Full wwPDB NMR Structure Validation Report (i)

Apr 26, 2016 – 03:57 PM BST

PDB ID	:	1MV3
Title	:	NMR STRUCTURE OF THE TUMOR SUPPRESSOR BIN1: ALTERNATIVE SPLICING IN MELANOMA AND INTERACTION WITH C-MYC
Authors	:	Pineda-Lucena, A.; Arrowsmith, C.H.
Deposited on	:	2002-09-24

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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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

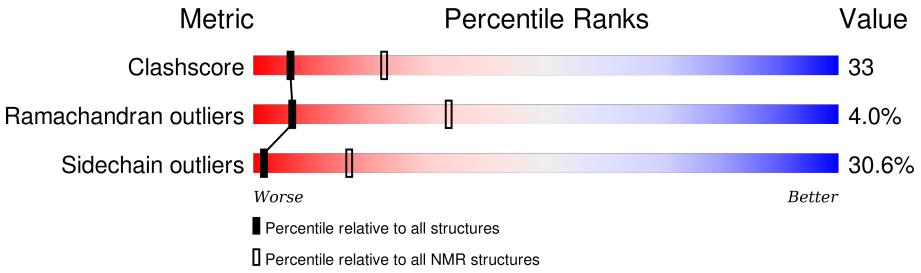
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	213	23% 22% 7% 48%

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:271-A:297 (27)	0.71	8
2	A:308-A:311, A:403-A:482 (84)	0.16	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 4 clusters and 4 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3107 atoms, of which 1525 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Myc box dependent interacting protein 1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	213	3107	990	1525	266	323	3	0

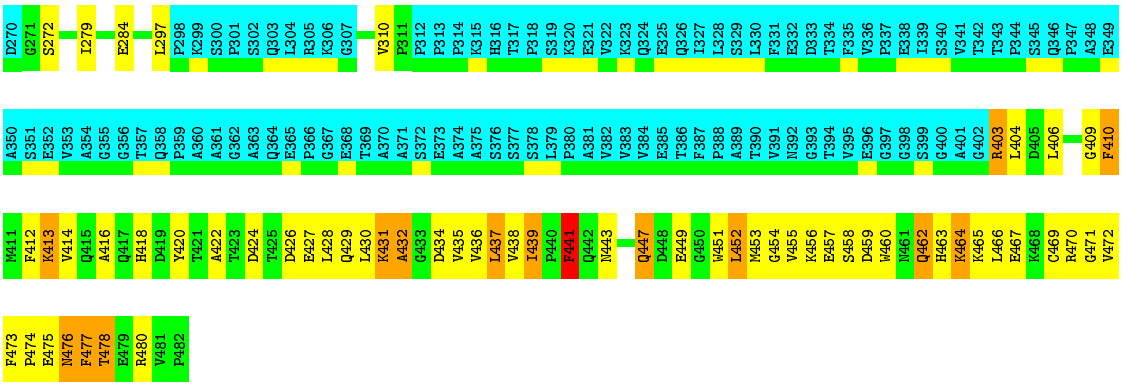
4 Residue-property plots

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: Myc box dependent interacting protein 1

Chain A:



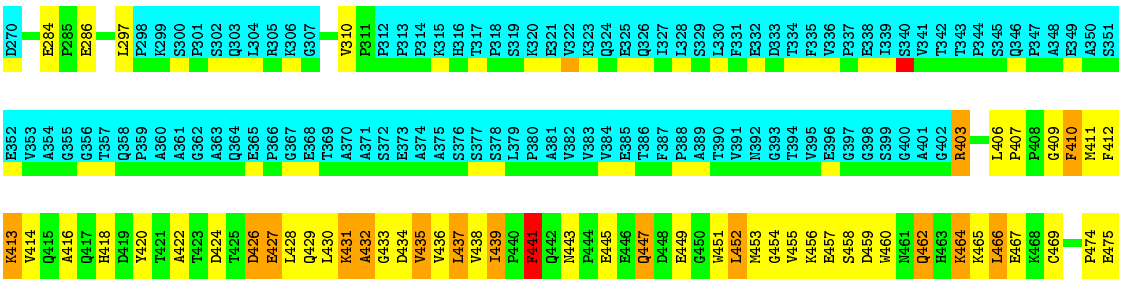
4.2 Scores per residue for each member of the ensemble

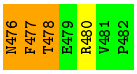
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Myc box dependent interacting protein 1

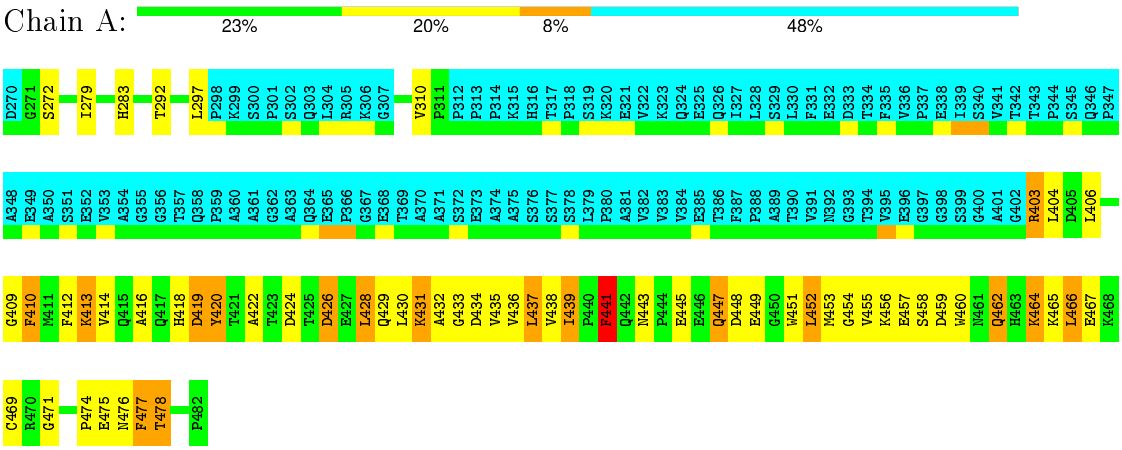
Chain A:





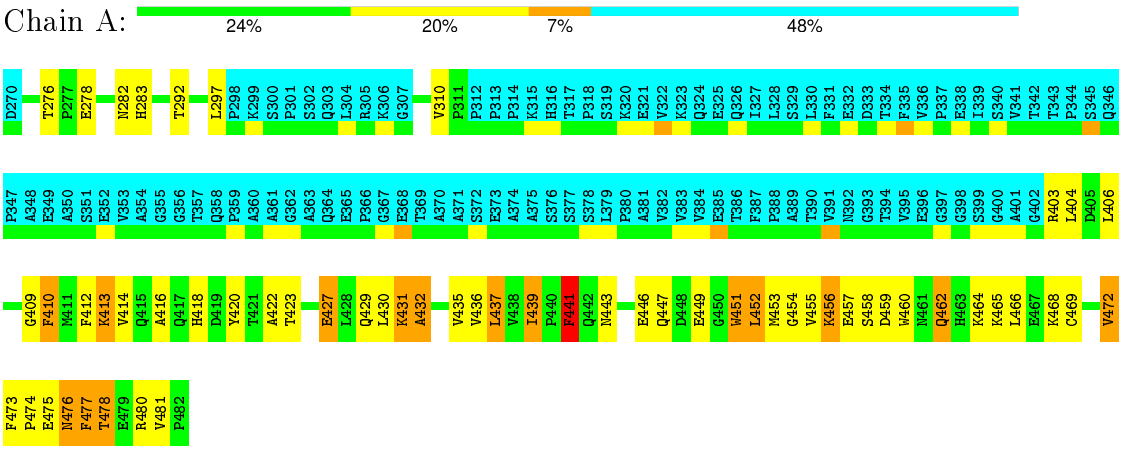
4.2.2 Score per residue for model 2 (medoid)

• Molecule 1: Myc box dependent interacting protein 1



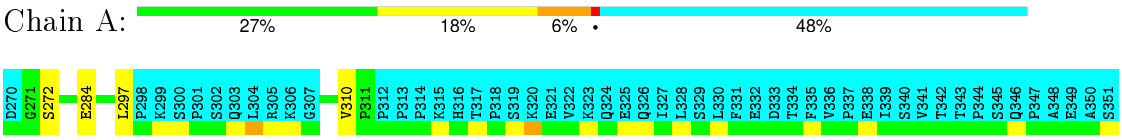
4.2.3 Score per residue for model 3

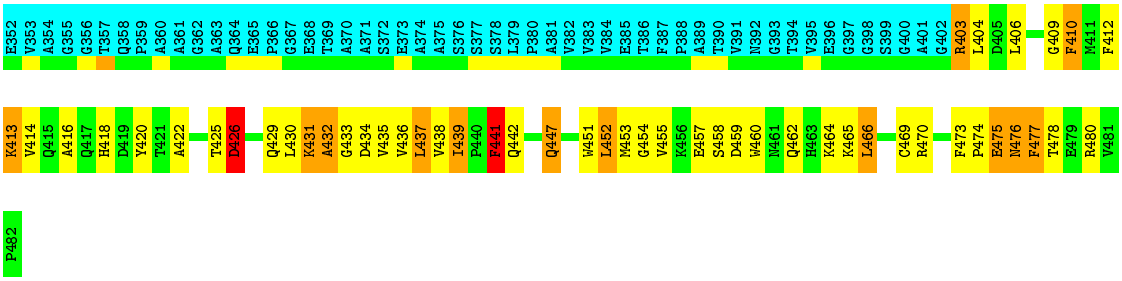
• Molecule 1: Myc box dependent interacting protein 1



4.2.4 Score per residue for model 4

• Molecule 1: Myc box dependent interacting protein 1

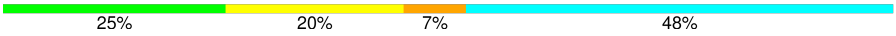


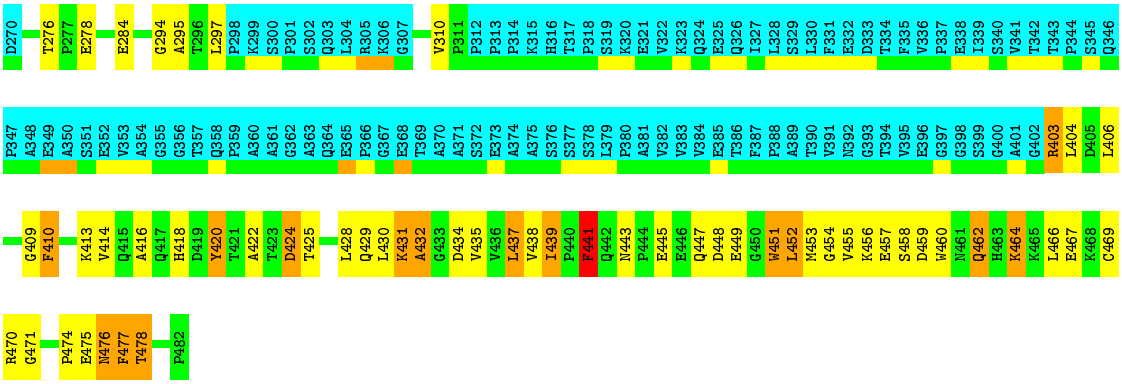


4.2.5 Score per residue for model 5

- Molecule 1: Myc box dependent interacting protein 1

Chain A:

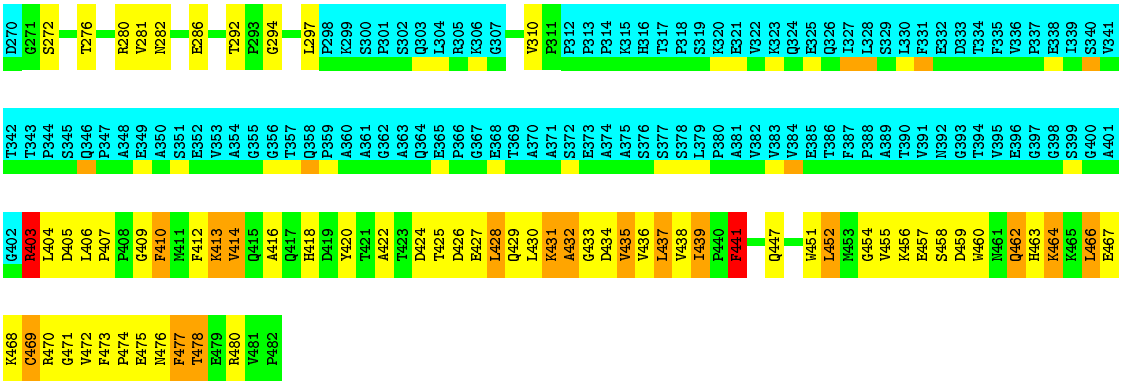




4.2.6 Score per residue for model 6

- Molecule 1: Myc box dependent interacting protein 1

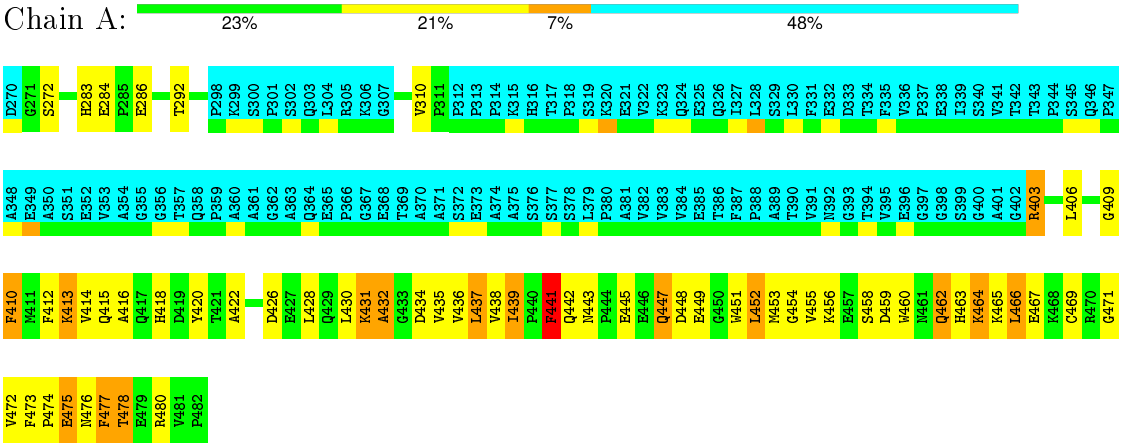
Chain A:



4.2.7 Score per residue for model 7

• Molecule 1: Myc box dependent interacting protein 1

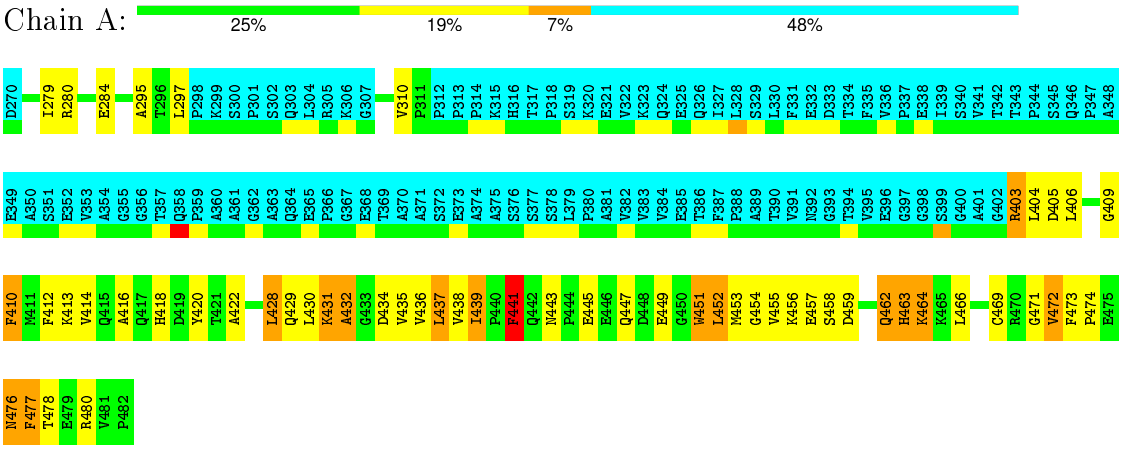
Chain A:



4.2.8 Score per residue for model 8

• Molecule 1: Myc box dependent interacting protein 1

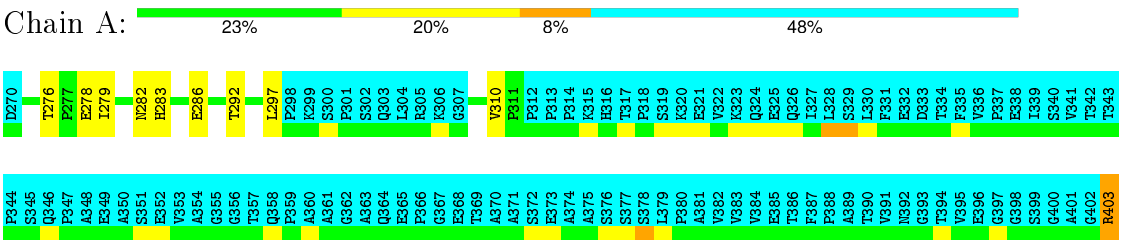
Chain A:

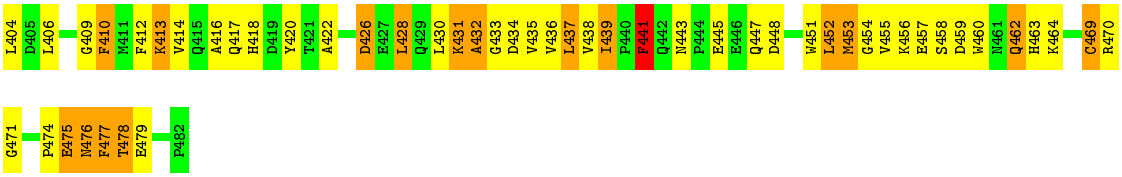


4.2.9 Score per residue for model 9

• Molecule 1: Myc box dependent interacting protein 1

Chain A:

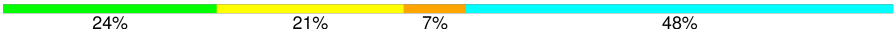


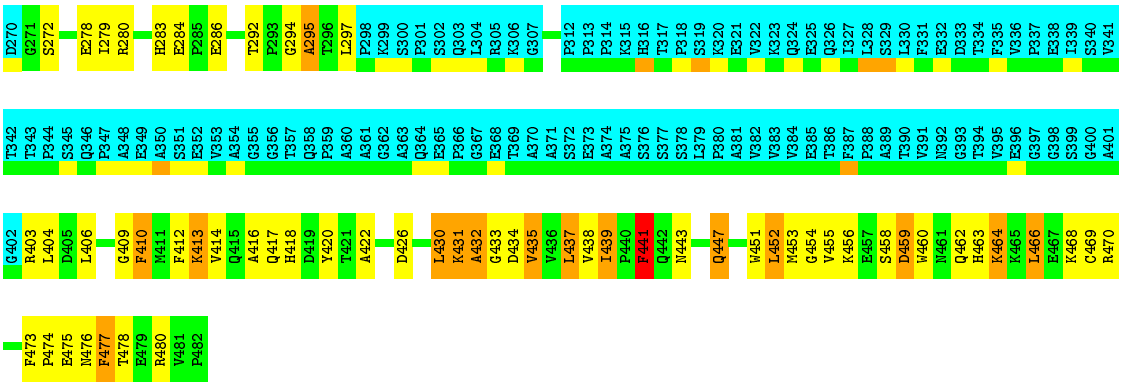


4.2.10 Score per residue for model 10

- Molecule 1: Myc box dependent interacting protein 1

Chain A:

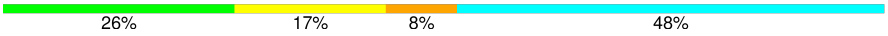


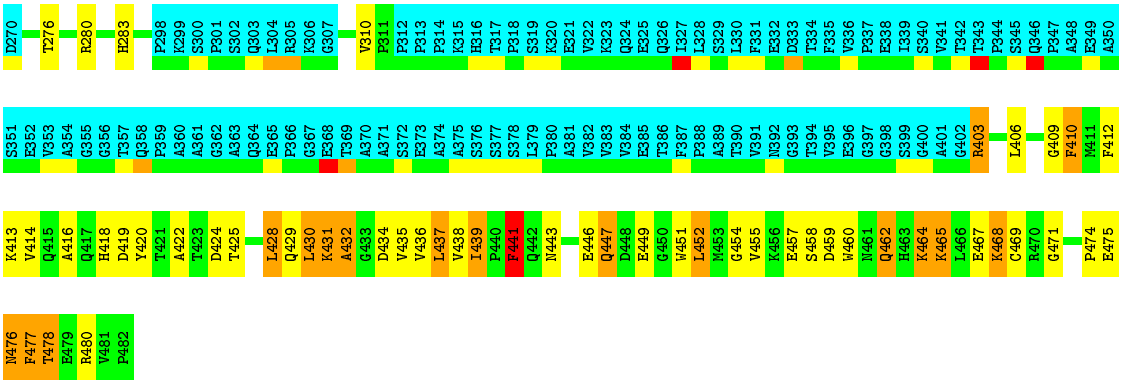


4.2.11 Score per residue for model 11

- Molecule 1: Myc box dependent interacting protein 1

Chain A:

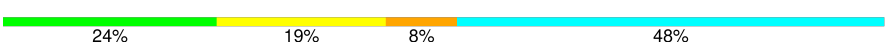


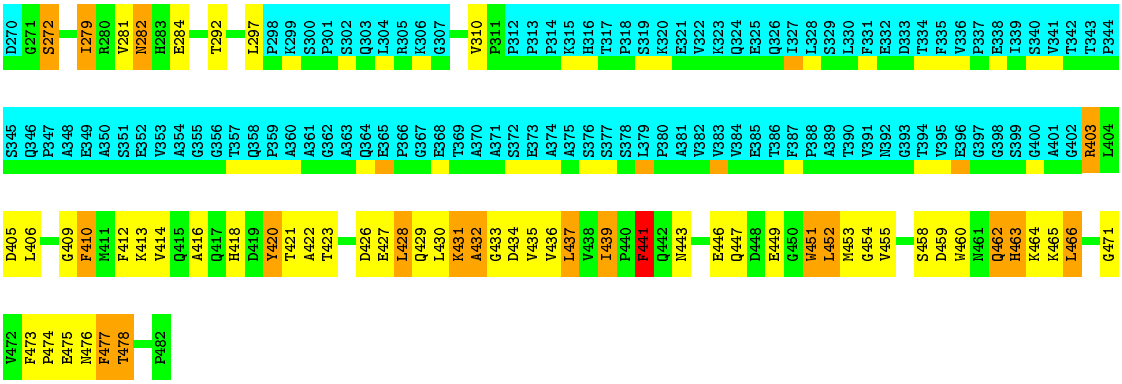


4.2.12 Score per residue for model 12

- Molecule 1: Myc box dependent interacting protein 1

Chain A:

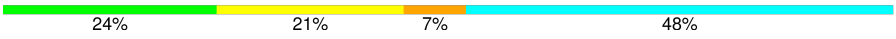


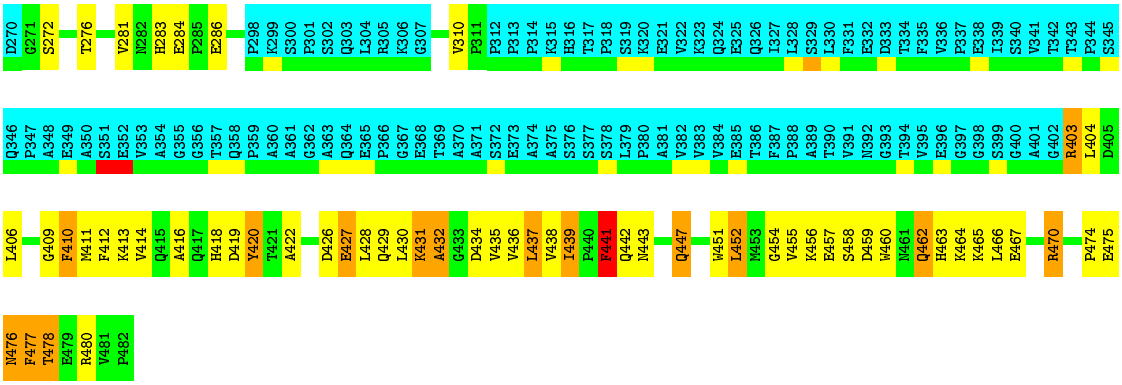


4.2.13 Score per residue for model 13

- Molecule 1: Myc box dependent interacting protein 1

Chain A:

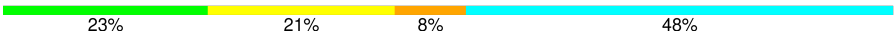


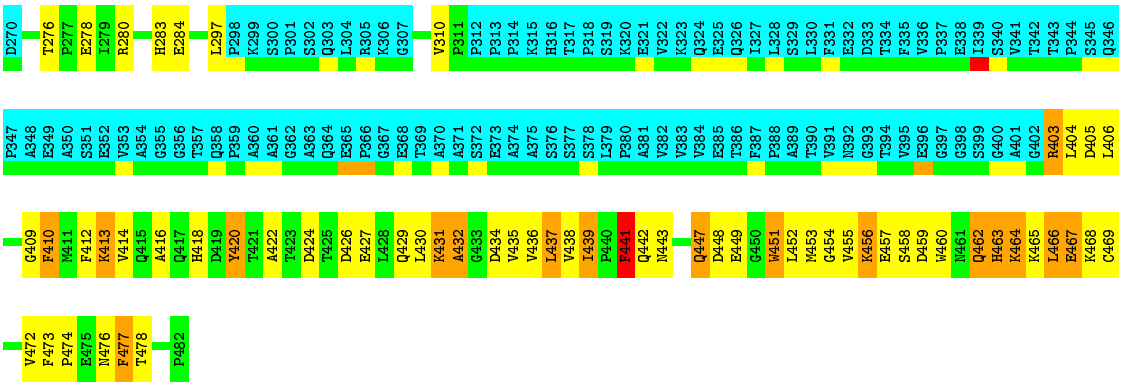


4.2.14 Score per residue for model 14

- Molecule 1: Myc box dependent interacting protein 1

Chain A:

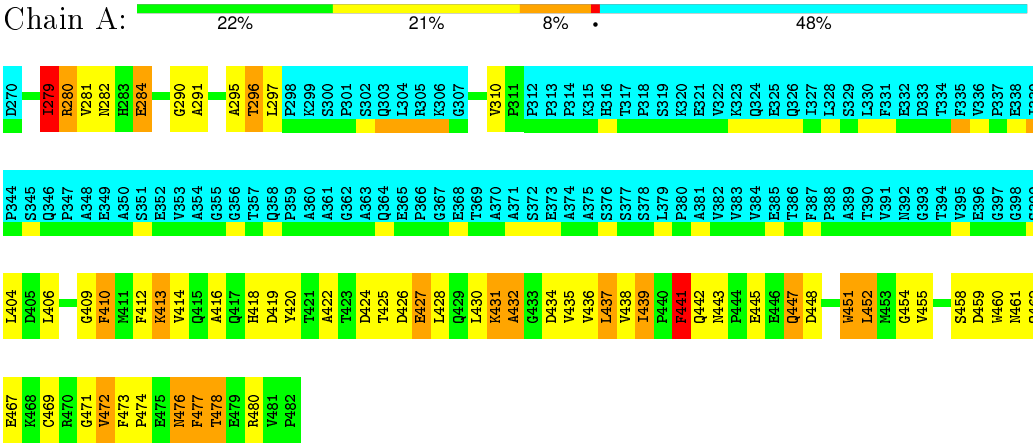




4.2.15 Score per residue for model 15

• Molecule 1: Myc box dependent interacting protein 1

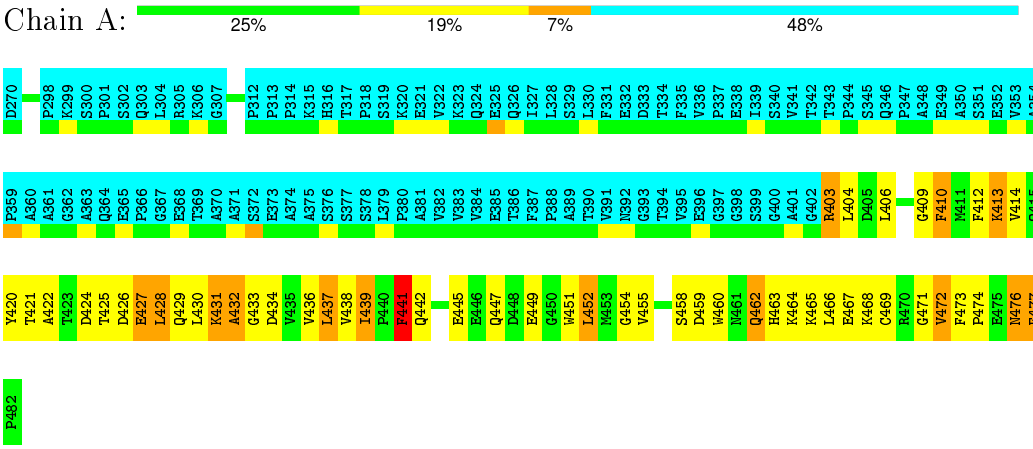
Chain A:



4.2.16 Score per residue for model 16

• Molecule 1: Myc box dependent interacting protein 1

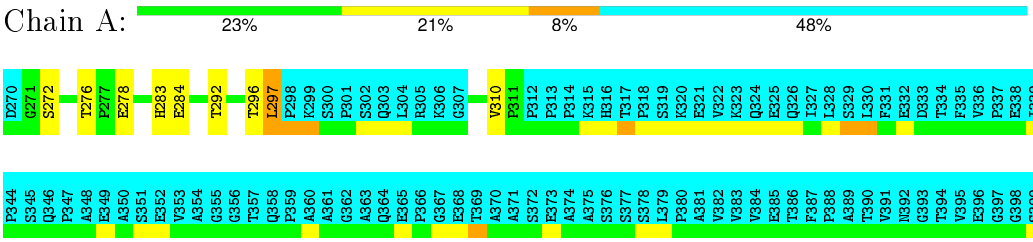
Chain A:

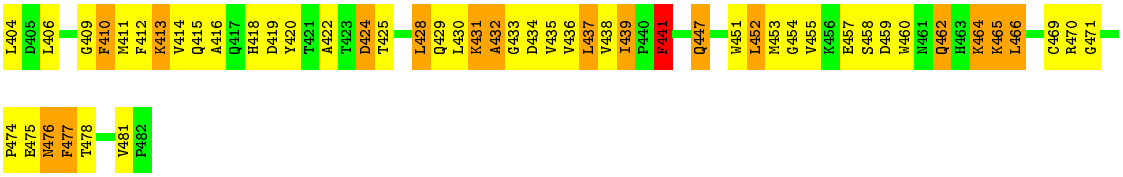


4.2.17 Score per residue for model 17

• Molecule 1: Myc box dependent interacting protein 1

Chain A:

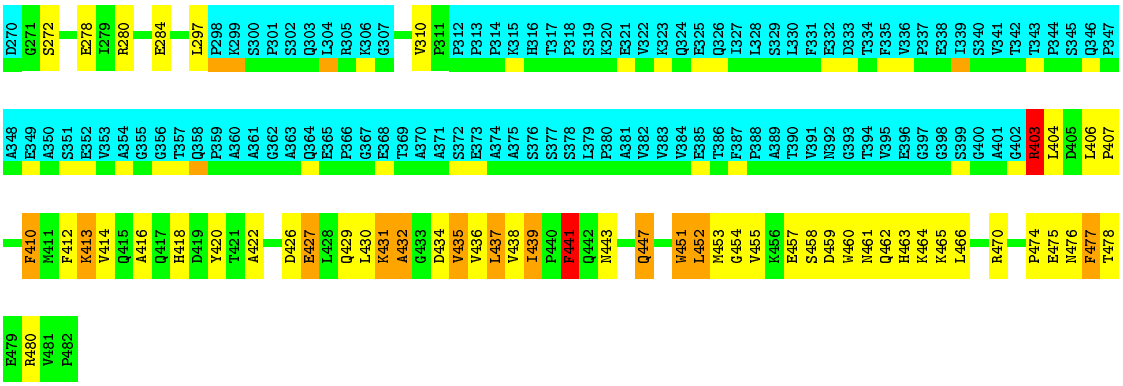




4.2.18 Score per residue for model 18

- Molecule 1: Myc box dependent interacting protein 1

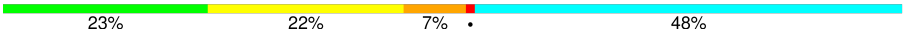
Chain A:

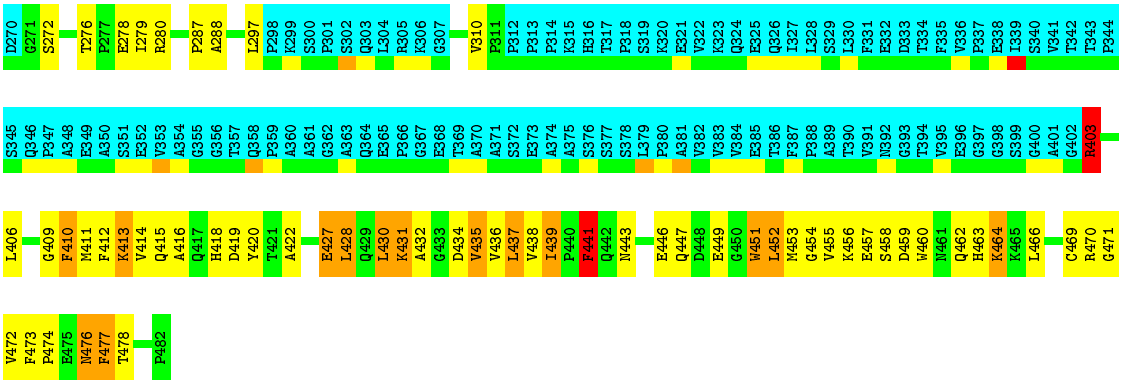


4.2.19 Score per residue for model 19

- Molecule 1: Myc box dependent interacting protein 1

Chain A:

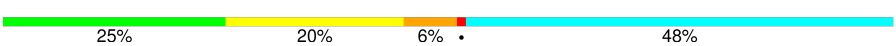


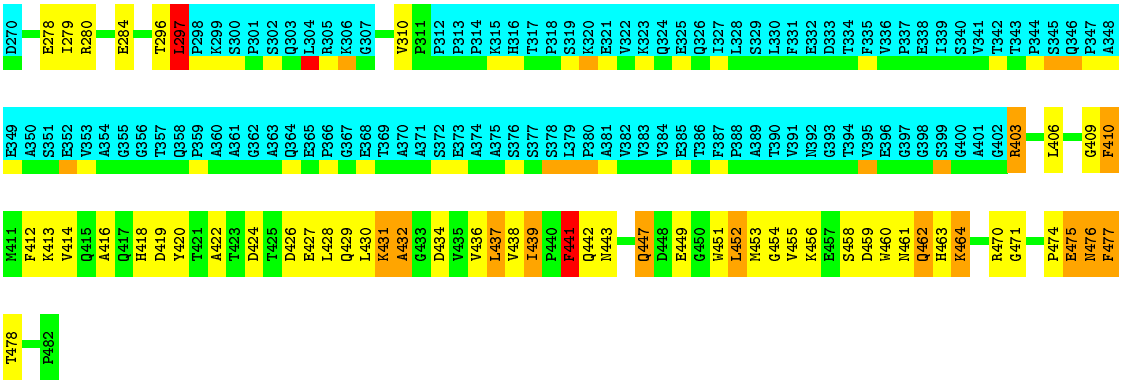


4.2.20 Score per residue for model 20

- Molecule 1: Myc box dependent interacting protein 1

Chain A:




D270 E278 I279 R280 E284 T296 L297 P298 K299 S300 P301 S302 Q303 L304 R305 K306 G307 V310 P311 P312 P313 P314 K315 H316 T317 P318 S319 K320 E321 V322 K323 Q324 E325 Q326 I327 L328 S329 L330 F331 E332 D333 T334 F335 V336 P337 E338 I339 S340 V341 T342 T343 P344 S345 Q346 P347 A348
E349 A350 S351 E352 V353 A354 G355 G356 T357 Q358 P359 A360 A361 G362 A363 Q364 E365 P366 G367 E368 T369 A370 A371 S372 E373 A374 A375 S376 S377 S378 L379 P380 A381 V382 V383 V384 E385 T386 F387 P388 A389 T390 V391 N392 G393 T394 V395 E396 G397 G398 S399 G400 A401 G402 R403 L406 G409 F410
M411 F412 K413 V414 Q415 A416 Q417 H418 D419 Y420 T421 A422 T423 D424 T425 D426 E427 L428 Q429 L430 K431 A432 G433 D434 V435 V436 L437 V438 I439 P440 F441 Q442 N443 Q447 D448 E449 G450 W451 L452 M453 G454 V455 K456 E457 S458 D459 W460 N461 Q462 H463 K464 R470 G471 P474 E475 N476 F477
T478 P482

5 Refinement protocol and experimental data overview

The models were refined using the following method: *TORSION ANGLE DYNAMICS*.

Of the 200 calculated structures, 20 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
DYANA	structure solution	1.5
DYANA	refinement	1.5

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	864	829	829	56±6
All	All	17280	16580	16580	1119

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 33.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:430:LEU:HD11	1:A:436:VAL:HG21	0.98	1.34	12	16
1:A:430:LEU:HD11	1:A:436:VAL:CG2	0.94	1.91	7	16
1:A:420:TYR:CE2	1:A:422:ALA:HB2	0.91	2.00	1	20
1:A:416:ALA:HB2	1:A:430:LEU:HD12	0.87	1.45	5	6
1:A:451:TRP:C	1:A:452:LEU:HD23	0.86	1.91	20	11
1:A:414:VAL:HG22	1:A:436:VAL:O	0.85	1.71	12	10
1:A:477:PHE:CD1	1:A:478:THR:HG23	0.84	2.07	19	20
1:A:455:VAL:HG22	1:A:459:ASP:HB2	0.82	1.52	17	15
1:A:420:TYR:CZ	1:A:422:ALA:HB2	0.81	2.10	19	20
1:A:437:LEU:HD13	1:A:460:TRP:CE3	0.78	2.14	13	16
1:A:416:ALA:HB2	1:A:430:LEU:HD23	0.76	1.57	10	2
1:A:413:LYS:HE3	1:A:435:VAL:HG13	0.75	1.59	7	1
1:A:452:LEU:HD11	1:A:475:GLU:HB2	0.73	1.58	3	9
1:A:455:VAL:HG22	1:A:459:ASP:CB	0.72	2.13	17	12

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:437:LEU:HG	1:A:455:VAL:HG13	0.72	1.60	12	15
1:A:422:ALA:HB1	1:A:427:GLU:CG	0.71	2.14	6	5
1:A:413:LYS:CE	1:A:435:VAL:HG13	0.71	2.16	7	1
1:A:412:PHE:CE1	1:A:438:VAL:HG21	0.69	2.22	14	1
1:A:416:ALA:HA	1:A:478:THR:HG22	0.69	1.64	16	20
1:A:429:GLN:C	1:A:430:LEU:HD22	0.68	2.09	8	14
1:A:422:ALA:HB1	1:A:427:GLU:HG3	0.68	1.64	6	4
1:A:437:LEU:HD23	1:A:437:LEU:N	0.68	2.04	18	11
1:A:437:LEU:CD1	1:A:460:TRP:CE3	0.67	2.77	13	14
1:A:292:THR:HG23	1:A:292:THR:O	0.67	1.89	3	2
1:A:403:ARG:CZ	1:A:460:TRP:CE2	0.66	2.79	6	1
1:A:416:ALA:HB2	1:A:430:LEU:CD2	0.65	2.21	19	2
1:A:430:LEU:HD11	1:A:436:VAL:HG23	0.65	1.69	7	2
1:A:295:ALA:O	1:A:296:THR:HG22	0.65	1.91	15	1
1:A:451:TRP:O	1:A:452:LEU:HD23	0.64	1.92	2	5
1:A:437:LEU:HD11	1:A:460:TRP:CE3	0.64	2.28	4	7
1:A:403:ARG:CZ	1:A:463:HIS:CG	0.63	2.81	8	2
1:A:414:VAL:CG1	1:A:438:VAL:HG23	0.63	2.24	9	16
1:A:477:PHE:HD1	1:A:478:THR:HG23	0.63	1.53	4	19
1:A:429:GLN:O	1:A:430:LEU:HD22	0.63	1.94	3	11
1:A:437:LEU:N	1:A:437:LEU:HD23	0.63	2.09	7	7
1:A:439:ILE:HD13	1:A:454:GLY:HA2	0.62	1.69	14	20
1:A:413:LYS:NZ	1:A:435:VAL:HG12	0.62	2.09	14	6
1:A:477:PHE:CG	1:A:477:PHE:O	0.62	2.52	14	13
1:A:466:LEU:HD23	1:A:467:GLU:N	0.61	2.11	1	3
1:A:477:PHE:O	1:A:477:PHE:CG	0.61	2.53	10	7
1:A:428:LEU:HD23	1:A:471:GLY:HA3	0.60	1.73	17	8
1:A:403:ARG:NH1	1:A:460:TRP:CD2	0.60	2.70	6	1
1:A:463:HIS:HA	1:A:466:LEU:HD22	0.59	1.73	12	1
1:A:279:ILE:HD13	1:A:280:ARG:N	0.59	2.12	15	1
1:A:452:LEU:HD23	1:A:452:LEU:N	0.58	2.14	11	4
1:A:310:VAL:HG13	1:A:476:ASN:HB2	0.58	1.74	8	15
1:A:294:GLY:O	1:A:295:ALA:HB2	0.58	1.98	10	1
1:A:403:ARG:NH1	1:A:460:TRP:CG	0.58	2.72	6	1
1:A:455:VAL:CG2	1:A:459:ASP:CB	0.57	2.82	19	19
1:A:414:VAL:HG11	1:A:438:VAL:HG23	0.57	1.76	9	9
1:A:431:LYS:O	1:A:432:ALA:C	0.57	2.43	7	19
1:A:477:PHE:CD1	1:A:477:PHE:O	0.57	2.57	14	10
1:A:441:PHE:CD1	1:A:441:PHE:N	0.56	2.73	6	8
1:A:435:VAL:HG23	1:A:457:GLU:CB	0.56	2.31	5	10
1:A:451:TRP:N	1:A:451:TRP:CD1	0.56	2.73	5	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:477:PHE:O	1:A:477:PHE:CD1	0.56	2.59	15	10
1:A:403:ARG:NH2	1:A:463:HIS:CE1	0.55	2.74	8	2
1:A:403:ARG:NE	1:A:463:HIS:CD2	0.55	2.74	8	2
1:A:428:LEU:HD13	1:A:471:GLY:HA3	0.55	1.77	7	4
1:A:428:LEU:HD23	1:A:471:GLY:CA	0.55	2.32	17	7
1:A:462:GLN:NE2	1:A:462:GLN:N	0.55	2.55	16	2
1:A:451:TRP:CD1	1:A:451:TRP:N	0.55	2.75	19	6
1:A:434:ASP:OD2	1:A:456:LYS:CD	0.55	2.55	5	3
1:A:423:THR:N	1:A:427:GLU:OE1	0.55	2.40	12	1
1:A:441:PHE:N	1:A:441:PHE:CD1	0.54	2.73	13	12
1:A:405:ASP:O	1:A:463:HIS:CD2	0.54	2.61	6	1
1:A:436:VAL:C	1:A:437:LEU:HD23	0.54	2.22	18	5
1:A:403:ARG:H	1:A:403:ARG:NE	0.54	2.01	15	5
1:A:430:LEU:HD13	1:A:434:ASP:OD2	0.54	2.03	12	10
1:A:451:TRP:CZ3	1:A:474:PRO:HG3	0.54	2.38	14	12
1:A:427:GLU:OE2	1:A:472:VAL:HG22	0.54	2.02	14	1
1:A:437:LEU:HD22	1:A:460:TRP:CE3	0.54	2.38	17	2
1:A:439:ILE:HD12	1:A:455:VAL:HG12	0.54	1.79	12	3
1:A:403:ARG:CZ	1:A:463:HIS:CD2	0.54	2.91	8	1
1:A:413:LYS:NZ	1:A:481:VAL:HG21	0.53	2.18	3	2
1:A:403:ARG:NH2	1:A:463:HIS:CD2	0.53	2.77	8	1
1:A:428:LEU:CD1	1:A:454:GLY:O	0.53	2.56	8	1
1:A:424:ASP:CB	1:A:427:GLU:OE1	0.53	2.56	6	2
1:A:413:LYS:HZ3	1:A:481:VAL:HG11	0.53	1.62	16	1
1:A:477:PHE:C	1:A:477:PHE:CD1	0.53	2.81	15	11
1:A:413:LYS:HE3	1:A:435:VAL:HG12	0.53	1.79	10	6
1:A:430:LEU:HD12	1:A:434:ASP:HB3	0.53	1.81	7	2
1:A:418:HIS:O	1:A:477:PHE:CZ	0.53	2.62	19	20
1:A:477:PHE:CD1	1:A:477:PHE:C	0.53	2.83	12	9
1:A:297:LEU:O	1:A:297:LEU:HD12	0.52	2.04	9	1
1:A:310:VAL:O	1:A:476:ASN:CB	0.52	2.57	7	17
1:A:403:ARG:HD2	1:A:460:TRP:CD1	0.52	2.39	1	10
1:A:276:THR:CG2	1:A:276:THR:O	0.52	2.57	14	2
1:A:296:THR:O	1:A:297:LEU:CB	0.52	2.56	20	1
1:A:403:ARG:NH2	1:A:463:HIS:NE2	0.52	2.58	8	1
1:A:403:ARG:CD	1:A:405:ASP:O	0.52	2.57	14	2
1:A:292:THR:O	1:A:292:THR:HG23	0.52	2.05	9	3
1:A:435:VAL:HG23	1:A:457:GLU:HB3	0.52	1.80	3	11
1:A:296:THR:O	1:A:297:LEU:HD12	0.52	2.03	17	1
1:A:451:TRP:CZ3	1:A:474:PRO:HD3	0.52	2.40	16	13
1:A:403:ARG:CZ	1:A:460:TRP:NE1	0.52	2.73	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:403:ARG:CD	1:A:460:TRP:CD1	0.51	2.94	5	5
1:A:310:VAL:HG13	1:A:310:VAL:O	0.51	2.06	6	6
1:A:461:ASN:N	1:A:461:ASN:ND2	0.51	2.59	15	2
1:A:452:LEU:CD1	1:A:473:PHE:CZ	0.51	2.94	12	4
1:A:403:ARG:NH2	1:A:460:TRP:CZ2	0.51	2.79	6	1
1:A:276:THR:HG23	1:A:276:THR:O	0.50	2.06	14	3
1:A:452:LEU:HD12	1:A:452:LEU:N	0.50	2.20	6	1
1:A:431:LYS:CD	1:A:434:ASP:OD1	0.50	2.59	20	2
1:A:477:PHE:CE1	1:A:478:THR:HG23	0.50	2.40	11	7
1:A:410:PHE:CZ	1:A:412:PHE:HA	0.50	2.42	11	17
1:A:403:ARG:NE	1:A:403:ARG:N	0.50	2.60	1	3
1:A:295:ALA:O	1:A:296:THR:CG2	0.50	2.59	15	1
1:A:403:ARG:CZ	1:A:403:ARG:O	0.50	2.60	9	2
1:A:462:GLN:N	1:A:462:GLN:NE2	0.50	2.60	9	1
1:A:430:LEU:CD1	1:A:434:ASP:OD2	0.50	2.60	9	6
1:A:441:PHE:CE2	1:A:447:GLN:HB2	0.50	2.41	4	15
1:A:429:GLN:O	1:A:456:LYS:CD	0.50	2.60	14	1
1:A:451:TRP:CE3	1:A:474:PRO:HD3	0.49	2.42	14	9
1:A:420:TYR:O	1:A:420:TYR:CD2	0.49	2.65	13	1
1:A:290:GLY:O	1:A:291:ALA:HB2	0.49	2.06	15	1
1:A:430:LEU:HD22	1:A:478:THR:CG2	0.49	2.37	10	1
1:A:403:ARG:N	1:A:403:ARG:NE	0.49	2.60	2	5
1:A:403:ARG:CG	1:A:405:ASP:O	0.49	2.61	8	2
1:A:414:VAL:HG11	1:A:438:VAL:CG2	0.49	2.36	9	5
1:A:292:THR:O	1:A:292:THR:CG2	0.49	2.59	2	1
1:A:430:LEU:CD1	1:A:436:VAL:CG2	0.49	2.88	12	2
1:A:292:THR:CG2	1:A:292:THR:O	0.49	2.60	3	2
1:A:310:VAL:O	1:A:310:VAL:HG13	0.49	2.08	8	6
1:A:413:LYS:NZ	1:A:437:LEU:CD2	0.48	2.76	9	2
1:A:427:GLU:OE1	1:A:427:GLU:CA	0.48	2.61	16	2
1:A:412:PHE:CZ	1:A:480:ARG:HD3	0.48	2.43	4	7
1:A:441:PHE:CD2	1:A:447:GLN:HB2	0.48	2.44	5	5
1:A:448:ASP:N	1:A:448:ASP:OD1	0.48	2.47	5	1
1:A:428:LEU:HD22	1:A:454:GLY:O	0.48	2.08	1	1
1:A:412:PHE:CE1	1:A:480:ARG:HD3	0.48	2.44	15	3
1:A:424:ASP:CB	1:A:427:GLU:CD	0.48	2.82	16	1
1:A:414:VAL:N	1:A:436:VAL:O	0.48	2.43	12	4
1:A:415:GLN:N	1:A:481:VAL:HG23	0.48	2.24	17	1
1:A:455:VAL:CG2	1:A:459:ASP:HB3	0.47	2.39	16	16
1:A:407:PRO:HA	1:A:463:HIS:CE1	0.47	2.44	18	1
1:A:472:VAL:CG2	1:A:473:PHE:N	0.47	2.77	16	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:420:TYR:HB3	1:A:477:PHE:CE2	0.47	2.45	12	2
1:A:420:TYR:HB3	1:A:477:PHE:CZ	0.47	2.44	19	2
1:A:462:GLN:C	1:A:464:LYS:N	0.47	2.68	17	20
1:A:447:GLN:NE2	1:A:451:TRP:O	0.47	2.48	7	11
1:A:403:ARG:NE	1:A:463:HIS:CG	0.47	2.82	14	2
1:A:448:ASP:OD1	1:A:451:TRP:CD1	0.47	2.67	9	1
1:A:431:LYS:O	1:A:433:GLY:N	0.46	2.49	4	9
1:A:411:MET:CE	1:A:438:VAL:CG1	0.46	2.93	13	3
1:A:413:LYS:CE	1:A:414:VAL:O	0.46	2.64	3	5
1:A:451:TRP:CE3	1:A:474:PRO:CD	0.46	2.98	5	6
1:A:455:VAL:CG2	1:A:459:ASP:HB2	0.46	2.39	12	6
1:A:413:LYS:CE	1:A:435:VAL:HG12	0.46	2.39	10	4
1:A:418:HIS:HB2	1:A:477:PHE:CE2	0.46	2.45	16	5
1:A:403:ARG:NH2	1:A:460:TRP:CE2	0.46	2.84	6	1
1:A:466:LEU:O	1:A:470:ARG:CG	0.46	2.63	6	3
1:A:437:LEU:CG	1:A:455:VAL:HG13	0.46	2.40	10	3
1:A:428:LEU:HD12	1:A:471:GLY:C	0.46	2.31	8	1
1:A:403:ARG:NE	1:A:403:ARG:H	0.46	2.08	5	1
1:A:437:LEU:CD2	1:A:437:LEU:N	0.46	2.75	1	5
1:A:412:PHE:CE1	1:A:414:VAL:HG12	0.46	2.46	17	1
1:A:415:GLN:NE2	1:A:434:ASP:O	0.46	2.49	7	2
1:A:420:TYR:CD2	1:A:420:TYR:O	0.46	2.69	1	1
1:A:452:LEU:H	1:A:452:LEU:HD12	0.46	1.71	6	1
1:A:407:PRO:N	1:A:463:HIS:NE2	0.46	2.64	6	1
1:A:413:LYS:HE3	1:A:437:LEU:HD23	0.46	1.88	17	2
1:A:278:GLU:O	1:A:279:ILE:HG23	0.45	2.12	20	1
1:A:435:VAL:CG2	1:A:457:GLU:CB	0.45	2.93	8	6
1:A:278:GLU:O	1:A:279:ILE:CG2	0.45	2.65	20	1
1:A:431:LYS:CE	1:A:434:ASP:OD2	0.45	2.64	17	2
1:A:294:GLY:O	1:A:295:ALA:CB	0.45	2.65	10	1
1:A:452:LEU:HD12	1:A:452:LEU:H	0.45	1.72	3	1
1:A:437:LEU:N	1:A:455:VAL:O	0.45	2.40	5	6
1:A:423:THR:C	1:A:427:GLU:OE1	0.45	2.55	12	1
1:A:276:THR:O	1:A:276:THR:HG23	0.45	2.12	6	1
1:A:452:LEU:CD1	1:A:473:PHE:CE1	0.45	3.00	10	2
1:A:403:ARG:NE	1:A:403:ARG:O	0.45	2.50	9	1
1:A:407:PRO:HB3	1:A:466:LEU:HD13	0.45	1.87	1	1
1:A:427:GLU:CD	1:A:427:GLU:C	0.45	2.75	15	1
1:A:459:ASP:O	1:A:462:GLN:N	0.44	2.50	17	8
1:A:427:GLU:C	1:A:427:GLU:CD	0.44	2.75	18	2
1:A:414:VAL:HG13	1:A:438:VAL:HG23	0.44	1.89	2	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:462:GLN:O	1:A:465:LYS:N	0.44	2.50	17	2
1:A:462:GLN:O	1:A:466:LEU:N	0.44	2.50	17	2
1:A:462:GLN:NE2	1:A:462:GLN:CA	0.44	2.79	16	1
1:A:465:LYS:O	1:A:468:LYS:CG	0.44	2.66	11	1
1:A:431:LYS:CE	1:A:434:ASP:OD1	0.44	2.66	20	1
1:A:427:GLU:CA	1:A:427:GLU:OE1	0.44	2.65	19	1
1:A:452:LEU:HD13	1:A:473:PHE:CZ	0.43	2.48	12	1
1:A:447:GLN:NE2	1:A:448:ASP:O	0.43	2.50	14	3
1:A:415:GLN:HB2	1:A:481:VAL:CG2	0.43	2.43	17	1
1:A:428:LEU:HD12	1:A:430:LEU:CD2	0.43	2.43	11	1
1:A:435:VAL:CG2	1:A:457:GLU:HB2	0.43	2.43	8	3
1:A:420:TYR:CG	1:A:420:TYR:O	0.43	2.69	19	1
1:A:460:TRP:O	1:A:463:HIS:N	0.43	2.50	20	1
1:A:448:ASP:OD1	1:A:449:GLU:N	0.43	2.50	2	1
1:A:452:LEU:CD2	1:A:452:LEU:N	0.43	2.80	11	1
1:A:431:LYS:CD	1:A:434:ASP:CG	0.43	2.87	13	2
1:A:415:GLN:CB	1:A:481:VAL:CG2	0.43	2.96	17	1
1:A:429:GLN:O	1:A:456:LYS:CE	0.43	2.67	3	2
1:A:411:MET:SD	1:A:438:VAL:HG12	0.43	2.54	17	2
1:A:281:VAL:CG1	1:A:282:ASN:N	0.43	2.81	12	2
1:A:412:PHE:CE2	1:A:480:ARG:HD3	0.43	2.48	8	1
1:A:409:GLY:O	1:A:410:PHE:C	0.43	2.57	12	19
1:A:405:ASP:HB2	1:A:463:HIS:CE1	0.43	2.48	12	1
1:A:411:MET:SD	1:A:438:VAL:CG1	0.43	3.07	17	1
1:A:294:GLY:O	1:A:295:ALA:HB3	0.43	2.13	5	1
1:A:410:PHE:CZ	1:A:412:PHE:CA	0.43	3.02	9	3
1:A:310:VAL:O	1:A:476:ASN:ND2	0.42	2.50	19	2
1:A:467:GLU:HA	1:A:470:ARG:CG	0.42	2.44	13	1
1:A:414:VAL:C	1:A:481:VAL:HG23	0.42	2.35	17	1
1:A:466:LEU:HD23	1:A:467:GLU:H	0.42	1.72	1	1
1:A:462:GLN:O	1:A:464:LYS:N	0.42	2.52	20	6
1:A:404:LEU:HD23	1:A:404:LEU:H	0.42	1.74	10	1
1:A:472:VAL:CG1	1:A:473:PHE:N	0.42	2.83	6	1
1:A:419:ASP:OD1	1:A:419:ASP:N	0.42	2.52	2	1
1:A:428:LEU:CD2	1:A:454:GLY:O	0.42	2.67	1	1
1:A:451:TRP:HA	1:A:473:PHE:O	0.42	2.15	14	2
1:A:447:GLN:CD	1:A:451:TRP:O	0.42	2.58	20	3
1:A:424:ASP:CB	1:A:427:GLU:HG2	0.42	2.45	20	2
1:A:431:LYS:CD	1:A:434:ASP:OD2	0.42	2.68	14	1
1:A:437:LEU:CD1	1:A:460:TRP:CD2	0.42	3.02	10	2
1:A:428:LEU:CB	1:A:472:VAL:O	0.42	2.67	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:466:LEU:HD21	1:A:470:ARG:HH21	0.42	1.74	4	1
1:A:437:LEU:HD13	1:A:460:TRP:CD2	0.42	2.50	9	2
1:A:462:GLN:HE21	1:A:462:GLN:N	0.42	2.13	16	1
1:A:428:LEU:HD13	1:A:471:GLY:CA	0.42	2.42	7	1
1:A:412:PHE:CZ	1:A:438:VAL:HG21	0.41	2.50	14	1
1:A:417:GLN:NE2	1:A:478:THR:O	0.41	2.53	10	2
1:A:426:ASP:O	1:A:426:ASP:CG	0.41	2.58	20	1
1:A:416:ALA:CA	1:A:478:THR:HG22	0.41	2.41	16	1
1:A:459:ASP:CG	1:A:469:CYS:SG	0.41	2.99	6	1
1:A:452:LEU:N	1:A:452:LEU:CD2	0.41	2.82	15	1
1:A:419:ASP:CG	1:A:419:ASP:O	0.41	2.58	20	2
1:A:403:ARG:HD2	1:A:463:HIS:CB	0.41	2.46	14	1
1:A:453:MET:HE3	1:A:471:GLY:O	0.41	2.15	9	1
1:A:435:VAL:HG23	1:A:457:GLU:HB2	0.41	1.91	5	1
1:A:413:LYS:HE3	1:A:437:LEU:CD2	0.41	2.45	17	1
1:A:434:ASP:CG	1:A:435:VAL:N	0.41	2.74	10	1
1:A:466:LEU:HD23	1:A:467:GLU:HG3	0.41	1.92	7	1
1:A:451:TRP:CZ3	1:A:474:PRO:CG	0.41	3.04	6	2
1:A:476:ASN:N	1:A:476:ASN:OD1	0.40	2.54	16	1
1:A:287:PRO:O	1:A:288:ALA:HB2	0.40	2.16	19	1
1:A:469:CYS:O	1:A:469:CYS:SG	0.40	2.78	9	1
1:A:425:THR:HG23	1:A:426:ASP:OD2	0.40	2.17	16	1
1:A:419:ASP:O	1:A:419:ASP:CG	0.40	2.60	19	1
1:A:431:LYS:HD3	1:A:434:ASP:CB	0.40	2.46	13	1
1:A:431:LYS:CD	1:A:434:ASP:HB2	0.40	2.47	11	1
1:A:281:VAL:HG12	1:A:282:ASN:N	0.40	2.31	12	1
1:A:437:LEU:HG	1:A:455:VAL:CG1	0.40	2.46	17	1
1:A:425:THR:O	1:A:426:ASP:OD1	0.40	2.40	4	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	110/213 (52%)	92±5 (84±4%)	14±4 (12±4%)	4±2 (4±1%)	6	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2200/4260 (52%)	1839 (84%)	273 (12%)	88 (4%)	6 33

All 15 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	410	PHE	20
1	A	441	PHE	20
1	A	432	ALA	19
1	A	426	ASP	12
1	A	403	ARG	3
1	A	279	ILE	3
1	A	295	ALA	2
1	A	284	GLU	2
1	A	294	GLY	1
1	A	272	SER	1
1	A	281	VAL	1
1	A	280	ARG	1
1	A	282	ASN	1
1	A	296	THR	1
1	A	297	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	94/173 (54%)	65±3 (69±3%)	29±3 (31±3%)	2 16
All	All	1880/3460 (54%)	1305 (69%)	575 (31%)	2 16

All 59 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	458	SER	20
1	A	413	LYS	20
1	A	439	ILE	20
1	A	452	LEU	20

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Mol	Chain	Res	Type	Models (Total)
1	A	403	ARG	20
1	A	441	PHE	20
1	A	431	LYS	20
1	A	406	LEU	20
1	A	437	LEU	20
1	A	477	PHE	20
1	A	466	LEU	16
1	A	443	ASN	16
1	A	469	CYS	16
1	A	462	GLN	15
1	A	453	MET	15
1	A	476	ASN	14
1	A	297	LEU	14
1	A	447	GLN	13
1	A	404	LEU	13
1	A	284	GLU	12
1	A	464	LYS	12
1	A	465	LYS	11
1	A	478	THR	11
1	A	449	GLU	11
1	A	272	SER	10
1	A	475	GLU	10
1	A	428	LEU	10
1	A	463	HIS	9
1	A	456	LYS	9
1	A	283	HIS	9
1	A	278	GLU	8
1	A	445	GLU	8
1	A	451	TRP	8
1	A	280	ARG	8
1	A	442	GLN	7
1	A	427	GLU	7
1	A	435	VAL	6
1	A	286	GLU	6
1	A	468	LYS	6
1	A	470	ARG	6
1	A	467	GLU	6
1	A	279	ILE	6
1	A	472	VAL	5
1	A	276	THR	5
1	A	420	TYR	5
1	A	480	ARG	4

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Mol	Chain	Res	Type	Models (Total)
1	A	419	ASP	4
1	A	426	ASP	4
1	A	430	LEU	3
1	A	282	ASN	3
1	A	446	GLU	3
1	A	421	THR	2
1	A	292	THR	2
1	A	424	ASP	2
1	A	423	THR	1
1	A	281	VAL	1
1	A	459	ASP	1
1	A	414	VAL	1
1	A	479	GLU	1

6.3.3 RNA

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates

There are no carbohydrates in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

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