



Full wwPDB NMR Structure Validation Report ⓘ

Mar 7, 2026 – 12:46 AM UTC

PDB ID : 1MV3 / pdb_00001mv3
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

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

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

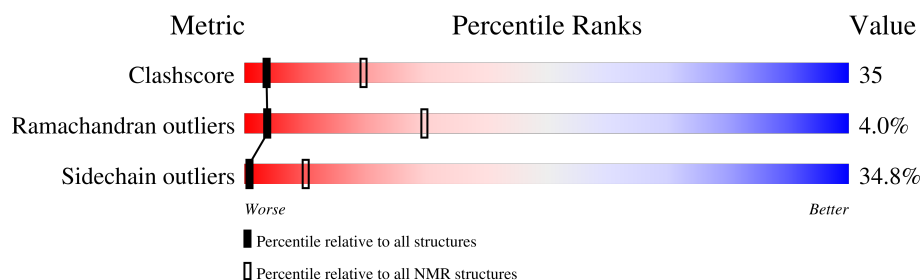
1 Overall quality at a glance

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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	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)	1.23	8
2	A:308-A:311, A:403-A:482 (84)	0.28	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.

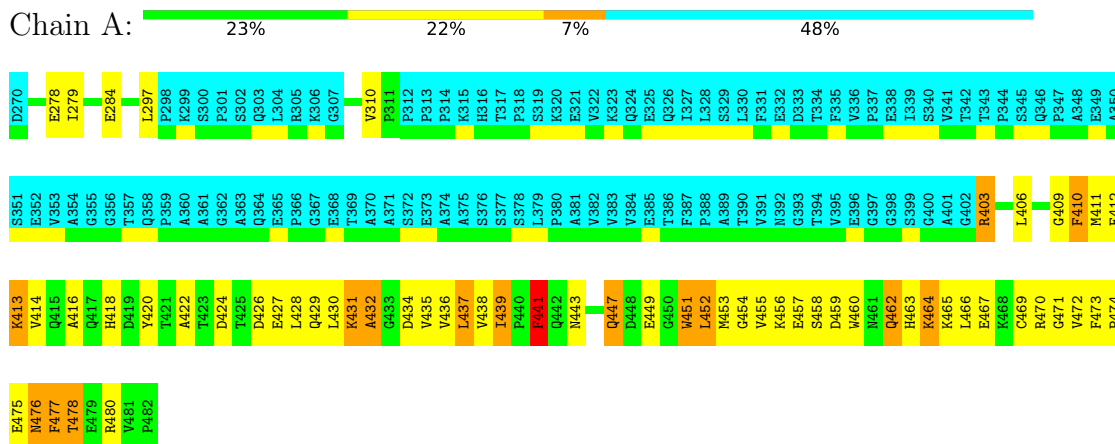
Mol	Chain	Residues	Atoms						Trace
1	A	213	Total	C	H	N	O	S	0
			3107	990	1525	266	323	3	

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide 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

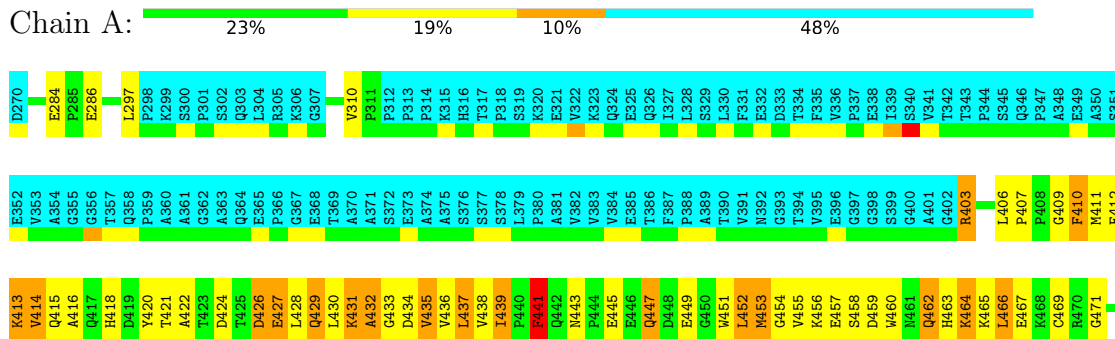


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

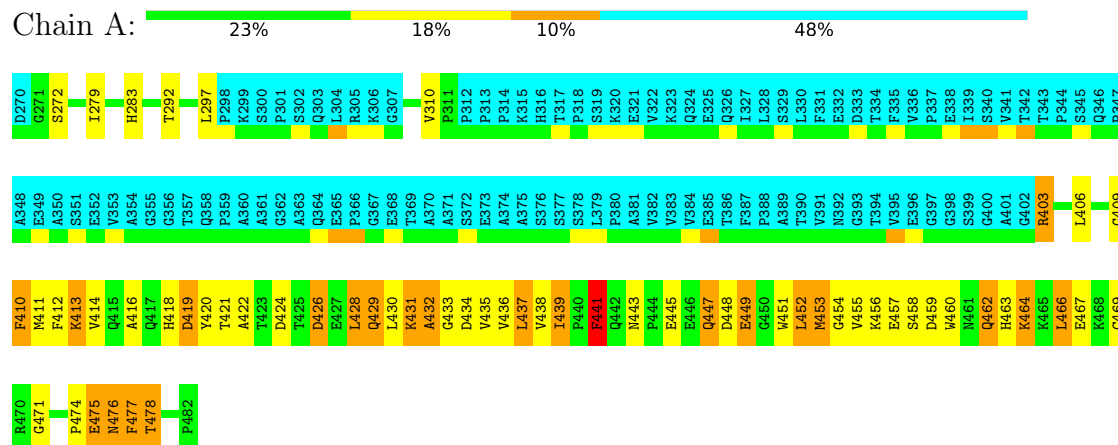
- Molecule 1: Myc box dependent interacting protein 1



P474
E475
N476
F477
T478
E479
R480
V481
P482

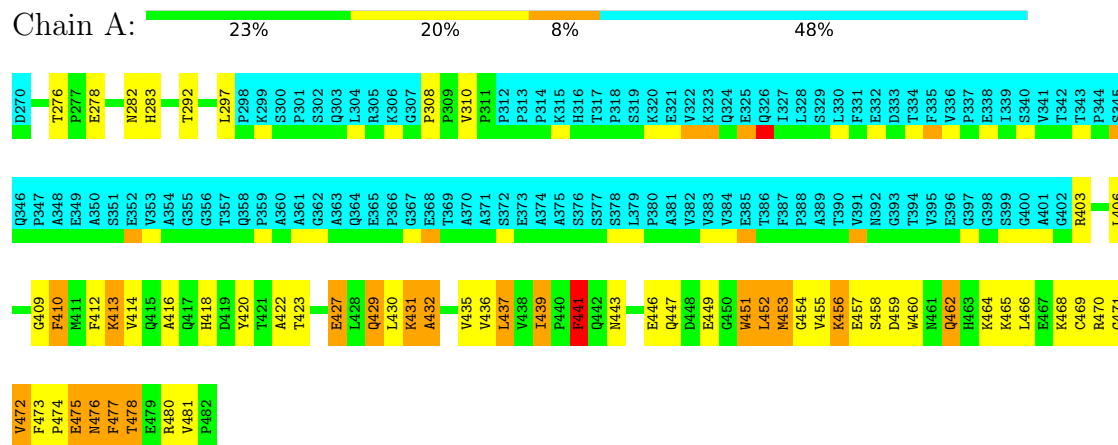
4.2.2 Score per residue for model 2 (medoid)

- Molecule 1: Myc box dependent interacting protein 1



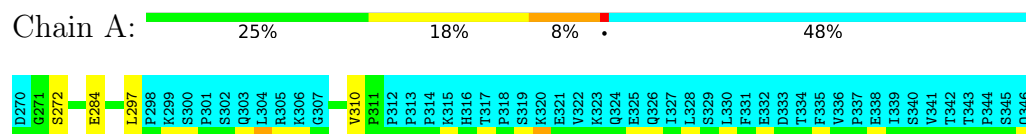
4.2.3 Score per residue for model 3

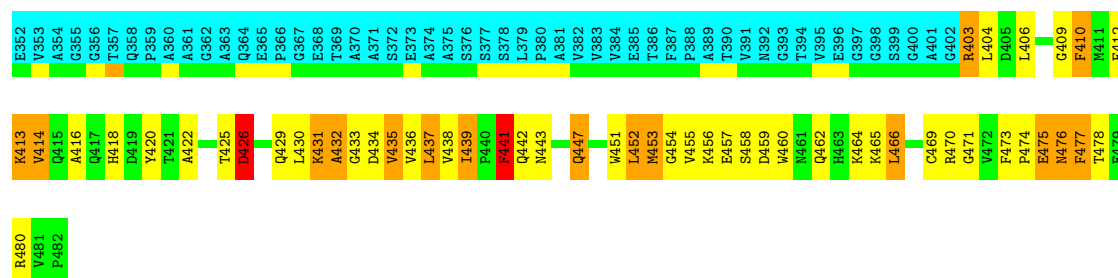
- Molecule 1: Myc box dependent interacting protein 1



4.2.4 Score per residue for model 4

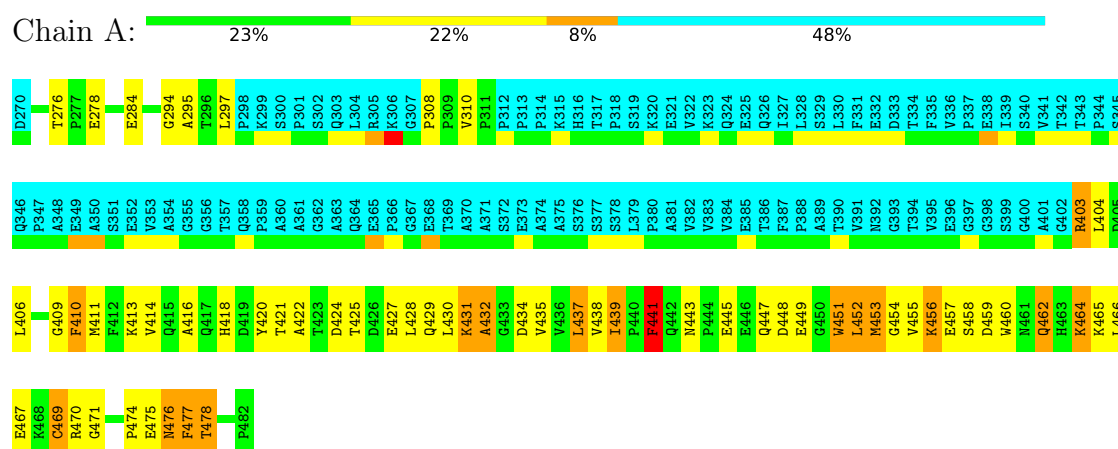
- Molecule 1: Myc box dependent interacting protein 1





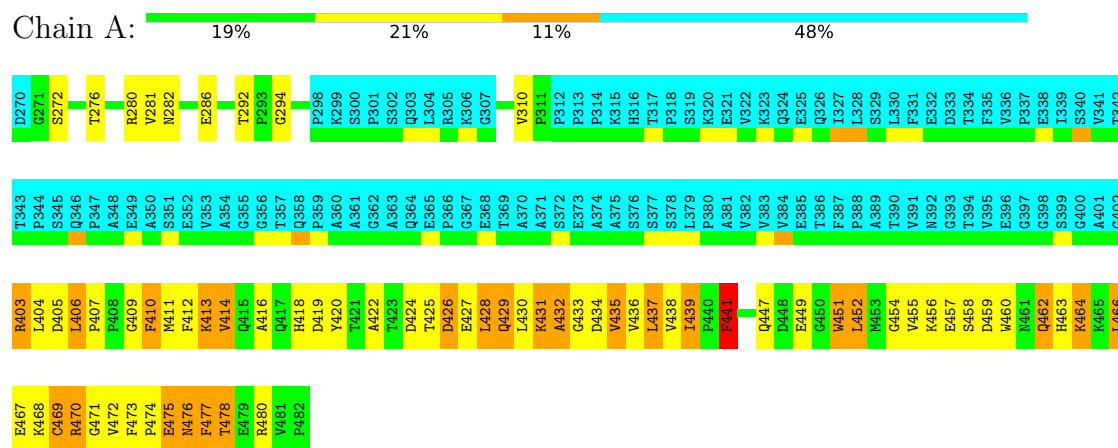
4.2.5 Score per residue for model 5

- Molecule 1: Myc box dependent interacting protein 1



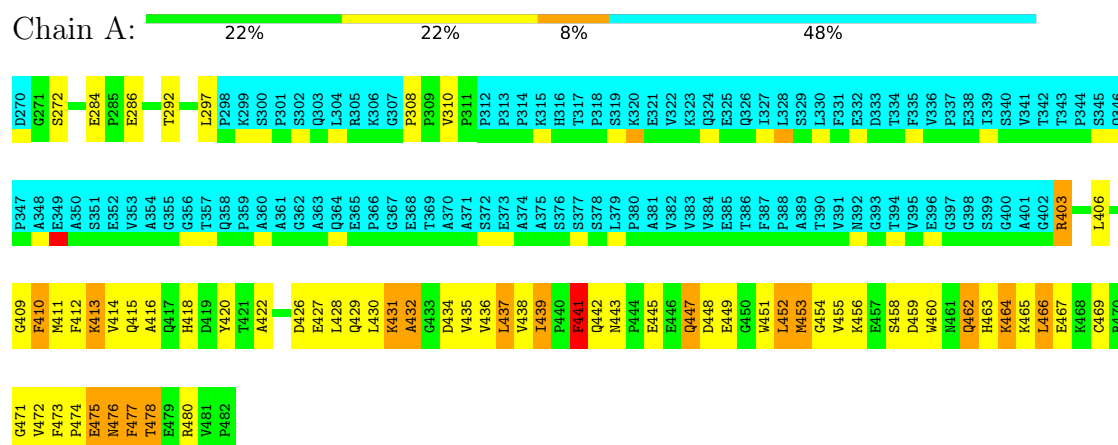
4.2.6 Score per residue for model 6

- Molecule 1: Myc box dependent interacting protein 1



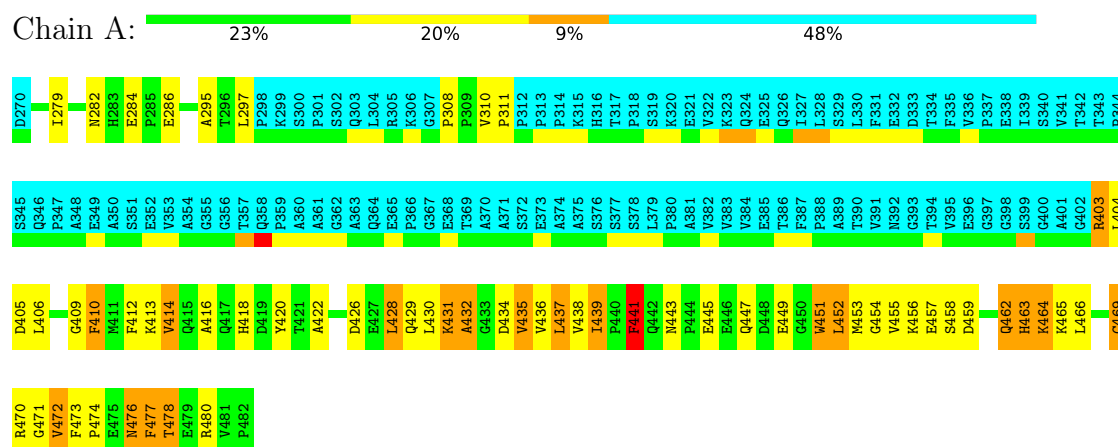
4.2.7 Score per residue for model 7

- Molecule 1: Myc box dependent interacting protein 1



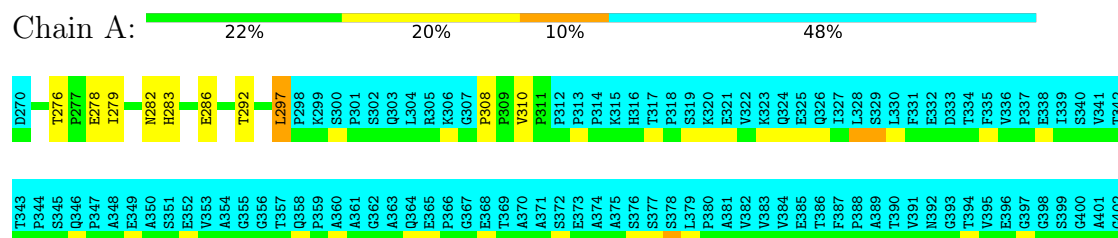
4.2.8 Score per residue for model 8

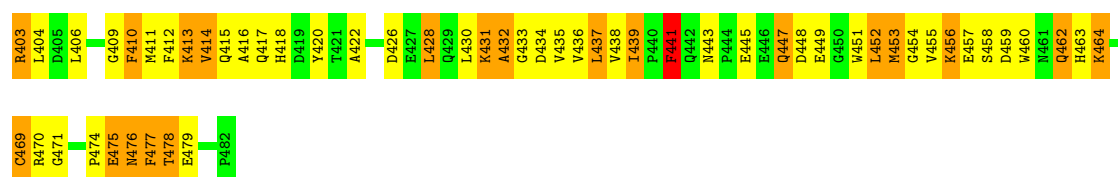
- Molecule 1: Myc box dependent interacting protein 1



4.2.9 Score per residue for model 9

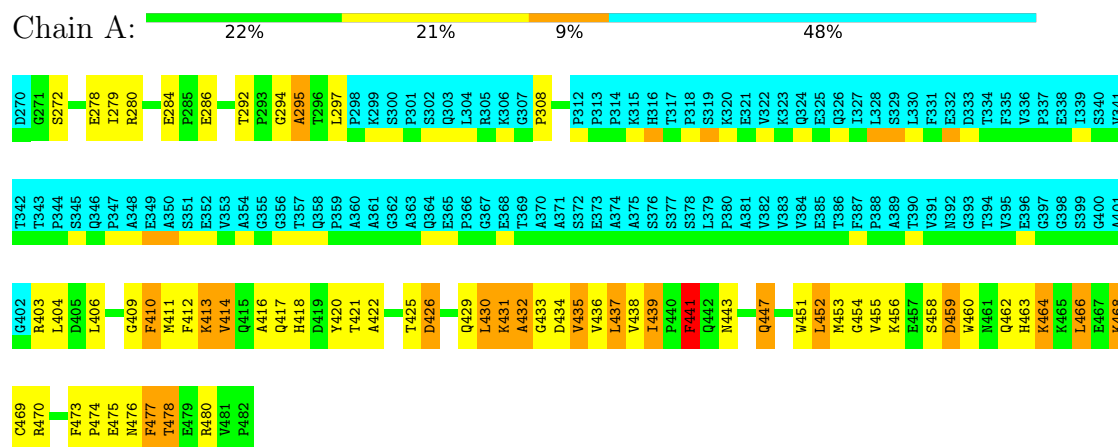
- Molecule 1: Myc box dependent interacting protein 1





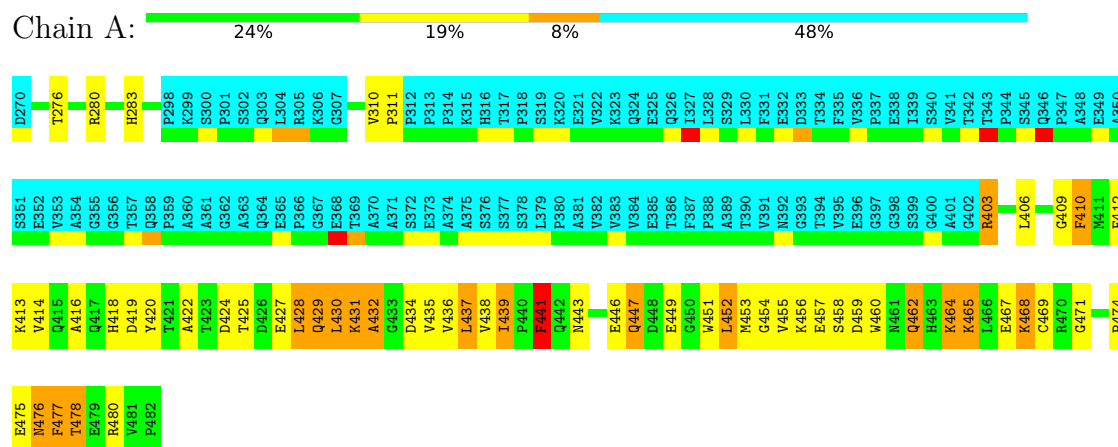
4.2.10 Score per residue for model 10

- Molecule 1: Myc box dependent interacting protein 1



4.2.11 Score per residue for model 11

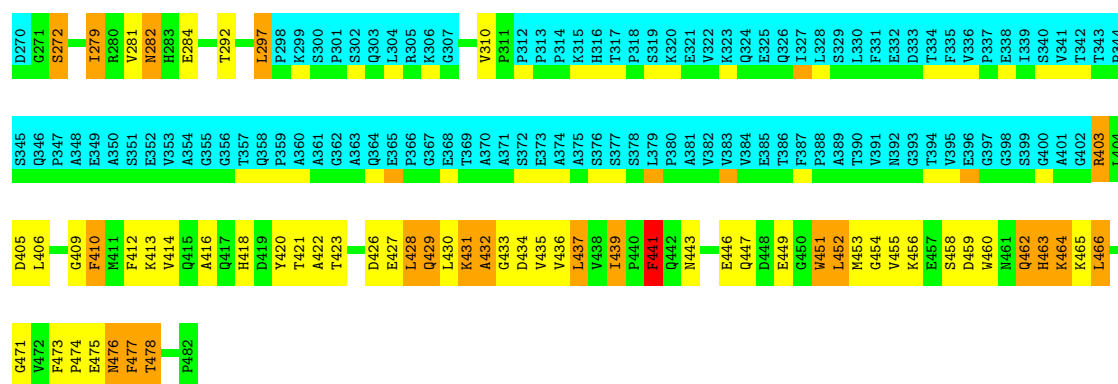
- Molecule 1: Myc box dependent interacting protein 1



4.2.12 Score per residue for model 12

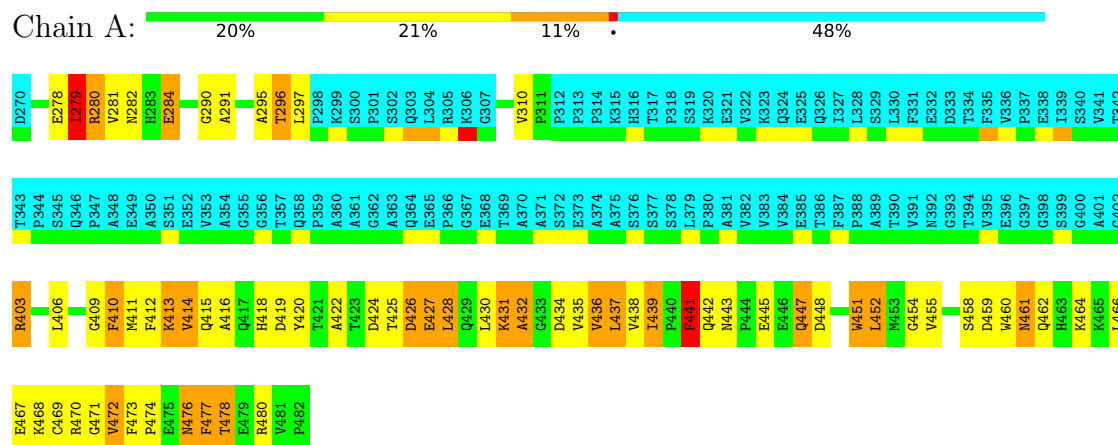
- Molecule 1: Myc box dependent interacting protein 1





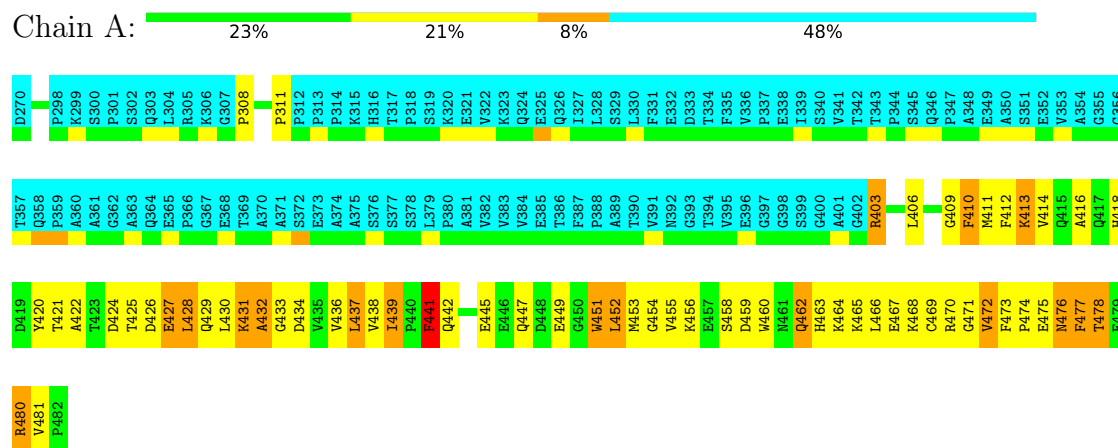
4.2.15 Score per residue for model 15

- Molecule 1: Myc box dependent interacting protein 1



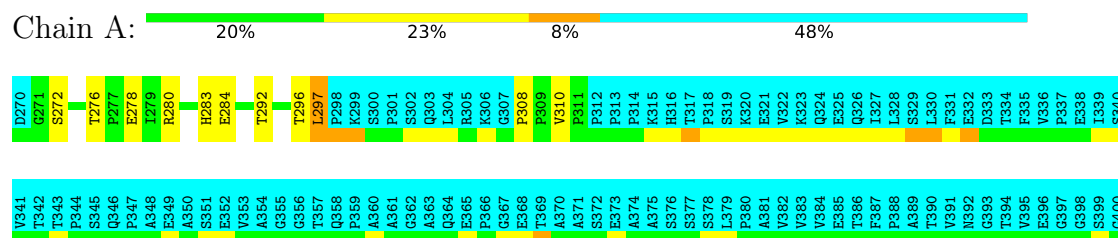
4.2.16 Score per residue for model 16

- Molecule 1: Myc box dependent interacting protein 1



4.2.17 Score per residue for model 17

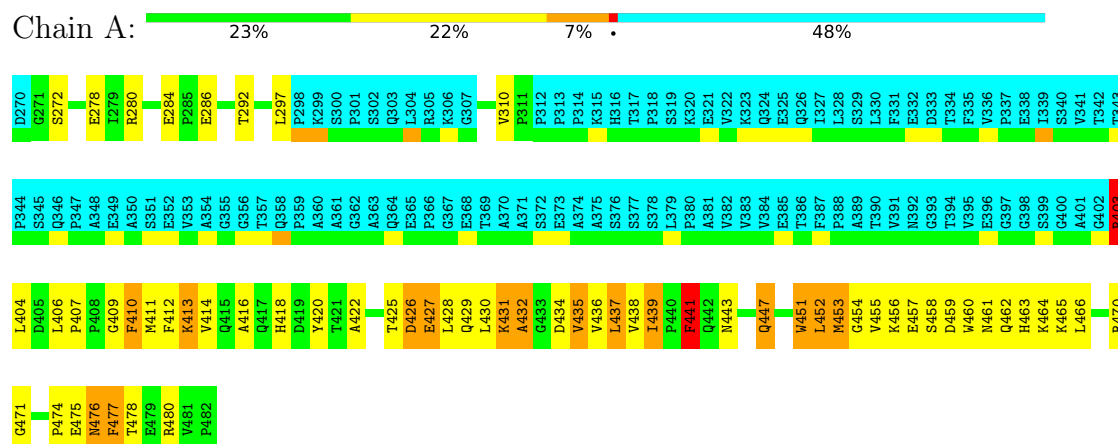
- Molecule 1: Myc box dependent interacting protein 1





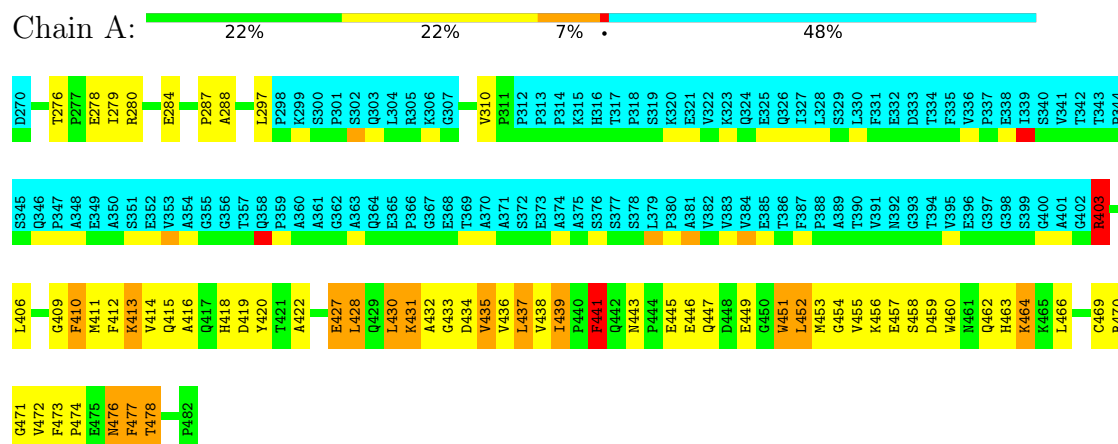
4.2.18 Score per residue for model 18

- Molecule 1: Myc box dependent interacting protein 1



4.2.19 Score per residue for model 19

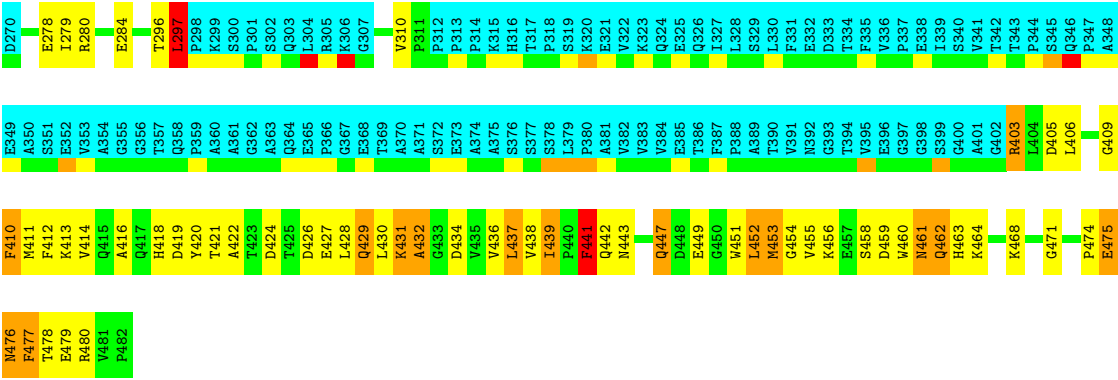
- Molecule 1: Myc box dependent interacting protein 1



4.2.20 Score per residue for model 20

- Molecule 1: 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.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.74±0.01	0±0/890 (0.0± 0.0%)	1.15±0.02	1±1/1217 (0.1± 0.1%)
All	All	0.74	0/17800 (0.0%)	1.15	14/24340 (0.1%)

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	311	PRO	O-C-N	7.29	124.58	121.15	16	3
1	A	308	PRO	O-C-N	7.23	124.55	121.15	7	9
1	A	297	LEU	O-C-N	5.40	124.51	121.27	12	2

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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	59±6
All	All	17280	16580	16580	1189

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 35.

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:451:TRP:C	1:A:452:LEU:HD23	0.91	1.91	20	11
1:A:416:ALA:HB2	1:A:430:LEU:HD12	0.87	1.45	5	6
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:429:GLN:C	1:A:430:LEU:HD22	0.73	2.09	8	15
1:A:455:VAL:HG22	1:A:459:ASP:CB	0.72	2.13	17	12
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:411:MET:HE3	1:A:438:VAL:CG1	0.69	2.18	1	12
1:A:416:ALA:HA	1:A:478:THR:HG22	0.69	1.64	16	20
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	16
1:A:437:LEU:CD1	1:A:460:TRP:CE3	0.67	2.77	13	14
1:A:292:THR:O	1:A:292:THR:HG23	0.67	1.89	3	5
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:413:LYS:NZ	1:A:435:VAL:HG12	0.62	2.09	14	6
1:A:439:ILE:HD13	1:A:454:GLY:HA2	0.62	1.69	14	20
1:A:477:PHE:CG	1:A:477:PHE:O	0.62	2.52	14	20
1:A:431:LYS:O	1:A:432:ALA:C	0.61	2.43	7	20
1:A:411:MET:HE3	1:A:438:VAL:HG12	0.61	1.72	7	14
1:A:466:LEU:HD23	1:A:467:GLU:N	0.61	2.11	1	3
1:A:428:LEU:HD23	1:A:471:GLY:HA3	0.60	1.73	17	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:453:MET:HE2	1:A:471:GLY:O	0.59	1.97	9	10
1:A:436:VAL:C	1:A:437:LEU:HD23	0.59	2.22	18	8
1:A:310:VAL:HG13	1:A:476:ASN:HB2	0.58	1.74	8	15
1:A:452:LEU:HD23	1:A:452:LEU:N	0.58	2.14	11	3
1:A:403:ARG:NH1	1:A:460:TRP:CG	0.58	2.72	6	1
1:A:477:PHE:CD1	1:A:477:PHE:C	0.58	2.81	15	20
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:477:PHE:CD1	1:A:477:PHE:O	0.57	2.57	14	20
1:A:441:PHE:CD1	1:A:441:PHE:N	0.56	2.73	6	20
1:A:294:GLY:O	1:A:295:ALA:HB2	0.56	1.98	10	1
1:A:435:VAL:HG23	1:A:457:GLU:CB	0.56	2.31	5	10
1:A:451:TRP:CD1	1:A:451:TRP:N	0.56	2.73	5	17
1:A:403:ARG:NH2	1:A:463:HIS:CE1	0.55	2.74	8	2
1:A:428:LEU:HD13	1:A:471:GLY:HA3	0.55	1.77	7	4
1:A:403:ARG:NE	1:A:463:HIS:CD2	0.55	2.74	8	2
1:A:428:LEU:HD23	1:A:471:GLY:CA	0.55	2.32	17	7
1:A:462:GLN:N	1:A:462:GLN:NE2	0.55	2.55	16	3
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:405:ASP:O	1:A:463:HIS:CD2	0.54	2.61	6	1
1:A:403:ARG:NE	1:A:403:ARG:H	0.54	2.01	15	6
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:427:GLU:CD	1:A:427:GLU:C	0.54	2.75	18	3
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: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:424:ASP:CB	1:A:427:GLU:CD	0.53	2.82	16	1
1:A:297:LEU:HD12	1:A:297:LEU:O	0.52	2.04	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:462:GLN:C	1:A:464:LYS:N	0.52	2.67	20	20
1:A:413:LYS:HZ3	1:A:481:VAL:HG11	0.52	1.63	16	1
1:A:276:THR:CG2	1:A:276:THR:O	0.52	2.57	14	1
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: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
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	12
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:431:LYS:CD	1:A:434:ASP:OD1	0.50	2.59	20	2
1:A:276:THR:HG23	1:A:276:THR:O	0.50	2.06	19	3
1:A:452:LEU:HD12	1:A:452:LEU:N	0.50	2.20	6	1
1:A:276:THR:O	1:A:276:THR:HG23	0.50	2.06	14	1
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:428:LEU:HD12	1:A:471:GLY:C	0.50	2.31	8	1
1:A:403:ARG:NE	1:A:403:ARG:N	0.50	2.60	1	8
1:A:295:ALA:O	1:A:296:THR:CG2	0.50	2.59	15	1
1:A:403:ARG:O	1:A:403:ARG:CZ	0.50	2.60	9	2
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:423:THR:C	1:A:427:GLU:OE1	0.50	2.55	12	1
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	2
1:A:430:LEU:HD22	1:A:478:THR:CG2	0.49	2.37	10	1
1:A:290:GLY:O	1:A:291:ALA:HB2	0.49	2.06	15	1
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	3
1:A:430:LEU:CD1	1:A:436:VAL:CG2	0.49	2.88	12	2
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	3
1:A:412:PHE:CZ	1:A:480:ARG:HD3	0.48	2.43	4	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:428:LEU:HD22	1:A:454:GLY:O	0.48	2.08	1	1
1:A:441:PHE:CD2	1:A:447:GLN:HB2	0.48	2.44	5	5
1:A:448:ASP:OD1	1:A:448:ASP:N	0.48	2.47	5	1
1:A:412:PHE:CE1	1:A:480:ARG:HD3	0.48	2.44	15	3
1:A:414:VAL:N	1:A:436:VAL:O	0.48	2.43	12	4
1:A:431:LYS:CD	1:A:434:ASP:CG	0.48	2.87	13	2
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:472:VAL:CG2	1:A:473:PHE:N	0.47	2.77	16	4
1:A:407:PRO:HA	1:A:463:HIS:CE1	0.47	2.44	18	1
1:A:409:GLY:O	1:A:410:PHE:C	0.47	2.57	12	20
1:A:420:TYR:HB3	1:A:477:PHE:CE2	0.47	2.45	12	2
1:A:414:VAL:C	1:A:481:VAL:HG23	0.47	2.35	17	1
1:A:420:TYR:HB3	1:A:477:PHE:CZ	0.47	2.44	19	2
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:447:GLN:CD	1:A:451:TRP:O	0.47	2.58	20	7
1:A:276:THR:O	1:A:276:THR:CG2	0.47	2.62	19	1
1:A:411:MET:CE	1:A:438:VAL:CG1	0.46	2.93	13	3
1:A:431:LYS:O	1:A:433:GLY:N	0.46	2.49	4	9
1:A:413:LYS:CE	1:A:414:VAL:O	0.46	2.64	3	5
1:A:461:ASN:N	1:A:461:ASN:ND2	0.46	2.59	15	2
1:A:451:TRP:CE3	1:A:474:PRO:CD	0.46	2.98	5	6
1:A:413:LYS:CE	1:A:435:VAL:HG12	0.46	2.39	10	4
1:A:455:VAL:CG2	1:A:459:ASP:HB2	0.46	2.39	12	6
1:A:426:ASP:O	1:A:426:ASP:CG	0.46	2.58	20	3
1:A:418:HIS:HB2	1:A:477:PHE:CE2	0.46	2.45	16	5
1:A:413:LYS:HZ2	1:A:435:VAL:HG12	0.46	1.70	15	1
1:A:466:LEU:O	1:A:470:ARG:CG	0.46	2.63	6	3
1:A:403:ARG:NH2	1:A:460:TRP:CE2	0.46	2.84	6	1
1:A:437:LEU:CG	1:A:455:VAL:HG13	0.46	2.40	10	3
1:A:437:LEU:N	1:A:437:LEU:CD2	0.46	2.75	1	5
1:A:415:GLN:NE2	1:A:434:ASP:O	0.46	2.49	7	2
1:A:412:PHE:CE1	1:A:414:VAL:HG12	0.46	2.46	17	1
1:A:452:LEU:HD12	1:A:452:LEU:H	0.46	1.71	6	2
1:A:459:ASP:CG	1:A:469:CYS:SG	0.46	2.99	6	4
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:419:ASP:CG	1:A:419:ASP:O	0.46	2.58	20	3
1:A:278:GLU:O	1:A:279:ILE:HG23	0.45	2.12	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:435:VAL:CG2	1:A:457:GLU:CB	0.45	2.93	8	6
1:A:434:ASP:CG	1:A:435:VAL:N	0.45	2.74	10	1
1:A:278:GLU:O	1:A:279:ILE:CG2	0.45	2.65	20	1
1:A:294:GLY:O	1:A:295:ALA:CB	0.45	2.65	10	1
1:A:431:LYS:CE	1:A:434:ASP:OD2	0.45	2.64	17	2
1:A:437:LEU:N	1:A:455:VAL:O	0.45	2.40	5	6
1:A:452:LEU:CD1	1:A:473:PHE:CE1	0.45	3.00	10	2
1:A:407:PRO:HB3	1:A:466:LEU:HD13	0.45	1.87	1	1
1:A:403:ARG:O	1:A:403:ARG:NE	0.45	2.50	9	1
1:A:425:THR:O	1:A:426:ASP:CG	0.45	2.60	18	4
1:A:459:ASP:O	1:A:462:GLN:N	0.44	2.49	9	8
1:A:414:VAL:HG13	1:A:438:VAL:HG23	0.44	1.89	2	4
1:A:279:ILE:CD1	1:A:279:ILE:C	0.44	2.90	15	1
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:411:MET:HE3	1:A:438:VAL:HG13	0.44	1.88	1	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:447:GLN:NE2	1:A:448:ASP:O	0.43	2.50	14	3
1:A:452:LEU:HD13	1:A:473:PHE:CZ	0.43	2.48	12	1
1:A:415:GLN:HB2	1:A:481:VAL:CG2	0.43	2.43	17	1
1:A:435:VAL:CG2	1:A:457:GLU:HB2	0.43	2.43	8	3
1:A:428:LEU:HD12	1:A:430:LEU:CD2	0.43	2.43	11	1
1:A:420:TYR:O	1:A:420:TYR:CG	0.43	2.69	19	1
1:A:448:ASP:OD1	1:A:449:GLU:N	0.43	2.50	2	1
1:A:431:LYS:CE	1:A:434:ASP:CG	0.43	2.91	17	1
1:A:460:TRP:O	1:A:463:HIS:N	0.43	2.50	20	1
1:A:452:LEU:N	1:A:452:LEU:CD2	0.43	2.80	11	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:294:GLY:O	1:A:295:ALA:HB3	0.43	2.13	5	1
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:410:PHE:CZ	1:A:412:PHE:CA	0.43	3.02	9	3
1:A:427:GLU:C	1:A:427:GLU:OE1	0.43	2.62	15	1
1:A:466:LEU:HD23	1:A:467:GLU:H	0.42	1.72	1	1
1:A:467:GLU:HA	1:A:470:ARG:CG	0.42	2.44	13	1
1:A:310:VAL:O	1:A:476:ASN:ND2	0.42	2.50	19	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:415:GLN:NE2	1:A:433:GLY:C	0.42	2.77	19	1
1:A:462:GLN:O	1:A:464:LYS:N	0.42	2.52	20	6
1:A:278:GLU:C	1:A:279:ILE:HG23	0.42	2.39	20	1
1:A:419:ASP:O	1:A:419:ASP:CG	0.42	2.61	6	1
1:A:404:LEU:H	1:A:404:LEU:HD23	0.42	1.74	10	1
1:A:428:LEU:CD2	1:A:454:GLY:O	0.42	2.67	1	1
1:A:419:ASP:OD1	1:A:419:ASP:N	0.42	2.52	2	1
1:A:472:VAL:CG1	1:A:473:PHE:N	0.42	2.83	6	1
1:A:437:LEU:N	1:A:437:LEU:HD23	0.42	2.30	5	2
1:A:451:TRP:HA	1:A:473:PHE:O	0.42	2.15	14	2
1:A:424:ASP:CB	1:A:427:GLU:HG2	0.42	2.45	20	2
1:A:428:LEU:CB	1:A:472:VAL:O	0.42	2.67	7	1
1:A:437:LEU:CD1	1:A:460:TRP:CD2	0.42	3.02	10	2
1:A:431:LYS:CD	1:A:434:ASP:OD2	0.42	2.68	14	1
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:428:LEU:HD13	1:A:471:GLY:CA	0.42	2.42	7	1
1:A:462:GLN:N	1:A:462:GLN:HE21	0.42	2.13	16	1
1:A:448:ASP:CG	1:A:451:TRP:HB2	0.42	2.39	5	1
1:A:448:ASP:CG	1:A:449:GLU:N	0.42	2.78	9	1
1:A:417:GLN:NE2	1:A:478:THR:O	0.41	2.53	10	2
1:A:412:PHE:CZ	1:A:438:VAL:HG21	0.41	2.50	14	1
1:A:462:GLN:NE2	1:A:462:GLN:CA	0.41	2.79	16	1
1:A:416:ALA:CA	1:A:478:THR:HG22	0.41	2.41	16	1
1:A:422:ALA:HB1	1:A:427:GLU:CD	0.41	2.41	12	1
1:A:279:ILE:HD13	1:A:279:ILE:C	0.41	2.40	15	1
1:A:406:LEU:C	1:A:463:HIS:NE2	0.41	2.78	6	1
1:A:450:GLY:C	1:A:451:TRP:CD1	0.41	2.98	13	1
1:A:435:VAL:HG23	1:A:457:GLU:HB2	0.41	1.91	5	1
1:A:403:ARG:HD2	1:A:463:HIS:CB	0.41	2.46	14	1
1:A:413:LYS:HE3	1:A:437:LEU:CD2	0.41	2.45	17	1
1:A:466:LEU:HD23	1:A:467:GLU:HG3	0.41	1.92	7	1
1:A:295:ALA:C	1:A:296:THR:HG22	0.41	2.41	15	1
1:A:451:TRP:CZ3	1:A:474:PRO:CG	0.41	3.04	6	2
1:A:424:ASP:HB2	1:A:427:GLU:CD	0.40	2.41	16	1
1:A:476:ASN:OD1	1:A:476:ASN:N	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:SG	1:A:469:CYS:O	0.40	2.78	9	1
1:A:425:THR:HG23	1:A:426:ASP:OD2	0.40	2.17	16	1
1:A:431:LYS:HD3	1:A:434:ASP:CB	0.40	2.46	13	1
1:A:466:LEU:C	1:A:468:LYS:N	0.40	2.79	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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

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	110/213 (52%)	92±5 (84±4%)	14±4 (12±4%)	4±2 (4±1%)	4	30
All	All	2200/4260 (52%)	1839 (84%)	273 (12%)	88 (4%)	4	30

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	280	ARG	1
1	A	294	GLY	1
1	A	272	SER	1
1	A	281	VAL	1
1	A	282	ASN	1
1	A	296	THR	1
1	A	297	LEU	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	94/173 (54%)	61±3 (65±3%)	33±3 (35±3%)	1	10
All	All	1880/3460 (54%)	1226 (65%)	654 (35%)	1	10

All 63 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	406	LEU	20
1	A	413	LYS	20
1	A	431	LYS	20
1	A	437	LEU	20
1	A	439	ILE	20
1	A	441	PHE	20
1	A	452	LEU	20
1	A	458	SER	20
1	A	476	ASN	20
1	A	477	PHE	20
1	A	403	ARG	19
1	A	443	ASN	18
1	A	453	MET	18
1	A	456	LYS	17
1	A	466	LEU	16
1	A	478	THR	16
1	A	297	LEU	15
1	A	462	GLN	15
1	A	469	CYS	15
1	A	475	GLU	15
1	A	449	GLU	14
1	A	284	GLU	13
1	A	447	GLN	13
1	A	428	LEU	13
1	A	464	LYS	12
1	A	465	LYS	12
1	A	427	GLU	11
1	A	463	HIS	11
1	A	451	TRP	11

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Mol	Chain	Res	Type	Models (Total)
1	A	421	THR	10
1	A	429	GLN	10
1	A	278	GLU	10
1	A	470	ARG	10
1	A	445	GLU	9
1	A	272	SER	9
1	A	286	GLU	8
1	A	414	VAL	8
1	A	435	VAL	8
1	A	468	LYS	8
1	A	283	HIS	7
1	A	404	LEU	7
1	A	442	GLN	7
1	A	280	ARG	7
1	A	279	ILE	6
1	A	467	GLU	6
1	A	276	THR	5
1	A	282	ASN	5
1	A	472	VAL	5
1	A	480	ARG	5
1	A	419	ASP	4
1	A	446	GLU	4
1	A	415	GLN	3
1	A	426	ASP	3
1	A	292	THR	3
1	A	430	LEU	3
1	A	479	GLU	2
1	A	461	ASN	2
1	A	423	THR	1
1	A	459	ASP	1
1	A	281	VAL	1
1	A	436	VAL	1
1	A	424	ASP	1
1	A	405	ASP	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 [i](#)

There are no oligosaccharides 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