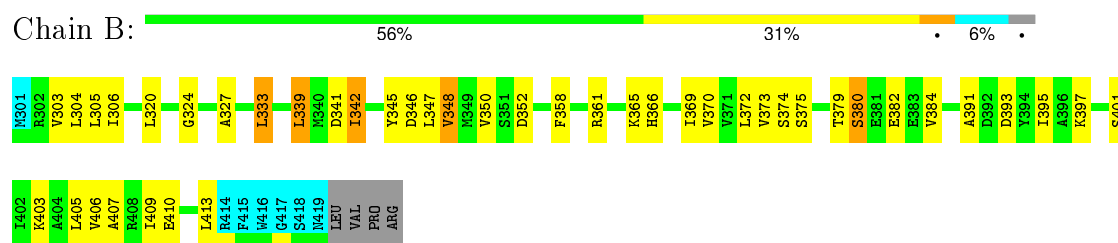


4.2.13 Score per residue for model 13

- Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

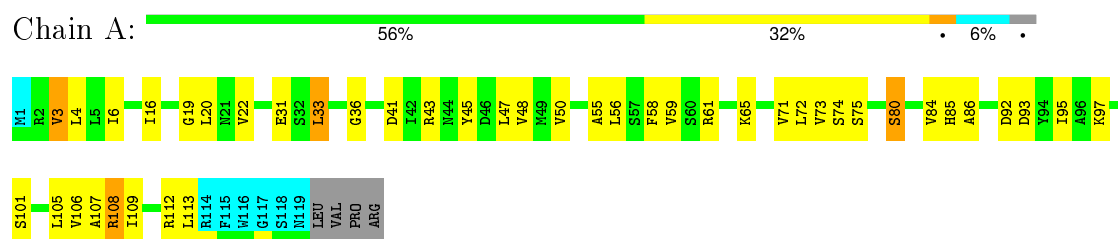


- Molecule 1: Putative TRANSCRIPTIONAL REGULATOR



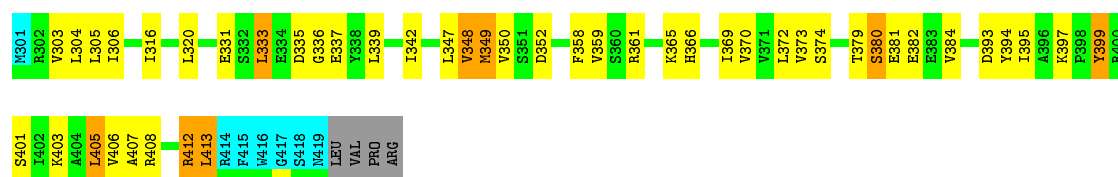
4.2.14 Score per residue for model 14

- Molecule 1: Putative TRANSCRIPTIONAL REGULATOR



- Molecule 1: Putative TRANSCRIPTIONAL REGULATOR





4.2.15 Score per residue for model 15

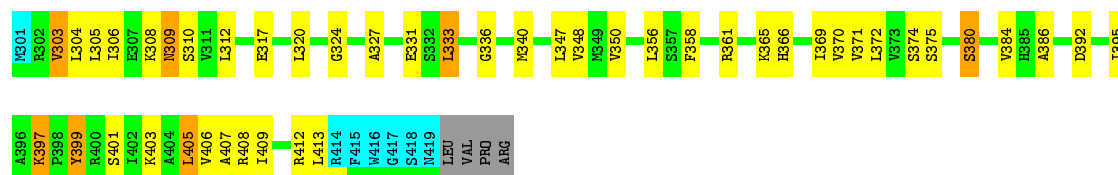
- Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

Chain A: 57% 31% 6%



- Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

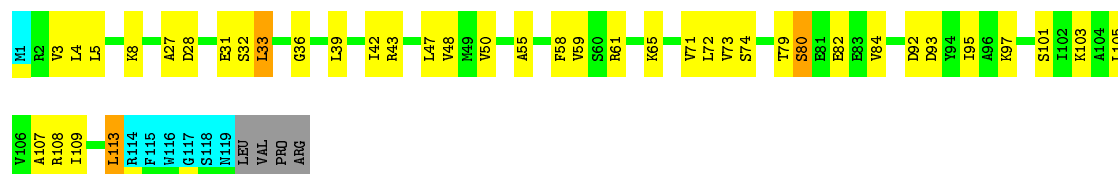
Chain B: 54% 32% 6% 6%



4.2.16 Score per residue for model 16

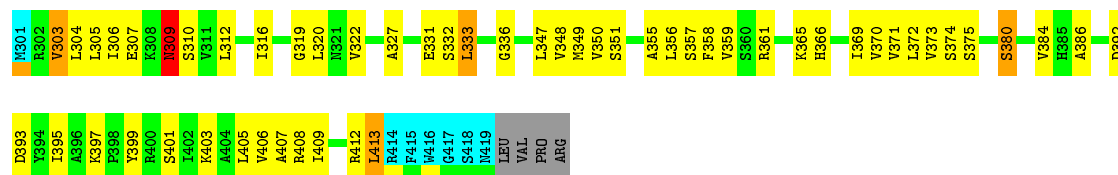
- Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

Chain A: 59% 30% 6%



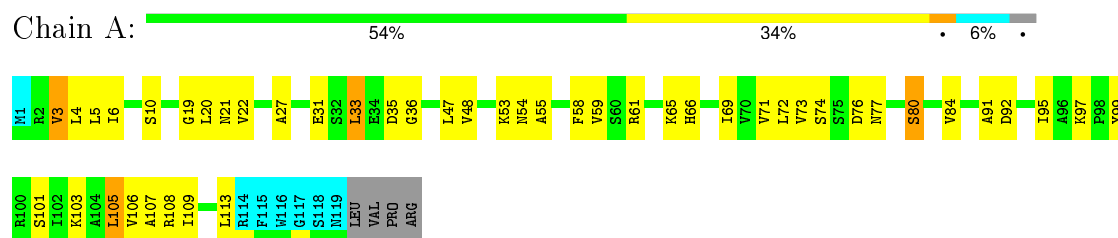
- Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

Chain B: 47% 40% 6%

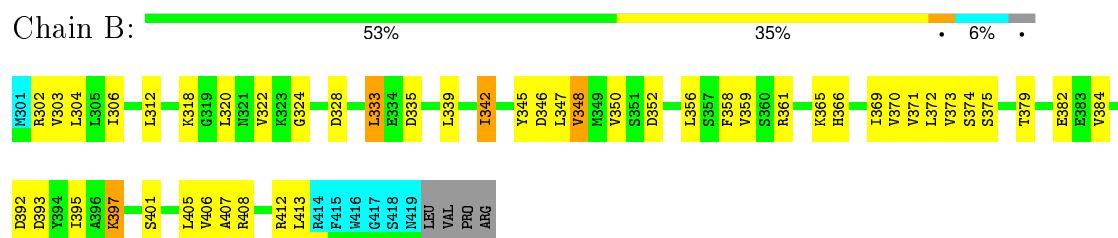


4.2.17 Score per residue for model 17

- Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

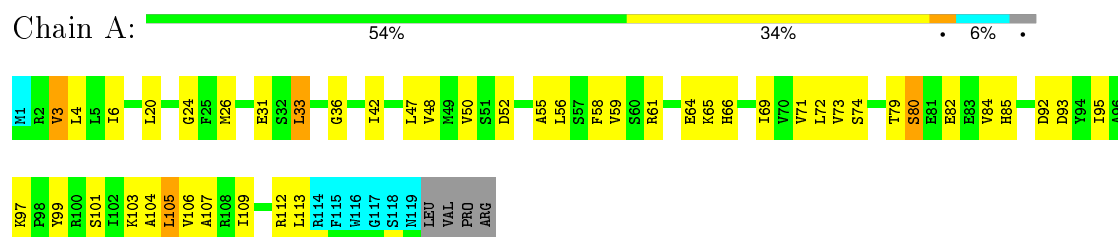


- Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

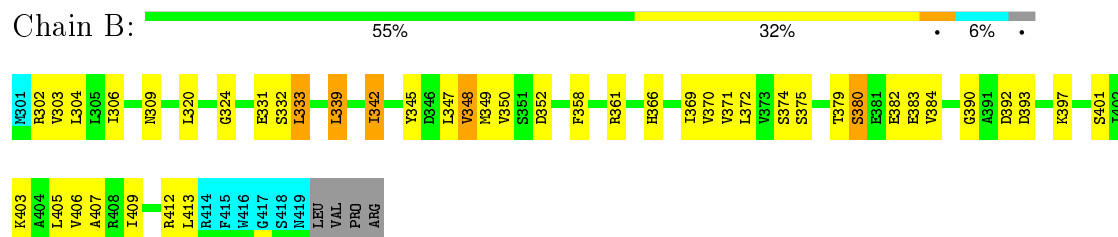


4.2.18 Score per residue for model 18

- Molecule 1: Putative TRANSCRIPTIONAL REGULATOR



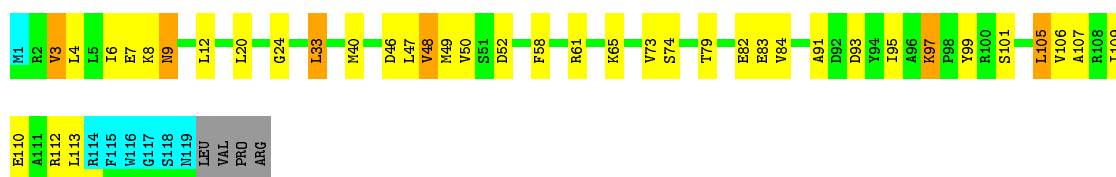
- Molecule 1: Putative TRANSCRIPTIONAL REGULATOR



4.2.19 Score per residue for model 19

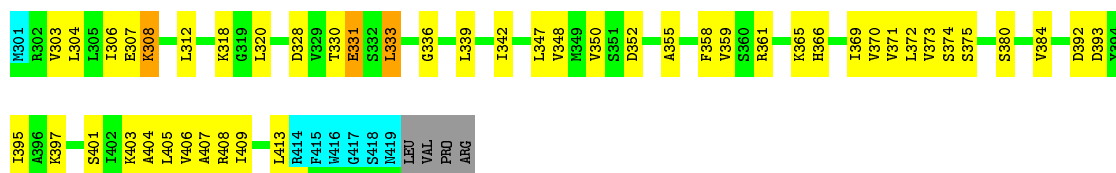
- Molecule 1: Putative TRANSCRIPTIONAL REGULATOR





- Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

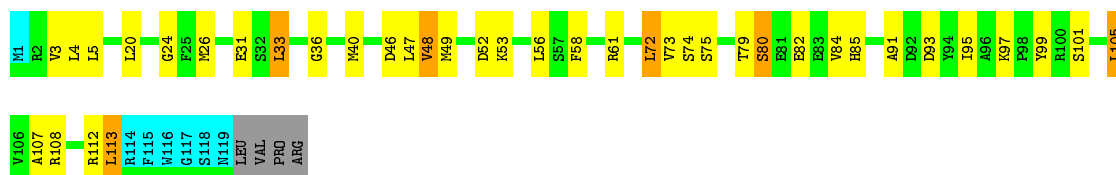
Chain B: 53% 36% 6%



4.2.20 Score per residue for model 20

- Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

Chain A: 59% 27% 5% 6%



- Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

Chain B: 58% 27% 7% 6%



5 Refinement protocol and experimental data overview ⓘ

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

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	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	878	886	886	27±5
1	B	878	886	886	29±4
All	All	35120	35440	35440	1038

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 15.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:347:LEU:HD23	1:B:413:LEU:HD11	0.90	1.39	15	2
1:B:303:VAL:HG13	1:B:347:LEU:HD12	0.89	1.45	8	14
1:A:3:VAL:HG13	1:A:47:LEU:HD12	0.87	1.43	5	11
1:B:347:LEU:HD11	1:B:372:LEU:HD12	0.83	1.48	19	12
1:A:72:LEU:HD22	1:A:95:ILE:HD11	0.79	1.54	13	12
1:A:20:LEU:HD21	1:A:109:ILE:HD13	0.78	1.56	15	10
1:A:95:ILE:HD13	1:A:105:LEU:HD21	0.77	1.56	2	19
1:B:320:LEU:HD23	1:B:406:VAL:HG22	0.75	1.57	5	5
1:B:305:LEU:HD11	1:B:316:ILE:HG21	0.74	1.59	14	3
1:A:47:LEU:HD23	1:A:113:LEU:HD11	0.74	1.57	4	3
1:B:333:LEU:H	1:B:333:LEU:HD13	0.73	1.43	9	1
1:B:372:LEU:HD22	1:B:395:ILE:HD11	0.72	1.61	9	11
1:A:47:LEU:HD11	1:A:72:LEU:HD12	0.70	1.63	4	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:109:ILE:O	1:A:113:LEU:HD12	0.70	1.87	19	2
1:A:4:LEU:HD23	1:A:48:VAL:HG23	0.67	1.66	5	3
1:B:395:ILE:HD13	1:B:405:LEU:HD21	0.67	1.67	20	10
1:B:347:LEU:CD2	1:B:409:ILE:HG23	0.67	2.20	20	2
1:B:320:LEU:HD21	1:B:409:ILE:HD13	0.66	1.66	2	6
1:B:304:LEU:HD21	1:B:336:GLY:HA3	0.66	1.67	14	14
1:A:47:LEU:HD23	1:A:113:LEU:HD21	0.66	1.67	20	4
1:A:84:VAL:HG12	1:B:407:ALA:CB	0.65	2.22	12	19
1:B:380:SER:O	1:B:384:VAL:HG22	0.65	1.92	18	14
1:A:107:ALA:CB	1:B:384:VAL:HG12	0.65	2.22	19	19
1:B:320:LEU:HD23	1:B:406:VAL:HG13	0.65	1.68	15	5
1:A:80:SER:O	1:A:84:VAL:HG22	0.64	1.91	12	16
1:B:366:HIS:O	1:B:369:ILE:HG22	0.64	1.93	19	20
1:A:4:LEU:HD21	1:A:36:GLY:HA3	0.64	1.68	10	13
1:A:72:LEU:HD21	1:A:108:ARG:CZ	0.64	2.23	14	1
1:A:47:LEU:HD13	1:A:48:VAL:N	0.64	2.08	10	20
1:B:303:VAL:CG1	1:B:347:LEU:HD12	0.63	2.22	8	12
1:A:45:TYR:CE1	1:A:69:ILE:HD12	0.63	2.28	10	3
1:B:347:LEU:HD23	1:B:413:LEU:CD2	0.63	2.23	16	7
1:B:347:LEU:HD13	1:B:348:VAL:N	0.62	2.10	18	17
1:A:66:HIS:O	1:A:69:ILE:HG22	0.62	1.95	12	13
1:B:333:LEU:HD13	1:B:358:PHE:HB2	0.62	1.72	10	19
1:A:33:LEU:HD13	1:A:58:PHE:HB2	0.61	1.71	4	19
1:B:303:VAL:HG21	1:B:320:LEU:HD13	0.61	1.71	19	2
1:B:304:LEU:HD21	1:B:336:GLY:CA	0.61	2.26	4	8
1:B:409:ILE:O	1:B:413:LEU:HD12	0.60	1.96	8	3
1:A:84:VAL:HG12	1:B:407:ALA:HB2	0.60	1.73	8	11
1:B:303:VAL:HG13	1:B:347:LEU:HB3	0.59	1.74	17	7
1:A:19:GLY:O	1:A:22:VAL:HG12	0.59	1.97	14	6
1:B:320:LEU:HD13	1:B:406:VAL:HG23	0.59	1.73	16	2
1:A:3:VAL:HG21	1:A:20:LEU:HD13	0.59	1.74	18	8
1:A:12:LEU:HD21	1:A:97:LYS:HE2	0.59	1.72	19	1
1:A:47:LEU:HD23	1:A:113:LEU:CD2	0.59	2.27	20	6
1:A:20:LEU:HD21	1:A:109:ILE:CD1	0.59	2.27	15	8
1:B:345:TYR:CE1	1:B:369:ILE:HD12	0.59	2.32	8	5
1:B:312:LEU:HD21	1:B:397:LYS:HE2	0.59	1.75	5	1
1:A:20:LEU:HG	1:A:106:VAL:HG22	0.59	1.75	14	3
1:A:4:LEU:HD21	1:A:36:GLY:CA	0.59	2.27	14	7
1:A:47:LEU:CD2	1:A:113:LEU:HD11	0.59	2.27	4	2
1:A:3:VAL:CG1	1:A:47:LEU:HD12	0.59	2.27	9	11
1:A:104:ALA:HB1	1:B:383:GLU:CD	0.59	2.18	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:305:LEU:HD23	1:B:327:ALA:HB1	0.58	1.73	12	4
1:B:347:LEU:HD22	1:B:370:VAL:HB	0.58	1.74	7	10
1:B:306:ILE:CG2	1:B:350:VAL:HG23	0.58	2.28	16	18
1:B:319:GLY:O	1:B:322:VAL:HG12	0.58	1.97	3	2
1:B:356:LEU:HD22	1:B:386:ALA:HA	0.58	1.76	11	5
1:A:72:LEU:HD22	1:A:95:ILE:CD1	0.58	2.28	13	2
1:B:316:ILE:HG23	1:B:405:LEU:HD23	0.58	1.75	7	7
1:B:304:LEU:HD11	1:B:336:GLY:CA	0.58	2.29	12	1
1:A:109:ILE:O	1:A:113:LEU:HD23	0.58	1.99	16	3
1:A:47:LEU:HD23	1:A:113:LEU:HD22	0.57	1.76	16	3
1:B:349:MET:HE1	1:B:405:LEU:HD11	0.57	1.75	14	2
1:A:45:TYR:CD1	1:A:69:ILE:HD12	0.57	2.35	12	3
1:A:4:LEU:HD21	1:A:36:GLY:HA2	0.57	1.76	14	4
1:B:370:VAL:HG21	1:B:413:LEU:HG	0.57	1.76	19	3
1:B:333:LEU:CD2	1:B:350:VAL:HG21	0.57	2.30	12	1
1:A:56:LEU:HD22	1:A:86:ALA:HA	0.57	1.75	8	2
1:A:6:ILE:CG2	1:A:50:VAL:HG23	0.57	2.29	11	9
1:B:303:VAL:HG12	1:B:347:LEU:HB3	0.56	1.77	19	1
1:A:104:ALA:HB1	1:B:383:GLU:OE1	0.56	2.00	10	2
1:B:305:LEU:HD11	1:B:316:ILE:CG2	0.56	2.30	14	1
1:A:83:GLU:OE1	1:B:404:ALA:HB1	0.56	2.01	19	4
1:B:347:LEU:HD11	1:B:372:LEU:CD1	0.56	2.30	9	2
1:B:320:LEU:HD21	1:B:409:ILE:CD1	0.56	2.31	4	11
1:B:409:ILE:O	1:B:413:LEU:HD23	0.55	2.00	11	1
1:A:59:VAL:HG11	1:A:73:VAL:CG1	0.55	2.31	18	8
1:B:355:ALA:O	1:B:359:VAL:HG13	0.55	2.02	16	3
1:B:305:LEU:HD21	1:B:327:ALA:HB1	0.55	1.78	11	4
1:B:305:LEU:CD2	1:B:327:ALA:HB1	0.55	2.32	13	9
1:A:20:LEU:HD23	1:A:106:VAL:HG13	0.55	1.79	11	7
1:A:107:ALA:HB2	1:B:384:VAL:HG12	0.55	1.79	9	9
1:A:55:ALA:O	1:A:59:VAL:HG22	0.54	2.01	10	9
1:A:73:VAL:HG21	1:A:91:ALA:HB2	0.54	1.80	20	9
1:B:316:ILE:HD13	1:B:349:MET:HE2	0.54	1.78	8	4
1:A:3:VAL:HG12	1:A:47:LEU:HB3	0.54	1.77	10	1
1:A:3:VAL:HA	1:A:47:LEU:O	0.54	2.02	10	4
1:A:105:LEU:O	1:A:109:ILE:HD12	0.54	2.02	14	1
1:B:347:LEU:HD13	1:B:370:VAL:CG1	0.54	2.32	19	2
1:A:3:VAL:HG13	1:A:47:LEU:HB3	0.54	1.80	6	6
1:B:347:LEU:CD1	1:B:372:LEU:HD12	0.54	2.29	19	2
1:A:71:VAL:HG23	1:A:92:ASP:H	0.53	1.63	16	9
1:A:49:MET:HE1	1:A:105:LEU:HD11	0.53	1.79	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:356:LEU:HD13	1:B:389:GLN:HG3	0.53	1.81	4	1
1:A:83:GLU:CD	1:B:404:ALA:HB1	0.53	2.24	6	2
1:A:20:LEU:HD23	1:A:106:VAL:HG22	0.53	1.79	7	4
1:A:47:LEU:HD23	1:A:113:LEU:CD1	0.53	2.33	9	2
1:B:320:LEU:HD21	1:B:409:ILE:HD12	0.52	1.81	1	2
1:B:304:LEU:HB3	1:B:348:VAL:HG12	0.52	1.81	17	4
1:B:320:LEU:CD2	1:B:406:VAL:HG22	0.52	2.34	6	3
1:B:339:LEU:O	1:B:339:LEU:HD12	0.52	2.03	8	5
1:B:306:ILE:HG23	1:B:331:GLU:O	0.52	2.05	19	1
1:B:372:LEU:CD2	1:B:395:ILE:HD11	0.52	2.35	20	2
1:A:71:VAL:HG23	1:A:92:ASP:N	0.52	2.19	7	12
1:A:16:ILE:HG23	1:A:105:LEU:HD23	0.52	1.81	14	1
1:A:4:LEU:HB3	1:A:48:VAL:HG12	0.51	1.83	12	1
1:B:349:MET:HE1	1:B:405:LEU:HD21	0.51	1.82	3	1
1:A:5:LEU:HD21	1:A:27:ALA:HB1	0.51	1.82	4	2
1:B:312:LEU:HD11	1:B:397:LYS:NZ	0.51	2.20	11	6
1:B:333:LEU:HD23	1:B:350:VAL:HG21	0.51	1.82	12	3
1:A:5:LEU:CD2	1:A:27:ALA:HB1	0.51	2.35	16	3
1:B:339:LEU:HD12	1:B:342:ILE:HG12	0.51	1.82	17	9
1:A:5:LEU:HD21	1:A:20:LEU:CD1	0.51	2.35	20	1
1:B:347:LEU:HD23	1:B:413:LEU:HD21	0.51	1.83	14	2
1:B:359:VAL:HG11	1:B:373:VAL:CG1	0.51	2.36	6	11
1:A:39:LEU:HD12	1:A:39:LEU:O	0.51	2.05	6	4
1:B:320:LEU:HD13	1:B:406:VAL:HG13	0.51	1.82	11	2
1:B:309:ASN:ND2	1:B:309:ASN:C	0.51	2.64	16	1
1:A:72:LEU:CD2	1:A:95:ILE:HD11	0.51	2.36	6	2
1:A:99:TYR:CE2	1:A:105:LEU:HD12	0.50	2.41	20	14
1:B:304:LEU:HD22	1:B:306:ILE:CD1	0.50	2.35	12	1
1:A:5:LEU:HD13	1:A:16:ILE:HB	0.50	1.81	2	2
1:B:347:LEU:HB2	1:B:413:LEU:HD23	0.50	1.83	20	1
1:B:355:ALA:O	1:B:359:VAL:HG22	0.50	2.05	11	8
1:B:345:TYR:CD1	1:B:369:ILE:HD12	0.50	2.41	18	4
1:B:347:LEU:HD12	1:B:348:VAL:H	0.50	1.65	19	2
1:A:3:VAL:HB	1:A:47:LEU:HD12	0.50	1.82	4	5
1:A:16:ILE:HD13	1:A:49:MET:CE	0.50	2.37	12	2
1:A:39:LEU:O	1:A:39:LEU:HD12	0.50	2.06	8	5
1:B:333:LEU:HD22	1:B:333:LEU:N	0.50	2.22	9	1
1:B:312:LEU:HD21	1:B:397:LYS:NZ	0.50	2.21	15	6
1:A:50:VAL:HG11	1:A:58:PHE:CD2	0.50	2.42	2	3
1:A:18:LYS:O	1:A:22:VAL:HG23	0.50	2.07	2	1
1:B:339:LEU:HD12	1:B:339:LEU:O	0.49	2.06	13	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:317:GLU:OE2	1:B:329:VAL:HG23	0.49	2.07	1	2
1:B:307:GLU:HG2	1:B:312:LEU:HD23	0.49	1.84	2	1
1:B:347:LEU:HD13	1:B:370:VAL:HG12	0.49	1.83	20	1
1:A:13:GLY:HA3	1:A:29:VAL:HG11	0.49	1.84	1	2
1:A:104:ALA:HB1	1:B:383:GLU:OE2	0.49	2.07	4	3
1:B:373:VAL:HG21	1:B:391:ALA:HB2	0.49	1.84	13	2
1:B:304:LEU:HD11	1:B:330:THR:HG21	0.49	1.84	11	1
1:A:79:THR:HG23	1:A:82:GLU:H	0.49	1.68	6	15
1:B:399:TYR:CE2	1:B:405:LEU:HD12	0.49	2.43	8	6
1:B:371:VAL:HG23	1:B:392:ASP:H	0.49	1.67	1	5
1:B:317:GLU:CD	1:B:329:VAL:HG23	0.48	2.28	10	2
1:A:6:ILE:HD13	1:A:33:LEU:HA	0.48	1.84	1	5
1:A:59:VAL:HG11	1:A:73:VAL:HG12	0.48	1.84	18	1
1:A:72:LEU:HD12	1:A:95:ILE:CD1	0.48	2.38	20	3
1:A:39:LEU:HD12	1:A:42:ILE:HG12	0.48	1.85	12	6
1:B:371:VAL:HG23	1:B:392:ASP:N	0.48	2.22	1	11
1:A:7:GLU:HG2	1:A:12:LEU:HD23	0.48	1.84	10	2
1:A:107:ALA:HB3	1:B:384:VAL:HG12	0.48	1.83	14	2
1:B:347:LEU:HD12	1:B:348:VAL:N	0.48	2.24	19	2
1:A:72:LEU:HD21	1:A:112:ARG:NH2	0.48	2.24	13	1
1:B:306:ILE:HB	1:B:350:VAL:HG23	0.48	1.86	16	2
1:A:16:ILE:HG22	1:A:20:LEU:HD11	0.47	1.86	7	1
1:A:12:LEU:HD11	1:A:97:LYS:NZ	0.47	2.24	6	1
1:B:394:TYR:O	1:B:395:ILE:HD13	0.47	2.09	14	1
1:B:347:LEU:HD13	1:B:347:LEU:C	0.47	2.30	4	6
1:A:19:GLY:O	1:A:106:VAL:HG21	0.47	2.08	3	1
1:B:312:LEU:HD21	1:B:397:LYS:HZ2	0.47	1.70	11	1
1:A:47:LEU:C	1:A:47:LEU:HD13	0.47	2.30	15	4
1:B:413:LEU:O	1:B:413:LEU:HD12	0.47	2.10	18	1
1:B:317:GLU:HG3	1:B:327:ALA:HB3	0.47	1.85	15	1
1:B:379:THR:HG23	1:B:382:GLU:H	0.47	1.69	13	13
1:B:333:LEU:HD22	1:B:358:PHE:CB	0.47	2.39	13	1
1:A:5:LEU:HD21	1:A:16:ILE:HG22	0.47	1.86	10	1
1:B:303:VAL:HG11	1:B:320:LEU:HD13	0.47	1.86	3	2
1:A:12:LEU:HD21	1:A:97:LYS:NZ	0.47	2.24	6	1
1:A:6:ILE:HB	1:A:50:VAL:HG23	0.47	1.85	19	5
1:B:405:LEU:HD12	1:B:408:ARG:HH22	0.47	1.70	2	1
1:B:347:LEU:HD22	1:B:409:ILE:HG23	0.47	1.86	19	2
1:B:347:LEU:HD22	1:B:413:LEU:HD11	0.47	1.87	19	1
1:A:47:LEU:HD23	1:A:113:LEU:HD23	0.47	1.87	13	1
1:A:20:LEU:CD2	1:A:106:VAL:HG22	0.46	2.40	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:303:VAL:HA	1:B:347:LEU:O	0.46	2.10	16	3
1:A:4:LEU:HD12	1:A:28:ASP:HB3	0.46	1.88	11	1
1:B:320:LEU:HD13	1:B:406:VAL:CG2	0.46	2.39	16	2
1:A:72:LEU:HD23	1:A:93:ASP:HB3	0.46	1.86	3	2
1:A:73:VAL:HG21	1:A:86:ALA:HB1	0.46	1.87	14	2
1:A:47:LEU:HD22	1:A:70:VAL:HB	0.46	1.86	2	2
1:B:333:LEU:HD21	1:B:354:ASN:HB2	0.46	1.87	7	1
1:B:405:LEU:O	1:B:409:ILE:HD12	0.46	2.11	16	3
1:A:39:LEU:HD12	1:A:42:ILE:CG1	0.46	2.41	1	1
1:A:48:VAL:O	1:A:48:VAL:HG13	0.46	2.10	10	2
1:B:370:VAL:HG22	1:B:412:ARG:NH1	0.45	2.27	14	1
1:A:4:LEU:CD2	1:A:6:ILE:HD11	0.45	2.41	19	1
1:B:303:VAL:HG21	1:B:320:LEU:HG	0.45	1.88	18	1
1:A:33:LEU:HD21	1:A:54:ASN:HB2	0.45	1.88	17	2
1:B:312:LEU:HD11	1:B:399:TYR:CE2	0.45	2.47	2	2
1:A:47:LEU:HD21	1:A:72:LEU:HD12	0.45	1.88	10	2
1:A:47:LEU:HD13	1:A:47:LEU:C	0.45	2.32	18	6
1:A:47:LEU:HD11	1:A:72:LEU:CD1	0.45	2.39	4	2
1:B:307:GLU:CG	1:B:309:ASN:ND2	0.45	2.79	16	1
1:A:39:LEU:HD21	1:A:45:TYR:OH	0.45	2.11	8	1
1:B:373:VAL:CG2	1:B:391:ALA:HB2	0.45	2.42	8	2
1:A:55:ALA:O	1:A:59:VAL:HG13	0.45	2.11	3	3
1:A:95:ILE:HD13	1:A:105:LEU:CD2	0.45	2.39	19	1
1:B:347:LEU:HD23	1:B:413:LEU:HD22	0.45	1.87	16	2
1:A:73:VAL:CG2	1:A:91:ALA:HB2	0.45	2.42	17	4
1:B:370:VAL:HG21	1:B:413:LEU:HB3	0.44	1.88	20	4
1:A:7:GLU:OE2	1:A:16:ILE:HD12	0.44	2.12	1	1
1:B:347:LEU:HD21	1:B:372:LEU:CD1	0.44	2.43	19	1
1:B:395:ILE:HD13	1:B:405:LEU:CD2	0.44	2.41	19	1
1:A:48:VAL:HG13	1:A:48:VAL:O	0.44	2.11	15	2
1:A:72:LEU:HD23	1:A:93:ASP:HB2	0.44	1.90	4	1
1:A:56:LEU:HD23	1:A:85:HIS:CD2	0.44	2.48	1	6
1:B:320:LEU:CD1	1:B:406:VAL:HG23	0.43	2.43	18	2
1:A:95:ILE:CD1	1:A:105:LEU:HD21	0.43	2.36	2	3
1:B:347:LEU:HD21	1:B:372:LEU:HD12	0.43	1.88	19	3
1:B:304:LEU:CB	1:B:348:VAL:HG12	0.43	2.44	13	1
1:A:72:LEU:HD21	1:A:112:ARG:HH22	0.43	1.72	13	1
1:B:308:LYS:HG2	1:B:331:GLU:O	0.43	2.13	19	1
1:B:348:VAL:HG21	1:B:358:PHE:HZ	0.43	1.73	16	2
1:B:347:LEU:C	1:B:347:LEU:HD13	0.43	2.34	3	3
1:B:307:GLU:OE1	1:B:312:LEU:HD23	0.43	2.14	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:306:ILE:CB	1:B:350:VAL:HG23	0.43	2.44	16	1
1:A:83:GLU:OE2	1:B:404:ALA:HB1	0.42	2.14	1	1
1:A:39:LEU:CD1	1:A:42:ILE:HD11	0.42	2.44	16	4
1:B:318:LYS:O	1:B:322:VAL:HG23	0.42	2.15	17	1
1:B:347:LEU:HD12	1:B:370:VAL:O	0.42	2.14	20	1
1:A:109:ILE:O	1:A:113:LEU:HD22	0.42	2.14	11	1
1:A:6:ILE:HD12	1:A:50:VAL:HB	0.42	1.90	1	1
1:B:333:LEU:HD22	1:B:334:GLU:N	0.42	2.30	9	1
1:A:71:VAL:HG22	1:A:92:ASP:OD2	0.42	2.13	17	1
1:A:70:VAL:HG11	1:A:112:ARG:HH11	0.42	1.73	11	1
1:B:370:VAL:HG11	1:B:412:ARG:HG2	0.42	1.90	15	1
1:B:333:LEU:HD12	1:B:350:VAL:HG21	0.42	1.91	9	1
1:B:305:LEU:HD21	1:B:316:ILE:HG22	0.42	1.91	6	1
1:B:309:ASN:O	1:B:310:SER:CB	0.42	2.68	15	1
1:A:33:LEU:HD22	1:A:58:PHE:CB	0.42	2.44	12	1
1:B:372:LEU:HD23	1:B:393:ASP:HB3	0.42	1.91	5	1
1:B:373:VAL:HG11	1:B:391:ALA:HB2	0.41	1.92	4	2
1:B:356:LEU:HD23	1:B:385:HIS:CD2	0.41	2.51	6	1
1:B:359:VAL:HG11	1:B:373:VAL:HG12	0.41	1.91	14	2
1:A:104:ALA:HB2	1:B:380:SER:HB2	0.41	1.91	11	1
1:B:304:LEU:HD23	1:B:348:VAL:HG13	0.41	1.91	10	1
1:B:304:LEU:HD11	1:B:336:GLY:HA2	0.41	1.93	12	1
1:A:3:VAL:HG13	1:A:47:LEU:CD1	0.41	2.37	7	1
1:A:48:VAL:HG21	1:A:58:PHE:HZ	0.41	1.76	18	2
1:B:347:LEU:HG	1:B:409:ILE:HG23	0.41	1.93	8	1
1:A:47:LEU:HD21	1:A:72:LEU:CD1	0.41	2.46	1	1
1:B:304:LEU:HD23	1:B:348:VAL:HG12	0.41	1.93	14	1
1:B:333:LEU:CD1	1:B:333:LEU:H	0.41	2.17	9	1
1:B:384:VAL:HG23	1:B:385:HIS:N	0.41	2.31	9	1
1:B:306:ILE:CG2	1:B:331:GLU:O	0.40	2.69	19	1
1:B:303:VAL:HB	1:B:347:LEU:HD12	0.40	1.91	11	1
1:B:348:VAL:HG13	1:B:348:VAL:O	0.40	2.15	8	1
1:A:72:LEU:HD23	1:A:93:ASP:CB	0.40	2.46	3	1
1:B:323:LYS:HE3	1:B:406:VAL:HG11	0.40	1.94	4	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	112/123 (91%)	102±2 (91±1%)	9±2 (8±1%)	1±1 (1±1%)	23	69
1	B	112/123 (91%)	102±1 (91±1%)	9±1 (8±1%)	1±1 (1±1%)	24	71
All	All	4480/4920 (91%)	4069 (91%)	363 (8%)	48 (1%)	23	69

All 7 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	B	324	GLY	14
1	A	24	GLY	12
1	A	9	ASN	9
1	B	309	ASN	6
1	B	390	GLY	3
1	A	90	GLY	3
1	A	45	TYR	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	98/108 (91%)	80±2 (81±2%)	18±2 (19±2%)	5	38
1	B	98/108 (91%)	79±2 (81±2%)	19±2 (19±2%)	5	37
All	All	3920/4320 (91%)	3178 (81%)	742 (19%)	5	38

All 106 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	B	401	SER	20
1	B	361	ARG	20
1	A	97	LYS	20
1	A	61	ARG	20
1	B	333	LEU	20
1	A	101	SER	20

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Mol	Chain	Res	Type	Models (Total)
1	A	74	SER	20
1	B	397	LYS	20
1	B	374	SER	20
1	A	33	LEU	20
1	B	393	ASP	19
1	B	375	SER	19
1	B	365	LYS	19
1	B	331	GLU	18
1	A	113	LEU	17
1	A	65	LYS	17
1	A	31	GLU	17
1	B	403	LYS	16
1	B	413	LEU	16
1	A	105	LEU	16
1	A	103	LYS	15
1	A	80	SER	15
1	A	93	ASP	15
1	B	352	ASP	15
1	A	75	SER	13
1	B	380	SER	12
1	A	112	ARG	12
1	A	108	ARG	12
1	B	408	ARG	11
1	B	348	VAL	9
1	A	3	VAL	8
1	A	35	ASP	8
1	A	46	ASP	8
1	B	346	ASP	7
1	A	26	MET	6
1	B	332	SER	6
1	A	52	ASP	6
1	A	48	VAL	6
1	A	42	ILE	6
1	B	349	MET	6
1	B	342	ILE	6
1	B	412	ARG	6
1	B	318	LYS	5
1	A	40	MET	5
1	A	9	ASN	5
1	A	110	GLU	5
1	B	337	GLU	5
1	B	358	PHE	5

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Mol	Chain	Res	Type	Models (Total)
1	B	405	LEU	5
1	B	340	MET	5
1	B	335	ASP	5
1	B	303	VAL	4
1	B	339	LEU	4
1	A	53	LYS	4
1	A	7	GLU	4
1	B	343	ARG	4
1	B	309	ASN	4
1	B	328	ASP	3
1	B	341	ASP	3
1	A	72	LEU	3
1	A	2	ARG	3
1	A	8	LYS	3
1	A	49	MET	3
1	A	100	ARG	3
1	B	399	TYR	3
1	B	410	GLU	3
1	B	302	ARG	3
1	B	353	LYS	3
1	A	64	GLU	3
1	A	43	ARG	3
1	B	347	LEU	2
1	A	67	SER	2
1	B	308	LYS	2
1	B	383	GLU	2
1	A	41	ASP	2
1	A	57	SER	2
1	B	368	SER	2
1	A	28	ASP	2
1	A	39	LEU	2
1	A	58	PHE	2
1	B	381	GLU	2
1	B	372	LEU	2
1	B	330	THR	2
1	A	18	LYS	2
1	A	21	ASN	2
1	A	76	ASP	2
1	A	99	TYR	1
1	B	321	ASN	1
1	B	369	ILE	1
1	B	376	ASP	1

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Mol	Chain	Res	Type	Models (Total)
1	A	68	SER	1
1	B	392	ASP	1
1	A	77	ASN	1
1	B	310	SER	1
1	B	357	SER	1
1	B	371	VAL	1
1	B	326	MET	1
1	A	83	GLU	1
1	A	37	GLU	1
1	B	356	LEU	1
1	B	351	SER	1
1	A	56	LEU	1
1	A	44	ASN	1
1	A	10	SER	1
1	B	304	LEU	1
1	A	32	SER	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 ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided