



Full wwPDB NMR Structure Validation Report ⓘ

May 29, 2020 – 04:36 am BST

PDB ID : 3ZTG
Title : Solution structure of the RING finger-like domain of Retinoblastoma Binding Protein-6 (RBBP6)
Authors : Kappo, M.A.; Ab, E.; Atkinson, R.A.; Faro, A.; Muleya, V.; Mulaudzi, T.; Poole, J.O.; McKenzie, J.M.; Pugh, D.J.R.
Deposited on : 2011-07-07

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:

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
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 : 2.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

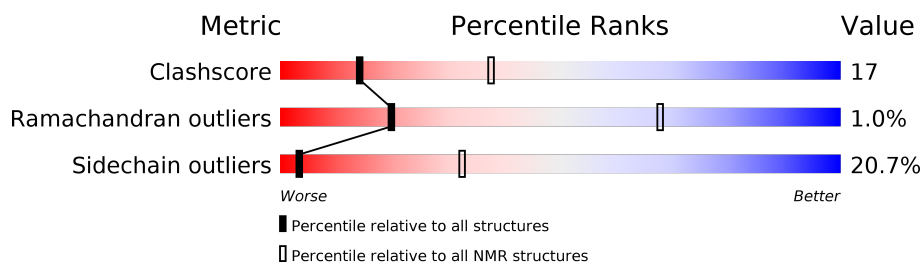
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 44%.

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	92	
1	B	92	

2 Ensemble composition and analysis

This entry contains 32 models. Model 17 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

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:253-A:322, B:255-B:319 (135)	0.17	17

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. No single-model clusters were found.

Cluster number	Models
1	4, 5, 6, 7, 8, 12, 14, 15, 16, 17, 18, 19, 21, 25, 27, 30, 31, 32
2	3, 9, 11, 23, 26, 28
3	1, 22, 24, 29
4	2, 10, 13, 20

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2674 atoms, of which 1252 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called E3 UBIQUITIN-PROTEIN LIGASE RBBP6.

Mol	Chain	Residues	Atoms						Trace
1	A	92	Total	C	H	N	O	S	0
			1335	435	626	122	143	9	
1	B	92	Total	C	H	N	O	S	0
			1335	435	626	122	143	9	

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	244	GLY	-	expression tag	UNP Q7Z6E9
A	245	PRO	-	expression tag	UNP Q7Z6E9
A	246	LEU	-	expression tag	UNP Q7Z6E9
A	247	GLY	-	expression tag	UNP Q7Z6E9
A	248	SER	-	expression tag	UNP Q7Z6E9
B	244	GLY	-	expression tag	UNP Q7Z6E9
B	245	PRO	-	expression tag	UNP Q7Z6E9
B	246	LEU	-	expression tag	UNP Q7Z6E9
B	247	GLY	-	expression tag	UNP Q7Z6E9
B	248	SER	-	expression tag	UNP Q7Z6E9

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

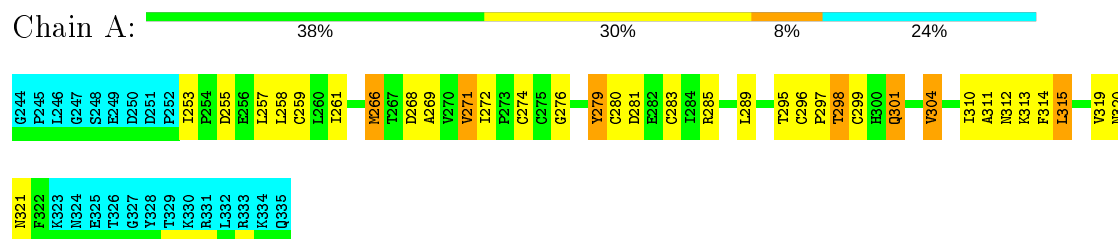
Mol	Chain	Residues	Atoms	
2	B	2	Total	Zn
			2	2
2	A	2	Total	Zn
			2	2

4 Residue-property plots

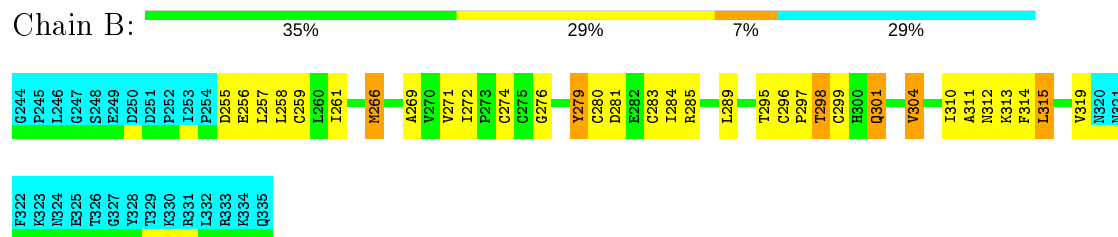
4.1 Average score per residue in the NMR ensemble

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: E3 UBIQUITIN-PROTEIN LIGASE RBBP6



- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

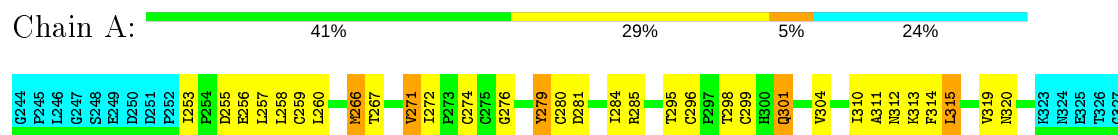


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

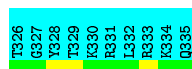
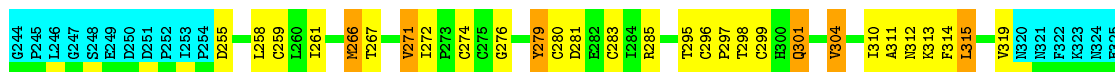
- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6





• Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

Chain B:



4.2.2 Score per residue for model 2

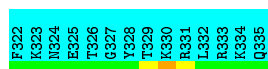
• Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

Chain A:



• Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

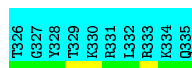
Chain B:



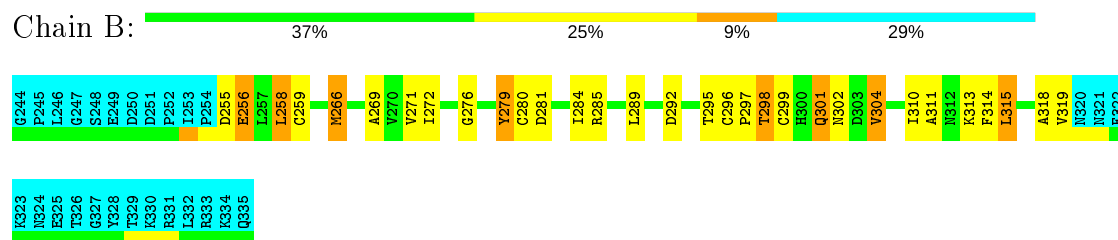
4.2.3 Score per residue for model 3

• Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

Chain A:

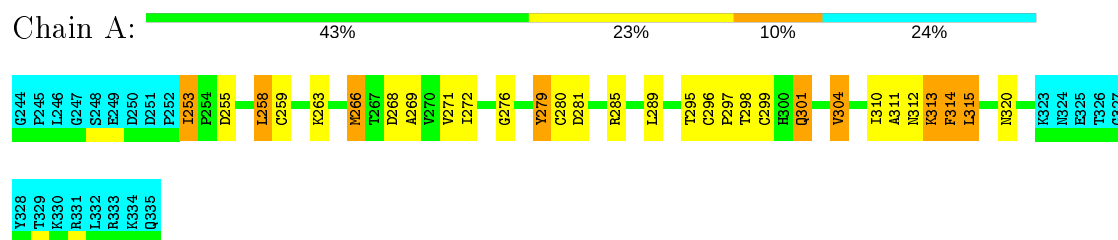


• Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

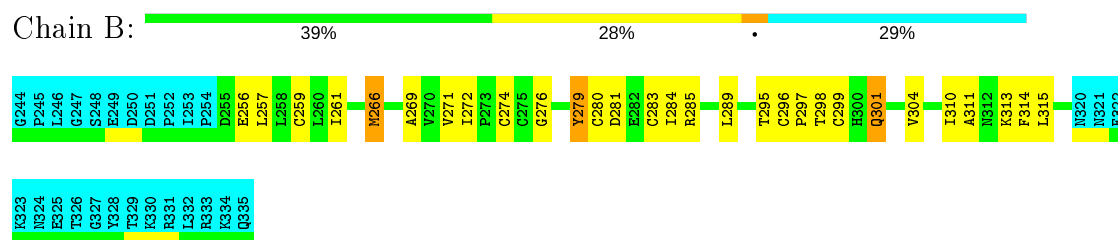


4.2.4 Score per residue for model 4

- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

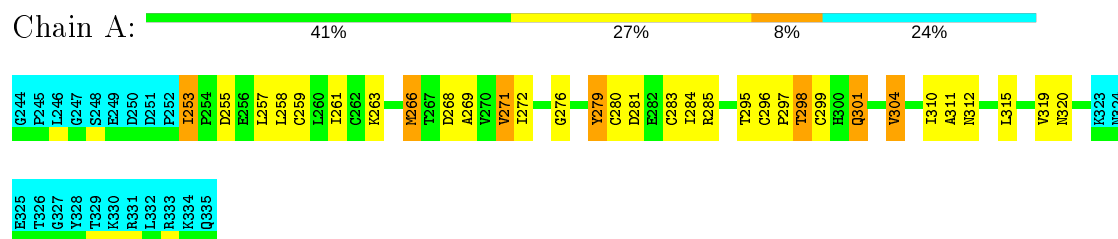


- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

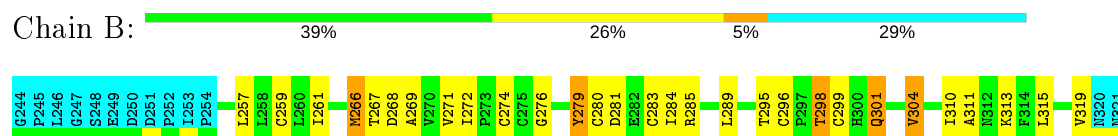


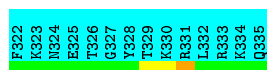
4.2.5 Score per residue for model 5

- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6



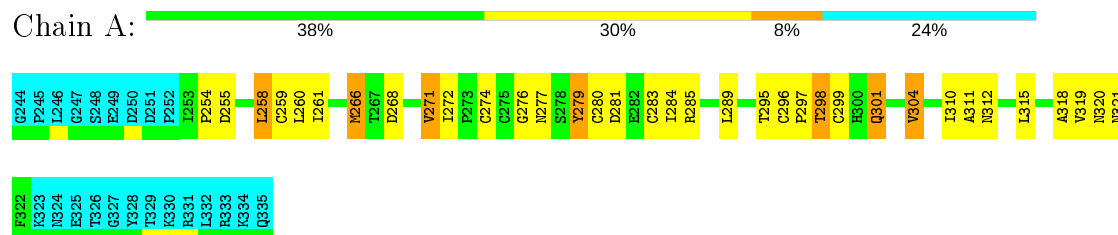
- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6



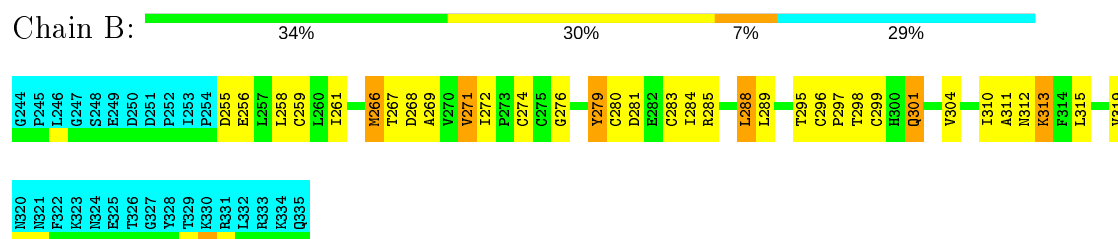


4.2.6 Score per residue for model 6

- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

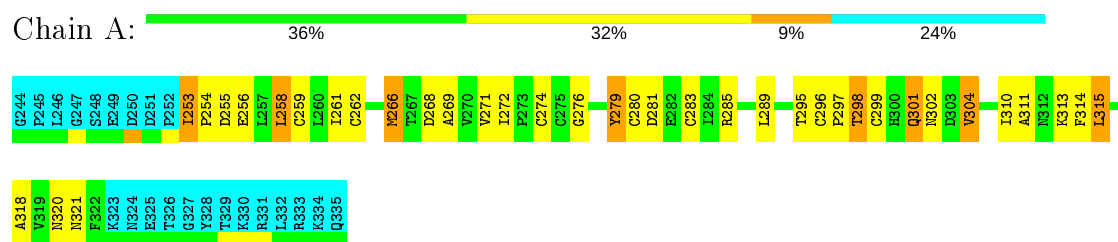


- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

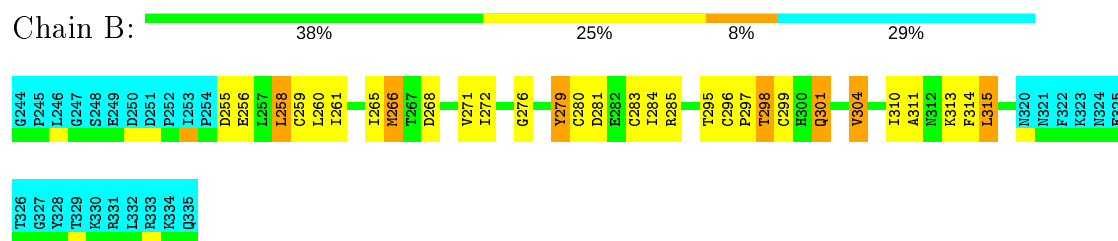


4.2.7 Score per residue for model 7

- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

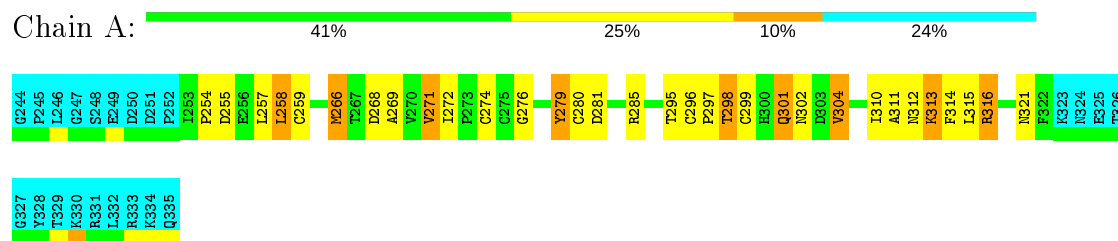


- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

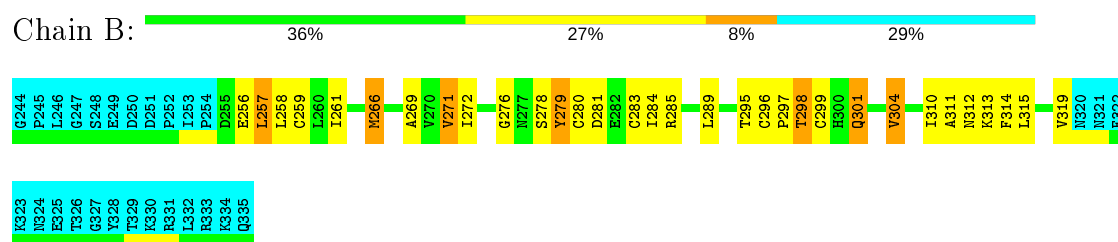


4.2.8 Score per residue for model 8

- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

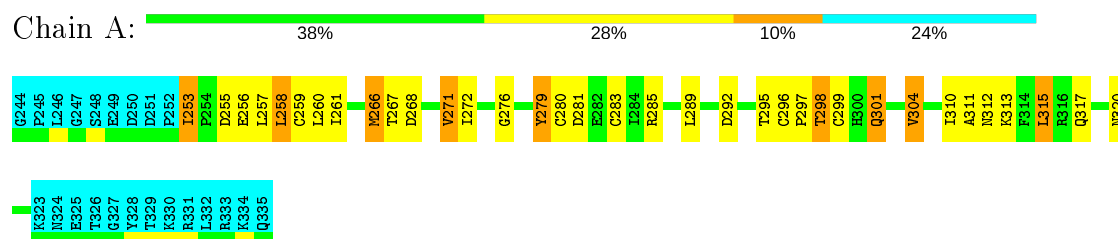


- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

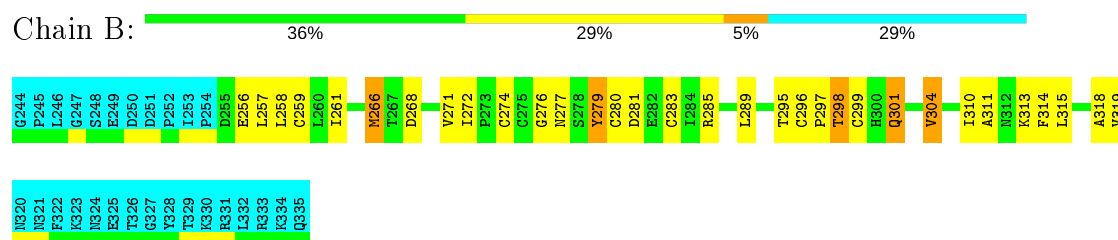


4.2.9 Score per residue for model 9

- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

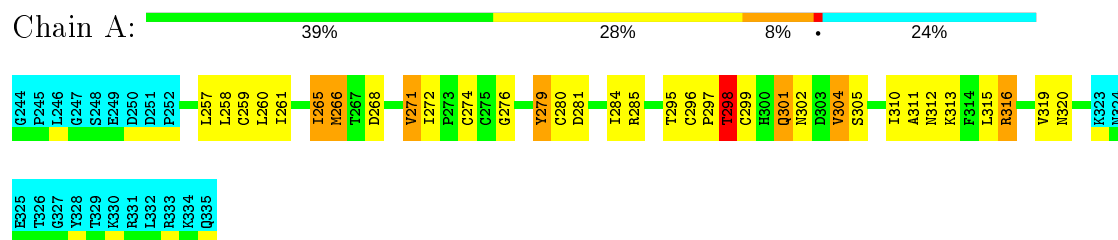


- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

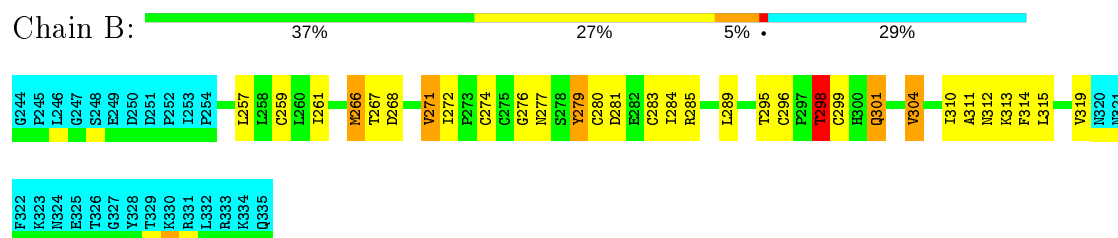


4.2.10 Score per residue for model 10

- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

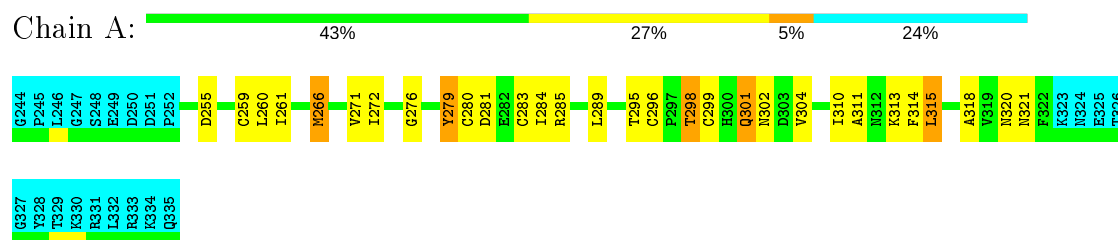


- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

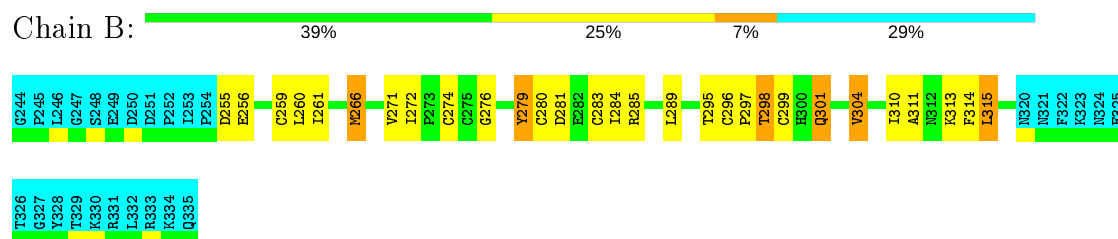


4.2.11 Score per residue for model 11

- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

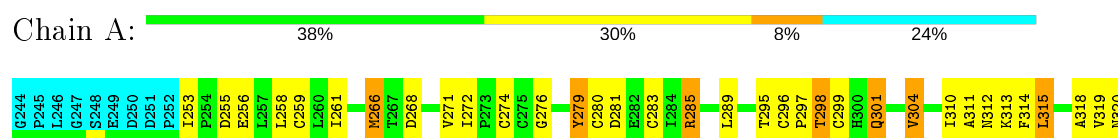


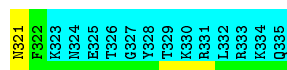
- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6



4.2.12 Score per residue for model 12

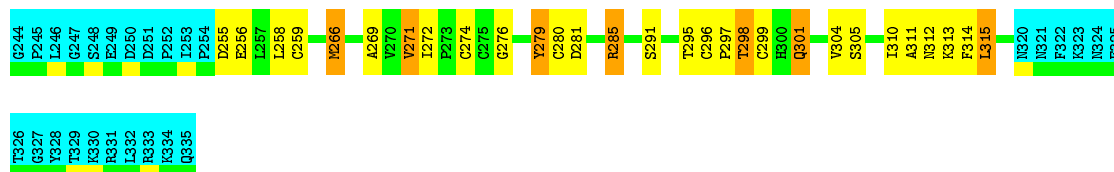
- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6





- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

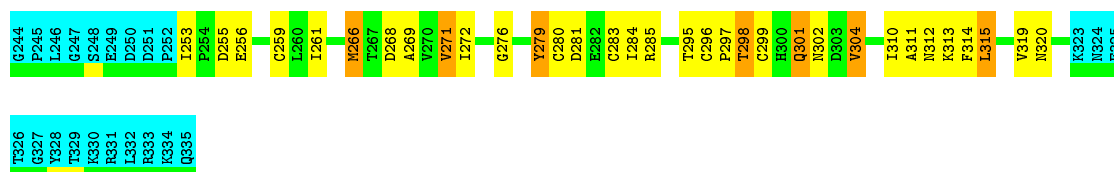
Chain B:



4.2.13 Score per residue for model 13

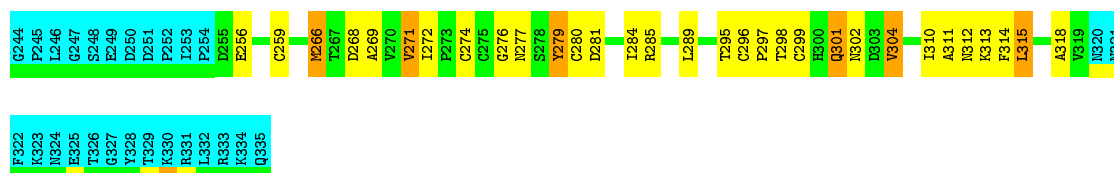
- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

Chain A:



- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

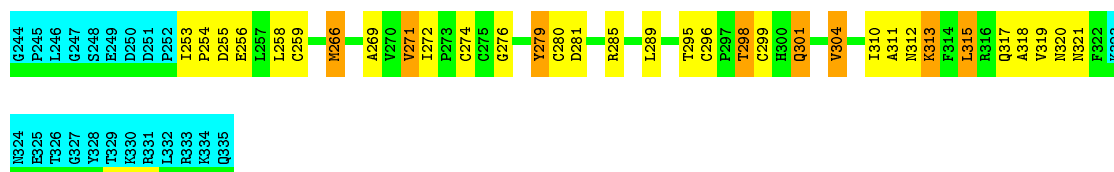
Chain B:



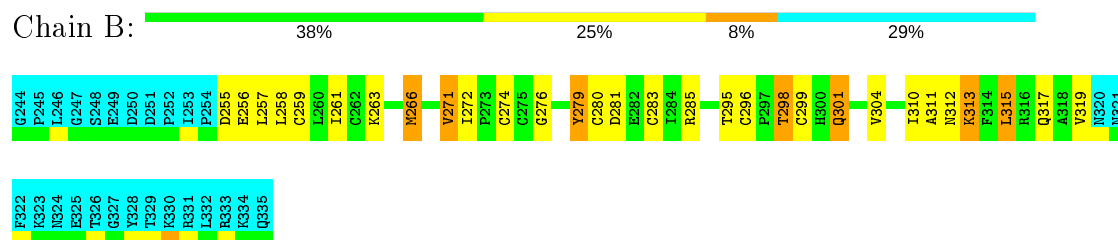
4.2.14 Score per residue for model 14

- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

Chain A:

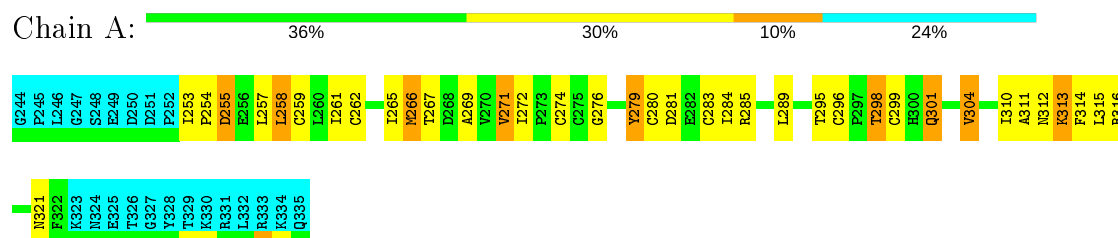


- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

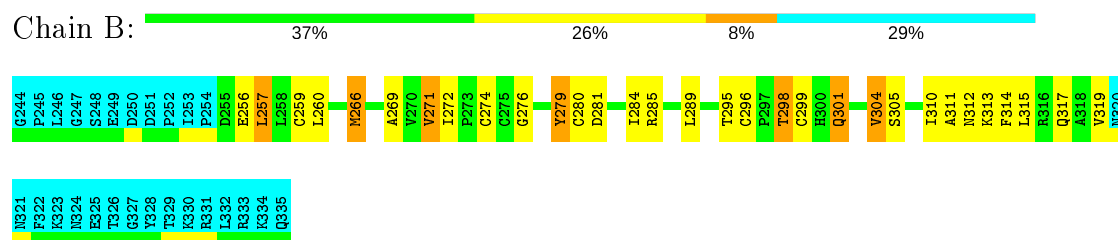


4.2.15 Score per residue for model 15

- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

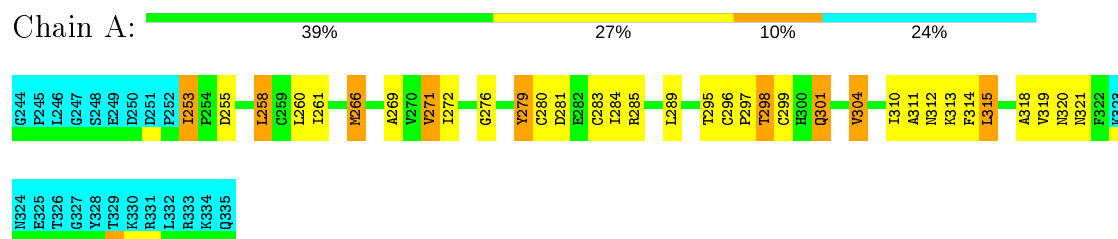


- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

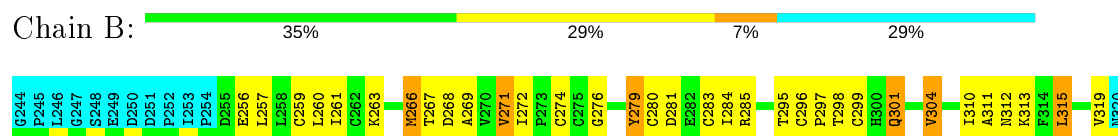


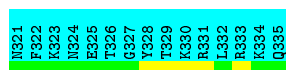
4.2.16 Score per residue for model 16

- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6



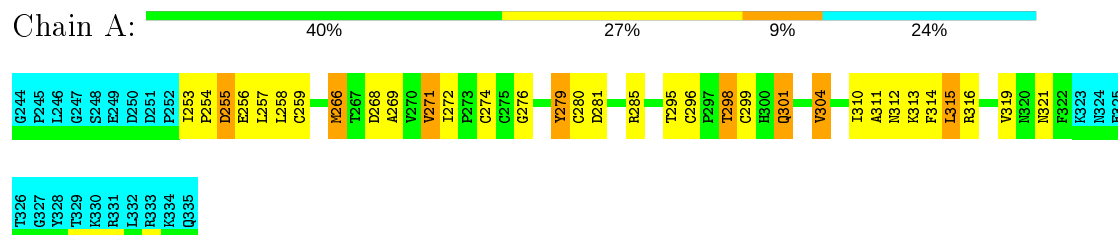
- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6



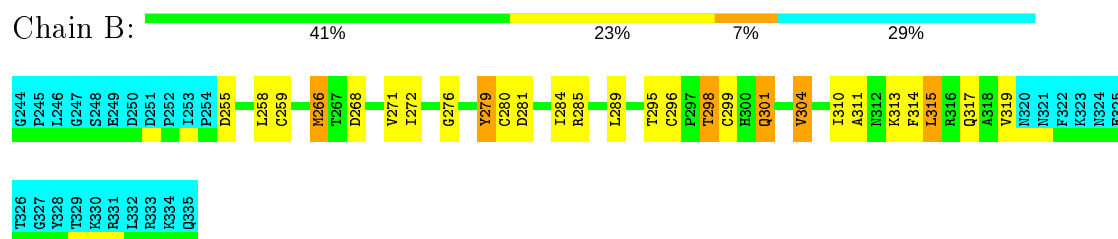


4.2.17 Score per residue for model 17 (medoid)

- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

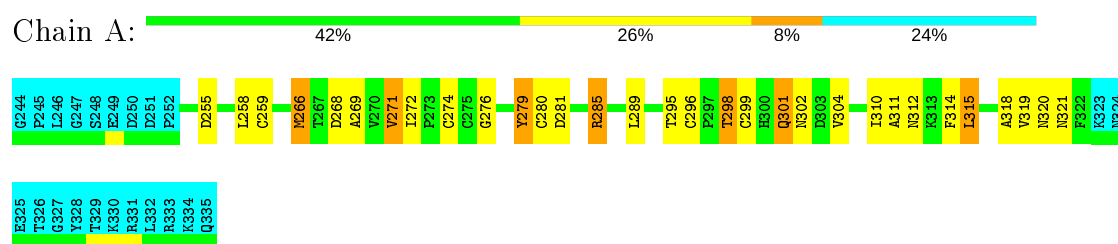


- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

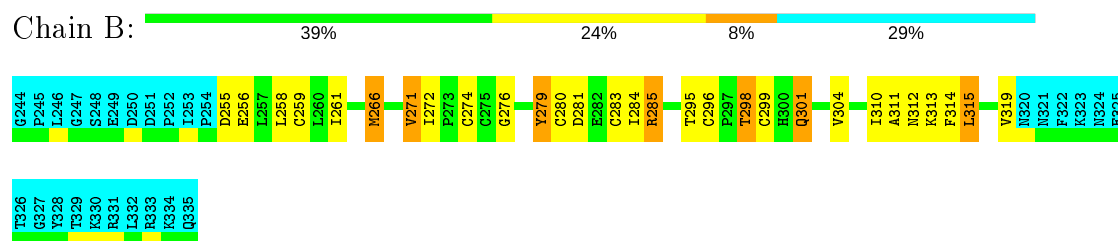


4.2.18 Score per residue for model 18

- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

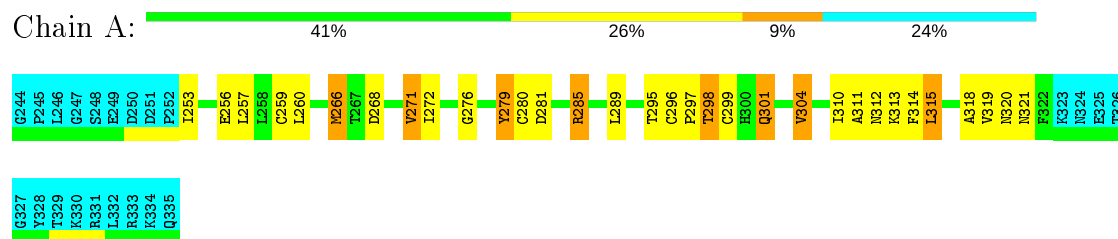


- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

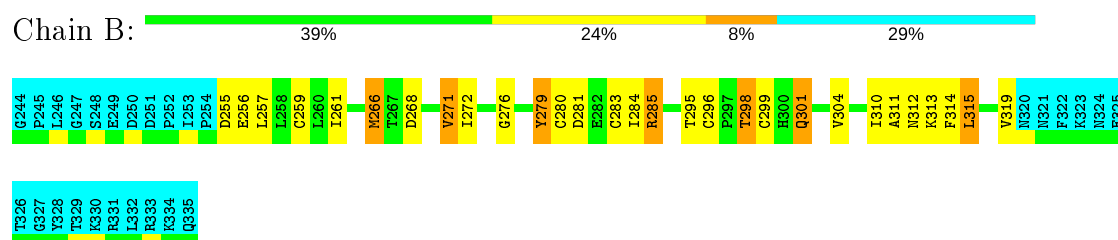


4.2.19 Score per residue for model 19

- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

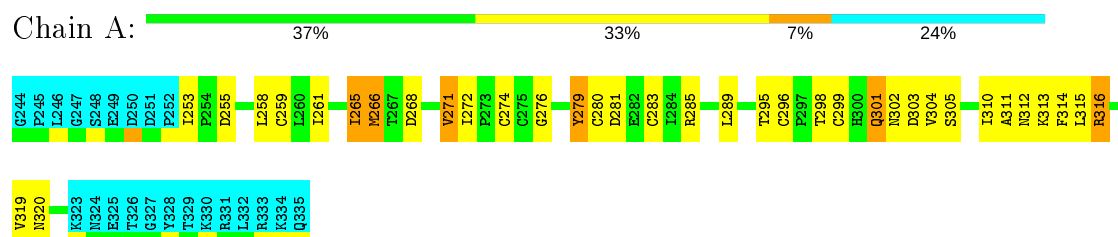


- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

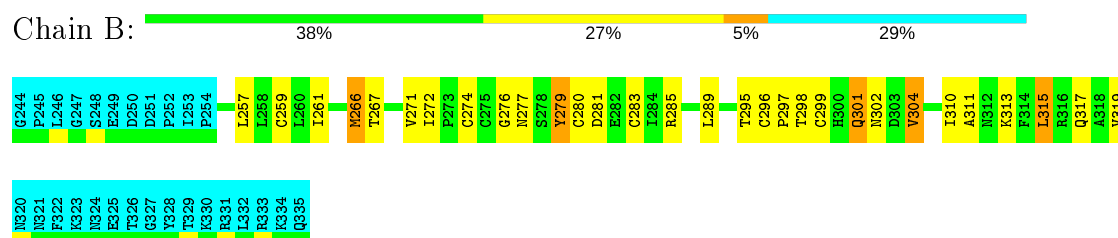


4.2.20 Score per residue for model 20

- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

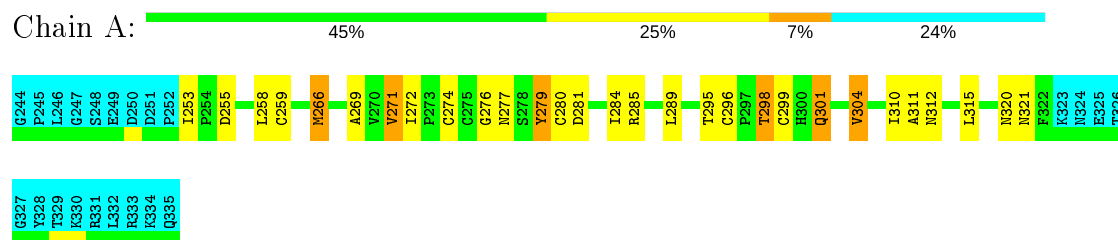


- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

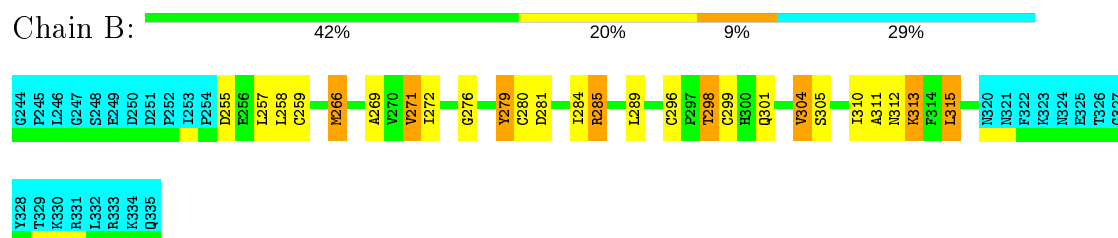


4.2.21 Score per residue for model 21

- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

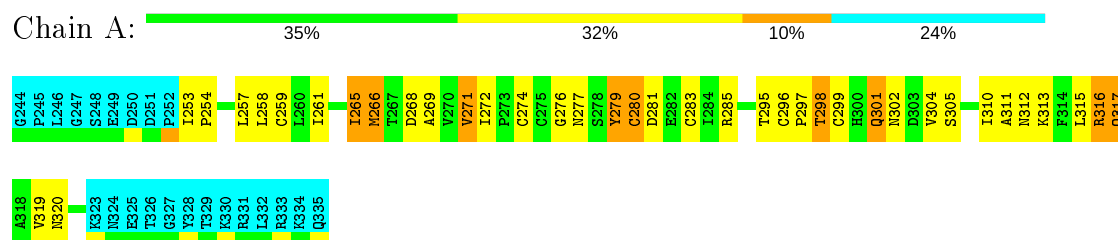


- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

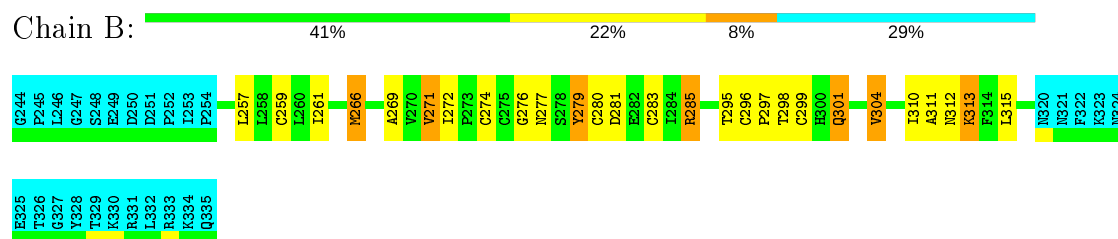


4.2.22 Score per residue for model 22

- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

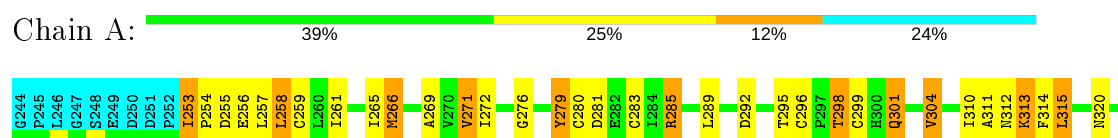


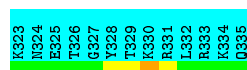
- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6



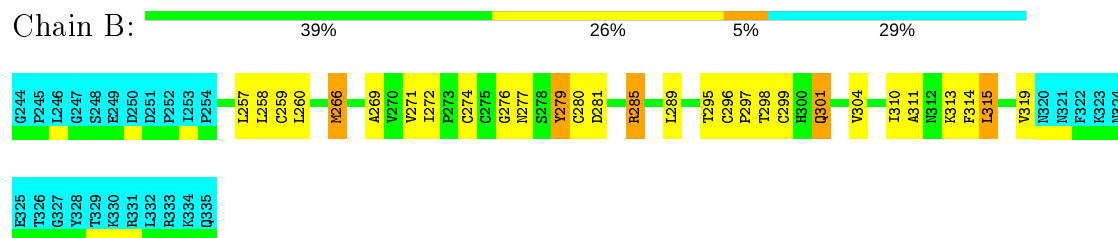
4.2.23 Score per residue for model 23

- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6



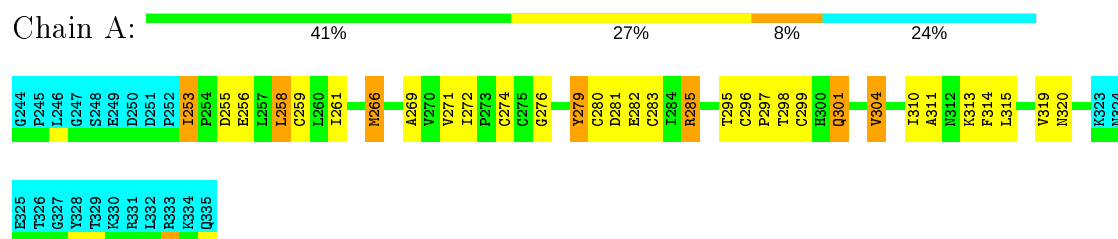


- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

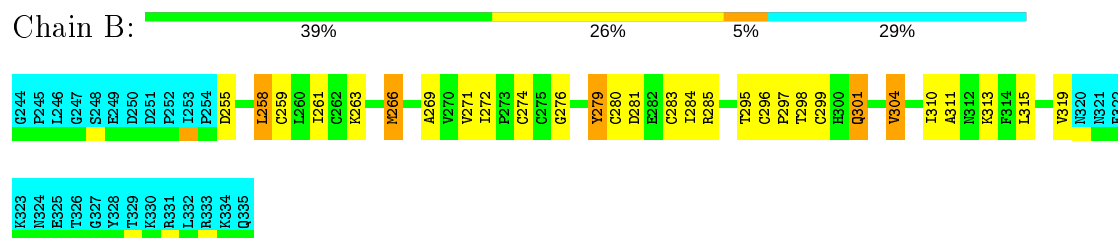


4.2.24 Score per residue for model 24

- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

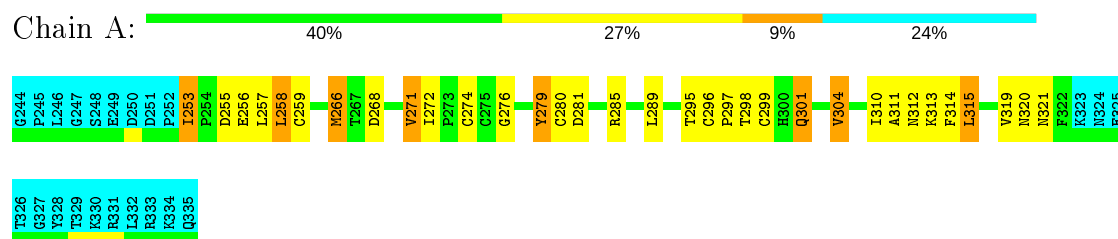


- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

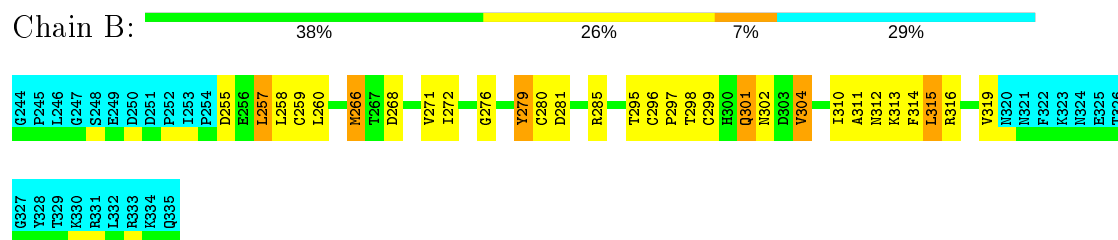


4.2.25 Score per residue for model 25

- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

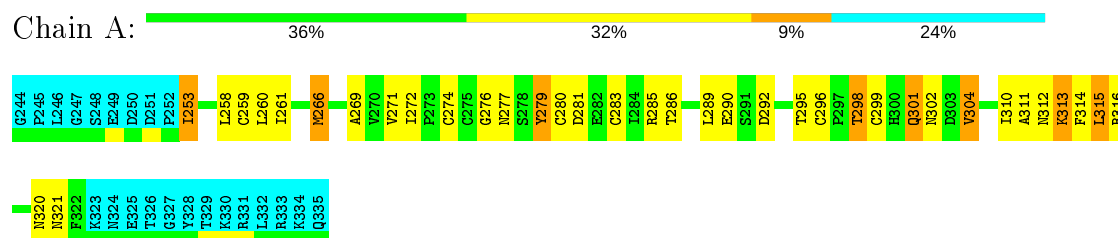


- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

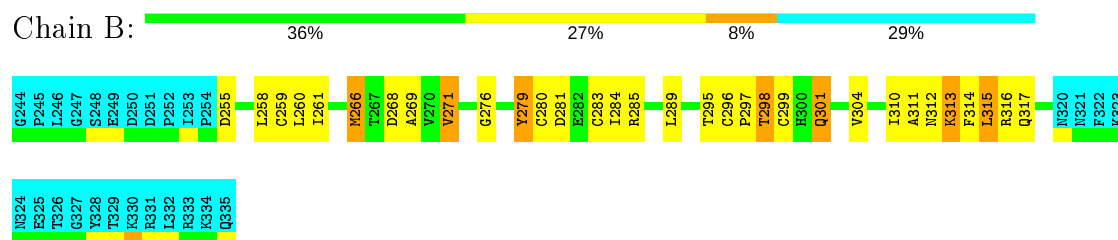


4.2.26 Score per residue for model 26

- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

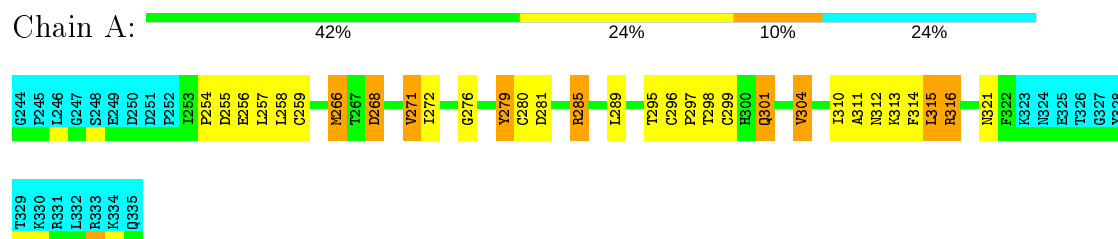


- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

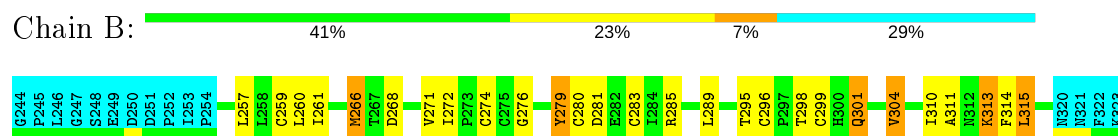


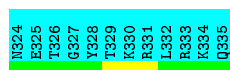
4.2.27 Score per residue for model 27

- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6



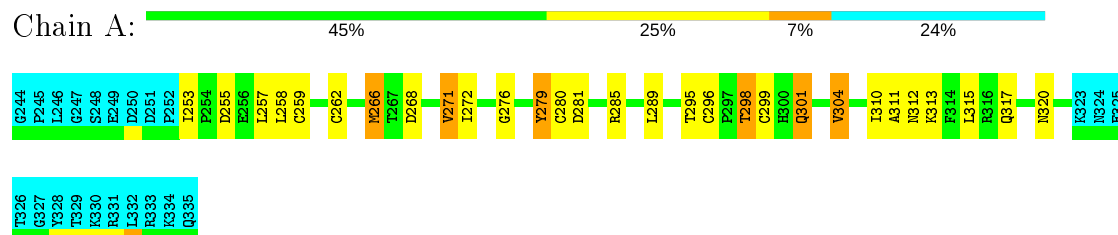
- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6



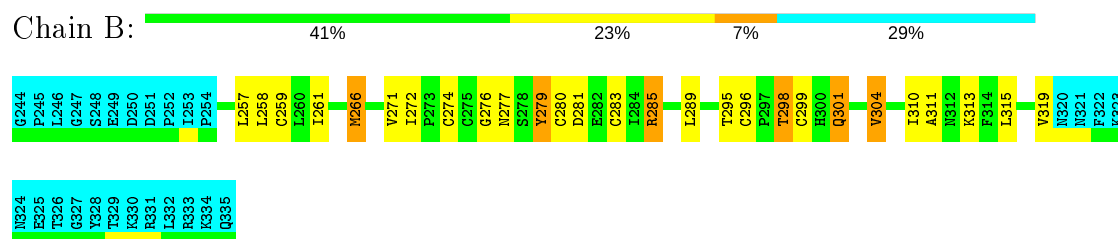


4.2.28 Score per residue for model 28

- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

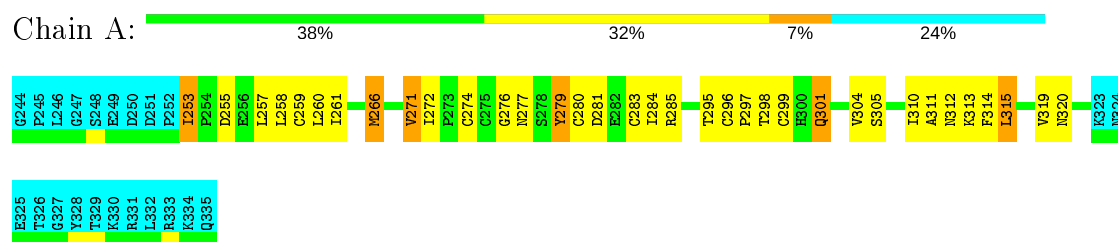


- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

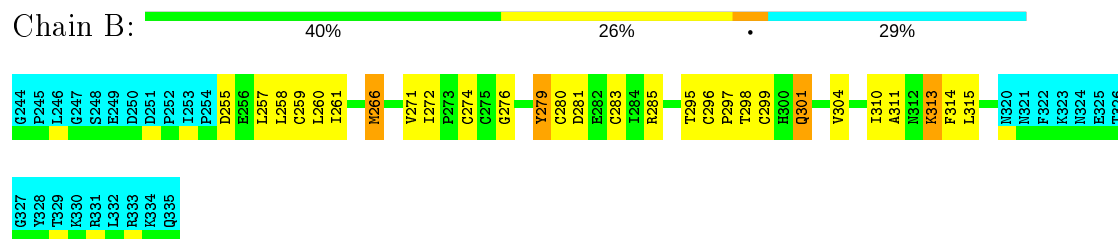


4.2.29 Score per residue for model 29

- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

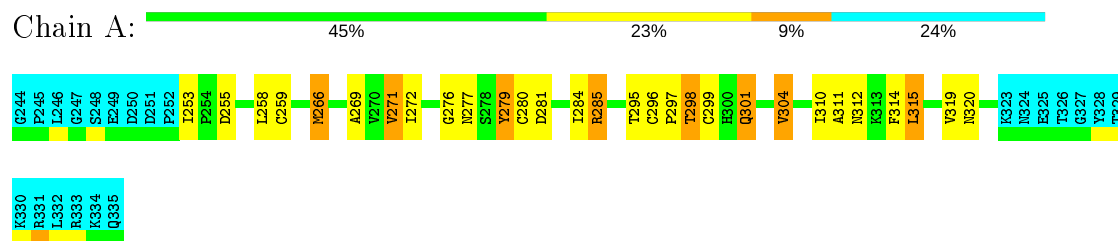


- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

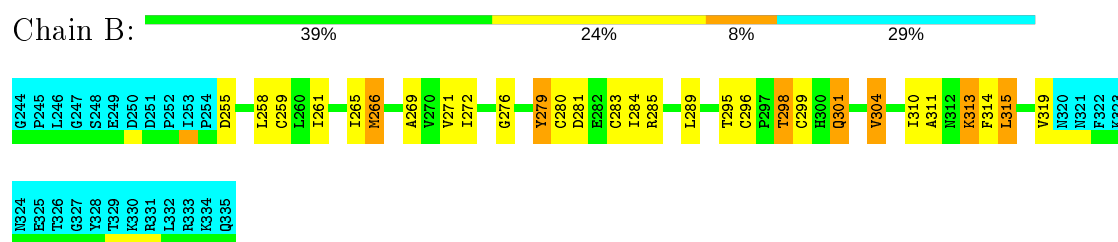


4.2.30 Score per residue for model 30

- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

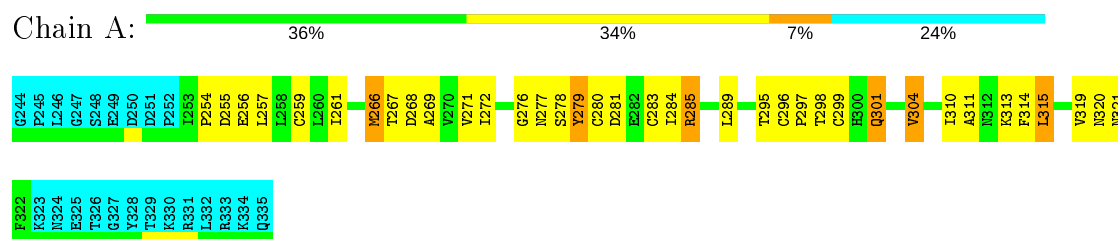


- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

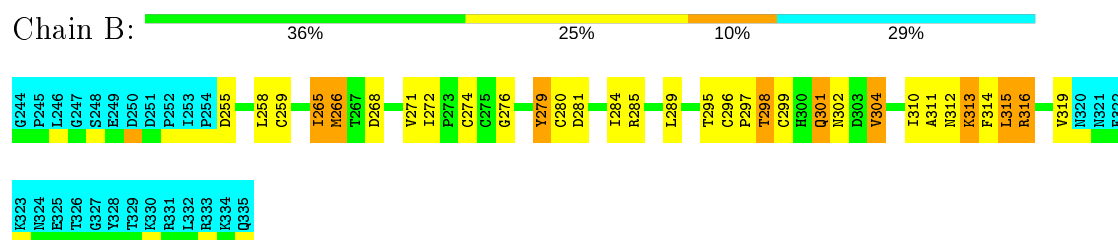


4.2.31 Score per residue for model 31

- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

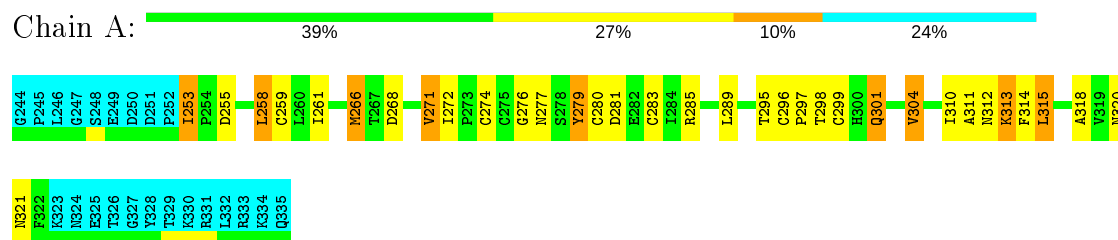


- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

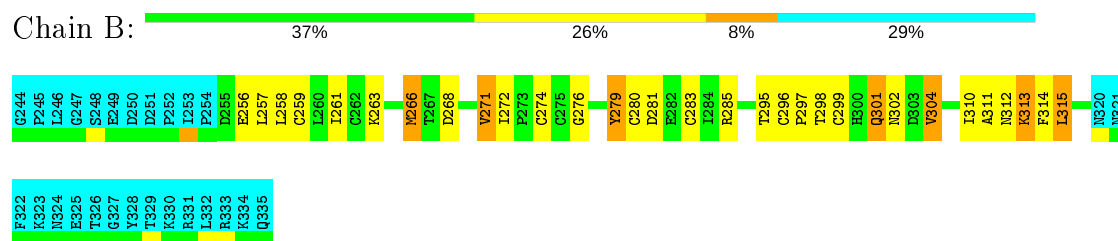


4.2.32 Score per residue for model 32

- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6



● Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6



5 Refinement protocol and experimental data overview

The models were refined using the following method: *CYANA FOLLOWED BY HADDOCK*.

Of the 400 calculated structures, 32 were deposited, based on the following criterion: *HADDOCK ENERGY*, *RAMACHANDRAN QUALITY*.

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

Software name	Classification	Version
CNS	refinement	2.1
CYANA	structure solution	
NMRVIEW	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)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	1027
Number of shifts mapped to atoms	1027
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	44%

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

6 Model quality ⓘ

6.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section:
ZN

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	535	454	510	20±3
1	B	493	420	471	19±2
All	All	33024	27968	31392	1118

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 17.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:266:MET:HB3	1:A:280:CYS:SG	0.80	2.15	31	32
1:B:266:MET:HB3	1:B:280:CYS:SG	0.80	2.16	20	32
1:B:296:CYS:SG	1:B:298:THR:HG22	0.75	2.21	24	32
1:A:271:VAL:HG22	1:A:312:ASN:HB2	0.75	1.57	28	24
1:A:296:CYS:SG	1:A:298:THR:HG22	0.74	2.23	3	32
1:A:253:ILE:HB	1:A:258:LEU:HD23	0.72	1.60	20	2
1:B:295:THR:HA	1:B:301:GLN:O	0.69	1.87	13	31
1:B:271:VAL:HG22	1:B:312:ASN:HB2	0.69	1.63	10	15
1:A:285:ARG:O	1:A:289:LEU:HG	0.67	1.90	23	19
1:A:261:ILE:HD12	1:A:283:CYS:HB3	0.66	1.68	22	18
1:A:295:THR:HA	1:A:301:GLN:O	0.66	1.90	2	32

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:285:ARG:O	1:B:289:LEU:HG	0.65	1.91	4	18
1:B:259:CYS:SG	1:B:279:TYR:HB3	0.65	2.31	13	32
1:B:284:ILE:O	1:B:288:LEU:HD23	0.65	1.90	6	1
1:A:311:ALA:O	1:B:276:GLY:HA3	0.63	1.93	8	32
1:B:269:ALA:HB3	1:B:315:LEU:HD12	0.61	1.72	15	4
1:B:257:LEU:HA	1:B:315:LEU:HD21	0.61	1.72	5	3
1:A:260:LEU:HD12	1:A:279:TYR:CE2	0.61	2.30	10	1
1:A:276:GLY:HA3	1:B:311:ALA:O	0.61	1.96	11	32
1:B:272:ILE:HD12	1:B:284:ILE:HD11	0.61	1.73	10	18
1:A:272:ILE:HD12	1:A:284:ILE:HD11	0.60	1.72	16	13
1:B:272:ILE:HD11	1:B:304:VAL:HG11	0.60	1.70	21	14
1:A:253:ILE:HB	1:A:258:LEU:HD13	0.60	1.72	26	12
1:A:318:ALA:HA	1:B:256:GLU:OE1	0.60	1.96	11	1
1:A:259:CYS:SG	1:A:279:TYR:HB3	0.60	2.37	24	30
1:B:261:ILE:HD12	1:B:283:CYS:HB3	0.59	1.73	22	23
1:A:318:ALA:HA	1:B:256:GLU:OE2	0.59	1.98	14	8
1:A:269:ALA:HB3	1:A:315:LEU:HD12	0.58	1.75	5	3
1:A:281:ASP:O	1:A:285:ARG:HB2	0.58	1.98	9	32
1:A:313:LYS:HD3	1:B:277:ASN:OD1	0.58	1.99	9	8
1:B:281:ASP:O	1:B:285:ARG:HB2	0.57	1.99	10	32
1:A:315:LEU:HD21	1:B:314:PHE:CD2	0.57	2.34	4	19
1:A:314:PHE:CD2	1:B:315:LEU:HD21	0.56	2.35	27	17
1:A:315:LEU:HD21	1:B:314:PHE:HD2	0.55	1.59	2	8
1:B:266:MET:O	1:B:319:VAL:HG11	0.55	2.01	5	20
1:A:272:ILE:HG12	1:A:274:CYS:SG	0.54	2.43	24	19
1:A:266:MET:O	1:A:319:VAL:HG11	0.54	2.03	24	16
1:A:254:PRO:O	1:A:258:LEU:HB2	0.54	2.02	17	5
1:A:313:LYS:HA	1:A:316:ARG:CD	0.53	2.34	10	3
1:B:272:ILE:HG12	1:B:274:CYS:SG	0.52	2.45	6	22
1:A:272:ILE:HD11	1:A:304:VAL:HG11	0.51	1.81	16	13
1:A:268:ASP:HA	1:A:316:ARG:NH1	0.50	2.21	8	2
1:A:314:PHE:HD2	1:B:315:LEU:HD21	0.50	1.66	27	5
1:A:257:LEU:HA	1:A:315:LEU:HD21	0.50	1.83	5	1
1:A:277:ASN:OD1	1:B:313:LYS:HD3	0.49	2.06	30	9
1:B:266:MET:SD	1:B:315:LEU:HD11	0.49	2.47	8	2
1:A:266:MET:SD	1:A:315:LEU:HD11	0.49	2.48	8	2
1:A:298:THR:CG2	1:A:299:CYS:N	0.49	2.75	2	32
1:A:313:LYS:O	1:A:317:GLN:HG2	0.49	2.08	14	1
1:B:298:THR:CG2	1:B:299:CYS:N	0.49	2.76	25	31
1:B:296:CYS:SG	1:B:297:PRO:HD2	0.49	2.48	13	21
1:A:296:CYS:SG	1:A:297:PRO:HD2	0.49	2.47	25	21

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:314:PHE:CD1	1:B:314:PHE:N	0.48	2.81	25	10
1:A:253:ILE:O	1:A:258:LEU:HD12	0.48	2.07	17	1
1:A:313:LYS:HA	1:A:316:ARG:HD2	0.48	1.86	10	2
1:A:311:ALA:HB1	1:A:316:ARG:HH21	0.48	1.68	27	1
1:A:266:MET:SD	1:A:269:ALA:HB2	0.48	2.48	26	16
1:A:314:PHE:CD1	1:A:314:PHE:N	0.47	2.82	15	7
1:A:255:ASP:OD1	1:B:317:GLN:HG3	0.47	2.09	17	2
1:A:261:ILE:CD1	1:A:283:CYS:HB3	0.47	2.39	22	1
1:A:272:ILE:CG1	1:A:304:VAL:HG11	0.47	2.39	7	13
1:A:259:CYS:HB2	1:A:266:MET:CG	0.47	2.40	2	14
1:B:257:LEU:HA	1:B:315:LEU:CD2	0.47	2.39	8	1
1:B:272:ILE:CD1	1:B:304:VAL:HG11	0.47	2.40	21	1
1:A:254:PRO:HB2	1:A:256:GLU:OE1	0.46	2.09	7	5
1:A:256:GLU:OE1	1:B:318:ALA:HA	0.46	2.09	13	1
1:B:298:THR:HG23	1:B:299:CYS:N	0.46	2.26	4	15
1:B:272:ILE:CG1	1:B:304:VAL:HG11	0.46	2.40	3	16
1:B:313:LYS:HA	1:B:316:ARG:HD2	0.46	1.88	26	2
1:B:274:CYS:HB3	1:B:304:VAL:HG13	0.46	1.88	1	1
1:A:314:PHE:N	1:A:314:PHE:CD1	0.46	2.83	4	7
1:A:312:ASN:ND2	1:A:315:LEU:HB2	0.46	2.26	15	2
1:B:266:MET:SD	1:B:269:ALA:HB2	0.45	2.52	13	12
1:B:314:PHE:N	1:B:314:PHE:CD1	0.45	2.84	9	8
1:A:253:ILE:CG2	1:A:265:ILE:HD12	0.45	2.41	20	1
1:B:261:ILE:HG13	1:B:279:TYR:CD2	0.45	2.47	10	1
1:B:259:CYS:HB2	1:B:266:MET:CG	0.45	2.41	10	13
1:A:313:LYS:O	1:A:317:GLN:HB2	0.45	2.11	22	1
1:B:313:LYS:O	1:B:317:GLN:HG2	0.45	2.12	14	1
1:B:279:TYR:OH	1:B:298:THR:HG21	0.45	2.12	1	5
1:B:285:ARG:O	1:B:289:LEU:HD13	0.45	2.11	11	2
1:B:312:ASN:CG	1:B:315:LEU:HB2	0.44	2.33	25	3
1:A:312:ASN:CG	1:A:315:LEU:HB2	0.44	2.33	14	6
1:A:260:LEU:HD12	1:A:279:TYR:HE2	0.44	1.73	29	3
1:A:256:GLU:OE2	1:B:318:ALA:HA	0.44	2.12	3	1
1:A:254:PRO:O	1:A:258:LEU:HB3	0.44	2.12	6	2
1:A:313:LYS:HB3	1:A:313:LYS:NZ	0.44	2.25	8	3
1:B:280:CYS:O	1:B:284:ILE:HG22	0.44	2.13	6	5
1:A:313:LYS:NZ	1:A:313:LYS:HB3	0.43	2.28	4	2
1:A:298:THR:HG23	1:A:299:CYS:N	0.43	2.28	19	17
1:A:279:TYR:OH	1:A:298:THR:HG21	0.43	2.13	32	8
1:B:261:ILE:CD1	1:B:283:CYS:HB3	0.43	2.42	10	1
1:A:312:ASN:O	1:A:316:ARG:HG2	0.43	2.14	26	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:253:ILE:HD12	1:A:265:ILE:HB	0.43	1.90	15	1
1:A:253:ILE:HB	1:A:258:LEU:CD1	0.42	2.43	25	2
1:B:314:PHE:N	1:B:314:PHE:HD1	0.42	2.12	25	1
1:B:312:ASN:ND2	1:B:315:LEU:HB2	0.42	2.29	8	1
1:B:269:ALA:HB3	1:B:315:LEU:CD1	0.42	2.43	15	1
1:A:253:ILE:HG21	1:A:265:ILE:HB	0.42	1.91	23	1
1:A:257:LEU:HA	1:A:315:LEU:CD2	0.42	2.45	5	1
1:B:260:LEU:HD12	1:B:279:TYR:HE2	0.41	1.75	15	3
1:A:312:ASN:ND2	1:A:315:LEU:HD23	0.41	2.31	27	1
1:B:313:LYS:NZ	1:B:313:LYS:HB3	0.41	2.28	27	1
1:A:279:TYR:OH	1:A:298:THR:CG2	0.41	2.69	22	13
1:A:286:THR:O	1:A:290:GLU:HG3	0.41	2.15	26	1
1:B:288:LEU:N	1:B:288:LEU:CD2	0.41	2.84	6	1
1:B:257:LEU:HA	1:B:315:LEU:HD11	0.41	1.91	21	2
1:B:279:TYR:OH	1:B:298:THR:CG2	0.41	2.69	4	5
1:B:296:CYS:HB3	1:B:301:GLN:H	0.41	1.75	10	1
1:A:314:PHE:HD1	1:A:314:PHE:N	0.41	2.13	15	1
1:A:285:ARG:O	1:A:289:LEU:HD13	0.41	2.16	4	1
1:B:304:VAL:HG12	1:B:305:SER:H	0.41	1.75	21	1
1:B:259:CYS:SG	1:B:261:ILE:HB	0.41	2.56	16	1
1:A:259:CYS:HB2	1:A:266:MET:HG3	0.41	1.93	2	2
1:A:261:ILE:HG13	1:A:279:TYR:CD2	0.40	2.50	10	1
1:A:260:LEU:HD13	1:A:298:THR:OG1	0.40	2.15	10	1
1:A:253:ILE:CD1	1:A:265:ILE:HB	0.40	2.46	3	1
1:A:256:GLU:HG2	1:B:318:ALA:CA	0.40	2.47	9	1
1:A:269:ALA:HB3	1:A:315:LEU:CD1	0.40	2.46	15	1
1:A:314:PHE:CB	1:B:315:LEU:HD21	0.40	2.47	16	1
1:A:253:ILE:CB	1:A:258:LEU:HD23	0.40	2.38	20	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	70/92 (76%)	62±1 (88±1%)	7±1 (11±1%)	1±1 (1±1%)	18	66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	65/92 (71%)	57±1 (87±1%)	8±1 (12±2%)	1±0 (1±1%)	21	69
All	All	4320/5888 (73%)	3796 (88%)	482 (11%)	42 (1%)	20	68

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

Mol	Chain	Res	Type	Models (Total)
1	A	298	THR	21
1	B	298	THR	18
1	A	304	VAL	2
1	A	303	ASP	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	64/83 (77%)	50±2 (78±2%)	14±2 (22±2%)	3	29
1	B	59/83 (71%)	48±1 (81±2%)	11±1 (19±2%)	4	36
All	All	3936/5312 (74%)	3122 (79%)	814 (21%)	3	32

All 59 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	B	301	GLN	32
1	B	279	TYR	32
1	B	266	MET	32
1	B	304	VAL	32
1	A	301	GLN	32
1	A	271	VAL	32
1	A	266	MET	32
1	B	310	ILE	32
1	B	271	VAL	32
1	B	313	LYS	32
1	A	279	TYR	32
1	A	310	ILE	32

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Mol	Chain	Res	Type	Models (Total)
1	A	304	VAL	32
1	A	315	LEU	29
1	A	320	ASN	28
1	B	315	LEU	28
1	A	255	ASP	28
1	A	258	LEU	21
1	A	313	LYS	20
1	A	253	ILE	20
1	A	268	ASP	18
1	A	321	ASN	17
1	B	257	LEU	17
1	B	255	ASP	17
1	A	257	LEU	15
1	B	268	ASP	14
1	B	258	LEU	13
1	A	302	ASN	11
1	A	285	ARG	9
1	A	316	ARG	7
1	B	285	ARG	7
1	A	256	GLU	6
1	B	267	THR	6
1	B	260	LEU	6
1	B	302	ASN	6
1	A	260	LEU	5
1	A	292	ASP	4
1	A	267	THR	4
1	A	305	SER	4
1	B	263	LYS	4
1	B	256	GLU	4
1	A	263	LYS	3
1	A	265	ILE	3
1	A	317	GLN	3
1	A	262	CYS	3
1	B	316	ARG	2
1	B	305	SER	2
1	A	298	THR	2
1	B	317	GLN	2
1	A	314	PHE	1
1	B	292	ASP	1
1	B	288	LEU	1
1	A	282	GLU	1
1	A	278	SER	1

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Mol	Chain	Res	Type	Models (Total)
1	A	280	CYS	1
1	B	265	ILE	1
1	B	291	SER	1
1	B	278	SER	1
1	B	298	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](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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 44% for the well-defined parts and 42% for the entire structure.

7.1 Chemical shift list 1

File name: input_cs.cif

Chemical shift list name: *rring-new.bmr.b.csh*

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	1027
Number of shifts mapped to atoms	1027
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	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
$^{13}\text{C}_\alpha$	92	-0.40 ± 0.17	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	88	-0.09 ± 0.19	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	83	-1.00 ± 0.19	Should be applied

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 44%, i.e. 688 atoms were assigned a chemical shift out of a possible 1557. 11 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	268/661 (41%)	134/263 (51%)	70/270 (26%)	64/128 (50%)
Sidechain	392/829 (47%)	241/481 (50%)	142/320 (44%)	9/28 (32%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	28/67 (42%)	18/39 (46%)	10/28 (36%)	0/0 (—%)
Overall	688/1557 (44%)	393/783 (50%)	222/618 (36%)	73/156 (47%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 42%, i.e. 908 atoms were assigned a chemical shift out of a possible 2180. 13 out of 26 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	350/896 (39%)	175/356 (49%)	92/368 (25%)	83/172 (48%)
Sidechain	524/1192 (44%)	323/698 (46%)	188/442 (43%)	13/52 (25%)
Aromatic	34/92 (37%)	22/52 (42%)	12/40 (30%)	0/0 (—%)
Overall	908/2180 (42%)	520/1106 (47%)	292/850 (34%)	96/224 (43%)

7.1.4 Statistically unusual chemical shifts ⓘ

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	335	GLN	CD	21.34	186.62 – 172.72	-113.9

7.1.5 Random Coil Index (RCI) plots ⓘ

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 A:

