



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 06:40 PM BST

PDB ID : 1YXE
Title : Structure and inter-domain interactions of domain II from the blood stage malarial protein, apical membrane antigen 1
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Deposited on : 2005-02-21

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

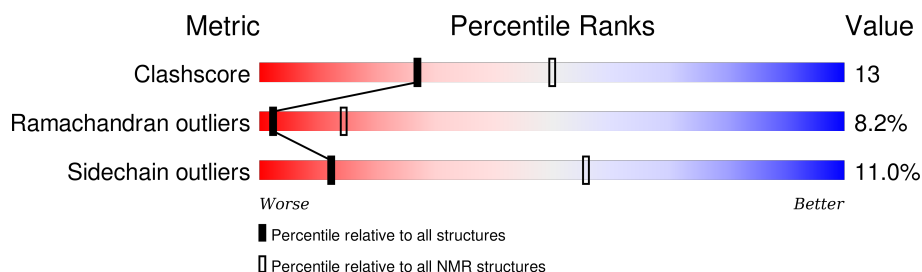
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 67%.

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	140	<div> <div>25%</div> <div>14%</div> <div>61%</div> </div>

2 Ensemble composition and analysis

This entry contains 20 models. Model 11 is the overall representative, medoid model (most similar to other models). The authors have identified model 12 as representative, based on the following criterion: *closest to the average*.

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:320-A:344, A:398-A:427 (55)	1.42	11

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

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

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

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2186 atoms, of which 1060 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called apical membrane antigen 1.

Mol	Chain	Residues	Atoms						Trace
1	A	140	Total	C	H	N	O	S	0
			2186	711	1060	197	212	6	

There are 12 discrepancies between the modelled and reference sequences:

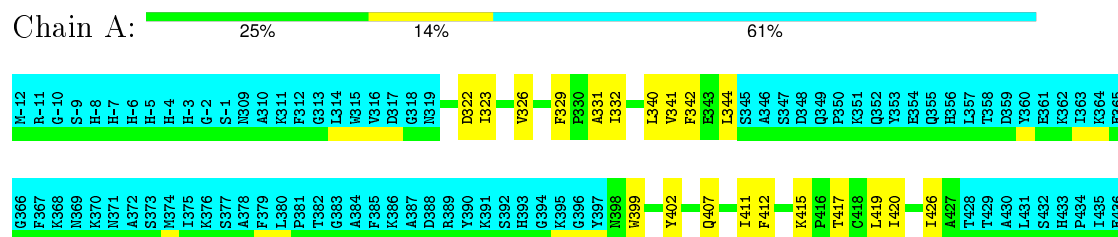
Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	MET	-	EXPRESSION TAG	UNP P22621
A	-11	ARG	-	EXPRESSION TAG	UNP P22621
A	-10	GLY	-	EXPRESSION TAG	UNP P22621
A	-9	SER	-	EXPRESSION TAG	UNP P22621
A	-8	HIS	-	EXPRESSION TAG	UNP P22621
A	-7	HIS	-	EXPRESSION TAG	UNP P22621
A	-6	HIS	-	EXPRESSION TAG	UNP P22621
A	-5	HIS	-	EXPRESSION TAG	UNP P22621
A	-4	HIS	-	EXPRESSION TAG	UNP P22621
A	-3	HIS	-	EXPRESSION TAG	UNP P22621
A	-2	GLY	-	EXPRESSION TAG	UNP P22621
A	-1	SER	-	EXPRESSION TAG	UNP P22621

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: apical membrane antigen 1

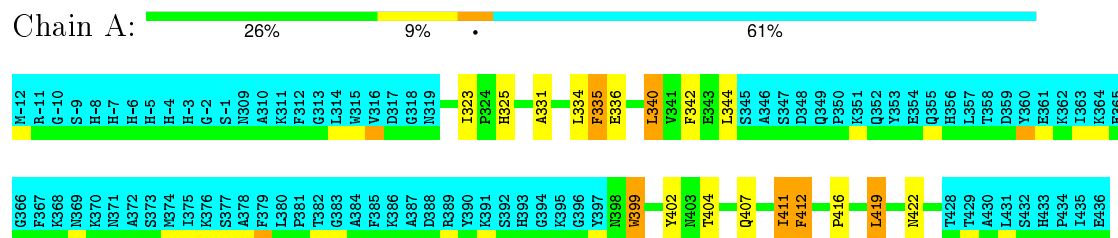


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

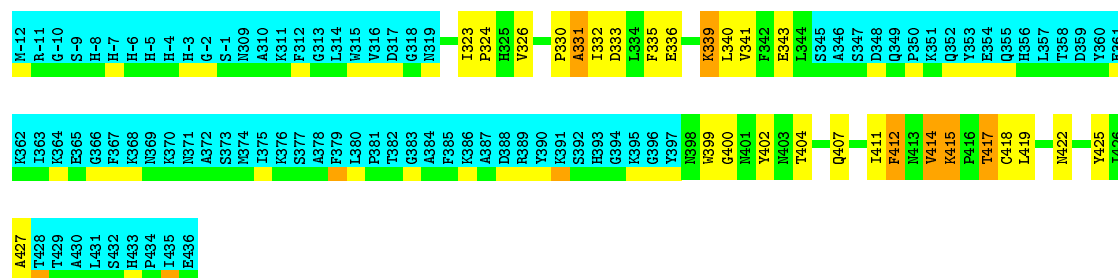
- Molecule 1: apical membrane antigen 1



4.2.2 Score per residue for model 2

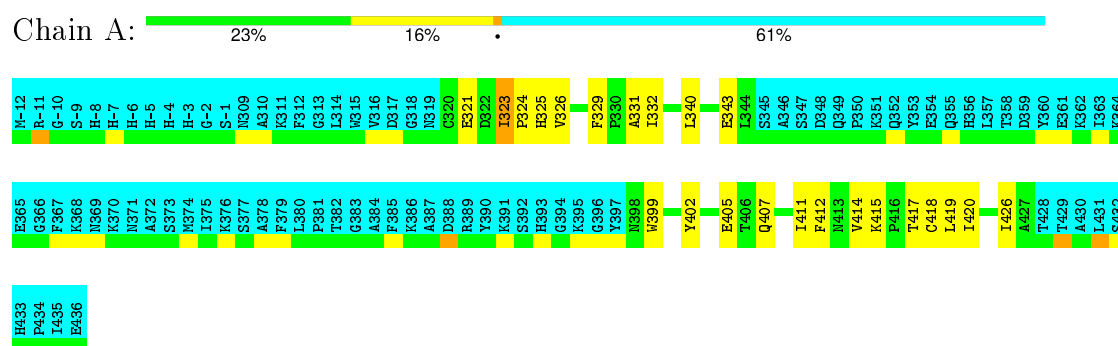
- Molecule 1: apical membrane antigen 1





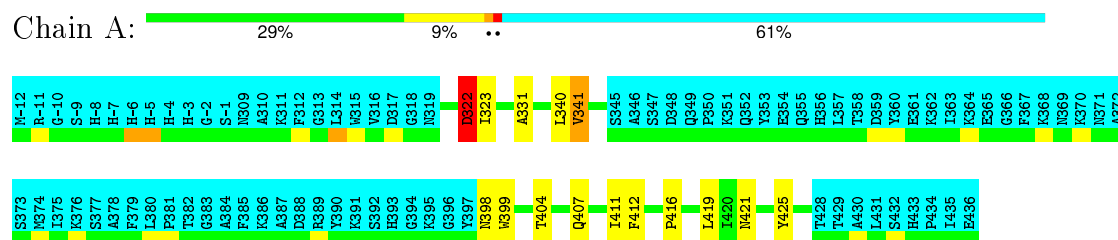
4.2.3 Score per residue for model 3

- Molecule 1: apical membrane antigen 1



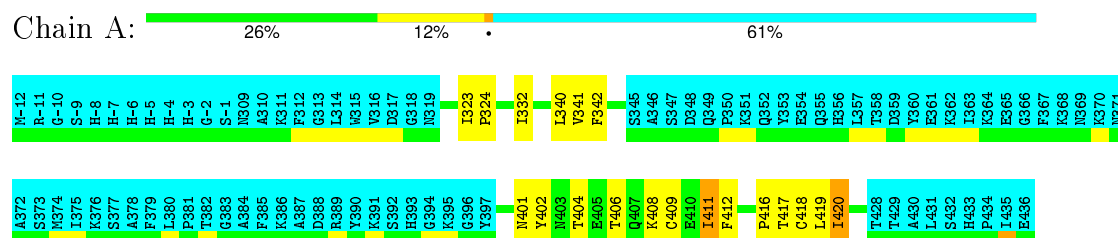
4.2.4 Score per residue for model 4

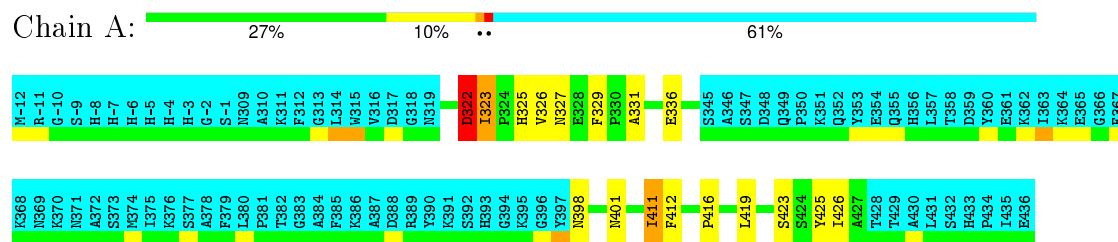
- Molecule 1: apical membrane antigen 1



4.2.5 Score per residue for model 5

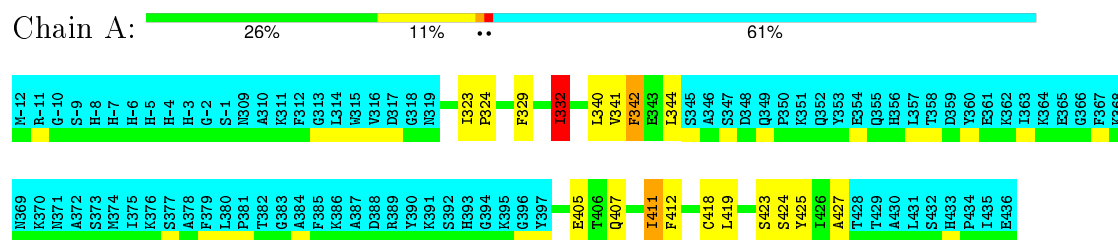
- Molecule 1: apical membrane antigen 1





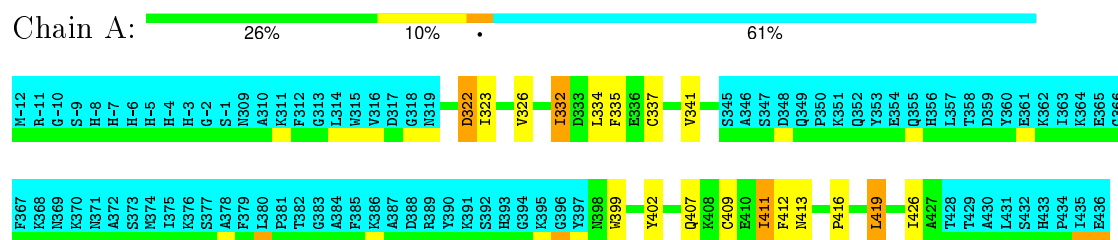
4.2.10 Score per residue for model 10

- Molecule 1: apical membrane antigen 1



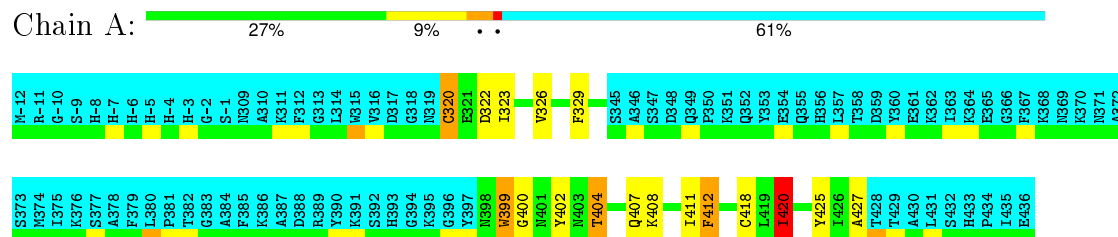
4.2.11 Score per residue for model 11 (medoid)

- Molecule 1: apical membrane antigen 1



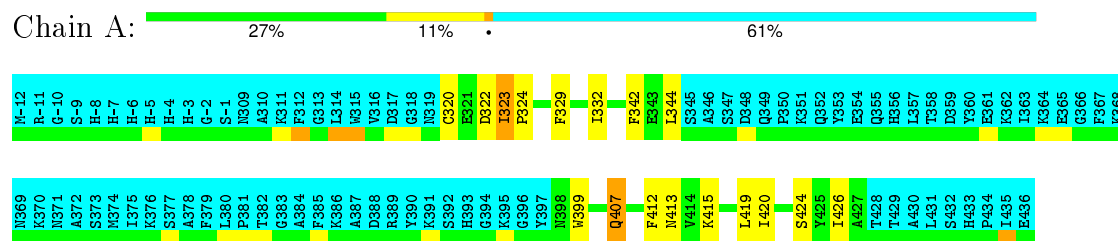
4.2.12 Score per residue for model 12

- Molecule 1: apical membrane antigen 1



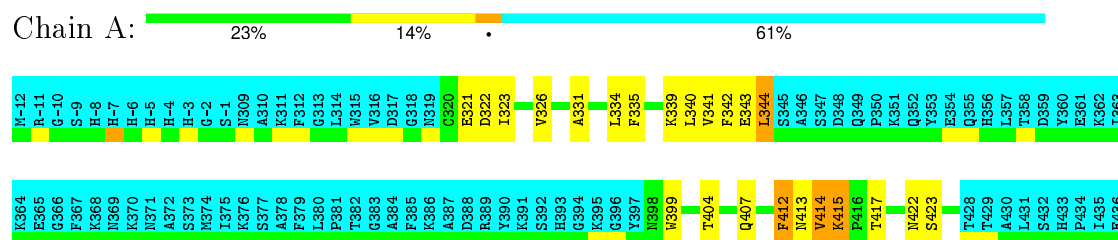
4.2.13 Score per residue for model 13

- Molecule 1: apical membrane antigen 1



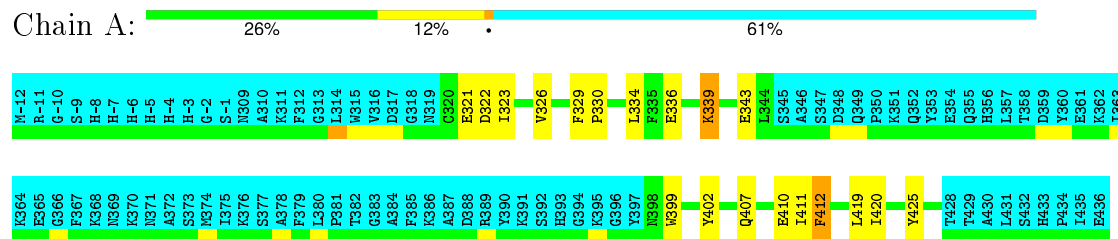
4.2.14 Score per residue for model 14

- Molecule 1: apical membrane antigen 1



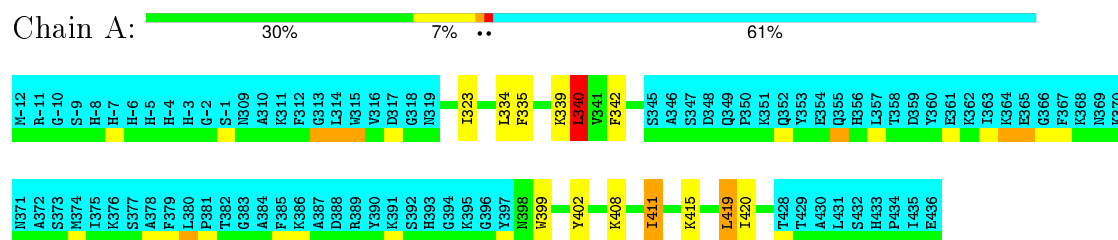
4.2.15 Score per residue for model 15

- Molecule 1: apical membrane antigen 1



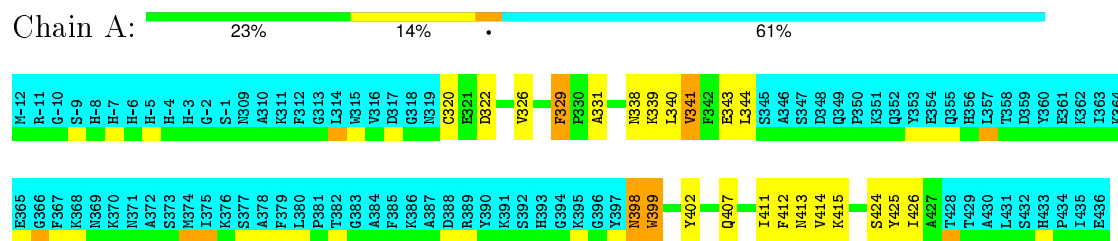
4.2.16 Score per residue for model 16

- Molecule 1: apical membrane antigen 1



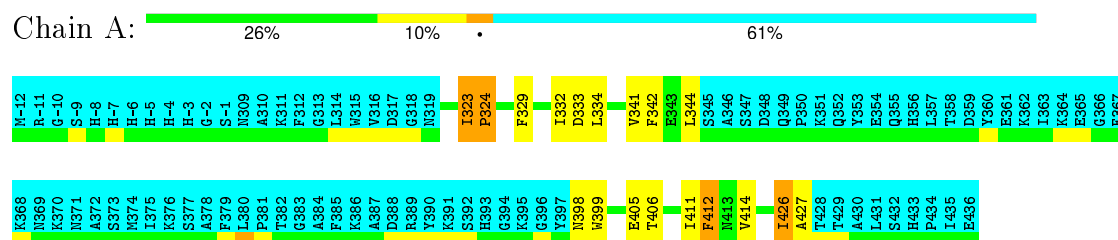
4.2.17 Score per residue for model 17

- Molecule 1: apical membrane antigen 1



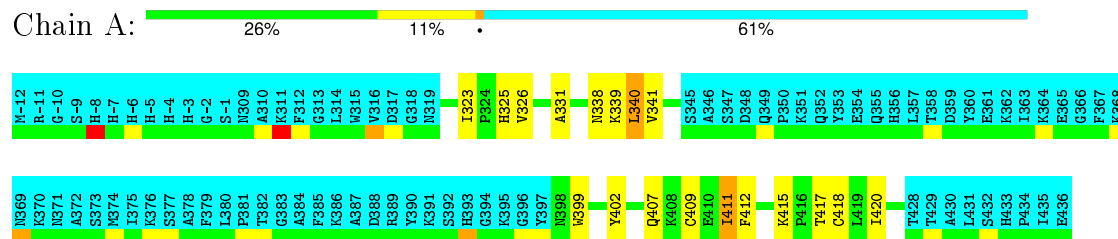
4.2.18 Score per residue for model 18

- Molecule 1: apical membrane antigen 1



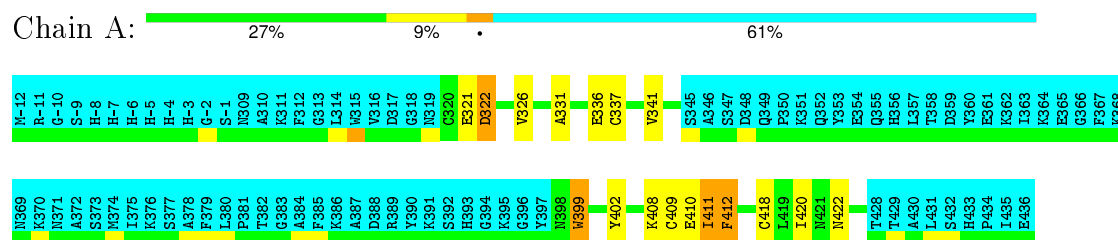
4.2.19 Score per residue for model 19

- Molecule 1: apical membrane antigen 1



4.2.20 Score per residue for model 20

- Molecule 1: apical membrane antigen 1



5 Refinement protocol and experimental data overview

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

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
X-PLOR	structure solution	NIH
X-PLOR	refinement	NIH

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)	BMRB entry 6510
Number of chemical shift lists	1
Total number of shifts	1325
Number of shifts mapped to atoms	1325
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	67%

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

6 Model quality ⓘ

6.1 Standard geometry ⓘ

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	447	417	417	11±4
All	All	8940	8340	8340	225

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 13.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:411:ILE:HD13	1:A:412:PHE:N	0.78	1.92	10	5
1:A:400:GLY:HA3	1:A:411:ILE:HD13	0.78	1.56	2	1
1:A:344:LEU:HD11	1:A:399:TRP:CZ3	0.75	2.16	6	1
1:A:326:VAL:HG12	1:A:412:PHE:CD1	0.73	2.18	2	3
1:A:323:ILE:HG21	1:A:420:ILE:HG21	0.72	1.60	5	1
1:A:326:VAL:HG12	1:A:412:PHE:CB	0.71	2.16	20	5
1:A:323:ILE:HD13	1:A:420:ILE:HG12	0.69	1.62	5	1
1:A:326:VAL:HG12	1:A:412:PHE:CE1	0.67	2.23	2	1
1:A:338:ASN:OD1	1:A:341:VAL:HG11	0.67	1.90	19	1
1:A:419:LEU:N	1:A:419:LEU:HD13	0.67	2.04	1	1
1:A:419:LEU:HD12	1:A:419:LEU:O	0.67	1.90	13	3
1:A:326:VAL:HG12	1:A:412:PHE:CG	0.67	2.24	15	8
1:A:425:TYR:CE2	1:A:427:ALA:HB3	0.66	2.25	12	3
1:A:344:LEU:HD11	1:A:399:TRP:CE3	0.66	2.25	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:400:GLY:CA	1:A:411:ILE:HD13	0.65	2.21	2	2
1:A:340:LEU:HD22	1:A:344:LEU:HD13	0.65	1.69	8	1
1:A:331:ALA:HB3	1:A:407:GLN:CG	0.64	2.21	19	1
1:A:340:LEU:N	1:A:340:LEU:HD13	0.63	2.08	19	1
1:A:340:LEU:HD22	1:A:344:LEU:CD1	0.63	2.24	8	1
1:A:322:ASP:HB3	1:A:323:ILE:HD13	0.63	1.68	9	1
1:A:426:ILE:HD12	1:A:427:ALA:N	0.62	2.08	18	1
1:A:400:GLY:CA	1:A:411:ILE:HG22	0.61	2.25	6	1
1:A:326:VAL:HG21	1:A:410:GLU:OE2	0.60	1.96	20	1
1:A:411:ILE:HD13	1:A:411:ILE:N	0.60	2.12	19	1
1:A:344:LEU:HD23	1:A:344:LEU:O	0.60	1.97	14	1
1:A:411:ILE:N	1:A:411:ILE:HD13	0.60	2.12	5	2
1:A:404:THR:HG21	1:A:408:LYS:CB	0.59	2.27	5	1
1:A:326:VAL:HG12	1:A:412:PHE:HB3	0.58	1.74	20	1
1:A:326:VAL:HG12	1:A:412:PHE:HB2	0.58	1.76	14	2
1:A:340:LEU:HB3	1:A:411:ILE:HG21	0.58	1.72	17	1
1:A:323:ILE:HD13	1:A:324:PRO:O	0.58	1.98	18	1
1:A:339:LYS:C	1:A:340:LEU:HD13	0.58	2.19	19	1
1:A:412:PHE:CE1	1:A:414:VAL:HG21	0.58	2.34	8	1
1:A:332:ILE:HD13	1:A:332:ILE:O	0.57	2.00	10	1
1:A:344:LEU:HD22	1:A:344:LEU:N	0.57	2.14	17	1
1:A:399:TRP:HA	1:A:426:ILE:HD13	0.57	1.75	13	1
1:A:331:ALA:HB3	1:A:407:GLN:HG3	0.56	1.75	19	1
1:A:418:CYS:SG	1:A:420:ILE:HG22	0.56	2.41	12	1
1:A:323:ILE:HG23	1:A:323:ILE:O	0.56	2.01	15	6
1:A:341:VAL:HG23	1:A:341:VAL:O	0.56	2.01	19	1
1:A:323:ILE:O	1:A:323:ILE:HG23	0.56	2.01	10	3
1:A:420:ILE:HG22	1:A:420:ILE:O	0.55	2.02	16	2
1:A:404:THR:HG23	1:A:404:THR:O	0.55	2.02	4	2
1:A:341:VAL:O	1:A:341:VAL:HG22	0.55	2.02	4	3
1:A:411:ILE:H	1:A:411:ILE:HD13	0.55	1.62	16	1
1:A:400:GLY:HA3	1:A:411:ILE:HG22	0.55	1.78	6	2
1:A:326:VAL:HG12	1:A:412:PHE:CD2	0.54	2.37	19	2
1:A:322:ASP:OD2	1:A:323:ILE:HG22	0.54	2.03	12	1
1:A:404:THR:O	1:A:404:THR:HG23	0.54	2.03	1	2
1:A:321:GLU:O	1:A:420:ILE:HD11	0.54	2.03	3	1
1:A:406:THR:O	1:A:406:THR:HG23	0.53	2.04	6	1
1:A:340:LEU:N	1:A:340:LEU:HD22	0.53	2.19	6	1
1:A:340:LEU:HD21	1:A:344:LEU:HD23	0.53	1.80	10	1
1:A:332:ILE:HD13	1:A:409:CYS:HB2	0.52	1.81	5	1
1:A:420:ILE:O	1:A:420:ILE:HG22	0.52	2.04	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:419:LEU:HD13	1:A:419:LEU:H	0.52	1.64	16	1
1:A:425:TYR:CZ	1:A:427:ALA:HB3	0.52	2.40	10	1
1:A:340:LEU:N	1:A:340:LEU:HD12	0.51	2.20	10	1
1:A:341:VAL:O	1:A:341:VAL:HG12	0.51	2.05	2	1
1:A:411:ILE:C	1:A:411:ILE:HD13	0.51	2.25	20	3
1:A:334:LEU:HD12	1:A:334:LEU:C	0.49	2.28	14	1
1:A:410:GLU:C	1:A:411:ILE:HD12	0.49	2.27	15	1
1:A:417:THR:O	1:A:417:THR:HG23	0.49	2.08	19	2
1:A:342:PHE:CD2	1:A:342:PHE:O	0.49	2.66	18	1
1:A:326:VAL:HG11	1:A:417:THR:HG21	0.48	1.83	2	1
1:A:411:ILE:HD13	1:A:411:ILE:C	0.48	2.26	9	2
1:A:332:ILE:HG21	1:A:407:GLN:HG3	0.48	1.85	13	1
1:A:339:LYS:O	1:A:340:LEU:HD22	0.48	2.07	2	2
1:A:323:ILE:HD13	1:A:323:ILE:C	0.48	2.29	18	1
1:A:411:ILE:HD12	1:A:411:ILE:N	0.48	2.23	15	2
1:A:340:LEU:CD1	1:A:344:LEU:HD23	0.48	2.38	1	1
1:A:340:LEU:HD12	1:A:343:GLU:CG	0.47	2.39	3	1
1:A:418:CYS:SG	1:A:420:ILE:HD12	0.47	2.49	3	1
1:A:426:ILE:C	1:A:426:ILE:HD12	0.47	2.30	18	1
1:A:402:TYR:CD1	1:A:402:TYR:N	0.47	2.83	2	5
1:A:334:LEU:HD12	1:A:335:PHE:N	0.47	2.24	14	1
1:A:419:LEU:HD13	1:A:419:LEU:N	0.47	2.24	16	1
1:A:344:LEU:HD21	1:A:399:TRP:CH2	0.47	2.45	6	1
1:A:400:GLY:HA2	1:A:411:ILE:HD13	0.47	1.86	12	1
1:A:401:ASN:ND2	1:A:412:PHE:CE2	0.47	2.83	5	1
1:A:331:ALA:HB1	1:A:336:GLU:HA	0.47	1.87	1	1
1:A:331:ALA:O	1:A:332:ILE:HD13	0.47	2.10	8	1
1:A:326:VAL:CG1	1:A:412:PHE:CE1	0.46	2.98	2	1
1:A:399:TRP:N	1:A:399:TRP:CD1	0.46	2.83	4	2
1:A:402:TYR:N	1:A:402:TYR:CD1	0.46	2.84	3	6
1:A:344:LEU:HD22	1:A:399:TRP:CH2	0.46	2.46	8	1
1:A:404:THR:HG21	1:A:408:LYS:HB2	0.46	1.87	5	2
1:A:412:PHE:CE1	1:A:414:VAL:CG2	0.45	3.00	8	1
1:A:323:ILE:CG2	1:A:420:ILE:HG21	0.45	2.37	5	1
1:A:341:VAL:HG23	1:A:343:GLU:H	0.45	1.70	17	1
1:A:419:LEU:CD1	1:A:419:LEU:N	0.45	2.75	1	1
1:A:411:ILE:HD13	1:A:411:ILE:H	0.45	1.71	19	1
1:A:399:TRP:CD1	1:A:399:TRP:N	0.45	2.84	3	8
1:A:323:ILE:HD13	1:A:420:ILE:CG1	0.45	2.37	5	1
1:A:340:LEU:N	1:A:340:LEU:HD23	0.45	2.27	16	1
1:A:402:TYR:CD2	1:A:409:CYS:CB	0.45	3.00	20	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:411:ILE:N	1:A:411:ILE:CD1	0.45	2.79	16	3
1:A:332:ILE:HD13	1:A:332:ILE:C	0.45	2.31	10	1
1:A:402:TYR:CE1	1:A:425:TYR:CE1	0.45	3.04	15	1
1:A:332:ILE:HG23	1:A:332:ILE:O	0.44	2.12	3	2
1:A:341:VAL:CG1	1:A:399:TRP:CH2	0.44	3.01	19	1
1:A:412:PHE:N	1:A:412:PHE:CD1	0.44	2.84	12	1
1:A:406:THR:O	1:A:407:GLN:C	0.44	2.56	6	1
1:A:329:PHE:CD1	1:A:331:ALA:HB3	0.44	2.47	8	1
1:A:323:ILE:CB	1:A:324:PRO:CD	0.44	2.96	3	1
1:A:417:THR:HG23	1:A:418:CYS:N	0.43	2.28	2	3
1:A:412:PHE:CD1	1:A:412:PHE:N	0.43	2.86	4	1
1:A:332:ILE:HG22	1:A:332:ILE:O	0.43	2.13	8	1
1:A:340:LEU:N	1:A:340:LEU:CD2	0.43	2.81	6	1
1:A:399:TRP:CH2	1:A:411:ILE:HD11	0.43	2.49	11	1
1:A:323:ILE:N	1:A:324:PRO:CD	0.43	2.81	2	1
1:A:326:VAL:CG1	1:A:412:PHE:CD1	0.43	2.99	2	1
1:A:327:ASN:CB	1:A:411:ILE:HD11	0.43	2.44	8	1
1:A:419:LEU:O	1:A:419:LEU:HD12	0.43	2.13	6	1
1:A:340:LEU:O	1:A:399:TRP:CZ2	0.43	2.71	17	1
1:A:412:PHE:CE1	1:A:415:LYS:O	0.43	2.71	2	1
1:A:339:LYS:N	1:A:340:LEU:HD23	0.43	2.28	16	1
1:A:426:ILE:O	1:A:426:ILE:HG22	0.43	2.14	3	2
1:A:411:ILE:N	1:A:411:ILE:HD12	0.42	2.29	3	2
1:A:419:LEU:HD22	1:A:419:LEU:N	0.42	2.29	3	1
1:A:325:HIS:CG	1:A:325:HIS:O	0.42	2.72	1	2
1:A:323:ILE:HB	1:A:324:PRO:CD	0.42	2.45	3	1
1:A:419:LEU:CD2	1:A:419:LEU:N	0.42	2.82	3	1
1:A:341:VAL:HG12	1:A:342:PHE:N	0.42	2.29	18	1
1:A:426:ILE:HG22	1:A:426:ILE:O	0.42	2.15	11	1
1:A:412:PHE:CE2	1:A:413:ASN:ND2	0.42	2.87	14	1
1:A:329:PHE:CE1	1:A:331:ALA:HB3	0.42	2.50	8	1
1:A:398:ASN:O	1:A:426:ILE:HD11	0.42	2.14	18	1
1:A:414:VAL:HG22	1:A:415:LYS:N	0.42	2.30	17	2
1:A:414:VAL:HG12	1:A:415:LYS:N	0.42	2.29	8	2
1:A:412:PHE:CZ	1:A:415:LYS:O	0.42	2.73	2	1
1:A:420:ILE:HG23	1:A:422:ASN:ND2	0.42	2.29	8	1
1:A:402:TYR:CD1	1:A:408:LYS:O	0.41	2.74	6	1
1:A:344:LEU:HD11	1:A:412:PHE:HA	0.41	1.93	18	1
1:A:340:LEU:CD1	1:A:340:LEU:N	0.41	2.79	19	1
1:A:412:PHE:CD2	1:A:413:ASN:OD1	0.41	2.74	17	1
1:A:341:VAL:HG13	1:A:342:PHE:N	0.41	2.30	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:414:VAL:HG12	1:A:426:ILE:HG21	0.41	1.91	7	1
1:A:420:ILE:HG23	1:A:420:ILE:O	0.41	2.16	19	1
1:A:399:TRP:O	1:A:399:TRP:CE3	0.41	2.74	15	2
1:A:414:VAL:HG22	1:A:427:ALA:HA	0.41	1.92	18	1
1:A:399:TRP:CD1	1:A:399:TRP:O	0.41	2.73	12	1
1:A:329:PHE:CD1	1:A:331:ALA:O	0.41	2.74	17	1
1:A:342:PHE:O	1:A:342:PHE:CD2	0.41	2.74	5	1
1:A:425:TYR:CD2	1:A:425:TYR:O	0.41	2.74	9	1
1:A:334:LEU:O	1:A:335:PHE:CD2	0.41	2.74	1	1
1:A:325:HIS:O	1:A:412:PHE:CE1	0.40	2.74	19	1
1:A:335:PHE:O	1:A:335:PHE:CD1	0.40	2.74	11	2
1:A:338:ASN:OD1	1:A:402:TYR:CE2	0.40	2.74	17	1
1:A:341:VAL:HG22	1:A:342:PHE:N	0.40	2.30	14	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	55/140 (39%)	35±3 (64±6%)	16±3 (28±5%)	5±2 (8±3%)	2	14
All	All	1100/2800 (39%)	700 (64%)	310 (28%)	90 (8%)	2	14

All 26 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	407	GLN	14
1	A	412	PHE	10
1	A	322	ASP	6
1	A	416	PRO	6
1	A	331	ALA	6
1	A	324	PRO	4
1	A	417	THR	4
1	A	342	PHE	4
1	A	341	VAL	4

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Mol	Chain	Res	Type	Models (Total)
1	A	399	TRP	3
1	A	332	ILE	3
1	A	343	GLU	3
1	A	420	ILE	3
1	A	426	ILE	3
1	A	414	VAL	2
1	A	336	GLU	2
1	A	330	PRO	2
1	A	398	ASN	2
1	A	413	ASN	2
1	A	335	PHE	1
1	A	427	ALA	1
1	A	323	ILE	1
1	A	339	LYS	1
1	A	340	LEU	1
1	A	423	SER	1
1	A	422	ASN	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	52/122 (43%)	46±1 (89±3%)	6±1 (11±3%)	12	56
All	All	1040/2440 (43%)	926 (89%)	114 (11%)	12	56

All 38 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	329	PHE	10
1	A	411	ILE	9
1	A	415	LYS	6
1	A	334	LEU	6
1	A	419	LEU	5
1	A	339	LYS	5
1	A	344	LEU	5
1	A	340	LEU	5

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Mol	Chain	Res	Type	Models (Total)
1	A	322	ASP	4
1	A	321	GLU	3
1	A	418	CYS	3
1	A	399	TRP	3
1	A	405	GLU	3
1	A	336	GLU	3
1	A	424	SER	3
1	A	335	PHE	3
1	A	323	ILE	3
1	A	320	CYS	3
1	A	423	SER	3
1	A	425	TYR	3
1	A	422	ASN	3
1	A	408	LYS	2
1	A	332	ILE	2
1	A	333	ASP	2
1	A	342	PHE	2
1	A	337	CYS	2
1	A	406	THR	2
1	A	421	ASN	1
1	A	404	THR	1
1	A	325	HIS	1
1	A	410	GLU	1
1	A	398	ASN	1
1	A	343	GLU	1
1	A	420	ILE	1
1	A	401	ASN	1
1	A	409	CYS	1
1	A	327	ASN	1
1	A	413	ASN	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.5 Carbohydrates [i](#)

There are no 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 67% for the well-defined parts and 70% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 6510

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	1325
Number of shifts mapped to atoms	1325
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
$^{13}\text{C}_\alpha$	134	-0.04 ± 0.17	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	122	0.35 ± 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}'$	127	0.14 ± 0.13	None needed (< 0.5 ppm)
^{15}N	128	0.24 ± 0.39	None needed (< 0.5 ppm)

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 67%, i.e. 454 atoms were assigned a chemical shift out of a possible 679. 1 out of 7 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	241/269 (90%)	100/107 (93%)	93/110 (85%)	48/52 (92%)
Sidechain	203/339 (60%)	127/198 (64%)	73/129 (57%)	3/12 (25%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	10/71 (14%)	9/38 (24%)	0/31 (0%)	1/2 (50%)
Overall	454/679 (67%)	236/343 (69%)	166/270 (61%)	52/66 (79%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 70%, i.e. 1210 atoms were assigned a chemical shift out of a possible 1729. 5 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	648/688 (94%)	259/274 (95%)	261/280 (93%)	128/134 (96%)
Sidechain	524/827 (63%)	297/491 (60%)	217/301 (72%)	10/35 (29%)
Aromatic	38/214 (18%)	36/116 (31%)	0/86 (0%)	2/12 (17%)
Overall	1210/1729 (70%)	592/881 (67%)	478/667 (72%)	140/181 (77%)

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	-11	ARG	NE	119.40	92.63 – 76.73	21.8

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:

