



Full wwPDB NMR Structure Validation Report ⓘ

Nov 21, 2016 – 05:57 PM EST

PDB ID : 2NBW
Title : Solution structure of the Rpn1 T1 site with the Rad23 UBL domain
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Deposited on : 2016-03-14

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-20028320
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028320

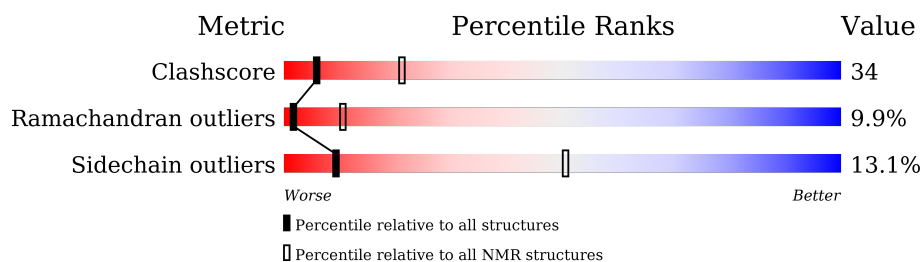
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 40%.

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	131	
2	B	78	

2 Ensemble composition and analysis

This entry contains 10 models. Model 3 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:497-A:607, B:1-B:75 (186)	0.67	3

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 1 single-model cluster was found.

Cluster number	Models
1	1, 3, 4, 5, 6, 8, 9
2	7, 10
Single-model clusters	2

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 3169 atoms, of which 1608 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called 26S proteasome regulatory subunit RPN1.

Mol	Chain	Residues	Atoms						Trace
1	A	131	Total	C	H	N	O	S	0
			1921	606	967	150	192	6	

- Molecule 2 is a protein called UV excision repair protein RAD23.

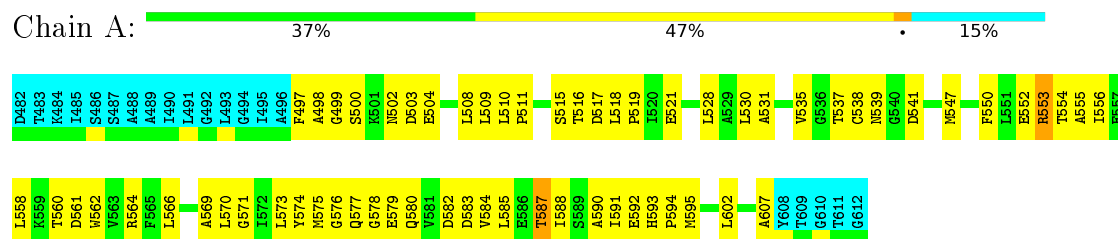
Mol	Chain	Residues	Atoms						Trace
2	B	78	Total	C	H	N	O	S	0
			1248	383	641	97	123	4	

4 Residue-property plots

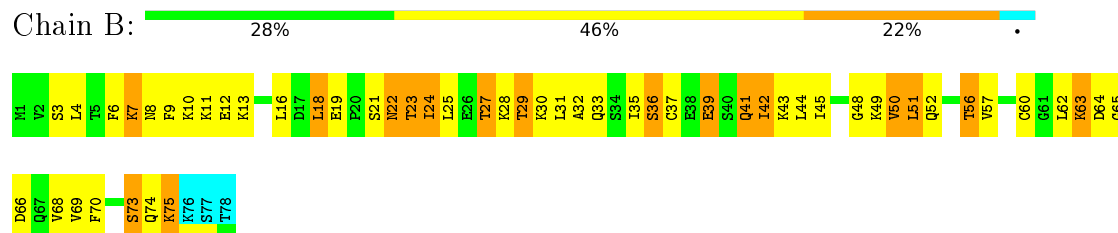
4.1 Average score per residue in the NMR ensemble

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: 26S proteasome regulatory subunit RPN1



- Molecule 2: UV excision repair protein RAD23

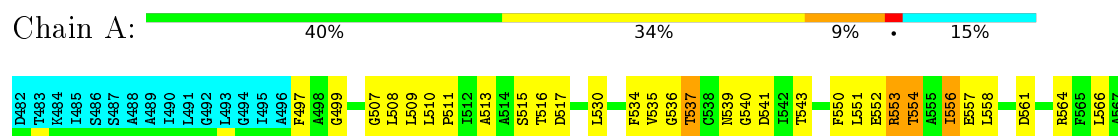


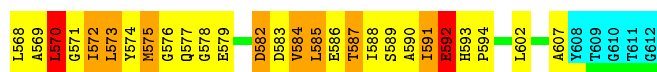
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

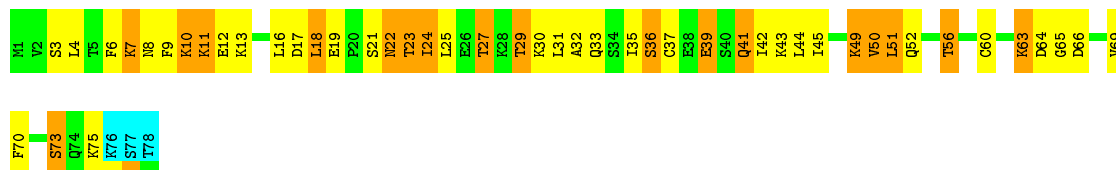
- Molecule 1: 26S proteasome regulatory subunit RPN1





- Molecule 2: UV excision repair protein RAD23

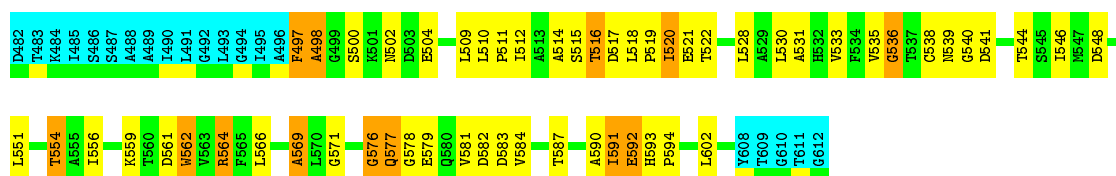
Chain B: 35% 38% 23%



4.2.2 Score per residue for model 2

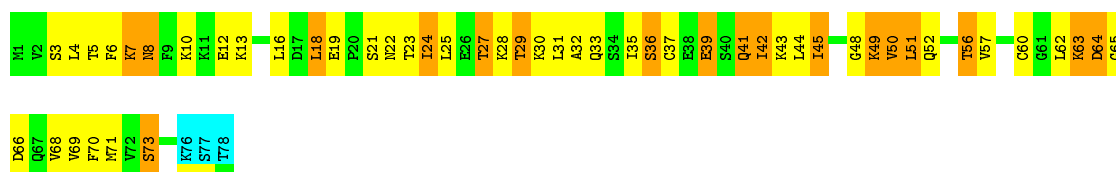
- Molecule 1: 26S proteasome regulatory subunit RPN1

Chain A: 42% 33% 10% 15%



- Molecule 2: UV excision repair protein RAD23

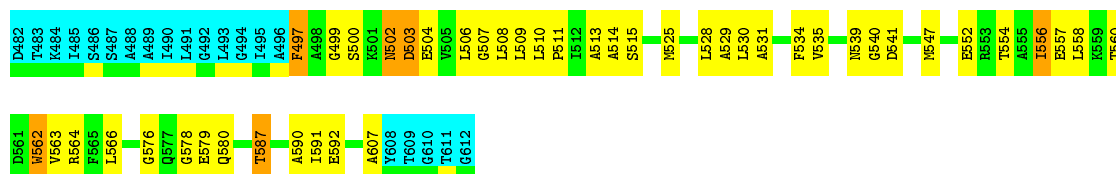
Chain B: 31% 42% 23%



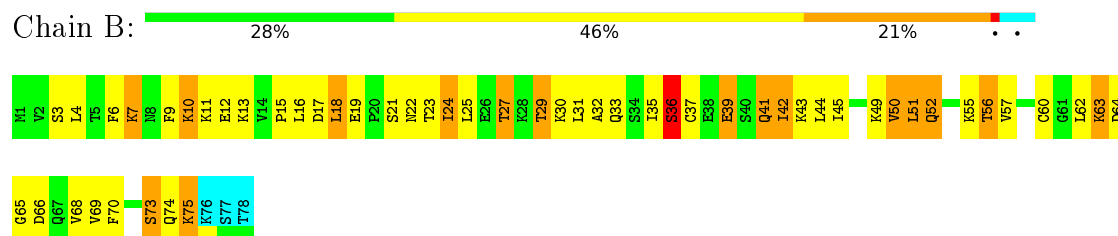
4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: 26S proteasome regulatory subunit RPN1

Chain A: 50% 30% 5% 15%

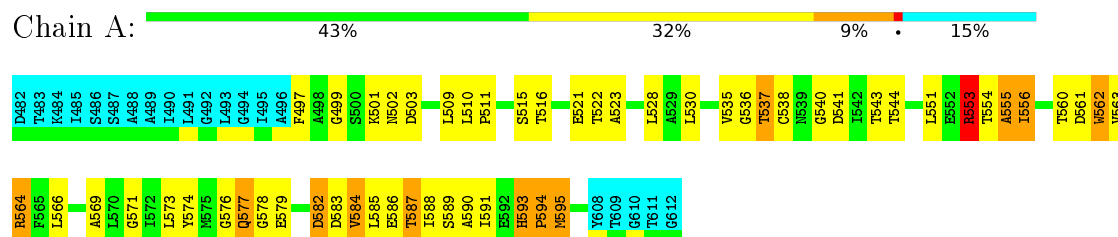


- Molecule 2: UV excision repair protein RAD23

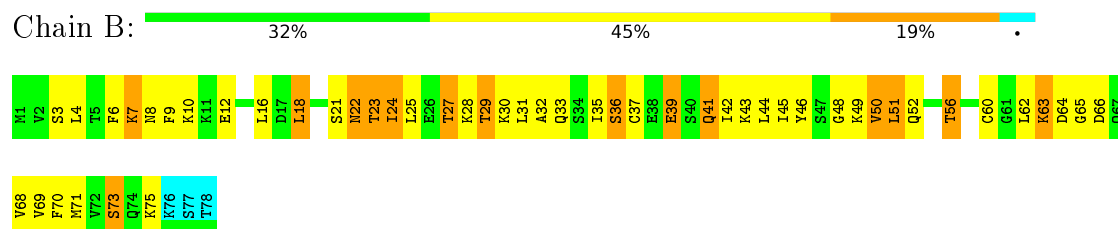


4.2.4 Score per residue for model 4

- Molecule 1: 26S proteasome regulatory subunit RPN1

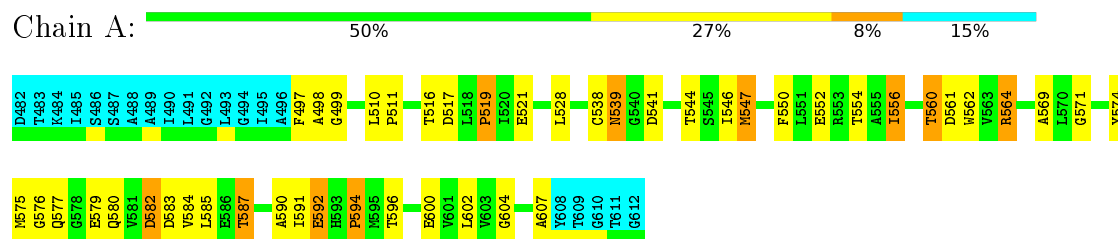


- Molecule 2: UV excision repair protein RAD23

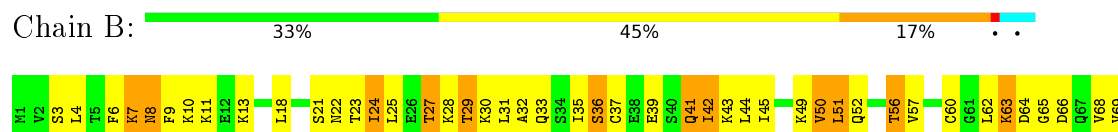


4.2.5 Score per residue for model 5

- Molecule 1: 26S proteasome regulatory subunit RPN1



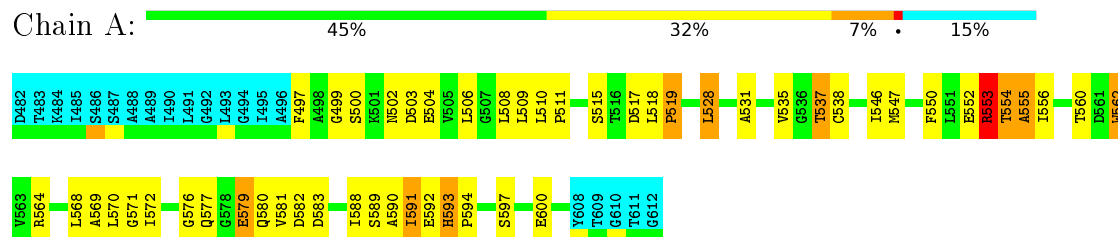
- Molecule 2: UV excision repair protein RAD23



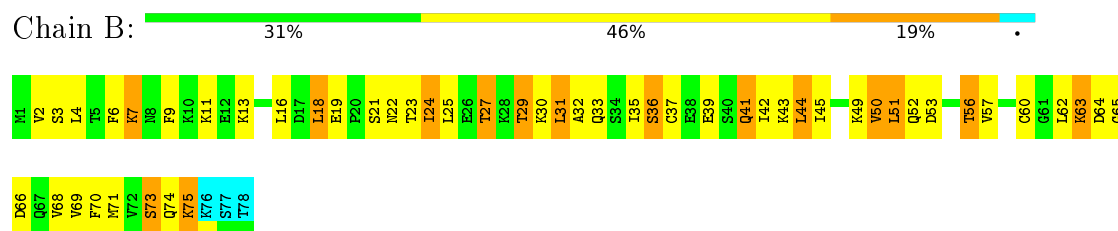


4.2.6 Score per residue for model 6

- Molecule 1: 26S proteasome regulatory subunit RPN1

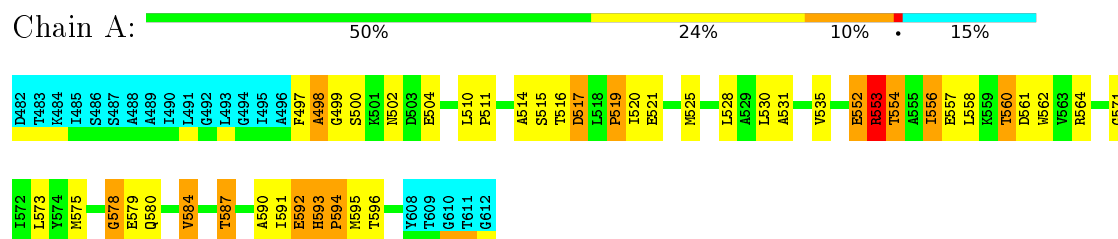


- Molecule 2: UV excision repair protein RAD23

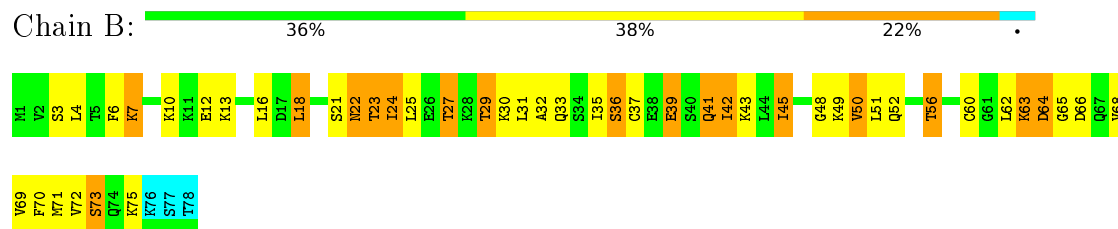


4.2.7 Score per residue for model 7

- Molecule 1: 26S proteasome regulatory subunit RPN1

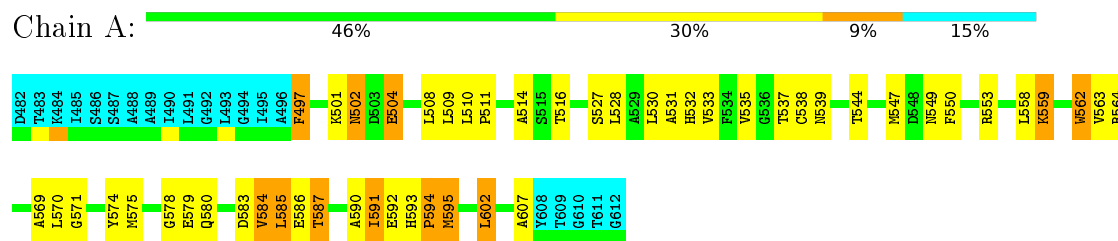


- Molecule 2: UV excision repair protein RAD23

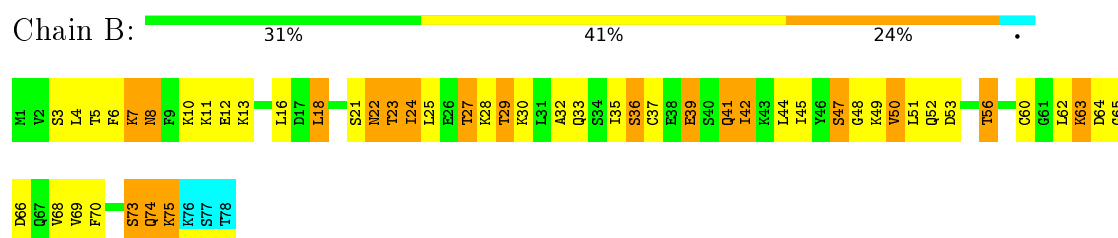


4.2.8 Score per residue for model 8

- Molecule 1: 26S proteasome regulatory subunit RPN1

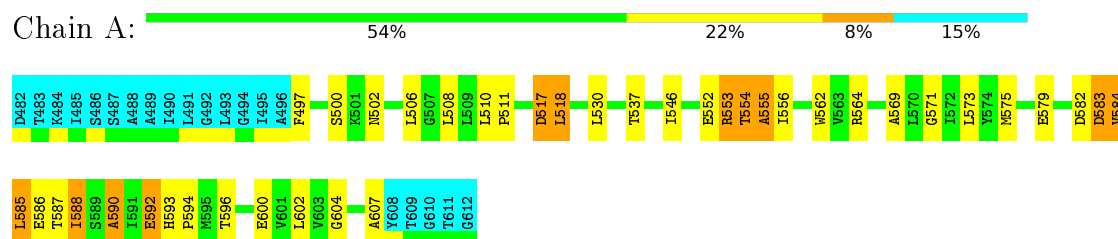


- Molecule 2: UV excision repair protein RAD23

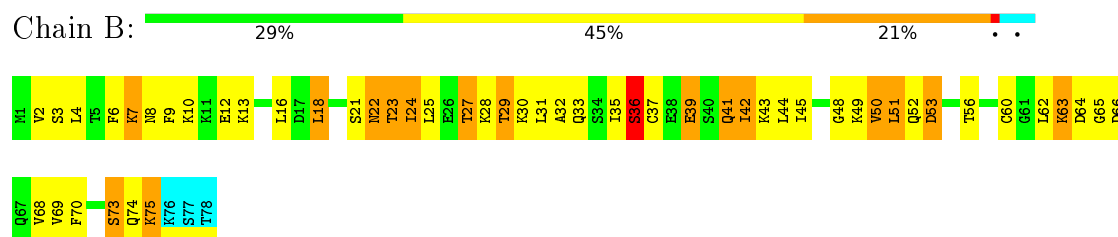


4.2.9 Score per residue for model 9

- Molecule 1: 26S proteasome regulatory subunit RPN1

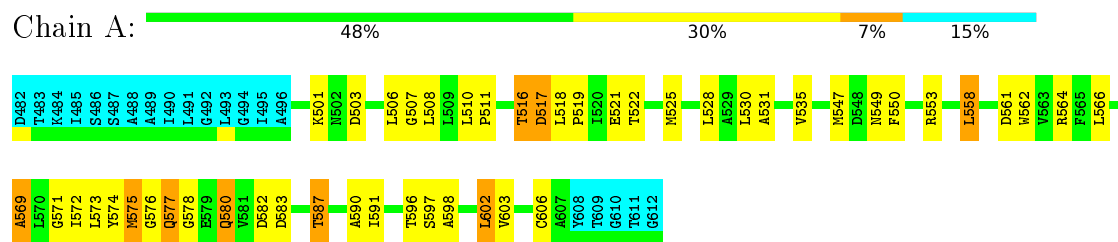


- Molecule 2: UV excision repair protein RAD23

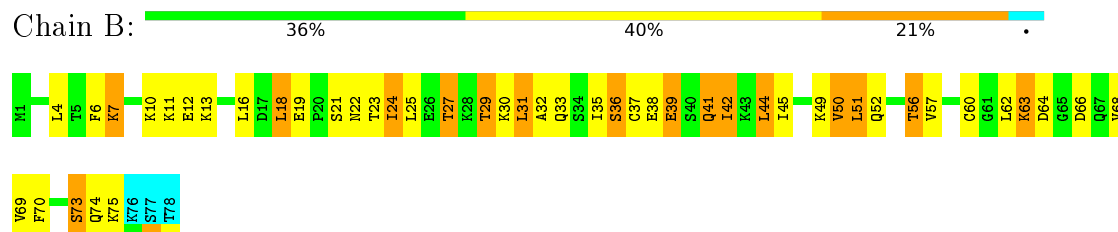


4.2.10 Score per residue for model 10

- Molecule 1: 26S proteasome regulatory subunit RPN1



● Molecule 2: UV excision repair protein RAD23



5 Refinement protocol and experimental data overview

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

Of the 50 calculated structures, 10 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
X-PLOR NIH	refinement	
X-PLOR NIH	structure solution	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	2nbw_cs.cif
Number of chemical shift lists	1
Total number of shifts	1177
Number of shifts mapped to atoms	1003
Number of unparsed shifts	0
Number of shifts with mapping errors	174
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	40%

No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

There are no covalent bond-length or bond-angle outliers.

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	1.6±0.5
All	All	0	16

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	564	ARG	Sidechain	10
1	A	553	ARG	Sidechain	6

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	820	826	826	38±5
2	B	584	616	616	61±6
All	All	14040	14420	14420	981

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 34.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:32:ALA:HB1	2:B:37:CYS:O	1.00	1.56	8	10
2:B:4:LEU:HD23	2:B:66:ASP:H	0.91	1.25	1	10
2:B:24:ILE:O	2:B:28:LYS:HG3	0.87	1.69	8	1
2:B:45:ILE:HG23	2:B:50:VAL:N	0.82	1.89	2	10
2:B:25:LEU:HD13	2:B:25:LEU:C	0.80	1.96	4	2
2:B:25:LEU:C	2:B:25:LEU:HD13	0.79	1.96	7	4
2:B:18:LEU:HD21	2:B:27:THR:OG1	0.77	1.80	2	10
2:B:24:ILE:HG21	2:B:52:GLN:O	0.70	1.85	5	4
2:B:4:LEU:HD23	2:B:66:ASP:N	0.70	2.00	1	10
1:A:554:THR:O	1:A:556:ILE:N	0.69	2.25	4	6
2:B:57:VAL:HG13	2:B:62:LEU:HB2	0.69	1.62	3	4
2:B:56:THR:OG1	2:B:57:VAL:N	0.69	2.24	10	5
2:B:51:LEU:HD21	2:B:60:CYS:SG	0.69	2.28	7	3
2:B:31:LEU:HD21	2:B:70:PHE:CD2	0.69	2.23	10	2
2:B:63:LYS:HD3	2:B:64:ASP:N	0.68	2.03	1	10
2:B:45:ILE:O	2:B:68:VAL:HG12	0.67	1.90	3	8
2:B:51:LEU:HD13	2:B:60:CYS:SG	0.66	2.30	10	2
2:B:74:GLN:O	2:B:75:LYS:C	0.65	2.33	9	4
2:B:42:ILE:O	2:B:42:ILE:HG22	0.64	1.92	2	5
2:B:63:LYS:CD	2:B:64:ASP:N	0.64	2.61	10	10
2:B:35:ILE:O	2:B:36:SER:CB	0.63	2.45	6	10
2:B:32:ALA:CB	2:B:37:CYS:O	0.63	2.44	2	9
2:B:50:VAL:HG13	2:B:50:VAL:O	0.62	1.95	4	4
2:B:8:ASN:ND2	2:B:10:LYS:H	0.61	1.93	5	2
2:B:50:VAL:O	2:B:50:VAL:HG13	0.61	1.94	2	5
2:B:51:LEU:HD22	2:B:60:CYS:SG	0.61	2.36	5	5
2:B:21:SER:O	2:B:22:ASN:C	0.61	2.39	8	10
2:B:25:LEU:C	2:B:25:LEU:HD23	0.61	2.16	6	2
2:B:43:LYS:O	2:B:45:ILE:HG13	0.60	1.96	7	8
2:B:25:LEU:O	2:B:29:THR:OG1	0.60	2.20	6	10
2:B:71:MET:SD	2:B:72:VAL:N	0.60	2.75	7	1
2:B:25:LEU:O	2:B:25:LEU:HD23	0.59	1.96	2	4
2:B:25:LEU:HD23	2:B:25:LEU:C	0.59	2.17	5	2
2:B:8:ASN:ND2	2:B:10:LYS:CE	0.59	2.66	1	2
2:B:7:LYS:O	2:B:70:PHE:CD1	0.59	2.55	9	10
2:B:25:LEU:C	2:B:25:LEU:CD1	0.59	2.70	7	4
2:B:45:ILE:O	2:B:68:VAL:CG1	0.59	2.50	8	9
1:A:575:MET:SD	1:A:576:GLY:N	0.58	2.76	1	1
2:B:45:ILE:O	2:B:69:VAL:O	0.58	2.21	2	10
2:B:45:ILE:HG22	2:B:49:LYS:N	0.58	2.13	2	10
2:B:41:GLN:NE2	2:B:73:SER:O	0.58	2.37	8	9
2:B:63:LYS:NZ	2:B:66:ASP:CG	0.58	2.57	4	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:18:LEU:HD21	2:B:27:THR:CB	0.58	2.27	5	4
1:A:590:ALA:O	1:A:592:GLU:N	0.57	2.37	1	2
2:B:25:LEU:CD1	2:B:25:LEU:C	0.57	2.72	1	2
1:A:593:HIS:N	1:A:594:PRO:CD	0.57	2.66	4	3
2:B:24:ILE:HD13	2:B:24:ILE:N	0.57	2.15	4	5
2:B:30:LYS:O	2:B:33:GLN:N	0.57	2.37	6	10
1:A:593:HIS:CE1	1:A:595:MET:SD	0.56	2.98	7	1
1:A:518:LEU:N	1:A:518:LEU:CD2	0.56	2.68	10	1
1:A:518:LEU:N	1:A:518:LEU:HD22	0.56	2.14	10	1
1:A:554:THR:C	1:A:556:ILE:N	0.56	2.58	4	7
1:A:562:TRP:CD1	1:A:563:VAL:N	0.55	2.74	3	1
2:B:63:LYS:HZ2	2:B:66:ASP:CG	0.55	2.05	1	4
2:B:3:SER:O	2:B:65:GLY:HA2	0.55	2.02	3	7
1:A:577:GLN:NE2	1:A:578:GLY:O	0.55	2.40	10	1
2:B:23:THR:OG1	2:B:24:ILE:N	0.55	2.40	8	4
1:A:510:LEU:CB	1:A:511:PRO:CD	0.55	2.85	6	9
1:A:592:GLU:O	1:A:593:HIS:CG	0.54	2.61	8	2
1:A:579:GLU:O	1:A:582:ASP:N	0.54	2.40	4	5
1:A:510:LEU:HB3	1:A:511:PRO:CD	0.54	2.32	10	2
2:B:8:ASN:N	2:B:8:ASN:OD1	0.54	2.40	4	1
2:B:6:PHE:CE2	2:B:44:LEU:HD11	0.54	2.37	10	2
1:A:558:LEU:N	1:A:558:LEU:CD2	0.54	2.71	1	1
2:B:7:LYS:HA	2:B:12:GLU:O	0.54	2.03	4	2
2:B:22:ASN:O	2:B:56:THR:CB	0.54	2.55	6	4
2:B:9:PHE:CD1	2:B:9:PHE:O	0.54	2.61	1	1
2:B:24:ILE:N	2:B:24:ILE:HD13	0.54	2.18	7	4
2:B:45:ILE:N	2:B:69:VAL:O	0.53	2.41	1	10
1:A:519:PRO:O	1:A:521:GLU:N	0.53	2.41	2	2
1:A:584:VAL:O	1:A:587:THR:N	0.53	2.41	9	6
2:B:6:PHE:CD1	2:B:16:LEU:HD12	0.53	2.39	9	8
1:A:566:LEU:N	1:A:566:LEU:HD12	0.53	2.19	10	1
2:B:45:ILE:HG22	2:B:49:LYS:H	0.53	1.63	5	10
1:A:497:PHE:O	1:A:497:PHE:CG	0.53	2.62	2	1
1:A:591:ILE:O	1:A:593:HIS:N	0.53	2.41	6	2
1:A:592:GLU:OE1	1:A:592:GLU:N	0.53	2.42	3	1
2:B:9:PHE:O	2:B:9:PHE:CD2	0.53	2.62	6	1
1:A:537:THR:OG1	1:A:538:CYS:N	0.53	2.41	6	2
1:A:582:ASP:OD1	1:A:583:ASP:N	0.53	2.41	10	7
1:A:560:THR:O	1:A:562:TRP:CZ3	0.53	2.62	3	1
1:A:570:LEU:O	1:A:574:TYR:CE2	0.53	2.62	8	1
1:A:558:LEU:N	1:A:558:LEU:HD22	0.53	2.18	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:42:ILE:O	2:B:42:ILE:CG2	0.53	2.56	2	1
2:B:63:LYS:CD	2:B:64:ASP:O	0.53	2.57	5	4
1:A:508:LEU:CD2	1:A:508:LEU:N	0.53	2.71	3	1
1:A:562:TRP:CD1	1:A:562:TRP:N	0.52	2.76	5	1
1:A:597:SER:O	1:A:600:GLU:N	0.52	2.42	6	1
2:B:63:LYS:HZ1	2:B:65:GLY:C	0.52	2.06	6	1
2:B:6:PHE:CD1	2:B:6:PHE:N	0.52	2.77	5	4
2:B:60:CYS:SG	2:B:62:LEU:HG	0.52	2.44	9	3
2:B:24:ILE:O	2:B:28:LYS:CG	0.52	2.52	8	1
2:B:63:LYS:NZ	2:B:66:ASP:OD1	0.52	2.43	8	1
1:A:540:GLY:O	1:A:543:THR:N	0.52	2.41	4	2
2:B:24:ILE:CG2	2:B:52:GLN:O	0.52	2.57	2	2
1:A:574:TYR:O	1:A:576:GLY:N	0.52	2.42	5	1
1:A:560:THR:O	1:A:562:TRP:CD1	0.52	2.63	6	1
2:B:25:LEU:HD13	2:B:25:LEU:O	0.52	2.03	10	2
1:A:527:SER:OG	1:A:528:LEU:N	0.52	2.42	8	1
2:B:49:LYS:O	2:B:50:VAL:C	0.52	2.48	7	10
1:A:587:THR:O	1:A:590:ALA:N	0.52	2.42	3	5
1:A:569:ALA:O	1:A:571:GLY:N	0.52	2.43	1	5
2:B:9:PHE:O	2:B:9:PHE:CD1	0.52	2.62	4	2
2:B:23:THR:HA	2:B:56:THR:HA	0.51	1.82	5	10
2:B:19:GLU:N	2:B:22:ASN:OD1	0.51	2.44	3	4
2:B:35:ILE:O	2:B:36:SER:OG	0.51	2.28	6	4
1:A:562:TRP:CG	1:A:563:VAL:N	0.51	2.78	4	2
1:A:588:ILE:O	1:A:590:ALA:N	0.51	2.44	4	2
1:A:596:THR:O	1:A:598:ALA:N	0.51	2.43	10	1
1:A:566:LEU:HD12	1:A:566:LEU:N	0.51	2.20	2	2
2:B:44:LEU:HD12	2:B:51:LEU:HD12	0.51	1.83	6	1
1:A:537:THR:O	1:A:538:CYS:SG	0.51	2.69	8	1
2:B:21:SER:O	2:B:22:ASN:O	0.51	2.29	8	5
2:B:42:ILE:HG22	2:B:42:ILE:O	0.50	2.06	5	2
1:A:553:ARG:O	1:A:554:THR:OG1	0.50	2.28	9	2
2:B:27:THR:CG2	2:B:44:LEU:CD2	0.50	2.89	9	4
1:A:503:ASP:OD1	1:A:503:ASP:N	0.50	2.43	6	1
2:B:27:THR:CG2	2:B:44:LEU:HD22	0.50	2.37	8	1
2:B:17:ASP:OD1	2:B:17:ASP:N	0.50	2.45	1	2
2:B:51:LEU:CD2	2:B:60:CYS:SG	0.50	3.00	9	3
1:A:508:LEU:HD22	1:A:508:LEU:N	0.50	2.20	3	1
1:A:554:THR:O	1:A:555:ALA:C	0.50	2.50	4	3
2:B:50:VAL:CG1	2:B:50:VAL:O	0.50	2.59	7	2
1:A:560:THR:OG1	1:A:561:ASP:N	0.50	2.45	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:579:GLU:O	1:A:582:ASP:OD2	0.50	2.30	4	6
1:A:530:LEU:C	1:A:530:LEU:HD23	0.50	2.27	3	2
1:A:590:ALA:CB	2:B:48:GLY:O	0.50	2.60	8	5
1:A:551:LEU:HD12	1:A:551:LEU:N	0.49	2.21	2	2
2:B:71:MET:SD	2:B:72:VAL:O	0.49	2.70	7	1
2:B:30:LYS:O	2:B:32:ALA:N	0.49	2.45	3	9
1:A:588:ILE:C	1:A:590:ALA:N	0.49	2.66	4	2
1:A:530:LEU:O	1:A:530:LEU:HD23	0.49	2.07	8	1
1:A:566:LEU:O	1:A:569:ALA:N	0.49	2.44	4	1
1:A:575:MET:SD	1:A:575:MET:O	0.49	2.70	10	1
2:B:25:LEU:O	2:B:25:LEU:HD13	0.49	2.05	1	4
2:B:63:LYS:CD	2:B:63:LYS:C	0.49	2.81	2	4
1:A:497:PHE:CE1	1:A:529:ALA:HB1	0.49	2.42	3	1
1:A:592:GLU:H	1:A:592:GLU:CD	0.49	2.11	9	1
1:A:594:PRO:O	1:A:596:THR:HG23	0.49	2.07	5	1
1:A:506:LEU:CD2	1:A:530:LEU:HD22	0.49	2.37	10	2
1:A:569:ALA:C	1:A:571:GLY:N	0.49	2.66	1	7
2:B:45:ILE:HG23	2:B:50:VAL:CA	0.49	2.37	7	7
1:A:510:LEU:O	1:A:514:ALA:N	0.49	2.45	7	2
1:A:510:LEU:HB3	1:A:511:PRO:HD3	0.49	1.85	10	1
1:A:538:CYS:O	1:A:539:ASN:ND2	0.49	2.46	8	1
1:A:572:ILE:O	1:A:574:TYR:N	0.49	2.45	1	1
2:B:63:LYS:NZ	2:B:65:GLY:C	0.49	2.67	6	1
1:A:497:PHE:C	1:A:499:GLY:N	0.49	2.66	5	3
1:A:547:MET:O	1:A:550:PHE:N	0.49	2.46	5	4
1:A:519:PRO:O	1:A:520:ILE:C	0.48	2.51	2	1
1:A:578:GLY:O	1:A:580:GLN:N	0.48	2.46	8	4
2:B:24:ILE:N	2:B:24:ILE:CD1	0.48	2.76	1	3
2:B:27:THR:CG2	2:B:44:LEU:HD21	0.48	2.38	9	3
1:A:553:ARG:HH11	1:A:556:ILE:CD1	0.48	2.22	4	1
1:A:515:SER:OG	1:A:516:THR:N	0.48	2.46	7	2
1:A:538:CYS:SG	1:A:580:GLN:OE1	0.48	2.70	5	1
2:B:27:THR:HG21	2:B:44:LEU:HD21	0.48	1.85	3	4
2:B:10:LYS:C	2:B:12:GLU:H	0.48	2.11	2	6
1:A:539:ASN:OD1	1:A:540:GLY:N	0.48	2.46	3	1
1:A:522:THR:HG23	1:A:523:ALA:N	0.48	2.24	4	1
2:B:44:LEU:O	2:B:51:LEU:N	0.48	2.47	3	7
2:B:24:ILE:CD1	2:B:24:ILE:N	0.48	2.76	4	2
1:A:592:GLU:N	1:A:592:GLU:CD	0.48	2.66	1	2
2:B:63:LYS:C	2:B:63:LYS:CD	0.48	2.82	1	6
1:A:592:GLU:CD	1:A:592:GLU:N	0.48	2.67	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:507:GLY:O	1:A:511:PRO:CG	0.48	2.62	3	1
1:A:528:LEU:HD23	1:A:528:LEU:O	0.48	2.08	6	1
2:B:28:LYS:NZ	2:B:39:GLU:OE1	0.48	2.46	5	1
1:A:539:ASN:OD1	1:A:541:ASP:N	0.47	2.46	2	1
2:B:39:GLU:CD	2:B:39:GLU:C	0.47	2.72	2	4
1:A:588:ILE:CG2	1:A:596:THR:OG1	0.47	2.62	9	1
2:B:7:LYS:C	2:B:70:PHE:CE1	0.47	2.87	7	7
2:B:41:GLN:OE1	2:B:75:LYS:O	0.47	2.32	6	1
2:B:3:SER:O	2:B:65:GLY:N	0.47	2.48	7	1
1:A:535:VAL:HG13	1:A:536:GLY:N	0.47	2.24	1	3
2:B:64:ASP:OD1	2:B:64:ASP:N	0.47	2.46	1	2
2:B:7:LYS:CE	2:B:69:VAL:HG13	0.47	2.39	6	2
1:A:544:THR:CG2	2:B:74:GLN:OE1	0.47	2.62	8	1
2:B:30:LYS:C	2:B:32:ALA:N	0.47	2.68	3	10
2:B:45:ILE:CG2	2:B:50:VAL:N	0.47	2.72	2	2
1:A:561:ASP:N	1:A:561:ASP:OD1	0.47	2.48	5	1
2:B:7:LYS:HE2	2:B:69:VAL:HG13	0.47	1.85	6	2
1:A:528:LEU:O	1:A:528:LEU:HD23	0.47	2.09	10	1
1:A:497:PHE:O	1:A:499:GLY:N	0.47	2.46	5	2
1:A:582:ASP:CG	1:A:583:ASP:N	0.47	2.68	1	1
1:A:552:GLU:OE2	2:B:75:LYS:NZ	0.47	2.48	5	1
1:A:507:GLY:C	1:A:508:LEU:HD12	0.47	2.30	1	2
1:A:510:LEU:O	1:A:513:ALA:HB3	0.47	2.09	1	1
2:B:52:GLN:OE1	2:B:55:LYS:NZ	0.47	2.41	3	1
1:A:500:SER:O	1:A:500:SER:OG	0.47	2.33	6	1
1:A:571:GLY:C	1:A:573:LEU:N	0.47	2.67	10	3
2:B:47:SER:OG	2:B:47:SER:O	0.47	2.29	8	1
1:A:558:LEU:N	1:A:558:LEU:HD12	0.47	2.25	3	1
1:A:557:GLU:CG	1:A:558:LEU:N	0.47	2.78	7	1
1:A:596:THR:C	1:A:598:ALA:N	0.47	2.67	10	1
1:A:554:THR:C	1:A:556:ILE:H	0.47	2.13	1	7
1:A:587:THR:HG21	2:B:71:MET:SD	0.47	2.49	4	1
2:B:4:LEU:CD2	2:B:66:ASP:H	0.47	2.16	5	1
1:A:571:GLY:O	1:A:573:LEU:N	0.46	2.48	10	3
1:A:510:LEU:N	1:A:511:PRO:HD2	0.46	2.25	10	5
2:B:41:GLN:HE21	2:B:73:SER:C	0.46	2.14	3	4
1:A:511:PRO:O	1:A:515:SER:N	0.46	2.48	2	2
1:A:530:LEU:HD23	1:A:530:LEU:C	0.46	2.31	7	3
2:B:7:LYS:CD	2:B:7:LYS:C	0.46	2.84	7	5
1:A:525:MET:C	1:A:525:MET:SD	0.46	2.94	3	1
2:B:7:LYS:C	2:B:7:LYS:CD	0.46	2.84	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:551:LEU:C	1:A:553:ARG:N	0.46	2.69	1	1
1:A:575:MET:SD	1:A:575:MET:C	0.46	2.94	10	2
2:B:21:SER:O	2:B:56:THR:HB	0.46	2.11	5	4
2:B:50:VAL:O	2:B:51:LEU:O	0.46	2.32	5	4
1:A:552:GLU:O	1:A:553:ARG:C	0.46	2.54	9	2
1:A:551:LEU:CD1	1:A:551:LEU:N	0.46	2.79	2	1
2:B:39:GLU:CD	2:B:39:GLU:O	0.46	2.54	2	3
1:A:551:LEU:O	1:A:553:ARG:N	0.46	2.49	1	1
1:A:584:VAL:O	1:A:586:GLU:N	0.46	2.49	9	3
1:A:538:CYS:SG	1:A:577:GLN:OE1	0.46	2.74	2	1
2:B:28:LYS:NZ	2:B:53:ASP:OD1	0.46	2.49	8	1
1:A:539:ASN:OD1	1:A:541:ASP:HB2	0.46	2.10	1	1
1:A:570:LEU:O	1:A:570:LEU:HD13	0.46	2.11	1	1
1:A:566:LEU:N	1:A:566:LEU:CD1	0.46	2.79	3	1
1:A:566:LEU:CD1	1:A:566:LEU:N	0.45	2.79	10	2
2:B:8:ASN:OD1	2:B:8:ASN:N	0.45	2.48	1	1
1:A:530:LEU:HD23	1:A:530:LEU:O	0.45	2.11	2	2
1:A:541:ASP:O	1:A:544:THR:OG1	0.45	2.33	5	2
1:A:595:MET:C	1:A:595:MET:SD	0.45	2.94	8	1
2:B:8:ASN:OD1	2:B:10:LYS:N	0.45	2.48	9	1
1:A:498:ALA:O	1:A:500:SER:N	0.45	2.50	7	1
2:B:8:ASN:ND2	2:B:10:LYS:CD	0.45	2.79	1	1
2:B:39:GLU:C	2:B:39:GLU:CD	0.45	2.75	8	2
1:A:519:PRO:C	1:A:521:GLU:N	0.45	2.69	5	3
1:A:602:LEU:HD23	1:A:602:LEU:C	0.45	2.32	9	2
1:A:552:GLU:O	1:A:553:ARG:O	0.45	2.33	7	1
2:B:6:PHE:CE2	2:B:44:LEU:HD21	0.45	2.46	8	1
1:A:572:ILE:C	1:A:574:TYR:N	0.45	2.69	1	1
2:B:41:GLN:NE2	2:B:75:LYS:O	0.45	2.49	4	1
2:B:8:ASN:ND2	2:B:8:ASN:H	0.45	2.09	8	2
1:A:528:LEU:HD23	1:A:528:LEU:C	0.45	2.32	3	4
1:A:541:ASP:OD1	1:A:541:ASP:N	0.45	2.48	3	1
1:A:600:GLU:O	1:A:604:GLY:N	0.45	2.50	9	2
1:A:582:ASP:C	1:A:582:ASP:OD1	0.45	2.54	6	3
1:A:578:GLY:C	1:A:580:GLN:N	0.45	2.70	8	3
2:B:22:ASN:O	2:B:56:THR:OG1	0.45	2.35	6	3
1:A:553:ARG:NH1	1:A:556:ILE:CD1	0.45	2.80	4	1
1:A:517:ASP:OD1	1:A:517:ASP:N	0.45	2.50	7	1
2:B:3:SER:HA	2:B:16:LEU:O	0.45	2.12	6	3
1:A:558:LEU:N	1:A:558:LEU:CD1	0.45	2.79	3	1
1:A:528:LEU:C	1:A:528:LEU:HD23	0.45	2.33	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:516:THR:OG1	1:A:517:ASP:N	0.44	2.50	10	2
1:A:561:ASP:OD1	1:A:561:ASP:N	0.44	2.51	2	1
1:A:531:ALA:O	1:A:535:VAL:N	0.44	2.49	3	6
1:A:502:ASN:C	1:A:504:GLU:H	0.44	2.16	3	4
1:A:503:ASP:N	1:A:503:ASP:OD1	0.44	2.49	3	1
1:A:562:TRP:O	1:A:564:ARG:N	0.44	2.50	5	2
1:A:560:THR:O	1:A:562:TRP:NE1	0.44	2.50	6	1
2:B:18:LEU:O	2:B:19:GLU:OE2	0.44	2.36	1	1
1:A:562:TRP:C	1:A:564:ARG:N	0.44	2.70	4	3
1:A:506:LEU:HD11	1:A:534:PHE:CZ	0.44	2.48	3	1
1:A:582:ASP:OD1	1:A:582:ASP:C	0.44	2.55	4	3
1:A:586:GLU:O	1:A:590:ALA:HB2	0.44	2.12	4	1
2:B:51:LEU:HD11	2:B:60:CYS:SG	0.44	2.53	1	1
1:A:595:MET:SD	1:A:595:MET:C	0.44	2.96	4	1
1:A:583:ASP:OD1	2:B:11:LYS:NZ	0.44	2.44	8	1
1:A:500:SER:OG	1:A:502:ASN:ND2	0.44	2.50	9	1
1:A:518:LEU:H	1:A:518:LEU:HD22	0.44	1.71	10	1
1:A:591:ILE:O	1:A:592:GLU:O	0.44	2.36	1	2
1:A:519:PRO:C	1:A:521:GLU:H	0.44	2.16	7	3
1:A:510:LEU:O	1:A:514:ALA:HB3	0.44	2.11	7	2
2:B:4:LEU:CD2	2:B:66:ASP:CB	0.44	2.96	2	3
2:B:39:GLU:OE2	2:B:39:GLU:O	0.44	2.36	7	2
1:A:584:VAL:O	1:A:587:THR:OG1	0.44	2.35	5	3
1:A:602:LEU:C	1:A:602:LEU:HD23	0.44	2.32	1	1
2:B:24:ILE:O	2:B:28:LYS:HB2	0.44	2.13	4	2
1:A:588:ILE:C	1:A:590:ALA:H	0.44	2.16	6	2
2:B:3:SER:O	2:B:65:GLY:CA	0.44	2.66	7	1
1:A:582:ASP:OD1	1:A:583:ASP:OD1	0.44	2.35	9	2
2:B:41:GLN:O	2:B:73:SER:OG	0.44	2.31	4	1
2:B:8:ASN:HD22	2:B:8:ASN:C	0.44	2.16	5	1
2:B:6:PHE:HE2	2:B:44:LEU:HD11	0.44	1.73	10	2
2:B:45:ILE:CA	2:B:69:VAL:O	0.44	2.65	2	7
2:B:25:LEU:C	2:B:25:LEU:CD2	0.44	2.86	2	2
1:A:558:LEU:O	1:A:559:LYS:O	0.44	2.36	8	1
2:B:39:GLU:O	2:B:39:GLU:OE2	0.44	2.36	9	2
1:A:589:SER:O	1:A:593:HIS:NE2	0.43	2.51	1	1
2:B:45:ILE:HD12	2:B:69:VAL:HG12	0.43	1.90	1	2
1:A:497:PHE:C	1:A:497:PHE:CD1	0.43	2.87	2	1
2:B:25:LEU:CD2	2:B:25:LEU:C	0.43	2.87	5	1
2:B:18:LEU:CD2	2:B:27:THR:OG1	0.43	2.66	8	1
2:B:70:PHE:O	2:B:71:MET:HG2	0.43	2.13	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:504:GLU:OE2	1:A:504:GLU:O	0.43	2.37	8	1
1:A:522:THR:O	1:A:525:MET:N	0.43	2.51	10	1
2:B:10:LYS:C	2:B:12:GLU:N	0.43	2.72	10	1
1:A:547:MET:SD	2:B:9:PHE:CZ	0.43	3.11	3	1
1:A:504:GLU:OE2	1:A:508:LEU:CD1	0.43	2.66	8	1
2:B:28:LYS:CE	2:B:39:GLU:OE1	0.43	2.66	5	1
1:A:506:LEU:O	1:A:510:LEU:CB	0.43	2.67	10	1
1:A:585:LEU:HD12	1:A:585:LEU:N	0.43	2.28	5	1
1:A:501:LYS:O	1:A:502:ASN:O	0.43	2.37	8	1
2:B:39:GLU:C	2:B:39:GLU:OE2	0.43	2.57	1	3
1:A:513:ALA:C	1:A:515:SER:H	0.43	2.17	3	1
2:B:45:ILE:CG2	2:B:49:LYS:N	0.43	2.82	3	3
2:B:39:GLU:OE2	2:B:39:GLU:C	0.43	2.57	4	2
2:B:7:LYS:CE	2:B:8:ASN:O	0.43	2.67	5	1
1:A:499:GLY:O	1:A:500:SER:OG	0.43	2.35	6	1
1:A:584:VAL:O	1:A:585:LEU:C	0.43	2.57	8	3
1:A:522:THR:CG2	1:A:523:ALA:N	0.43	2.82	4	1
1:A:579:GLU:C	1:A:581:VAL:N	0.43	2.72	2	1
2:B:50:VAL:O	2:B:50:VAL:CG1	0.43	2.66	2	1
2:B:45:ILE:C	2:B:69:VAL:O	0.43	2.57	7	3
1:A:501:LYS:O	1:A:502:ASN:OD1	0.43	2.36	4	1
1:A:539:ASN:N	1:A:539:ASN:HD22	0.43	2.12	5	1
1:A:517:ASP:O	1:A:518:LEU:O	0.43	2.36	9	1
2:B:74:GLN:O	2:B:75:LYS:O	0.43	2.35	9	1
1:A:553:ARG:O	1:A:555:ALA:N	0.43	2.51	6	2
2:B:56:THR:O	2:B:60:CYS:SG	0.43	2.75	10	1
1:A:509:LEU:O	1:A:510:LEU:C	0.42	2.56	3	4
2:B:28:LYS:HB3	2:B:39:GLU:HB2	0.42	1.91	2	1
2:B:62:LEU:HD21	2:B:68:VAL:HG22	0.42	1.90	7	3
1:A:562:TRP:CD2	1:A:563:VAL:N	0.42	2.87	8	1
2:B:45:ILE:HA	2:B:50:VAL:HA	0.42	1.91	2	3
1:A:562:TRP:CE3	1:A:566:LEU:HD22	0.42	2.48	4	1
2:B:24:ILE:HG23	2:B:44:LEU:CD2	0.42	2.44	5	1
2:B:63:LYS:NZ	2:B:64:ASP:O	0.42	2.31	6	1
1:A:579:GLU:O	1:A:581:VAL:N	0.42	2.52	2	1
2:B:4:LEU:HD22	2:B:66:ASP:HB3	0.42	1.91	6	2
1:A:497:PHE:C	1:A:499:GLY:H	0.42	2.18	4	2
1:A:590:ALA:O	1:A:591:ILE:C	0.42	2.58	6	1
1:A:592:GLU:O	1:A:593:HIS:CD2	0.42	2.73	8	1
1:A:550:PHE:CE1	1:A:566:LEU:HD21	0.42	2.50	1	1
2:B:56:THR:O	2:B:60:CYS:N	0.42	2.49	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:502:ASN:C	1:A:504:GLU:N	0.42	2.72	2	2
1:A:509:LEU:HD23	1:A:509:LEU:C	0.42	2.35	8	1
1:A:576:GLY:O	1:A:577:GLN:O	0.42	2.38	2	1
1:A:549:ASN:HD22	1:A:549:ASN:N	0.42	2.12	8	1
2:B:6:PHE:HB3	2:B:70:PHE:CD1	0.42	2.50	8	1
1:A:579:GLU:CB	2:B:11:LYS:NZ	0.42	2.83	5	2
1:A:497:PHE:CZ	1:A:533:VAL:HG21	0.42	2.50	2	1
2:B:44:LEU:HD12	2:B:70:PHE:HB2	0.42	1.92	9	1
1:A:544:THR:O	1:A:548:ASP:OD2	0.41	2.37	2	1
2:B:51:LEU:O	2:B:52:GLN:OE1	0.41	2.38	4	1
1:A:595:MET:CG	1:A:596:THR:N	0.41	2.82	7	1
1:A:602:LEU:C	1:A:602:LEU:CD1	0.41	2.88	8	1
1:A:499:GLY:O	1:A:500:SER:CB	0.41	2.68	6	1
1:A:591:ILE:HG22	1:A:593:HIS:CE1	0.41	2.50	8	1
2:B:27:THR:HG21	2:B:44:LEU:CD2	0.41	2.45	8	2
2:B:49:LYS:O	2:B:51:LEU:N	0.41	2.53	5	2
1:A:590:ALA:HB1	2:B:48:GLY:O	0.41	2.16	4	1
2:B:60:CYS:SG	2:B:62:LEU:CD1	0.41	3.08	9	1
1:A:603:VAL:O	1:A:606:CYS:O	0.41	2.38	10	1
1:A:535:VAL:CG1	1:A:536:GLY:N	0.41	2.82	4	2
2:B:15:PRO:O	2:B:16:LEU:HG	0.41	2.14	3	1
1:A:506:LEU:C	1:A:508:LEU:N	0.41	2.74	9	1
2:B:8:ASN:ND2	2:B:10:LYS:N	0.41	2.67	5	1
1:A:549:ASN:N	1:A:549:ASN:HD22	0.41	2.12	10	1
1:A:549:ASN:N	1:A:549:ASN:ND2	0.41	2.68	10	1
1:A:568:LEU:O	1:A:572:ILE:N	0.41	2.54	6	2
1:A:506:LEU:C	1:A:508:LEU:H	0.41	2.19	9	1
1:A:584:VAL:C	1:A:586:GLU:N	0.41	2.73	9	2
1:A:512:ILE:C	1:A:514:ALA:N	0.41	2.74	2	1
1:A:539:ASN:CG	1:A:540:GLY:N	0.41	2.74	2	1
2:B:46:TYR:CB	2:B:51:LEU:HD21	0.41	2.46	4	1
1:A:534:PHE:CD2	1:A:537:THR:OG1	0.41	2.71	1	1
1:A:579:GLU:O	1:A:580:GLN:C	0.41	2.59	6	1
1:A:558:LEU:C	1:A:558:LEU:HD12	0.41	2.36	10	1
1:A:579:GLU:CB	2:B:11:LYS:HZ3	0.41	2.28	1	1
1:A:530:LEU:CD2	1:A:530:LEU:C	0.41	2.89	3	1
2:B:10:LYS:O	2:B:11:LYS:HB2	0.41	2.15	3	1
1:A:585:LEU:N	1:A:585:LEU:HD12	0.41	2.30	4	1
1:A:577:GLN:O	1:A:581:VAL:HG23	0.41	2.16	6	1
2:B:43:LYS:N	2:B:71:MET:O	0.41	2.52	6	1
1:A:506:LEU:O	1:A:508:LEU:N	0.41	2.54	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:516:THR:O	1:A:517:ASP:O	0.41	2.39	7	1
2:B:41:GLN:NE2	2:B:73:SER:C	0.41	2.75	7	1
1:A:532:HIS:O	1:A:535:VAL:CG1	0.41	2.69	8	1
1:A:602:LEU:CD1	1:A:602:LEU:C	0.41	2.88	10	1
1:A:531:ALA:O	1:A:535:VAL:CA	0.41	2.69	6	1
1:A:571:GLY:O	1:A:572:ILE:C	0.40	2.57	1	1
1:A:566:LEU:H	1:A:566:LEU:CD1	0.40	2.29	3	1
2:B:53:ASP:OD1	2:B:53:ASP:N	0.40	2.54	9	2
1:A:602:LEU:C	1:A:602:LEU:HD13	0.40	2.36	8	1
1:A:571:GLY:C	1:A:573:LEU:H	0.40	2.20	10	1
1:A:500:SER:N	1:A:502:ASN:HD21	0.40	2.15	3	1
1:A:517:ASP:CG	1:A:518:LEU:N	0.40	2.74	2	1
1:A:592:GLU:CD	1:A:592:GLU:H	0.40	2.19	2	1
1:A:497:PHE:CD1	1:A:497:PHE:N	0.40	2.84	5	1
1:A:573:LEU:O	1:A:575:MET:N	0.40	2.54	7	1
1:A:594:PRO:C	1:A:596:THR:H	0.40	2.20	9	1
1:A:602:LEU:CD2	1:A:602:LEU:C	0.40	2.90	9	1
2:B:51:LEU:CD1	2:B:60:CYS:SG	0.40	3.09	1	1
2:B:8:ASN:H	2:B:8:ASN:ND2	0.40	2.14	5	1
1:A:518:LEU:O	1:A:519:PRO:O	0.40	2.40	6	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	111/131 (85%)	64±5 (58±4%)	34±3 (30±3%)	13±3 (12±2%)	1	7
2	B	74/78 (95%)	59±1 (80±2%)	10±1 (14±2%)	5±1 (7±1%)	3	18
All	All	1850/2090 (89%)	1230 (66%)	437 (24%)	183 (10%)	2	10

All 57 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	50	VAL	10

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Mol	Chain	Res	Type	Models (Total)
2	B	31	LEU	9
2	B	36	SER	9
1	A	591	ILE	8
2	B	51	LEU	8
1	A	562	TRP	8
1	A	594	PRO	7
1	A	592	GLU	6
1	A	576	GLY	5
1	A	517	ASP	5
2	B	75	LYS	5
1	A	607	ALA	5
2	B	22	ASN	5
1	A	584	VAL	5
1	A	579	GLU	4
1	A	537	THR	4
2	B	56	THR	4
1	A	516	THR	4
1	A	578	GLY	4
1	A	577	GLN	4
1	A	552	GLU	3
1	A	555	ALA	3
1	A	585	LEU	3
1	A	575	MET	3
1	A	560	THR	3
1	A	561	ASP	3
1	A	519	PRO	3
1	A	498	ALA	3
1	A	589	SER	2
1	A	570	LEU	2
1	A	572	ILE	2
1	A	559	LYS	2
1	A	574	TYR	2
1	A	554	THR	2
1	A	588	ILE	2
1	A	557	GLU	2
1	A	569	ALA	2
1	A	520	ILE	2
1	A	573	LEU	2
1	A	580	GLN	1
1	A	499	GLY	1
1	A	515	SER	1
1	A	590	ALA	1

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Mol	Chain	Res	Type	Models (Total)
1	A	525	MET	1
1	A	502	ASN	1
1	A	553	ARG	1
1	A	501	LYS	1
1	A	602	LEU	1
1	A	593	HIS	1
1	A	500	SER	1
1	A	518	LEU	1
1	A	597	SER	1
1	A	497	PHE	1
1	A	521	GLU	1
1	A	533	VAL	1
1	A	514	ALA	1
1	A	536	GLY	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	89/102 (87%)	84±1 (94±2%)	5±1 (6±2%)	28 73
2	B	71/74 (96%)	56±2 (78±3%)	16±2 (22±3%)	4 32
All	All	1600/1760 (91%)	1391 (87%)	209 (13%)	9 50

All 56 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	24	ILE	10
2	B	42	ILE	10
2	B	27	THR	10
2	B	63	LYS	10
2	B	41	GLN	10
2	B	29	THR	10
2	B	73	SER	10
2	B	7	LYS	10
2	B	13	LYS	9
2	B	18	LEU	9

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Mol	Chain	Res	Type	Models (Total)
2	B	39	GLU	9
1	A	587	THR	7
2	B	52	GLN	6
2	B	56	THR	5
2	B	23	THR	5
1	A	556	ILE	5
1	A	546	ILE	4
2	B	8	ASN	3
1	A	554	THR	3
2	B	75	LYS	3
2	B	36	SER	3
2	B	11	LYS	3
1	A	582	ASP	3
1	A	553	ARG	3
1	A	503	ASP	3
2	B	44	LEU	3
1	A	595	MET	2
2	B	45	ILE	2
2	B	49	LYS	2
2	B	10	LYS	2
1	A	575	MET	2
2	B	2	VAL	2
1	A	602	LEU	2
1	A	593	HIS	2
1	A	509	LEU	2
2	B	64	ASP	2
1	A	497	PHE	2
1	A	577	GLN	2
2	B	5	THR	2
1	A	522	THR	1
1	A	592	GLU	1
1	A	530	LEU	1
1	A	558	LEU	1
1	A	570	LEU	1
1	A	504	GLU	1
1	A	528	LEU	1
1	A	502	ASN	1
2	B	71	MET	1
2	B	74	GLN	1
1	A	547	MET	1
1	A	583	ASP	1
2	B	47	SER	1

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Mol	Chain	Res	Type	Models (Total)
2	B	53	ASP	1
1	A	539	ASN	1
2	B	9	PHE	1
1	A	516	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

The completeness of assignment taking into account all chemical shift lists is 40% for the well-defined parts and 37% for the entire structure.

7.1 Chemical shift list 1

File name: 2nbw_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1177
Number of shifts mapped to atoms	1003
Number of unparsed shifts	0
Number of shifts with mapping errors	174
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- Residue not found in structure. All 174 occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
B	82	SER	C	174.653	0.0	1
B	88	LEU	HD13	0.909	0.0	2
B	85	VAL	N	121.117	0.0	1
B	84	SER	H	8.283	0.0	1
B	88	LEU	N	121.846	0.0	1
B	88	LEU	CB	41.583	0.0	1
B	87	LYS	C	177.35	0.0	1
B	92	LEU	HD23	0.835	0.0	2
B	94	HIS	H	8.18	0.0	1
B	92	LEU	HD22	0.835	0.0	2
B	83	SER	HB3	3.894	0.0	2
B	90	ALA	H	8.023	0.0	1
B	92	LEU	HD12	0.889	0.0	2
B	91	ALA	H	7.95	0.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
B	86	ASP	CB	40.752	0.0	1
B	91	ALA	C	178.1	0.0	1
B	85	VAL	HG23	0.938	0.0	2
B	81	ASN	ND2	113.877	0.0	1
B	81	ASN	HD22	7.756	0.0	2
B	81	ASN	HB3	2.789	0.0	2
B	80	PRO	C	177.067	0.0	1
B	93	GLU	CG	35.958	0.0	1
B	88	LEU	HD11	0.909	0.0	2
B	93	GLU	HB2	1.897	0.0	2
B	81	ASN	C	175.519	0.0	1
B	81	ASN	H	8.52	0.0	1
B	89	ALA	H	8.001	0.0	1
B	92	LEU	CG	26.676	0.0	1
B	88	LEU	H	8.101	0.0	1
B	86	ASP	N	123.029	0.0	1
B	80	PRO	HA	4.423	0.0	1
B	80	PRO	HB2	2.3	0.0	2
B	88	LEU	CG	26.959	0.0	1
B	81	ASN	HB2	2.863	0.0	2
B	80	PRO	CG	26.959	0.0	1
B	90	ALA	CA	52.833	0.0	1
B	87	LYS	HB3	1.773	0.0	2
B	80	PRO	CA	63.802	0.0	1
B	87	LYS	CA	57.052	0.0	1
B	80	PRO	HG2	2.015	0.0	2
B	93	GLU	H	8.061	0.0	1
B	87	LYS	HD2	1.664	0.0	2
B	83	SER	HA	4.491	0.0	1
B	89	ALA	HB3	1.395	0.0	2
B	92	LEU	HG	1.641	0.0	1
B	87	LYS	HE3	2.986	0.0	2
B	91	ALA	CB	18.802	0.0	1
B	87	LYS	HE2	2.986	0.0	2
B	89	ALA	CB	18.521	0.0	1
B	89	ALA	N	123.573	0.0	1
B	81	ASN	CB	38.771	0.0	1
B	93	GLU	HB3	1.897	0.0	2
B	90	ALA	CB	19.084	0.0	1
B	83	SER	CB	63.802	0.0	1
B	82	SER	HB3	3.875	0.0	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
B	94	HIS	HA	4.565	0.0	1
B	87	LYS	HG3	1.417	0.0	2
B	92	LEU	CD2	23.298	0.0	2
B	82	SER	HB2	3.875	0.0	2
B	93	GLU	HA	4.16	0.0	1
B	94	HIS	HB3	2.98	0.0	2
B	93	GLU	N	120.382	0.0	1
B	88	LEU	HG	1.62	0.0	1
B	94	HIS	C	174.955	0.0	1
B	93	GLU	HG2	2.205	0.0	2
B	85	VAL	HG22	0.938	0.0	2
B	83	SER	HB2	3.894	0.0	2
B	80	PRO	HB3	1.966	0.0	2
B	92	LEU	C	177.584	0.0	1
B	79	ASP	H	8.28	0.0	1
B	80	PRO	CD	50.583	0.0	1
B	85	VAL	HG11	0.931	0.0	2
B	87	LYS	CD	28.927	0.0	1
B	79	ASP	CB	41.205	0.0	1
B	87	LYS	CB	32.583	0.0	1
B	79	ASP	HB3	2.574	0.0	2
B	94	HIS	CB	30.333	0.0	1
B	91	ALA	HB2	1.394	0.0	2
B	89	ALA	C	178.382	0.0	1
B	87	LYS	HD3	1.664	0.0	2
B	84	SER	CB	63.523	0.0	1
B	85	VAL	CG2	20.483	0.0	2
B	93	GLU	CB	30.052	0.0	1
B	91	ALA	HA	4.232	0.0	1
B	79	ASP	N	124.382	0.0	1
B	88	LEU	CD2	23.302	0.0	2
B	88	LEU	C	177.798	0.0	1
B	82	SER	N	115.818	0.0	1
B	94	HIS	HB2	3.057	0.0	2
B	80	PRO	HG3	2.015	0.0	2
B	94	HIS	CA	55.927	0.0	1
B	89	ALA	HB2	1.395	0.0	2
B	84	SER	N	117.712	0.0	1
B	92	LEU	HA	4.24	0.0	1
B	92	LEU	HD11	0.889	0.0	2
B	87	LYS	H	8.172	0.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
B	88	LEU	CA	55.646	0.0	1
B	88	LEU	HB2	1.713	0.0	2
B	92	LEU	N	120.154	0.0	1
B	86	ASP	HB3	2.612	0.0	2
B	81	ASN	CA	53.396	0.0	1
B	91	ALA	HB3	1.394	0.0	2
B	85	VAL	HG12	0.931	0.0	2
B	90	ALA	HB1	1.395	0.0	2
B	93	GLU	HG3	2.121	0.0	2
B	91	ALA	HB1	1.394	0.0	2
B	86	ASP	H	8.269	0.0	1
B	88	LEU	HD12	0.909	0.0	2
B	81	ASN	HD21	6.95	0.0	2
B	81	ASN	N	117.478	0.0	1
B	82	SER	H	8.023	0.0	1
B	82	SER	HA	4.402	0.0	1
B	81	ASN	HA	4.736	0.0	1
B	88	LEU	HD22	0.851	0.0	2
B	83	SER	N	117.494	0.0	1
B	79	ASP	C	175.013	0.0	1
B	84	SER	CA	58.461	0.0	1
B	92	LEU	CA	55.109	0.0	1
B	89	ALA	HA	4.189	0.0	1
B	85	VAL	CB	32.518	0.0	1
B	79	ASP	CA	52.087	0.0	1
B	86	ASP	CA	54.546	0.0	1
B	93	GLU	CA	56.771	0.0	1
B	88	LEU	HA	4.261	0.0	1
B	87	LYS	HB2	1.858	0.0	2
B	85	VAL	HA	4.062	0.0	1
B	92	LEU	CB	42.159	0.0	1
B	87	LYS	HA	4.196	0.0	1
B	92	LEU	HB2	1.644	0.0	2
B	80	PRO	CB	32.021	0.0	1
B	85	VAL	HG13	0.931	0.0	2
B	90	ALA	N	121.852	0.0	1
B	85	VAL	C	176.142	0.0	1
B	88	LEU	CD1	24.709	0.0	2
B	84	SER	C	174.886	0.0	1
B	94	HIS	N	119.338	0.0	1
B	79	ASP	HB2	2.774	0.0	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
B	83	SER	H	8.331	0.0	1
B	86	ASP	HB2	2.713	0.0	2
B	91	ALA	CA	52.552	0.0	1
B	89	ALA	CA	53.389	0.0	1
B	85	VAL	H	8.034	0.0	1
B	88	LEU	HD21	0.851	0.0	2
B	88	LEU	HD23	0.851	0.0	2
B	82	SER	CB	63.802	0.0	1
B	86	ASP	C	176.766	0.0	1
B	80	PRO	HD2	3.889	0.0	2
B	93	GLU	C	176.308	0.0	1
B	92	LEU	HD13	0.889	0.0	2
B	90	ALA	HA	4.232	0.0	1
B	85	VAL	HG21	0.938	0.0	2
B	92	LEU	HD21	0.835	0.0	2
B	92	LEU	HB3	1.519	0.0	2
B	87	LYS	HG2	1.476	0.0	2
B	87	LYS	CE	41.865	0.0	1
B	82	SER	CA	58.739	0.0	1
B	90	ALA	C	178.119	0.0	1
B	85	VAL	HB	2.098	0.0	1
B	87	LYS	CG	24.709	0.0	1
B	83	SER	C	174.662	0.0	1
B	88	LEU	HB3	1.592	0.0	2
B	90	ALA	HB2	1.395	0.0	2
B	92	LEU	H	7.928	0.0	1
B	85	VAL	CG1	20.885	0.0	2
B	91	ALA	N	121.781	0.0	1
B	79	ASP	HA	4.878	0.0	1
B	86	ASP	HA	4.565	0.0	1
B	83	SER	CA	58.458	0.0	1
B	92	LEU	CD1	24.987	0.0	2
B	90	ALA	HB3	1.395	0.0	2
B	80	PRO	HD3	3.835	0.0	2
B	87	LYS	N	121.906	0.0	1
B	89	ALA	HB1	1.395	0.0	2
B	85	VAL	CA	62.889	0.0	1

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	94	-0.01 ± 0.08	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	91	0.12 ± 0.14	None needed (< 0.5 ppm)
$^{13}\text{C}'$	94	-0.05 ± 0.27	None needed (< 0.5 ppm)
^{15}N	90	0.42 ± 0.33	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 40%, i.e. 862 atoms were assigned a chemical shift out of a possible 2166. 0 out of 38 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	369/920 (40%)	147/367 (40%)	150/372 (40%)	72/181 (40%)
Sidechain	478/1141 (42%)	297/658 (45%)	174/452 (38%)	7/31 (23%)
Aromatic	15/105 (14%)	15/57 (26%)	0/45 (0%)	0/3 (0%)
Overall	862/2166 (40%)	459/1082 (42%)	324/869 (37%)	79/215 (37%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 37%, i.e. 894 atoms were assigned a chemical shift out of a possible 2398. 0 out of 40 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	384/1035 (37%)	153/413 (37%)	156/418 (37%)	75/204 (37%)
Sidechain	495/1250 (40%)	308/720 (43%)	180/497 (36%)	7/33 (21%)
Aromatic	15/113 (13%)	15/61 (25%)	0/49 (0%)	0/3 (0%)
Overall	894/2398 (37%)	476/1194 (40%)	336/964 (35%)	82/240 (34%)

7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain B:

