



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 03:59 PM BST

PDB ID : 1MV0
Title : NMR STRUCTURE OF THE TUMOR SUPPRESSOR BIN1: ALTERNATIVE SPLICING IN MELANOMA AND INTERACTION WITH C-MYC
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Deposited on : 2002-09-24

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

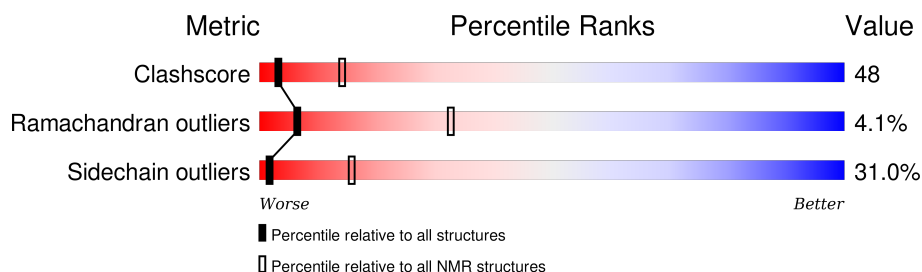
1 Overall quality at a glance

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	14	
2	B	81	

2 Ensemble composition and analysis

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:59-A:63, B:406-B:441, B:448-B:482 (76)	0.14	1

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 3 clusters and 1 single-model cluster was found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1502 atoms, of which 741 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Myc proto-oncogene protein.

Mol	Chain	Residues	Atoms					Trace
1	A	14	Total	C	H	N	O	0
			215	65	112	20	18	

- Molecule 2 is a protein called Myc box-dependent-interacting protein 1.

Mol	Chain	Residues	Atoms						Trace
2	B	81	Total	C	H	N	O	S	0
			1287	418	629	111	126	3	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	465	LYS	GLU	SEE REMARK 999	UNP O00499

4 Residue-property plots

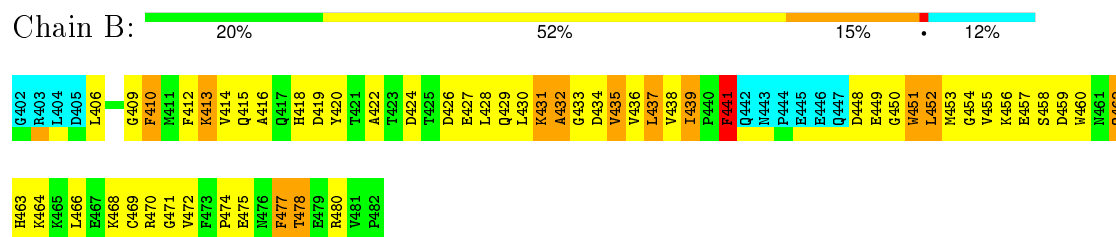
4.1 Average score per residue in the NMR ensemble

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 proto-oncogene protein



- Molecule 2: Myc box-dependent-interacting protein 1

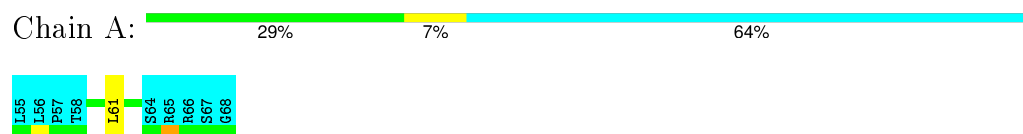


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

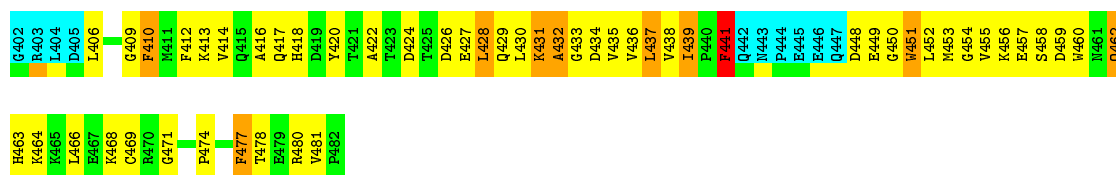
4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Myc proto-oncogene protein



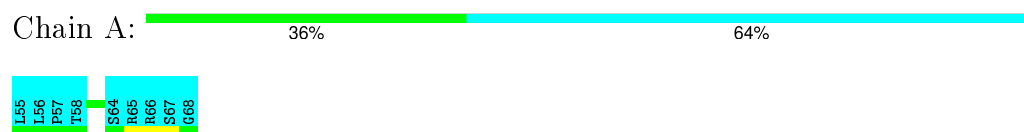
- Molecule 2: Myc box-dependent-interacting protein 1



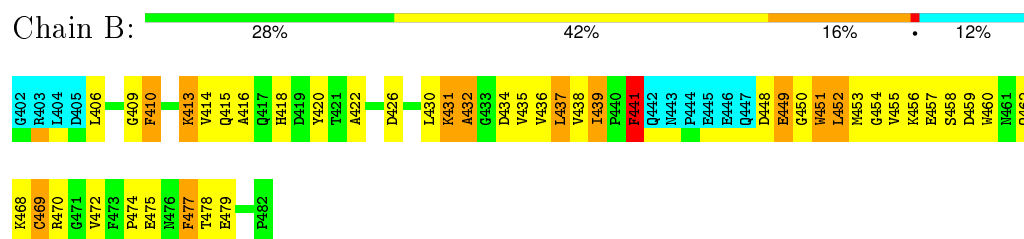


4.2.2 Score per residue for model 2

- Molecule 1: Myc proto-oncogene protein

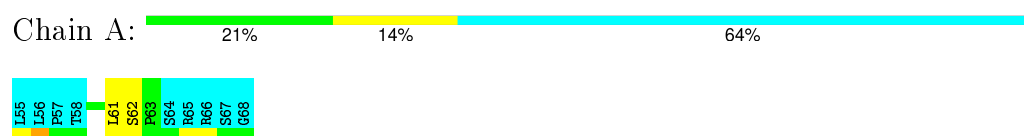


- Molecule 2: Myc box-dependent-interacting protein 1

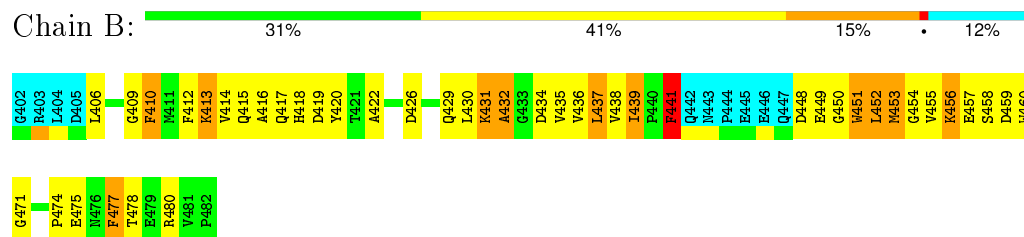


4.2.3 Score per residue for model 3

- Molecule 1: Myc proto-oncogene protein



- Molecule 2: Myc box-dependent-interacting protein 1

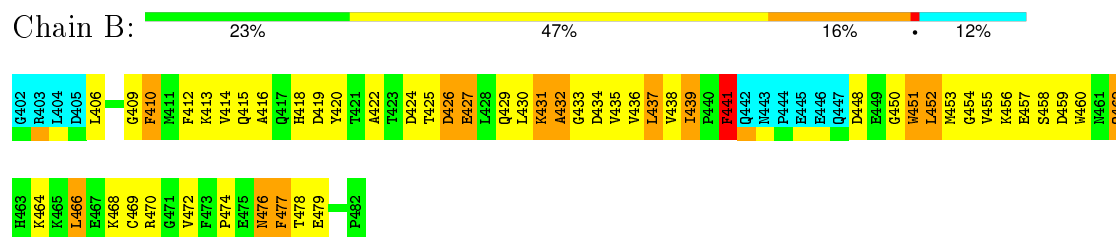


4.2.4 Score per residue for model 4

- Molecule 1: Myc proto-oncogene protein

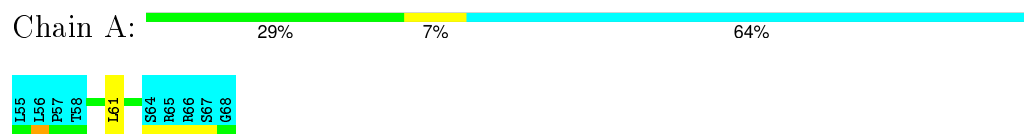


- Molecule 2: Myc box-dependent-interacting protein 1

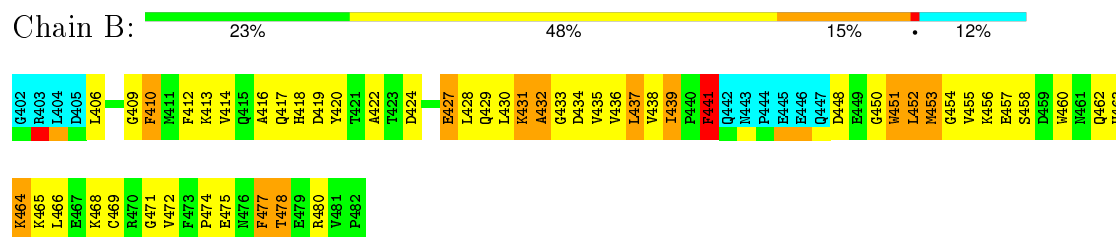


4.2.5 Score per residue for model 5

- Molecule 1: Myc proto-oncogene protein

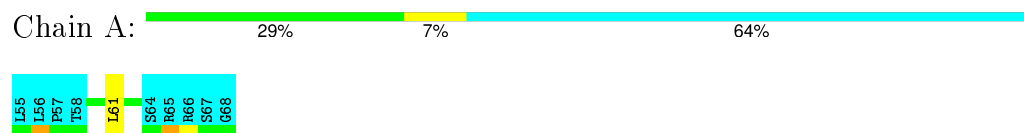


- Molecule 2: Myc box-dependent-interacting protein 1



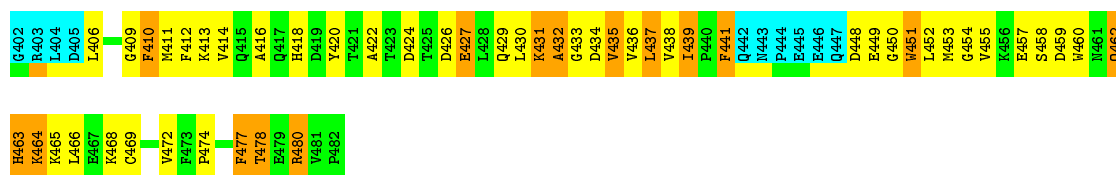
4.2.6 Score per residue for model 6

- Molecule 1: Myc proto-oncogene protein



- Molecule 2: Myc box-dependent-interacting protein 1



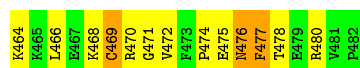
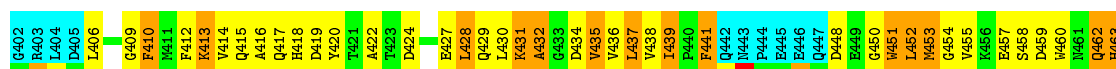


4.2.7 Score per residue for model 7

- Molecule 1: Myc proto-oncogene protein



- Molecule 2: Myc box-dependent-interacting protein 1

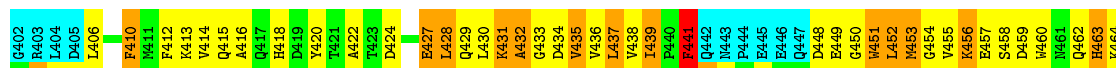


4.2.8 Score per residue for model 8

- Molecule 1: Myc proto-oncogene protein



- Molecule 2: Myc box-dependent-interacting protein 1

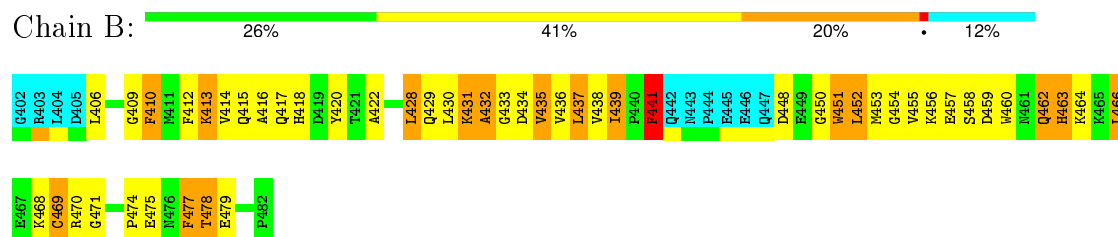


4.2.9 Score per residue for model 9

- Molecule 1: Myc proto-oncogene protein

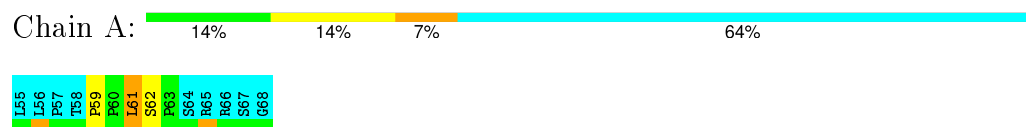


- Molecule 2: Myc box-dependent-interacting protein 1

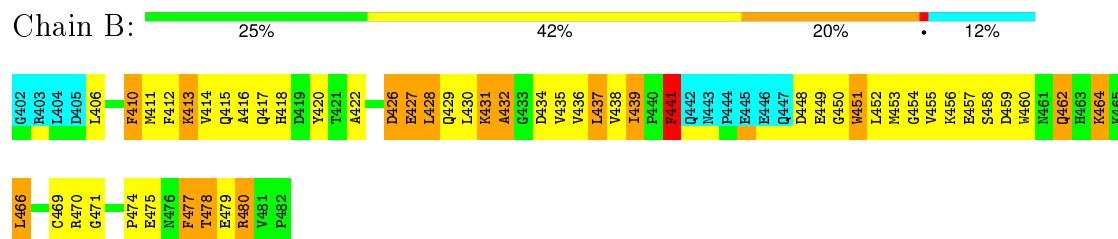


4.2.10 Score per residue for model 10

- Molecule 1: Myc proto-oncogene protein



- Molecule 2: Myc box-dependent-interacting protein 1



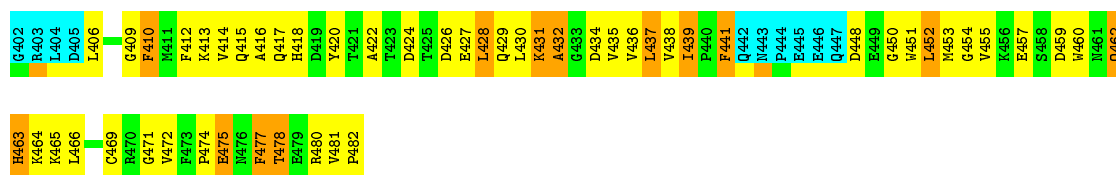
4.2.11 Score per residue for model 11

- Molecule 1: Myc proto-oncogene protein



- Molecule 2: Myc box-dependent-interacting protein 1



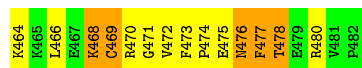
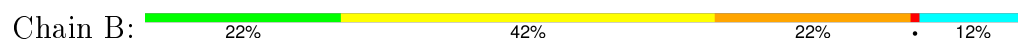


4.2.12 Score per residue for model 12

- Molecule 1: Myc proto-oncogene protein



- Molecule 2: Myc box-dependent-interacting protein 1

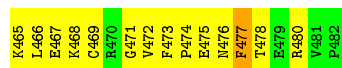
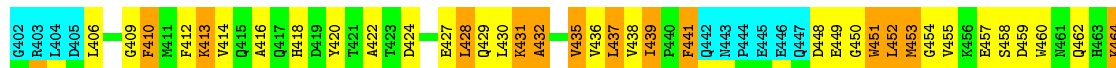


4.2.13 Score per residue for model 13

- Molecule 1: Myc proto-oncogene protein

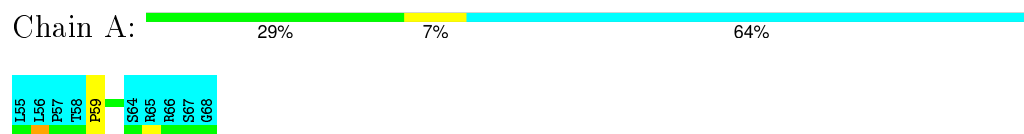


- Molecule 2: Myc box-dependent-interacting protein 1

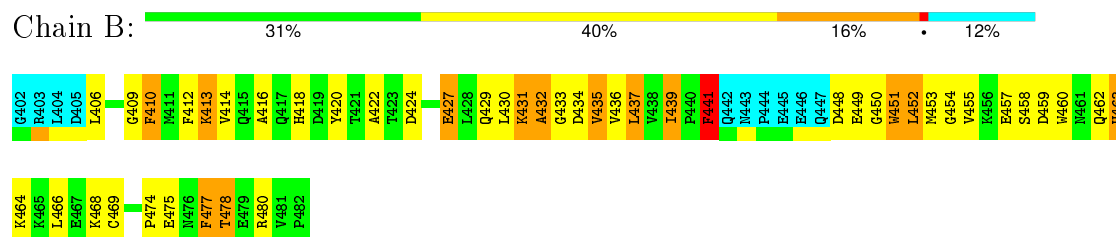


4.2.14 Score per residue for model 14

- Molecule 1: Myc proto-oncogene protein

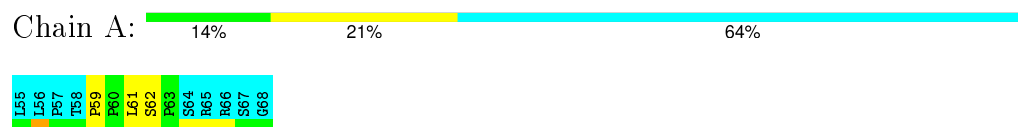


- Molecule 2: Myc box-dependent-interacting protein 1

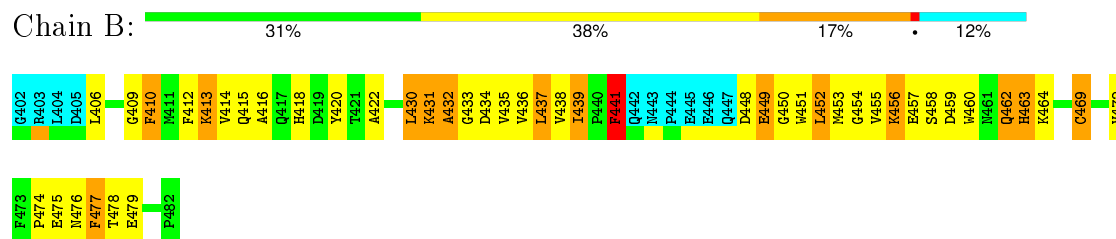


4.2.15 Score per residue for model 15

- Molecule 1: Myc proto-oncogene protein

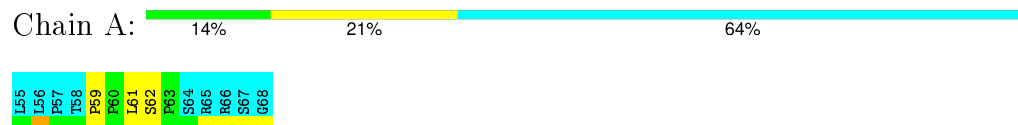


- Molecule 2: Myc box-dependent-interacting protein 1



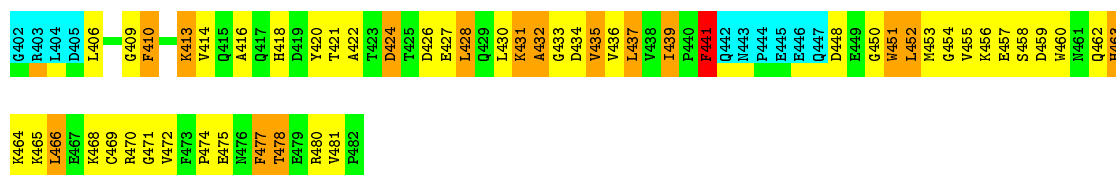
4.2.16 Score per residue for model 16

- Molecule 1: Myc proto-oncogene protein



- Molecule 2: Myc box-dependent-interacting protein 1



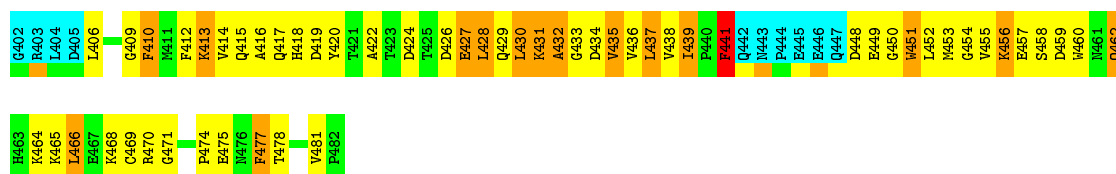
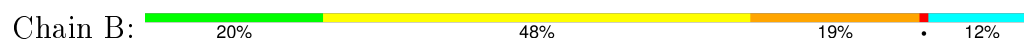


4.2.17 Score per residue for model 17

- Molecule 1: Myc proto-oncogene protein



- Molecule 2: Myc box-dependent-interacting protein 1

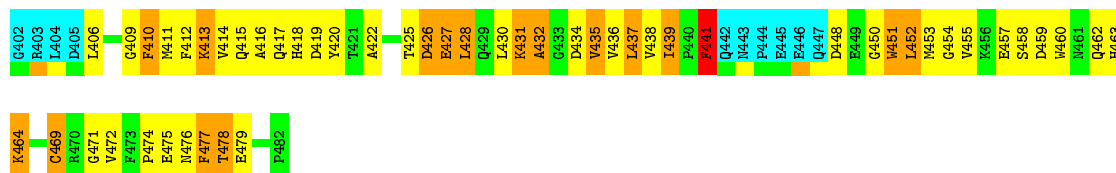


4.2.18 Score per residue for model 18

- Molecule 1: Myc proto-oncogene protein

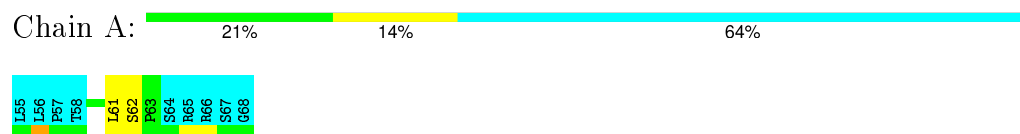


- Molecule 2: Myc box-dependent-interacting protein 1

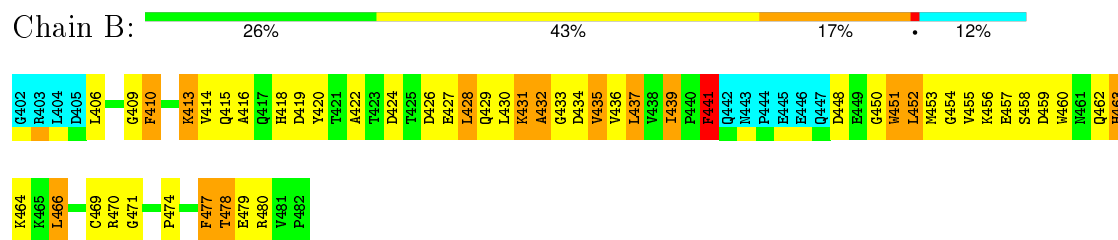


4.2.19 Score per residue for model 19

- Molecule 1: Myc proto-oncogene protein

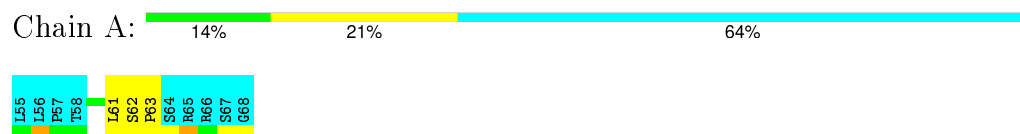


- Molecule 2: Myc box-dependent-interacting protein 1

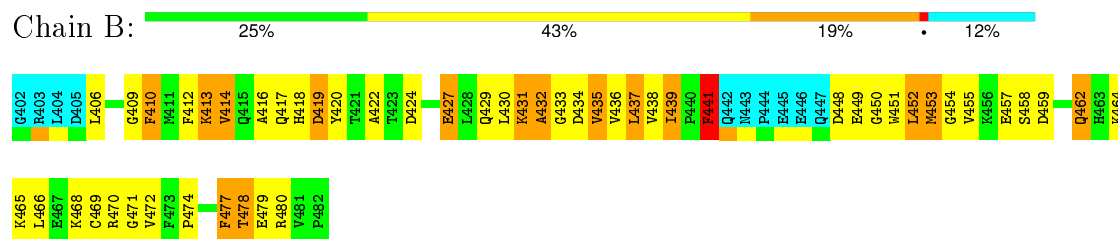


4.2.20 Score per residue for model 20

- Molecule 1: Myc proto-oncogene protein



- Molecule 2: Myc box-dependent-interacting protein 1



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	35	37	37	1±1
2	B	576	557	557	57±4
All	All	12220	11880	11880	1150

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 48.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:416:ALA:HB2	2:B:430:LEU:HD12	1.08	1.19	19	9
2:B:420:TYR:CE2	2:B:422:ALA:HB2	1.01	1.91	11	20
2:B:430:LEU:HD11	2:B:436:VAL:HG21	1.00	1.32	13	17
2:B:477:PHE:CD1	2:B:478:THR:HG23	0.90	2.01	9	20
2:B:430:LEU:HD11	2:B:436:VAL:CG2	0.90	1.96	7	17
2:B:451:TRP:C	2:B:452:LEU:HD23	0.88	1.90	14	13
2:B:414:VAL:HG22	2:B:436:VAL:O	0.86	1.69	18	13
2:B:455:VAL:HG22	2:B:459:ASP:HB2	0.83	1.50	18	11
2:B:416:ALA:CB	2:B:430:LEU:HD12	0.83	2.03	19	3
2:B:455:VAL:HG22	2:B:459:ASP:CB	0.81	2.05	7	8
2:B:420:TYR:CZ	2:B:422:ALA:HB2	0.81	2.11	15	20
2:B:437:LEU:HG	2:B:455:VAL:HG13	0.76	1.57	13	16
2:B:428:LEU:HD23	2:B:471:GLY:HA3	0.76	1.58	11	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:416:ALA:HB2	2:B:430:LEU:HD23	0.76	1.58	15	2
2:B:430:LEU:HD21	2:B:436:VAL:HG21	0.73	1.59	17	1
2:B:452:LEU:HD21	2:B:475:GLU:CB	0.71	2.14	16	7
2:B:436:VAL:HG22	2:B:456:LYS:HG3	0.70	1.61	12	4
2:B:416:ALA:HA	2:B:478:THR:HG22	0.70	1.63	9	14
2:B:429:GLN:O	2:B:430:LEU:HD22	0.69	1.88	11	14
2:B:437:LEU:N	2:B:437:LEU:HD23	0.69	2.03	13	4
2:B:422:ALA:HB1	2:B:427:GLU:HG3	0.68	1.65	12	4
2:B:437:LEU:HD13	2:B:460:TRP:CE3	0.68	2.24	15	17
2:B:429:GLN:C	2:B:430:LEU:HD22	0.68	2.09	1	11
2:B:413:LYS:HE2	2:B:435:VAL:HG12	0.67	1.66	17	1
2:B:437:LEU:HD23	2:B:437:LEU:N	0.67	2.03	9	11
2:B:422:ALA:HB1	2:B:427:GLU:CG	0.67	2.19	12	4
2:B:477:PHE:HD1	2:B:478:THR:HG23	0.67	1.50	6	19
2:B:437:LEU:CD1	2:B:460:TRP:CE3	0.66	2.79	2	16
2:B:414:VAL:CG1	2:B:438:VAL:HG23	0.66	2.21	20	16
2:B:452:LEU:HD21	2:B:475:GLU:HB3	0.66	1.68	16	7
2:B:416:ALA:HB2	2:B:430:LEU:CD1	0.64	2.11	19	2
2:B:477:PHE:CE1	2:B:478:THR:HG23	0.64	2.27	9	7
2:B:416:ALA:HB2	2:B:430:LEU:CD2	0.64	2.21	15	2
2:B:448:ASP:OD2	2:B:451:TRP:CD1	0.63	2.51	15	17
2:B:477:PHE:O	2:B:477:PHE:CG	0.63	2.51	13	15
2:B:413:LYS:HE3	2:B:435:VAL:HG12	0.62	1.72	12	9
2:B:430:LEU:HD13	2:B:434:ASP:OD2	0.62	1.95	4	5
2:B:439:ILE:HD13	2:B:454:GLY:HA2	0.62	1.71	19	20
2:B:439:ILE:HD12	2:B:455:VAL:HG12	0.61	1.72	6	9
2:B:414:VAL:HG11	2:B:438:VAL:HG23	0.61	1.72	17	4
2:B:477:PHE:O	2:B:477:PHE:CD1	0.60	2.55	12	11
2:B:477:PHE:CG	2:B:477:PHE:O	0.60	2.54	9	5
2:B:412:PHE:CZ	2:B:438:VAL:HG21	0.59	2.32	8	1
2:B:412:PHE:CE1	2:B:438:VAL:HG21	0.59	2.32	4	3
2:B:477:PHE:C	2:B:477:PHE:CD1	0.59	2.76	12	11
2:B:441:PHE:CD1	2:B:441:PHE:N	0.59	2.71	8	13
2:B:441:PHE:N	2:B:441:PHE:CD1	0.58	2.69	17	7
2:B:463:HIS:C	2:B:463:HIS:CD2	0.58	2.77	9	1
2:B:435:VAL:HG23	2:B:457:GLU:CB	0.58	2.28	13	19
2:B:455:VAL:CG2	2:B:459:ASP:CB	0.57	2.82	15	17
2:B:413:LYS:NZ	2:B:435:VAL:HG12	0.57	2.14	14	2
2:B:451:TRP:CE3	2:B:474:PRO:HD3	0.57	2.35	11	20
1:A:61:LEU:HD12	1:A:61:LEU:C	0.57	2.19	10	1
2:B:451:TRP:O	2:B:452:LEU:HD23	0.56	1.99	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:451:TRP:N	2:B:451:TRP:CD1	0.55	2.74	10	12
2:B:413:LYS:CE	2:B:435:VAL:HG12	0.55	2.31	17	6
2:B:418:HIS:HB2	2:B:477:PHE:CE2	0.55	2.37	13	20
2:B:452:LEU:N	2:B:452:LEU:HD23	0.55	2.16	5	1
2:B:451:TRP:CZ3	2:B:474:PRO:HD3	0.54	2.37	4	20
2:B:451:TRP:CZ3	2:B:474:PRO:HG3	0.54	2.37	5	20
2:B:449:GLU:O	2:B:449:GLU:CG	0.54	2.55	1	3
2:B:414:VAL:HG13	2:B:438:VAL:HG23	0.54	1.79	4	4
2:B:450:GLY:C	2:B:451:TRP:CD1	0.54	2.81	10	20
2:B:428:LEU:HD23	2:B:471:GLY:CA	0.54	2.31	11	10
2:B:431:LYS:O	2:B:432:ALA:C	0.54	2.46	13	20
2:B:477:PHE:CD1	2:B:477:PHE:C	0.54	2.80	11	8
2:B:452:LEU:HD23	2:B:452:LEU:N	0.54	2.16	14	1
2:B:463:HIS:CD2	2:B:463:HIS:C	0.53	2.81	15	2
2:B:451:TRP:CE3	2:B:474:PRO:CD	0.53	2.92	3	20
2:B:477:PHE:CD1	2:B:477:PHE:O	0.52	2.63	13	9
2:B:434:ASP:OD2	2:B:456:LYS:CD	0.52	2.57	10	3
2:B:435:VAL:HG23	2:B:457:GLU:HB3	0.52	1.81	17	20
2:B:451:TRP:CD1	2:B:451:TRP:N	0.52	2.78	19	8
2:B:437:LEU:CD1	2:B:460:TRP:CD2	0.52	2.93	17	2
2:B:429:GLN:O	2:B:456:LYS:CE	0.52	2.58	3	1
2:B:437:LEU:CG	2:B:455:VAL:HG13	0.52	2.34	14	5
2:B:462:GLN:N	2:B:462:GLN:NE2	0.52	2.58	12	1
2:B:430:LEU:CD1	2:B:434:ASP:OD2	0.51	2.58	9	4
2:B:410:PHE:CZ	2:B:412:PHE:HA	0.51	2.41	6	14
2:B:452:LEU:HD11	2:B:475:GLU:OE1	0.51	2.06	15	6
2:B:416:ALA:CA	2:B:478:THR:HG22	0.51	2.34	9	1
2:B:452:LEU:HD11	2:B:475:GLU:HB2	0.51	1.81	11	3
2:B:429:GLN:O	2:B:456:LYS:CD	0.50	2.60	17	3
2:B:453:MET:HE2	2:B:471:GLY:O	0.50	2.07	20	5
2:B:414:VAL:CG1	2:B:438:VAL:CG2	0.49	2.91	4	2
2:B:424:ASP:CB	2:B:427:GLU:OE1	0.49	2.60	8	2
2:B:430:LEU:HD21	2:B:436:VAL:CG2	0.49	2.36	17	1
2:B:435:VAL:HG23	2:B:457:GLU:HB2	0.49	1.85	1	3
2:B:466:LEU:O	2:B:470:ARG:CG	0.49	2.61	19	7
2:B:436:VAL:C	2:B:437:LEU:HD23	0.49	2.28	13	2
2:B:431:LYS:O	2:B:433:GLY:N	0.49	2.46	14	13
2:B:412:PHE:CZ	2:B:480:ARG:HD3	0.49	2.43	6	5
2:B:427:GLU:N	2:B:427:GLU:OE1	0.48	2.45	14	1
2:B:431:LYS:CE	2:B:434:ASP:CG	0.48	2.82	11	5
2:B:427:GLU:CA	2:B:427:GLU:OE1	0.48	2.60	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:448:ASP:OD2	2:B:451:TRP:CG	0.48	2.67	15	4
2:B:430:LEU:CD1	2:B:436:VAL:CG2	0.48	2.85	9	3
2:B:462:GLN:NE2	2:B:462:GLN:N	0.48	2.62	6	2
2:B:452:LEU:HD21	2:B:475:GLU:HB2	0.48	1.83	16	1
1:A:63:PRO:CD	2:B:448:ASP:OD1	0.47	2.62	7	2
2:B:427:GLU:OE1	2:B:427:GLU:CA	0.47	2.60	5	1
2:B:427:GLU:C	2:B:427:GLU:CD	0.47	2.74	17	4
2:B:437:LEU:HD13	2:B:460:TRP:CD2	0.47	2.44	17	1
2:B:418:HIS:HB2	2:B:477:PHE:CD2	0.47	2.44	18	10
2:B:415:GLN:NE2	2:B:434:ASP:O	0.47	2.48	4	8
2:B:476:ASN:OD1	2:B:476:ASN:N	0.47	2.48	4	3
2:B:437:LEU:N	2:B:437:LEU:CD2	0.47	2.72	13	2
1:A:59:PRO:HG2	2:B:451:TRP:CZ2	0.47	2.45	10	6
2:B:431:LYS:O	2:B:434:ASP:N	0.47	2.48	16	1
2:B:462:GLN:C	2:B:464:LYS:N	0.47	2.68	19	20
2:B:455:VAL:CG2	2:B:459:ASP:HB3	0.47	2.40	3	12
2:B:414:VAL:N	2:B:436:VAL:O	0.46	2.43	11	6
2:B:414:VAL:HG11	2:B:438:VAL:CG2	0.46	2.40	2	3
2:B:437:LEU:CD2	2:B:437:LEU:N	0.46	2.72	9	6
2:B:431:LYS:CE	2:B:434:ASP:OD2	0.46	2.64	18	2
2:B:431:LYS:CD	2:B:434:ASP:OD1	0.46	2.64	8	1
2:B:412:PHE:CE1	2:B:480:ARG:HD3	0.46	2.45	7	3
2:B:454:GLY:HA3	2:B:473:PHE:CE1	0.46	2.45	13	2
2:B:437:LEU:HD11	2:B:460:TRP:CE3	0.46	2.45	9	5
2:B:411:MET:CE	2:B:438:VAL:CG1	0.46	2.94	6	1
2:B:448:ASP:OD1	2:B:449:GLU:N	0.45	2.49	15	2
2:B:437:LEU:N	2:B:455:VAL:O	0.45	2.39	14	11
2:B:420:TYR:CD2	2:B:420:TYR:O	0.45	2.69	20	1
2:B:455:VAL:CG2	2:B:459:ASP:HB2	0.45	2.41	19	9
2:B:415:GLN:HB2	2:B:481:VAL:HG21	0.45	1.87	17	1
2:B:435:VAL:CG2	2:B:457:GLU:CB	0.45	2.95	7	15
2:B:451:TRP:CZ3	2:B:474:PRO:CG	0.45	3.00	5	15
1:A:62:SER:CB	2:B:448:ASP:OD2	0.45	2.65	3	5
2:B:452:LEU:HD11	2:B:475:GLU:CD	0.44	2.32	9	3
2:B:418:HIS:O	2:B:432:ALA:N	0.44	2.50	16	1
2:B:415:GLN:O	2:B:479:GLU:N	0.44	2.48	15	2
2:B:430:LEU:HD11	2:B:436:VAL:HG23	0.44	1.82	7	2
2:B:466:LEU:HD12	2:B:470:ARG:HG2	0.44	1.89	16	1
2:B:418:HIS:O	2:B:477:PHE:CZ	0.44	2.71	18	11
2:B:451:TRP:CH2	2:B:474:PRO:HG3	0.44	2.48	12	6
2:B:435:VAL:CG2	2:B:457:GLU:HB2	0.44	2.42	18	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:436:VAL:HG22	2:B:456:LYS:HG2	0.44	1.89	15	1
2:B:462:GLN:NE2	2:B:462:GLN:CA	0.44	2.79	12	2
2:B:412:PHE:CE2	2:B:414:VAL:HG12	0.44	2.48	8	1
2:B:463:HIS:O	2:B:466:LEU:HD23	0.43	2.13	5	2
2:B:477:PHE:CE1	2:B:478:THR:CG2	0.43	3.00	9	1
2:B:468:LYS:N	2:B:468:LYS:CD	0.43	2.80	12	1
2:B:413:LYS:CE	2:B:414:VAL:O	0.43	2.67	16	3
2:B:424:ASP:CB	2:B:427:GLU:HB2	0.43	2.44	8	11
2:B:411:MET:CE	2:B:438:VAL:HG12	0.43	2.44	10	1
2:B:451:TRP:CZ3	2:B:474:PRO:CD	0.43	3.02	4	10
2:B:412:PHE:CE1	2:B:438:VAL:HG11	0.43	2.49	8	1
2:B:436:VAL:HG13	2:B:455:VAL:O	0.43	2.13	17	2
2:B:437:LEU:CD2	2:B:460:TRP:CE3	0.43	3.01	17	1
2:B:412:PHE:CE2	2:B:480:ARG:CD	0.43	3.02	8	1
2:B:419:ASP:CG	2:B:419:ASP:O	0.43	2.57	19	2
2:B:481:VAL:HG13	2:B:482:PRO:HD2	0.43	1.89	11	1
2:B:409:GLY:O	2:B:410:PHE:C	0.43	2.57	16	18
2:B:448:ASP:O	2:B:451:TRP:O	0.43	2.37	3	12
2:B:419:ASP:O	2:B:419:ASP:CG	0.43	2.57	17	4
2:B:414:VAL:HG22	2:B:436:VAL:C	0.43	2.30	18	2
2:B:434:ASP:OD1	2:B:435:VAL:N	0.42	2.52	16	1
2:B:411:MET:SD	2:B:438:VAL:HG12	0.42	2.54	18	1
2:B:425:THR:O	2:B:426:ASP:CG	0.42	2.58	18	1
2:B:414:VAL:HA	2:B:481:VAL:HG23	0.42	1.91	16	2
2:B:436:VAL:HG22	2:B:456:LYS:CG	0.42	2.44	2	1
2:B:459:ASP:CB	2:B:469:CYS:SG	0.42	3.08	15	3
2:B:463:HIS:ND1	2:B:463:HIS:O	0.42	2.52	19	1
2:B:410:PHE:CZ	2:B:412:PHE:CA	0.42	3.02	6	4
2:B:416:ALA:HB3	2:B:434:ASP:H	0.42	1.74	16	1
2:B:439:ILE:HD12	2:B:455:VAL:CG1	0.42	2.42	8	2
2:B:417:GLN:NE2	2:B:479:GLU:CD	0.42	2.73	18	1
2:B:413:LYS:CE	2:B:435:VAL:CG1	0.41	2.98	17	1
2:B:413:LYS:HG2	2:B:437:LEU:HD22	0.41	1.90	9	1
2:B:453:MET:HE3	2:B:471:GLY:O	0.41	2.15	3	1
2:B:466:LEU:O	2:B:470:ARG:N	0.41	2.49	19	1
2:B:412:PHE:CE2	2:B:480:ARG:HD2	0.41	2.50	8	1
2:B:431:LYS:CE	2:B:434:ASP:OD1	0.41	2.68	8	1
2:B:459:ASP:O	2:B:462:GLN:N	0.41	2.54	15	1
2:B:420:TYR:CG	2:B:420:TYR:O	0.41	2.72	14	1
2:B:430:LEU:CD2	2:B:436:VAL:HG21	0.41	2.41	17	1
2:B:460:TRP:O	2:B:463:HIS:N	0.41	2.51	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:459:ASP:CG	2:B:469:CYS:SG	0.41	2.99	18	3
2:B:453:MET:CE	2:B:471:GLY:O	0.41	2.69	7	1
2:B:425:THR:O	2:B:426:ASP:OD1	0.41	2.39	4	1
2:B:452:LEU:CD2	2:B:452:LEU:N	0.41	2.82	5	1
2:B:428:LEU:HD22	2:B:454:GLY:O	0.41	2.16	5	1
2:B:462:GLN:O	2:B:464:LYS:N	0.41	2.54	6	2
2:B:422:ALA:HB1	2:B:427:GLU:HB2	0.41	1.93	10	1
2:B:450:GLY:O	2:B:476:ASN:ND2	0.41	2.54	15	1
2:B:436:VAL:HG13	2:B:455:VAL:C	0.40	2.36	17	1
2:B:459:ASP:OD2	2:B:469:CYS:SG	0.40	2.79	12	1
2:B:415:GLN:HB2	2:B:481:VAL:CG2	0.40	2.47	17	1
2:B:455:VAL:HG23	2:B:459:ASP:CB	0.40	2.47	20	2
2:B:413:LYS:HE3	2:B:435:VAL:CG1	0.40	2.46	20	1
2:B:419:ASP:OD2	2:B:432:ALA:HB2	0.40	2.17	20	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	5/14 (36%)	5±0 (100±0%)	0±0 (0±0%)	0±0 (0±0%)	100	100
2	B	70/81 (86%)	63±1 (90±1%)	4±1 (6±2%)	3±1 (4±1%)	6	30
All	All	1500/1900 (79%)	1359 (91%)	79 (5%)	62 (4%)	6	33

All 4 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	432	ALA	20
2	B	410	PHE	20
2	B	441	PHE	16
2	B	426	ASP	6

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	5/13 (38%)	4±0 (83±7%)	1±0 (17±7%)	6	42
2	B	63/72 (88%)	43±3 (68±4%)	20±3 (32±4%)	1	14
All	All	1360/1700 (80%)	938 (69%)	422 (31%)	2	16

All 38 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)
2	B	477	PHE	20
2	B	441	PHE	20
2	B	437	LEU	20
2	B	452	LEU	20
2	B	413	LYS	20
2	B	431	LYS	20
2	B	453	MET	20
2	B	439	ILE	20
2	B	406	LEU	20
2	B	458	SER	19
2	B	469	CYS	19
1	A	61	LEU	17
2	B	451	TRP	16
2	B	466	LEU	15
2	B	468	LYS	14
2	B	462	GLN	12
2	B	435	VAL	12
2	B	463	HIS	12
2	B	428	LEU	11
2	B	478	THR	11
2	B	427	GLU	10
2	B	456	LYS	9
2	B	480	ARG	9
2	B	465	LYS	9
2	B	449	GLU	8
2	B	464	LYS	6
2	B	426	ASP	6
2	B	479	GLU	5

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Mol	Chain	Res	Type	Models (Total)
2	B	476	ASN	4
2	B	424	ASP	4
2	B	475	GLU	3
2	B	419	ASP	3
2	B	430	LEU	2
2	B	415	GLN	2
2	B	414	VAL	1
2	B	470	ARG	1
2	B	459	ASP	1
2	B	421	THR	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided