



Full wwPDB NMR Structure Validation Report ⓘ

Sep 15, 2021 – 01:15 pm BST

PDB ID : 7BBB
Title : Solution structure of C-terminal RecA and RRM domains of the DEAD box helicase DbpA
Authors : Wurm, J.P.; Sprangers, R.
Deposited on : 2020-12-17

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

MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.23.1
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.1

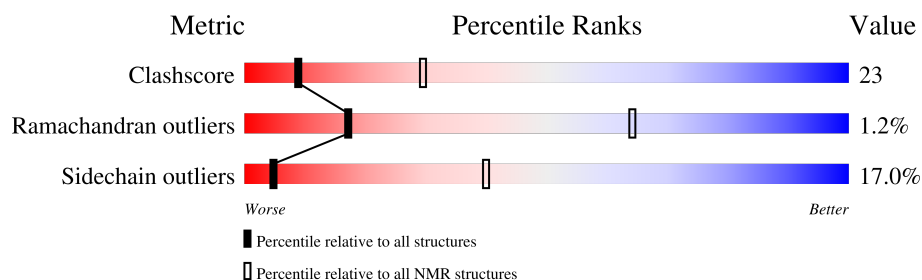
1 Overall quality at a glance

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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	251	

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:216-A:333, A:338-A:368, A:375-A:457 (232)	0.30	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 1 clusters. No single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3823 atoms, of which 1932 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called ATP-dependent RNA helicase DbpA.

Mol	Chain	Residues	Atoms						Trace
1	A	251	Total	C	H	N	O	S	0
			3823	1180	1932	348	353	10	

There are 2 discrepancies between the modelled and reference sequences:

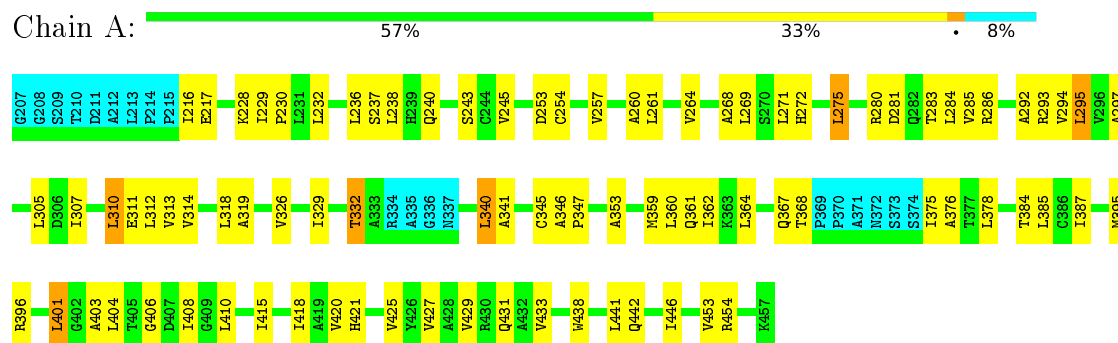
Chain	Residue	Modelled	Actual	Comment	Reference
A	207	GLY	-	cloning artifact	UNP P21693
A	208	GLY	-	cloning artifact	UNP P21693

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: ATP-dependent RNA helicase DbpA

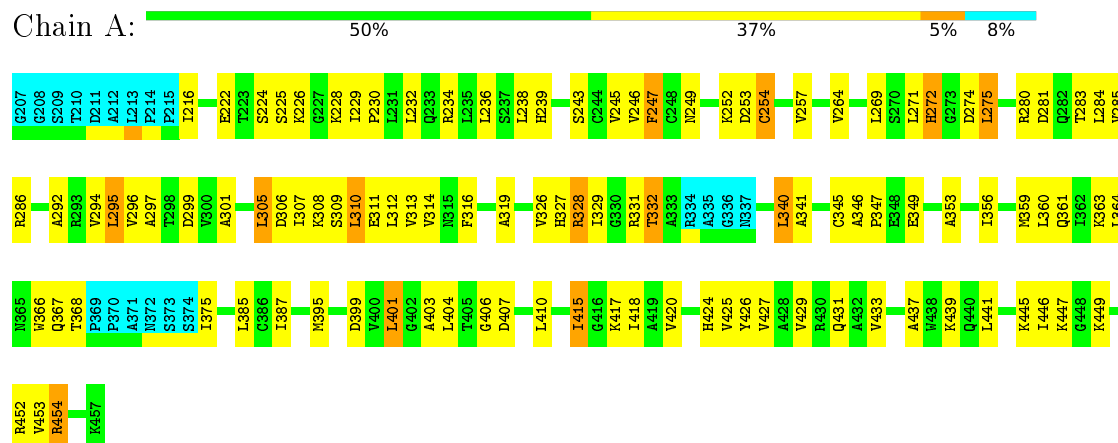


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

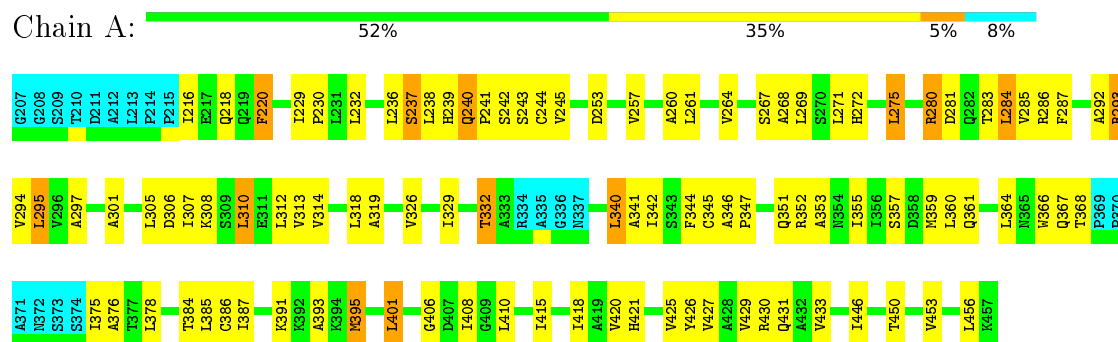
4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: ATP-dependent RNA helicase DbpA



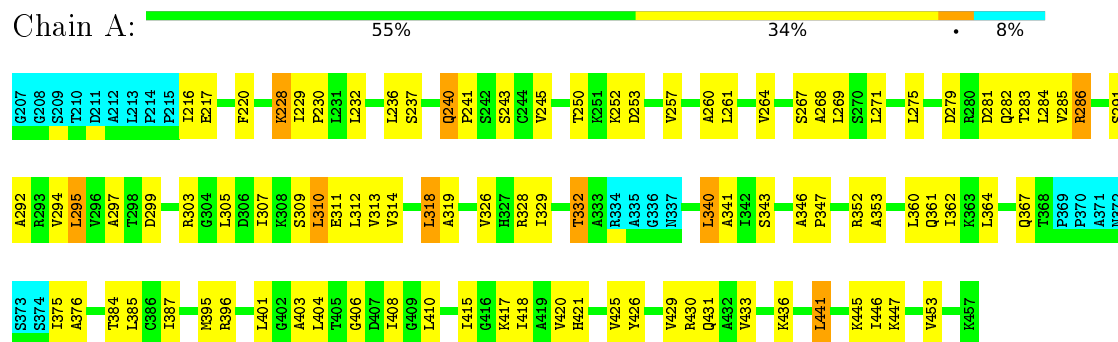
4.2.2 Score per residue for model 2

- Molecule 1: ATP-dependent RNA helicase DbpA



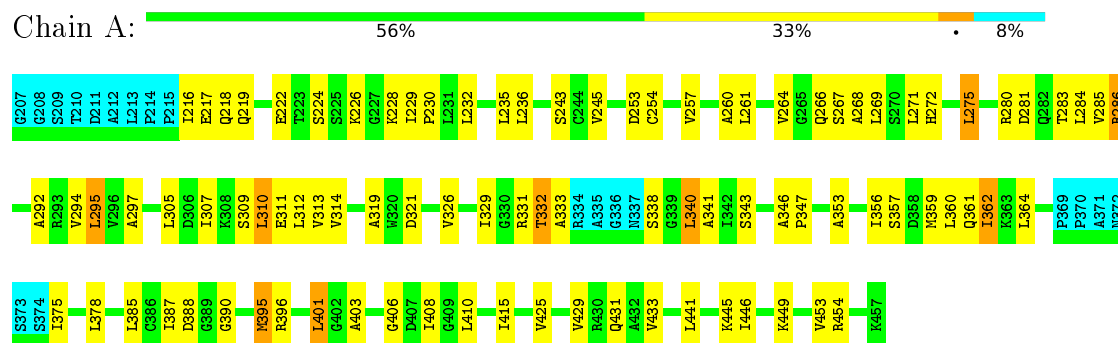
4.2.3 Score per residue for model 3

- Molecule 1: ATP-dependent RNA helicase DbpA



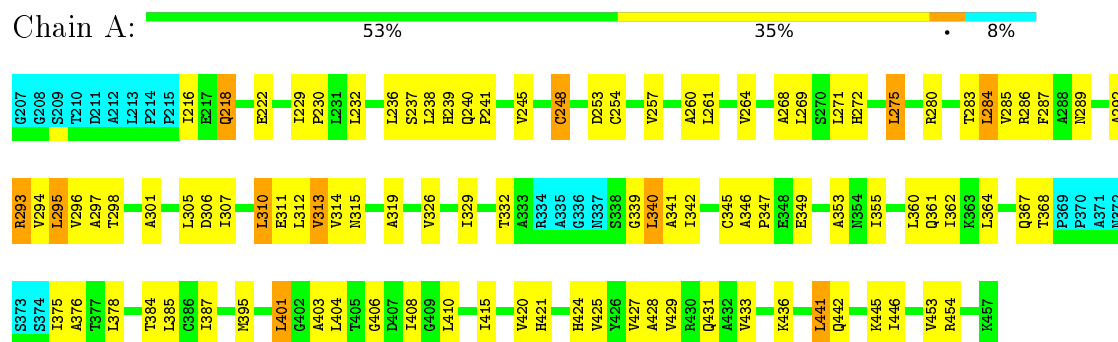
4.2.4 Score per residue for model 4

- Molecule 1: ATP-dependent RNA helicase DbpA



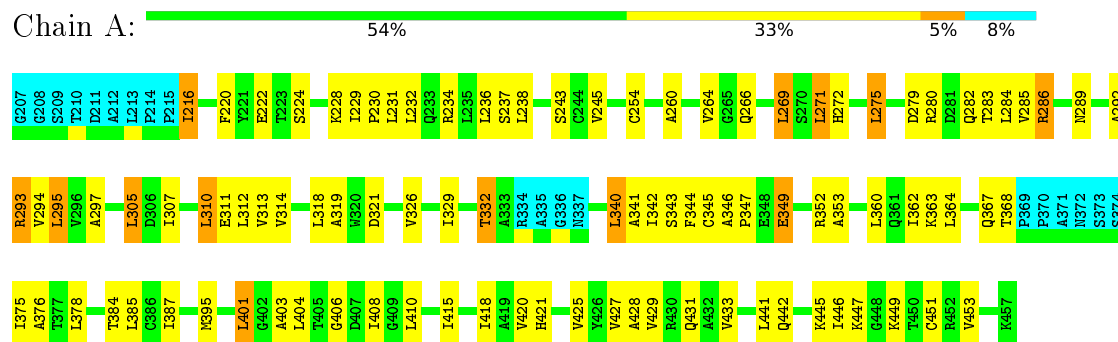
4.2.8 Score per residue for model 8

- Molecule 1: ATP-dependent RNA helicase DbpA



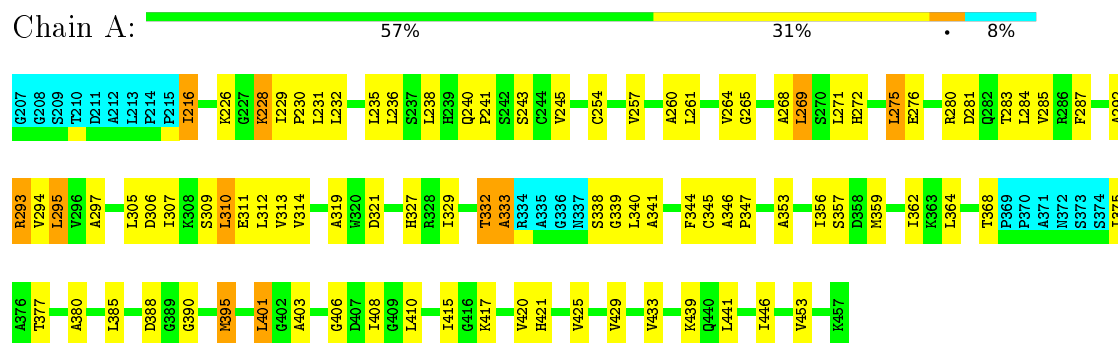
4.2.9 Score per residue for model 9

- Molecule 1: ATP-dependent RNA helicase DbpA



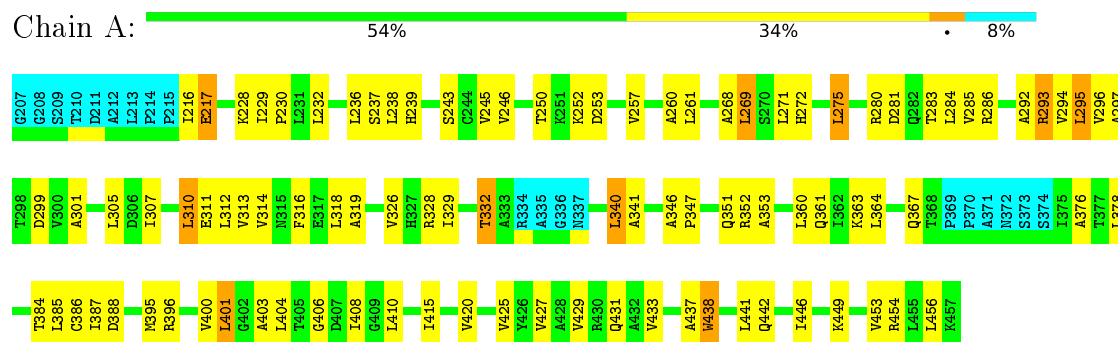
4.2.10 Score per residue for model 10

- Molecule 1: ATP-dependent RNA helicase DbpA



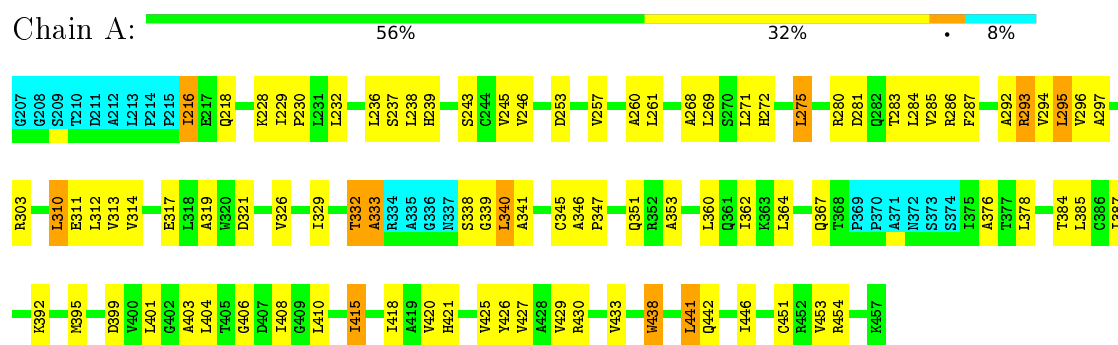
4.2.11 Score per residue for model 11

- Molecule 1: ATP-dependent RNA helicase DbpA



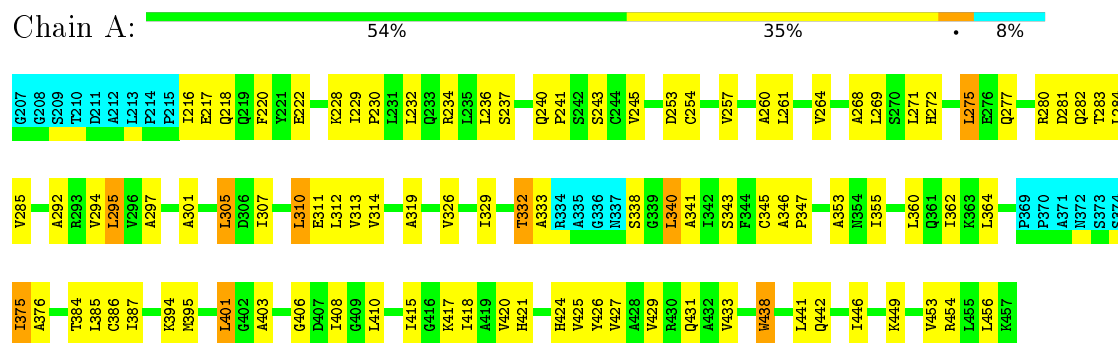
4.2.12 Score per residue for model 12

- Molecule 1: ATP-dependent RNA helicase DbpA



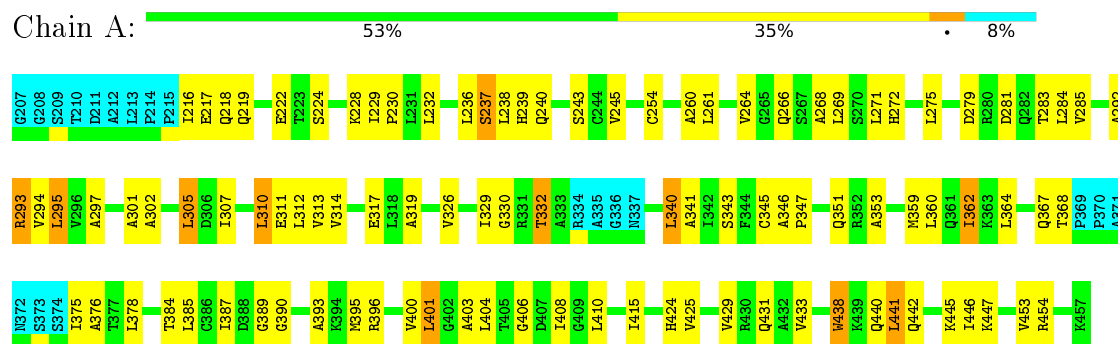
4.2.13 Score per residue for model 13

- Molecule 1: ATP-dependent RNA helicase DbpA



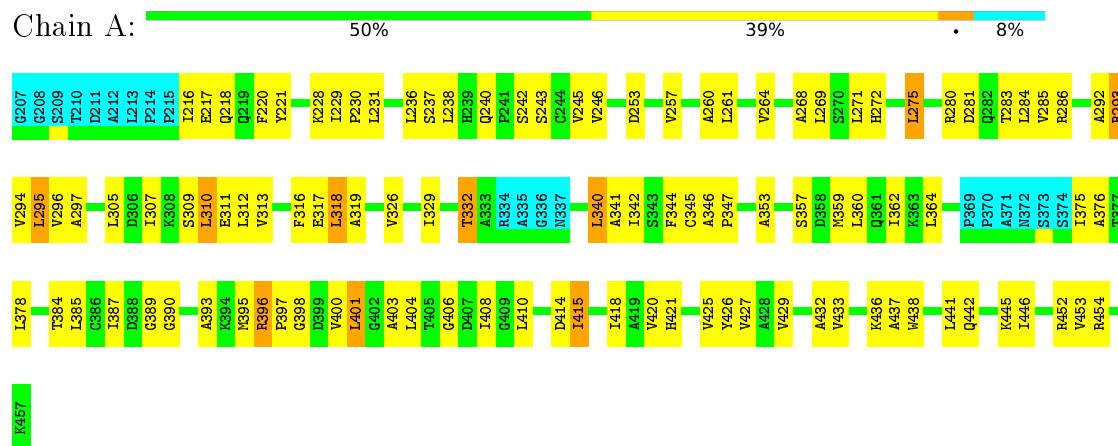
4.2.14 Score per residue for model 14

- Molecule 1: ATP-dependent RNA helicase DbpA



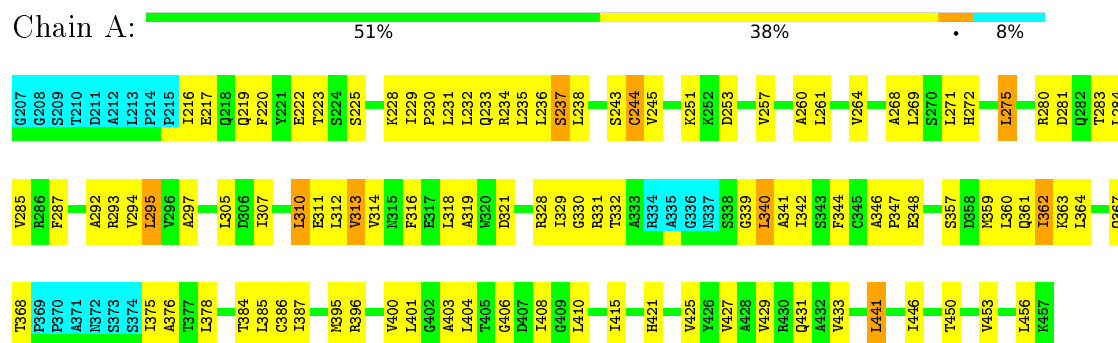
4.2.15 Score per residue for model 15

- Molecule 1: ATP-dependent RNA helicase DbpA



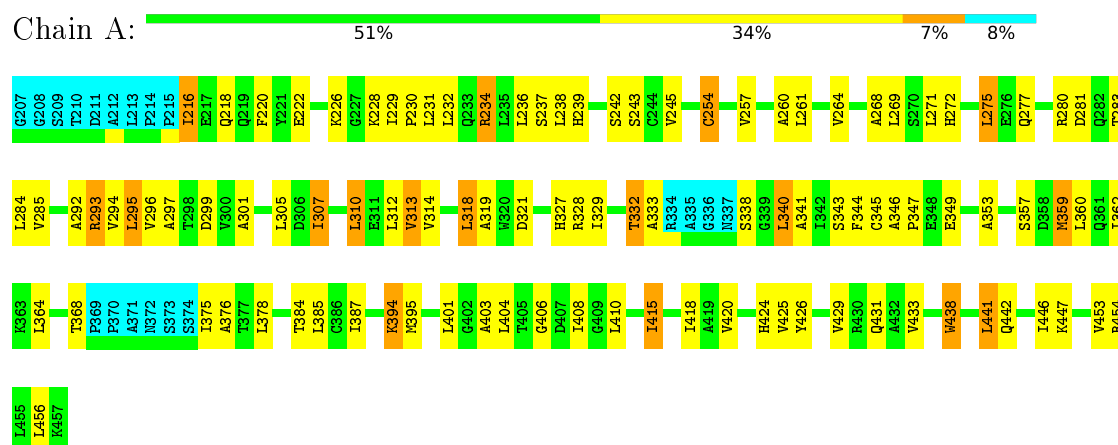
4.2.16 Score per residue for model 16

- Molecule 1: ATP-dependent RNA helicase DbpA



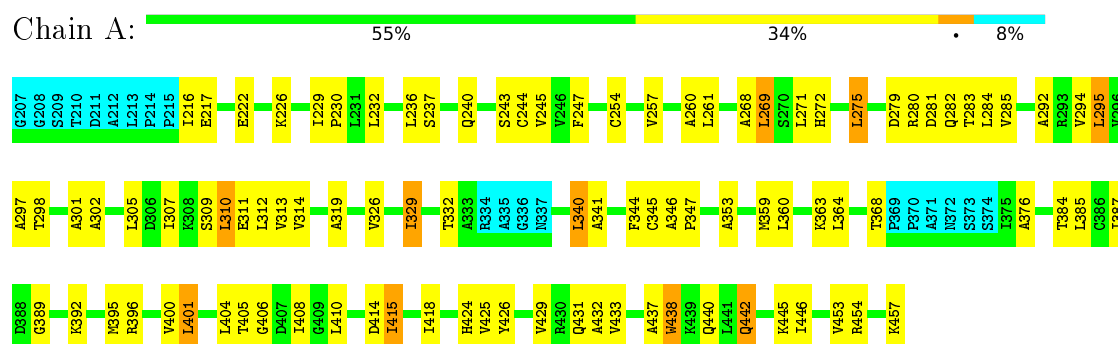
4.2.17 Score per residue for model 17

- Molecule 1: ATP-dependent RNA helicase DbpA



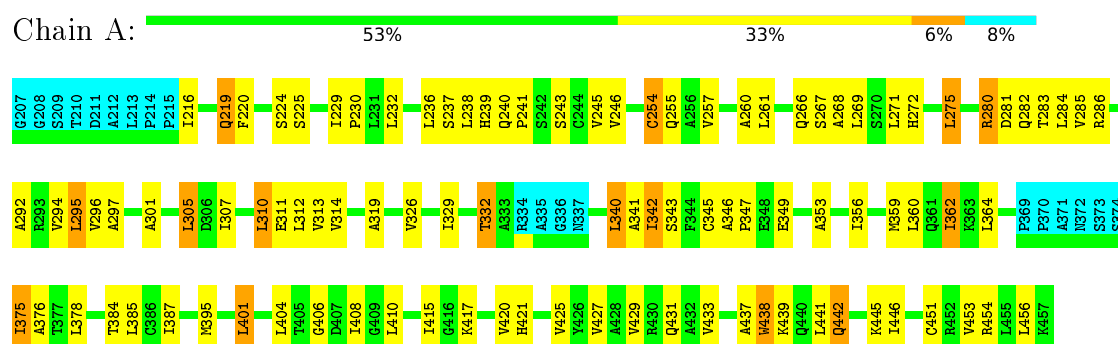
4.2.18 Score per residue for model 18

- Molecule 1: ATP-dependent RNA helicase DbpA



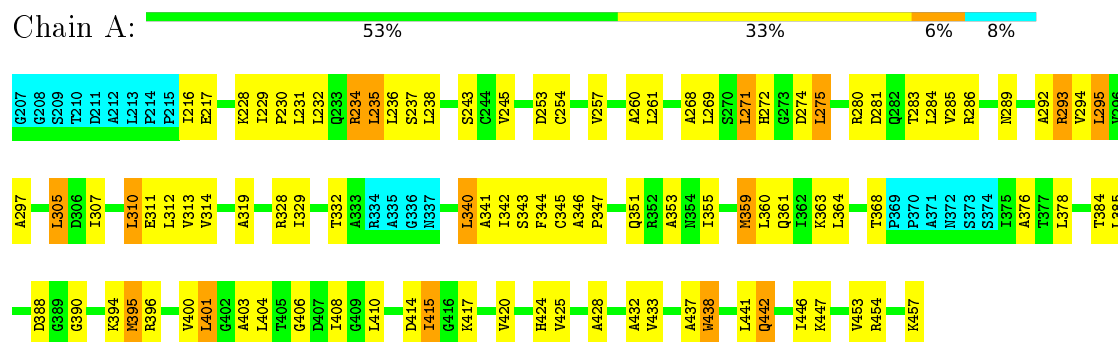
4.2.19 Score per residue for model 19

- Molecule 1: ATP-dependent RNA helicase DbpA



4.2.20 Score per residue for model 20

- Molecule 1: ATP-dependent RNA helicase DbpA



5 Refinement protocol and experimental data overview ⓘ

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
CYANA	structure calculation	3.98.5

No chemical shift data was provided.

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	1768	1818	1818	83±7
All	All	35360	36360	36360	1668

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 23.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:329:ILE:HG21	1:A:341:ALA:HB2	1.05	1.27	2	17
1:A:441:LEU:HD23	1:A:453:VAL:HG21	1.05	1.29	8	9
1:A:310:LEU:HD13	1:A:313:VAL:HG22	1.04	1.30	1	17
1:A:441:LEU:HD13	1:A:453:VAL:HG21	1.02	1.28	15	9
1:A:264:VAL:HG11	1:A:375:ILE:HD11	1.01	1.32	9	7
1:A:269:LEU:HD21	1:A:295:LEU:HD12	0.90	1.41	9	1
1:A:326:VAL:HG11	1:A:360:LEU:HD21	0.89	1.45	14	11
1:A:264:VAL:HG11	1:A:375:ILE:HD13	0.84	1.49	15	6
1:A:216:ILE:HD12	1:A:329:ILE:HD12	0.83	1.48	7	8
1:A:271:LEU:HB2	1:A:283:THR:HG21	0.82	1.52	9	1
1:A:216:ILE:HD11	1:A:329:ILE:HD12	0.80	1.52	15	9
1:A:236:LEU:HD13	1:A:294:VAL:HG21	0.79	1.54	6	20
1:A:269:LEU:HD12	1:A:283:THR:HG23	0.79	1.53	1	18
1:A:408:ILE:HD11	1:A:441:LEU:HD13	0.78	1.54	8	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:305:LEU:HD11	1:A:307:ILE:HD13	0.76	1.56	19	2
1:A:231:LEU:HD23	1:A:344:PHE:CE2	0.74	2.17	16	2
1:A:403:ALA:HB2	1:A:446:ILE:HG23	0.73	1.60	17	16
1:A:404:LEU:HD22	1:A:415:ILE:HD11	0.73	1.61	18	7
1:A:216:ILE:HG23	1:A:329:ILE:HD12	0.72	1.57	1	8
1:A:305:LEU:HD11	1:A:307:ILE:HD12	0.72	1.59	16	14
1:A:395:MET:SD	1:A:425:VAL:HG11	0.72	2.24	15	3
1:A:269:LEU:HD12	1:A:283:THR:CG2	0.71	2.15	8	18
1:A:329:ILE:HD13	1:A:341:ALA:HB2	0.71	1.62	8	3
1:A:269:LEU:HD13	1:A:286:ARG:CG	0.70	2.17	8	2
1:A:272:HIS:O	1:A:275:LEU:HD22	0.70	1.87	12	18
1:A:216:ILE:CD1	1:A:329:ILE:HD12	0.69	2.17	15	9
1:A:438:TRP:CE3	1:A:453:VAL:HB	0.69	2.22	15	10
1:A:326:VAL:CG2	1:A:360:LEU:HD11	0.69	2.18	1	15
1:A:313:VAL:HG21	1:A:329:ILE:HG22	0.69	1.63	12	12
1:A:229:ILE:HD12	1:A:260:ALA:CB	0.69	2.18	2	19
1:A:275:LEU:HD21	1:A:280:ARG:CB	0.69	2.18	15	9
1:A:395:MET:HG2	1:A:425:VAL:HG21	0.69	1.65	4	4
1:A:353:ALA:HB1	1:A:364:LEU:HD13	0.68	1.62	20	11
1:A:229:ILE:HD12	1:A:260:ALA:HB2	0.68	1.63	5	18
1:A:441:LEU:CD2	1:A:453:VAL:HG21	0.68	2.15	12	9
1:A:261:LEU:CD2	1:A:268:ALA:HB2	0.68	2.18	2	16
1:A:293:ARG:NH1	1:A:380:ALA:HB2	0.68	2.01	10	1
1:A:231:LEU:HD23	1:A:344:PHE:CD2	0.67	2.25	9	3
1:A:329:ILE:HG21	1:A:341:ALA:CB	0.67	2.18	17	18
1:A:232:LEU:HD13	1:A:314:VAL:HG11	0.66	1.64	16	19
1:A:286:ARG:NE	1:A:292:ALA:HB3	0.66	2.05	9	1
1:A:326:VAL:HG21	1:A:360:LEU:HD11	0.66	1.67	18	12
1:A:289:ASN:ND2	1:A:428:ALA:HB1	0.66	2.05	8	1
1:A:231:LEU:HD23	1:A:344:PHE:CZ	0.65	2.25	15	1
1:A:353:ALA:O	1:A:364:LEU:HD11	0.65	1.91	1	15
1:A:245:VAL:HB	1:A:310:LEU:HD11	0.65	1.68	17	16
1:A:264:VAL:HG11	1:A:375:ILE:CD1	0.65	2.21	17	12
1:A:441:LEU:HD23	1:A:453:VAL:CG2	0.65	2.16	20	7
1:A:313:VAL:CG2	1:A:329:ILE:HG22	0.64	2.22	17	12
1:A:261:LEU:HD22	1:A:268:ALA:HB2	0.64	1.68	5	11
1:A:253:ASP:O	1:A:257:VAL:HG23	0.64	1.92	12	13
1:A:275:LEU:HD11	1:A:280:ARG:HA	0.64	1.70	13	11
1:A:220:PHE:CE1	1:A:364:LEU:HD22	0.64	2.27	16	6
1:A:387:ILE:HD11	1:A:427:VAL:HG12	0.64	1.69	9	8
1:A:235:LEU:CD1	1:A:342:ILE:HG21	0.64	2.23	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:351:GLN:NE2	1:A:355:ILE:HG23	0.63	2.08	20	1
1:A:420:VAL:HG22	1:A:425:VAL:HG23	0.63	1.70	8	10
1:A:305:LEU:HD11	1:A:307:ILE:CD1	0.63	2.23	10	14
1:A:396:ARG:O	1:A:400:VAL:HG23	0.63	1.92	14	3
1:A:310:LEU:HD12	1:A:332:THR:OG1	0.63	1.94	16	17
1:A:237:SER:HB3	1:A:376:ALA:HB3	0.63	1.71	16	3
1:A:216:ILE:CG1	1:A:329:ILE:HD12	0.63	2.24	4	8
1:A:216:ILE:O	1:A:216:ILE:HG23	0.63	1.93	12	7
1:A:237:SER:CB	1:A:376:ALA:HB3	0.62	2.24	20	16
1:A:286:ARG:CZ	1:A:292:ALA:HB3	0.62	2.24	9	1
1:A:271:LEU:HG	1:A:301:ALA:HB1	0.62	1.70	14	9
1:A:275:LEU:HD21	1:A:280:ARG:HB3	0.62	1.70	17	4
1:A:232:LEU:HD22	1:A:316:PHE:CZ	0.62	2.30	16	1
1:A:360:LEU:HB3	1:A:362:ILE:HD12	0.62	1.70	16	1
1:A:269:LEU:HD22	1:A:292:ALA:CB	0.62	2.24	1	18
1:A:245:VAL:HG22	1:A:295:LEU:HD22	0.62	1.72	5	10
1:A:269:LEU:HD11	1:A:287:PHE:HB2	0.62	1.71	8	3
1:A:285:VAL:CG2	1:A:384:THR:HG21	0.62	2.25	18	12
1:A:293:ARG:CD	1:A:378:LEU:HD23	0.62	2.25	12	5
1:A:269:LEU:N	1:A:269:LEU:HD23	0.61	2.10	11	18
1:A:314:VAL:HG13	1:A:344:PHE:CE1	0.61	2.30	9	2
1:A:275:LEU:HD21	1:A:280:ARG:HB2	0.61	1.73	8	12
1:A:293:ARG:HH12	1:A:380:ALA:HB2	0.61	1.56	7	1
1:A:231:LEU:HD23	1:A:344:PHE:CE1	0.61	2.30	15	1
1:A:269:LEU:HD21	1:A:292:ALA:HB3	0.61	1.72	5	1
1:A:403:ALA:CB	1:A:446:ILE:HG23	0.61	2.25	12	14
1:A:395:MET:CE	1:A:446:ILE:HG21	0.60	2.26	2	2
1:A:420:VAL:HG22	1:A:425:VAL:CG2	0.60	2.26	8	11
1:A:438:TRP:O	1:A:438:TRP:CE3	0.60	2.54	20	3
1:A:310:LEU:CD1	1:A:313:VAL:HG22	0.59	2.20	1	1
1:A:346:ALA:HB1	1:A:347:PRO:HD2	0.59	1.73	16	20
1:A:410:LEU:HD13	1:A:433:VAL:CG2	0.59	2.27	10	7
1:A:269:LEU:CD1	1:A:283:THR:HG23	0.59	2.27	9	1
1:A:275:LEU:HD11	1:A:280:ARG:CA	0.59	2.28	13	9
1:A:318:LEU:HD22	1:A:352:ARG:CD	0.59	2.27	3	1
1:A:410:LEU:HD22	1:A:433:VAL:HB	0.58	1.75	7	20
1:A:220:PHE:CE2	1:A:353:ALA:HB2	0.58	2.33	9	2
1:A:271:LEU:HD23	1:A:297:ALA:CB	0.58	2.29	12	14
1:A:271:LEU:HB3	1:A:297:ALA:HB2	0.58	1.76	10	17
1:A:216:ILE:HD11	1:A:329:ILE:HB	0.58	1.75	12	1
1:A:433:VAL:HG12	1:A:436:LYS:NZ	0.58	2.13	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:293:ARG:HG2	1:A:378:LEU:HD23	0.58	1.76	17	3
1:A:275:LEU:HD22	1:A:279:ASP:CB	0.58	2.28	14	2
1:A:401:LEU:CD1	1:A:415:ILE:HG21	0.58	2.28	10	5
1:A:387:ILE:HG12	1:A:453:VAL:HG22	0.58	1.74	1	16
1:A:219:GLN:HB2	1:A:342:ILE:HG22	0.58	1.74	5	2
1:A:228:LYS:NZ	1:A:232:LEU:HD22	0.58	2.13	10	1
1:A:364:LEU:HD22	1:A:366:TRP:CZ2	0.57	2.35	2	1
1:A:228:LYS:HE3	1:A:257:VAL:HG22	0.57	1.74	3	2
1:A:238:LEU:HD12	1:A:239:HIS:N	0.57	2.14	8	9
1:A:269:LEU:HD11	1:A:283:THR:HG23	0.57	1.75	9	1
1:A:229:ILE:HD12	1:A:260:ALA:HB3	0.57	1.76	18	10
1:A:408:ILE:HD11	1:A:441:LEU:CD1	0.57	2.30	14	7
1:A:275:LEU:HD21	1:A:280:ARG:CG	0.57	2.29	19	3
1:A:312:LEU:HD11	1:A:342:ILE:HD11	0.57	1.77	19	2
1:A:326:VAL:HG11	1:A:360:LEU:CD2	0.57	2.29	8	5
1:A:293:ARG:HD3	1:A:378:LEU:HD23	0.57	1.75	12	2
1:A:219:GLN:HG3	1:A:340:LEU:HD11	0.56	1.77	4	2
1:A:245:VAL:HG13	1:A:295:LEU:HD23	0.56	1.76	17	6
1:A:268:ALA:HA	1:A:294:VAL:O	0.56	2.00	5	1
1:A:318:LEU:HD13	1:A:349:GLU:OE2	0.56	2.00	17	1
1:A:269:LEU:HD23	1:A:269:LEU:O	0.56	1.99	9	1
1:A:217:GLU:HB3	1:A:340:LEU:HD22	0.56	1.76	15	2
1:A:438:TRP:CE2	1:A:442:GLN:NE2	0.56	2.74	19	3
1:A:326:VAL:HG22	1:A:360:LEU:HD11	0.56	1.77	4	8
1:A:293:ARG:HD2	1:A:378:LEU:HD23	0.56	1.76	14	5
1:A:356:ILE:O	1:A:360:LEU:HD12	0.56	2.01	1	3
1:A:390:GLY:H	1:A:425:VAL:HG23	0.56	1.61	14	5
1:A:408:ILE:HG21	1:A:437:ALA:HA	0.56	1.77	18	6
1:A:245:VAL:CG2	1:A:310:LEU:HD11	0.56	2.30	8	7
1:A:295:LEU:HD23	1:A:295:LEU:O	0.56	2.01	18	18
1:A:395:MET:HE3	1:A:446:ILE:HG21	0.56	1.78	2	1
1:A:408:ILE:CD1	1:A:441:LEU:HD13	0.56	2.31	5	6
1:A:333:ALA:HB1	1:A:338:SER:OG	0.56	2.01	10	3
1:A:235:LEU:CD1	1:A:342:ILE:HD13	0.55	2.32	20	2
1:A:236:LEU:CD1	1:A:294:VAL:HG21	0.55	2.31	10	14
1:A:353:ALA:HB1	1:A:364:LEU:CD1	0.55	2.31	1	12
1:A:326:VAL:CG1	1:A:360:LEU:HD21	0.55	2.31	4	3
1:A:234:ARG:O	1:A:238:LEU:HD13	0.55	2.02	16	2
1:A:217:GLU:HB2	1:A:340:LEU:HD22	0.55	1.77	18	8
1:A:404:LEU:HD23	1:A:410:LEU:HD12	0.55	1.78	16	5
1:A:318:LEU:HD23	1:A:352:ARG:HB3	0.55	1.78	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:395:MET:SD	1:A:425:VAL:HG21	0.55	2.41	14	1
1:A:312:LEU:HD12	1:A:313:VAL:N	0.55	2.17	19	20
1:A:446:ILE:HD12	1:A:451:CYS:SG	0.55	2.41	9	3
1:A:360:LEU:CB	1:A:362:ILE:HD12	0.55	2.32	19	2
1:A:438:TRP:CZ3	1:A:453:VAL:HB	0.54	2.37	19	10
1:A:234:ARG:HD3	1:A:238:LEU:HD23	0.54	1.78	17	1
1:A:281:ASP:O	1:A:285:VAL:HG13	0.54	2.02	13	18
1:A:385:LEU:HD11	1:A:429:VAL:HG21	0.54	1.78	14	19
1:A:438:TRP:CE3	1:A:438:TRP:O	0.54	2.60	11	7
1:A:244:CYS:SG	1:A:294:VAL:HG22	0.54	2.42	5	2
1:A:385:LEU:HD22	1:A:453:VAL:HG11	0.54	1.77	1	4
1:A:401:LEU:HD11	1:A:415:ILE:HG21	0.54	1.78	10	7
1:A:269:LEU:HD23	1:A:295:LEU:HA	0.54	1.80	9	1
1:A:233:GLN:HB3	1:A:375:ILE:HD11	0.54	1.79	7	1
1:A:235:LEU:HD11	1:A:342:ILE:HD13	0.54	1.80	20	2
1:A:387:ILE:HG23	1:A:453:VAL:HG22	0.54	1.77	9	1
1:A:364:LEU:HD13	1:A:366:TRP:CZ2	0.54	2.37	2	1
1:A:237:SER:HB2	1:A:376:ALA:HB3	0.54	1.78	9	10
1:A:216:ILE:HG12	1:A:329:ILE:HD12	0.54	1.80	4	3
1:A:314:VAL:HG13	1:A:344:PHE:CD1	0.53	2.37	16	2
1:A:386:CYS:SG	1:A:456:LEU:HD21	0.53	2.44	11	4
1:A:387:ILE:HD11	1:A:427:VAL:CG1	0.53	2.34	15	9
1:A:269:LEU:HD21	1:A:295:LEU:CD1	0.53	2.26	9	1
1:A:236:LEU:HD13	1:A:294:VAL:CG2	0.53	2.34	16	5
1:A:269:LEU:HD22	1:A:286:ARG:HD2	0.53	1.78	9	1
1:A:404:LEU:HD23	1:A:410:LEU:CD1	0.53	2.34	16	1
1:A:245:VAL:HG22	1:A:295:LEU:CD2	0.53	2.33	5	2
1:A:305:LEU:HD21	1:A:307:ILE:CG1	0.53	2.33	14	1
1:A:387:ILE:HB	1:A:425:VAL:HG13	0.53	1.79	16	3
1:A:313:VAL:HB	1:A:329:ILE:HG22	0.53	1.79	18	2
1:A:340:LEU:HD13	1:A:341:ALA:N	0.53	2.19	12	15
1:A:305:LEU:HD21	1:A:307:ILE:CG2	0.53	2.34	17	1
1:A:318:LEU:HD12	1:A:352:ARG:HG2	0.52	1.81	11	2
1:A:245:VAL:HG23	1:A:310:LEU:HD21	0.52	1.81	17	4
1:A:272:HIS:HA	1:A:301:ALA:HB2	0.52	1.81	14	6
1:A:410:LEU:HD13	1:A:433:VAL:HG21	0.52	1.79	10	4
1:A:269:LEU:HD11	1:A:295:LEU:HD12	0.52	1.81	18	1
1:A:281:ASP:O	1:A:285:VAL:HG22	0.52	2.05	7	3
1:A:312:LEU:HD11	1:A:342:ILE:CD1	0.52	2.34	19	2
1:A:275:LEU:HD11	1:A:280:ARG:CB	0.52	2.34	12	2
1:A:401:LEU:CD2	1:A:415:ILE:HG21	0.52	2.34	8	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:305:LEU:HD21	1:A:307:ILE:HG13	0.52	1.81	14	1
1:A:269:LEU:HB3	1:A:283:THR:HG23	0.52	1.80	5	1
1:A:269:LEU:HD13	1:A:286:ARG:HG2	0.52	1.80	20	2
1:A:246:VAL:HB	1:A:296:VAL:HG13	0.52	1.81	11	3
1:A:269:LEU:HD13	1:A:286:ARG:HD2	0.52	1.82	1	5
1:A:275:LEU:HD22	1:A:279:ASP:HB3	0.52	1.81	14	2
1:A:353:ALA:HB1	1:A:366:TRP:CZ2	0.52	2.40	2	1
1:A:394:LYS:O	1:A:394:LYS:CG	0.52	2.58	17	1
1:A:247:PHE:CE1	1:A:302:ALA:HB3	0.52	2.40	18	1
1:A:275:LEU:HD23	1:A:275:LEU:O	0.51	2.04	12	7
1:A:271:LEU:HD23	1:A:297:ALA:HB1	0.51	1.82	19	6
1:A:359:MET:HE3	1:A:360:LEU:HD13	0.51	1.82	17	2
1:A:453:VAL:CG1	1:A:454:ARG:N	0.51	2.74	14	11
1:A:216:ILE:HG22	1:A:216:ILE:O	0.51	2.05	1	1
1:A:438:TRP:CE3	1:A:438:TRP:HA	0.51	2.40	18	3
1:A:216:ILE:HD12	1:A:329:ILE:CD1	0.51	2.36	14	1
1:A:329:ILE:CG2	1:A:341:ALA:HB2	0.51	2.20	2	3
1:A:218:GLN:OE1	1:A:362:ILE:HD11	0.51	2.06	4	1
1:A:414:ASP:OD2	1:A:432:ALA:HB3	0.51	2.06	15	4
1:A:385:LEU:HD11	1:A:429:VAL:CG2	0.51	2.35	4	12
1:A:217:GLU:CB	1:A:340:LEU:HD22	0.51	2.35	18	7
1:A:229:ILE:N	1:A:230:PRO:HD2	0.50	2.21	17	20
1:A:408:ILE:CG2	1:A:410:LEU:HD21	0.50	2.37	12	16
1:A:312:LEU:HD13	1:A:340:LEU:HD12	0.50	1.83	18	4
1:A:269:LEU:HD21	1:A:292:ALA:CB	0.50	2.37	5	1
1:A:302:ALA:HA	1:A:305:LEU:HD13	0.50	1.83	14	1
1:A:318:LEU:HD22	1:A:352:ARG:HD3	0.50	1.84	3	1
1:A:312:LEU:HD11	1:A:342:ILE:HD12	0.50	1.83	15	1
1:A:265:GLY:O	1:A:377:THR:HG23	0.50	2.06	7	2
1:A:233:GLN:HB3	1:A:375:ILE:HD13	0.50	1.82	16	1
1:A:245:VAL:HG21	1:A:307:ILE:HD11	0.50	1.84	17	1
1:A:254:CYS:HA	1:A:296:VAL:HG11	0.49	1.83	19	5
1:A:420:VAL:HA	1:A:425:VAL:HG23	0.49	1.82	17	8
1:A:360:LEU:HB2	1:A:362:ILE:HD12	0.49	1.83	19	1
1:A:375:ILE:HD13	1:A:376:ALA:O	0.49	2.07	19	1
1:A:307:ILE:HG21	1:A:332:THR:OG1	0.49	2.06	14	1
1:A:312:LEU:HD12	1:A:313:VAL:H	0.49	1.67	2	15
1:A:269:LEU:HD12	1:A:283:THR:HG22	0.49	1.84	18	2
1:A:264:VAL:HG21	1:A:375:ILE:HD11	0.49	1.85	1	1
1:A:261:LEU:HD23	1:A:268:ALA:HB2	0.49	1.82	2	2
1:A:272:HIS:CE1	1:A:298:THR:HG21	0.49	2.42	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:269:LEU:HD22	1:A:269:LEU:N	0.49	2.22	5	1
1:A:269:LEU:HD13	1:A:286:ARG:HB3	0.49	1.83	4	3
1:A:223:THR:HG21	1:A:231:LEU:HD22	0.48	1.85	16	1
1:A:264:VAL:CG1	1:A:375:ILE:HD11	0.48	2.34	16	1
1:A:329:ILE:HD13	1:A:341:ALA:CB	0.48	2.36	8	2
1:A:236:LEU:HD21	1:A:244:CYS:SG	0.48	2.48	2	2
1:A:269:LEU:HD13	1:A:286:ARG:CD	0.48	2.38	9	2
1:A:404:LEU:HB3	1:A:410:LEU:HD12	0.48	1.84	9	2
1:A:362:ILE:HD12	1:A:362:ILE:O	0.48	2.08	6	6
1:A:216:ILE:HD12	1:A:339:GLY:CA	0.48	2.39	12	2
1:A:228:LYS:HE2	1:A:257:VAL:HG22	0.48	1.86	10	1
1:A:357:SER:HB2	1:A:362:ILE:HD12	0.48	1.85	10	1
1:A:218:GLN:OE1	1:A:341:ALA:HB3	0.48	2.08	15	1
1:A:333:ALA:HB1	1:A:338:SER:HB2	0.48	1.85	17	3
1:A:257:VAL:O	1:A:261:LEU:HD13	0.47	2.09	12	9
1:A:404:LEU:CD1	1:A:427:VAL:HG21	0.47	2.39	5	4
1:A:266:GLN:NE2	1:A:378:LEU:HD13	0.47	2.24	19	4
1:A:216:ILE:HD13	1:A:339:GLY:HA3	0.47	1.85	16	1
1:A:293:ARG:CG	1:A:378:LEU:HD23	0.47	2.38	17	1
1:A:220:PHE:CE1	1:A:353:ALA:HB1	0.47	2.43	5	1
1:A:401:LEU:HD21	1:A:415:ILE:HG21	0.47	1.84	8	3
1:A:248:CYS:SG	1:A:298:THR:HG22	0.47	2.50	8	1
1:A:286:ARG:CD	1:A:292:ALA:HB3	0.47	2.38	9	1
1:A:216:ILE:HG23	1:A:329:ILE:CD1	0.47	2.40	7	6
1:A:400:VAL:O	1:A:404:LEU:HD12	0.47	2.09	11	2
1:A:438:TRP:CE3	1:A:438:TRP:CA	0.47	2.98	18	3
1:A:289:ASN:ND2	1:A:289:ASN:O	0.47	2.48	8	1
1:A:229:ILE:HG23	1:A:260:ALA:CB	0.47	2.40	15	2
1:A:318:LEU:HD12	1:A:352:ARG:CG	0.47	2.40	11	1
1:A:397:PRO:N	1:A:420:VAL:HG21	0.46	2.25	15	1
1:A:364:LEU:HB3	1:A:366:TRP:CZ2	0.46	2.45	2	1
1:A:433:VAL:HG12	1:A:436:LYS:HZ2	0.46	1.70	8	1
1:A:438:TRP:CZ2	1:A:453:VAL:O	0.46	2.69	17	7
1:A:344:PHE:CD1	1:A:344:PHE:O	0.46	2.69	20	2
1:A:312:LEU:HD11	1:A:342:ILE:HG13	0.46	1.87	2	1
1:A:390:GLY:N	1:A:425:VAL:HG23	0.46	2.25	14	1
1:A:245:VAL:CB	1:A:310:LEU:HD11	0.46	2.41	17	2
1:A:362:ILE:O	1:A:362:ILE:HD13	0.46	2.11	4	2
1:A:216:ILE:O	1:A:216:ILE:CG2	0.46	2.62	12	2
1:A:438:TRP:CZ2	1:A:442:GLN:NE2	0.46	2.84	20	3
1:A:312:LEU:HD11	1:A:342:ILE:CG1	0.45	2.41	19	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:235:LEU:HD23	1:A:235:LEU:O	0.45	2.11	16	1
1:A:437:ALA:O	1:A:441:LEU:HD12	0.45	2.11	1	1
1:A:312:LEU:CD1	1:A:340:LEU:HD12	0.45	2.40	19	1
1:A:221:TYR:CD2	1:A:342:ILE:HG23	0.45	2.47	15	1
1:A:269:LEU:CD1	1:A:295:LEU:HD12	0.45	2.41	18	1
1:A:404:LEU:HA	1:A:408:ILE:HD12	0.45	1.88	9	1
1:A:353:ALA:HB1	1:A:366:TRP:HZ2	0.45	1.72	2	1
1:A:246:VAL:HG23	1:A:294:VAL:HG13	0.45	1.87	1	2
1:A:385:LEU:HD22	1:A:453:VAL:CG1	0.45	2.42	9	3
1:A:329:ILE:O	1:A:332:THR:HG22	0.45	2.11	16	2
1:A:284:LEU:HD12	1:A:306:ASP:HB3	0.45	1.89	8	1
1:A:216:ILE:HD13	1:A:339:GLY:CA	0.45	2.41	16	2
1:A:218:GLN:CG	1:A:341:ALA:HB3	0.45	2.41	8	1
1:A:238:LEU:C	1:A:238:LEU:HD12	0.45	2.32	9	3
1:A:218:GLN:HB3	1:A:364:LEU:HD23	0.45	1.88	14	1
1:A:387:ILE:HG23	1:A:453:VAL:CG2	0.45	2.41	9	2
1:A:438:TRP:HA	1:A:438:TRP:HE3	0.45	1.72	18	3
1:A:250:THR:HG22	1:A:253:ASP:OD2	0.45	2.12	3	1
1:A:404:LEU:CD2	1:A:415:ILE:HD11	0.45	2.41	7	2
1:A:313:VAL:CG1	1:A:329:ILE:HG22	0.45	2.42	14	1
1:A:318:LEU:HD12	1:A:352:ARG:HB3	0.44	1.89	2	1
1:A:340:LEU:HD12	1:A:342:ILE:HG13	0.44	1.88	8	4
1:A:266:GLN:CD	1:A:378:LEU:HD13	0.44	2.33	19	1
1:A:420:VAL:HA	1:A:425:VAL:HG13	0.44	1.88	20	1
1:A:232:LEU:CD1	1:A:314:VAL:HG11	0.44	2.39	16	1
1:A:269:LEU:CB	1:A:295:LEU:HD12	0.44	2.42	5	1
1:A:359:MET:CE	1:A:360:LEU:HD13	0.44	2.42	20	1
1:A:408:ILE:HG22	1:A:410:LEU:HD21	0.44	1.90	4	3
1:A:384:THR:HB	1:A:456:LEU:HD12	0.44	1.89	17	4
1:A:250:THR:HG23	1:A:253:ASP:H	0.44	1.72	11	1
1:A:229:ILE:CB	1:A:230:PRO:CD	0.44	2.96	12	15
1:A:269:LEU:N	1:A:269:LEU:CD2	0.44	2.80	11	6
1:A:395:MET:SD	1:A:400:VAL:HG22	0.44	2.53	7	2
1:A:216:ILE:HD11	1:A:330:GLY:HA2	0.44	1.88	14	2
1:A:245:VAL:CG2	1:A:307:ILE:HD11	0.44	2.42	17	1
1:A:433:VAL:O	1:A:437:ALA:HB2	0.44	2.13	19	2
1:A:221:TYR:HB3	1:A:231:LEU:HD21	0.43	1.88	15	1
1:A:405:THR:HG22	1:A:410:LEU:O	0.43	2.12	18	1
1:A:418:ILE:HG23	1:A:426:TYR:O	0.43	2.13	18	10
1:A:321:ASP:OD1	1:A:324:VAL:HG13	0.43	2.12	6	1
1:A:245:VAL:HG23	1:A:287:PHE:CZ	0.43	2.48	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:390:GLY:H	1:A:425:VAL:HG12	0.43	1.72	7	2
1:A:396:ARG:CB	1:A:397:PRO:HD2	0.43	2.44	15	2
1:A:410:LEU:HD22	1:A:433:VAL:CB	0.43	2.44	12	7
1:A:269:LEU:HD23	1:A:294:VAL:O	0.43	2.14	8	1
1:A:389:GLY:CA	1:A:393:ALA:HB2	0.43	2.43	15	2
1:A:342:ILE:HG22	1:A:344:PHE:CE2	0.43	2.49	2	1
1:A:385:LEU:HB2	1:A:427:VAL:HG13	0.43	1.90	9	2
1:A:313:VAL:CB	1:A:329:ILE:HG22	0.43	2.44	17	2
1:A:293:ARG:CZ	1:A:380:ALA:HB2	0.43	2.43	10	1
1:A:245:VAL:HG21	1:A:307:ILE:CD1	0.43	2.44	17	1
1:A:453:VAL:HG12	1:A:454:ARG:N	0.42	2.29	18	4
1:A:216:ILE:HD11	1:A:329:ILE:CD1	0.42	2.43	8	1
1:A:404:LEU:HB3	1:A:415:ILE:HD11	0.42	1.91	19	1
1:A:318:LEU:HD23	1:A:349:GLU:OE2	0.42	2.13	9	1
1:A:246:VAL:HG23	1:A:294:VAL:CG1	0.42	2.44	1	1
1:A:420:VAL:HG22	1:A:425:VAL:HG13	0.42	1.90	5	2
1:A:240:GLN:N	1:A:241:PRO:CD	0.42	2.82	2	7
1:A:401:LEU:HD22	1:A:418:ILE:HD11	0.42	1.91	9	1
1:A:247:PHE:HE1	1:A:302:ALA:HB3	0.42	1.74	18	1
1:A:357:SER:HB3	1:A:364:LEU:HD21	0.42	1.92	2	3
1:A:329:ILE:CD1	1:A:341:ALA:HB2	0.42	2.40	8	1
1:A:318:LEU:HD23	1:A:349:GLU:OE1	0.42	2.14	9	1
1:A:287:PHE:CB	1:A:295:LEU:HD13	0.42	2.44	12	1
1:A:326:VAL:HG21	1:A:360:LEU:HD21	0.42	1.92	13	1
1:A:220:PHE:HB3	1:A:366:TRP:CE3	0.42	2.49	2	1
1:A:293:ARG:HG3	1:A:294:VAL:N	0.42	2.30	2	1
1:A:385:LEU:HB3	1:A:453:VAL:HG13	0.42	1.92	4	6
1:A:282:GLN:O	1:A:285:VAL:CG2	0.42	2.68	9	1
1:A:220:PHE:CE2	1:A:318:LEU:HD11	0.42	2.50	15	1
1:A:289:ASN:CG	1:A:428:ALA:HB2	0.42	2.35	20	1
1:A:293:ARG:NE	1:A:294:VAL:HG23	0.42	2.30	2	1
1:A:289:ASN:ND2	1:A:428:ALA:HB2	0.42	2.30	9	1
1:A:302:ALA:O	1:A:305:LEU:HD22	0.42	2.13	14	1
1:A:375:ILE:HD12	1:A:376:ALA:O	0.42	2.15	16	1
1:A:247:PHE:CE2	1:A:328:ARG:HG2	0.41	2.50	1	1
1:A:293:ARG:NH1	1:A:378:LEU:HD13	0.41	2.30	2	1
1:A:393:ALA:HB3	1:A:395:MET:SD	0.41	2.55	2	1
1:A:360:LEU:O	1:A:361:GLN:HG2	0.41	2.15	11	1
1:A:231:LEU:HD21	1:A:344:PHE:CD2	0.41	2.51	17	1
1:A:389:GLY:HA3	1:A:395:MET:HE3	0.41	1.92	18	1
1:A:229:ILE:HB	1:A:230:PRO:HD3	0.41	1.91	9	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:284:LEU:HD21	1:A:305:LEU:HD12	0.41	1.91	2	1
1:A:285:VAL:HG21	1:A:384:THR:HG21	0.41	1.93	12	1
1:A:387:ILE:HG21	1:A:446:ILE:CD1	0.41	2.44	3	1
1:A:357:SER:HA	1:A:362:ILE:HD11	0.41	1.91	15	1
1:A:216:ILE:CG2	1:A:329:ILE:HD12	0.41	2.44	13	1
1:A:305:LEU:N	1:A:305:LEU:HD23	0.41	2.30	19	1
1:A:305:LEU:HD21	1:A:307:ILE:HB	0.41	1.93	9	2
1:A:408:ILE:HG23	1:A:440:GLN:HB2	0.41	1.91	18	1
1:A:441:LEU:HD21	1:A:446:ILE:HD11	0.41	1.93	20	1
1:A:229:ILE:HG22	1:A:230:PRO:N	0.41	2.29	1	1
1:A:395:MET:HG3	1:A:400:VAL:HG22	0.41	1.91	5	2
1:A:229:ILE:N	1:A:230:PRO:CD	0.41	2.84	17	3
1:A:318:LEU:HD23	1:A:352:ARG:CB	0.40	2.46	5	1
1:A:216:ILE:HB	1:A:339:GLY:O	0.40	2.16	8	1
1:A:285:VAL:HG23	1:A:286:ARG:N	0.40	2.32	8	1
1:A:264:VAL:HG11	1:A:375:ILE:HD12	0.40	1.93	13	1
1:A:247:PHE:O	1:A:316:PHE:HB3	0.40	2.16	1	1
1:A:267:SER:O	1:A:293:ARG:CG	0.40	2.69	2	1
1:A:396:ARG:HB3	1:A:397:PRO:HD2	0.40	1.93	5	1
1:A:261:LEU:O	1:A:264:VAL:HG22	0.40	2.16	10	1
1:A:420:VAL:HG22	1:A:425:VAL:CG1	0.40	2.47	20	1
1:A:362:ILE:HD12	1:A:362:ILE:C	0.40	2.37	17	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	231/251 (92%)	218±3 (94±1%)	10±3 (4±1%)	3±1 (1±0%)	17	64
All	All	4620/5020 (92%)	4356 (94%)	207 (4%)	57 (1%)	17	64

All 9 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	319	ALA	20
1	A	406	GLY	20
1	A	309	SER	6
1	A	305	LEU	3
1	A	216	ILE	3
1	A	333	ALA	2
1	A	366	TRP	1
1	A	308	LYS	1
1	A	398	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	188/201 (94%)	156±5 (83±3%)	32±5 (17±3%)	5	40
All	All	3760/4020 (94%)	3121 (83%)	639 (17%)	5	40

All 108 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	284	LEU	20
1	A	295	LEU	20
1	A	310	LEU	20
1	A	340	LEU	20
1	A	401	LEU	20
1	A	243	SER	19
1	A	332	THR	19
1	A	275	LEU	18
1	A	311	GLU	17
1	A	395	MET	16
1	A	228	LYS	15
1	A	345	CYS	15
1	A	431	GLN	14
1	A	421	HIS	13
1	A	367	GLN	12
1	A	368	THR	12
1	A	293	ARG	12

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Mol	Chain	Res	Type	Models (Total)
1	A	442	GLN	12
1	A	254	CYS	11
1	A	359	MET	11
1	A	222	GLU	10
1	A	361	GLN	10
1	A	415	ILE	10
1	A	445	LYS	10
1	A	424	HIS	9
1	A	417	LYS	8
1	A	343	SER	8
1	A	441	LEU	8
1	A	438	TRP	8
1	A	234	ARG	7
1	A	447	LYS	7
1	A	240	GLN	7
1	A	321	ASP	7
1	A	328	ARG	6
1	A	363	LYS	6
1	A	449	LYS	6
1	A	351	GLN	6
1	A	318	LEU	6
1	A	396	ARG	6
1	A	224	SER	5
1	A	226	LYS	5
1	A	218	GLN	5
1	A	267	SER	5
1	A	282	GLN	5
1	A	286	ARG	5
1	A	388	ASP	5
1	A	299	ASP	4
1	A	331	ARG	4
1	A	349	GLU	4
1	A	242	SER	4
1	A	355	ILE	4
1	A	362	ILE	4
1	A	305	LEU	4
1	A	394	LYS	4
1	A	269	LEU	4
1	A	225	SER	3
1	A	252	LYS	3
1	A	306	ASP	3
1	A	308	LYS	3

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Mol	Chain	Res	Type	Models (Total)
1	A	327	HIS	3
1	A	439	LYS	3
1	A	452	ARG	3
1	A	454	ARG	3
1	A	237	SER	3
1	A	430	ARG	3
1	A	450	THR	3
1	A	384	THR	3
1	A	235	LEU	3
1	A	219	GLN	3
1	A	457	LYS	3
1	A	357	SER	3
1	A	375	ILE	3
1	A	313	VAL	3
1	A	317	GLU	3
1	A	272	HIS	2
1	A	274	ASP	2
1	A	309	SER	2
1	A	399	ASP	2
1	A	280	ARG	2
1	A	307	ILE	2
1	A	303	ARG	2
1	A	342	ILE	2
1	A	251	LYS	2
1	A	315	ASN	2
1	A	436	LYS	2
1	A	271	LEU	2
1	A	279	ASP	2
1	A	316	PHE	2
1	A	392	LYS	2
1	A	277	GLN	2
1	A	247	PHE	1
1	A	249	ASN	1
1	A	407	ASP	1
1	A	220	PHE	1
1	A	391	LYS	1
1	A	291	SER	1
1	A	278	ARG	1
1	A	248	CYS	1
1	A	276	GLU	1
1	A	356	ILE	1
1	A	217	GLU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	216	ILE	1
1	A	440	GLN	1
1	A	244	CYS	1
1	A	348	GLU	1
1	A	329	ILE	1
1	A	255	GLN	1
1	A	231	LEU	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 monosaccharides 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