



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 03:36 PM UTC

PDB ID : 1YXE / pdb_00001yxe
Title : Structure and inter-domain interactions of domain II from the blood stage malarial protein, apical membrane antigen 1
Authors : Feng, Z.P.; Keizer, D.W.; Stevenson, R.A.; Yao, S.; Babon, J.J.; Murphy, V.J.; Anders, R.F.; Norton, R.S.
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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

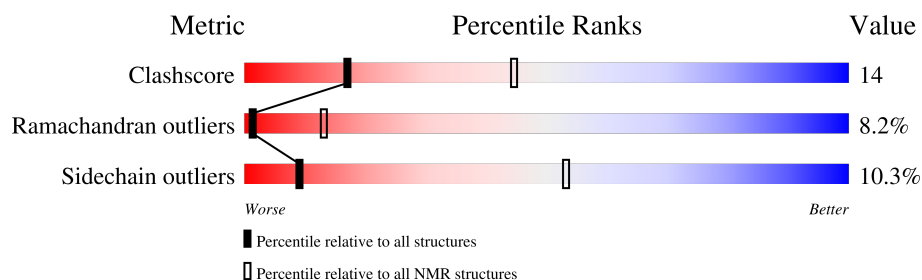
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	140	26% 14% 61%

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)	2.45	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:

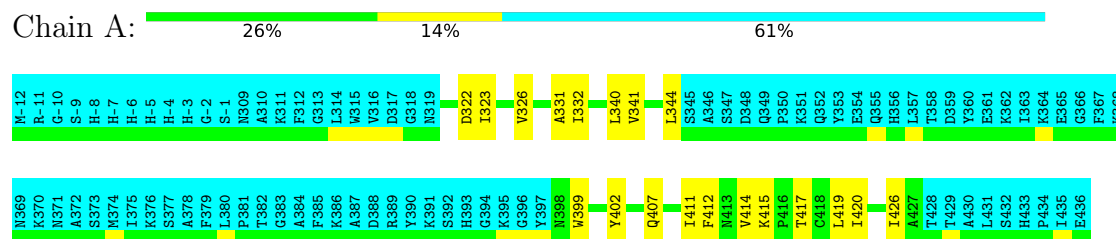
Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	MET	-	expression tag	UNP P22621
A	-11	ARG	-	expression tag	UNP P22621
A	-10	GLY	-	expression tag	UNP P22621
A	-9	SER	-	expression tag	UNP P22621
A	-8	HIS	-	expression tag	UNP P22621
A	-7	HIS	-	expression tag	UNP P22621
A	-6	HIS	-	expression tag	UNP 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, 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: apical membrane antigen 1

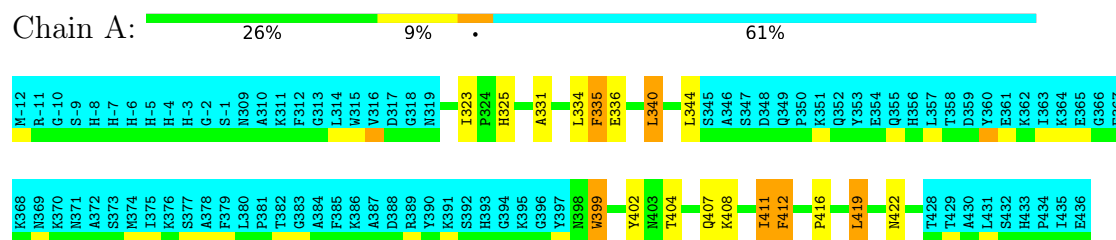


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

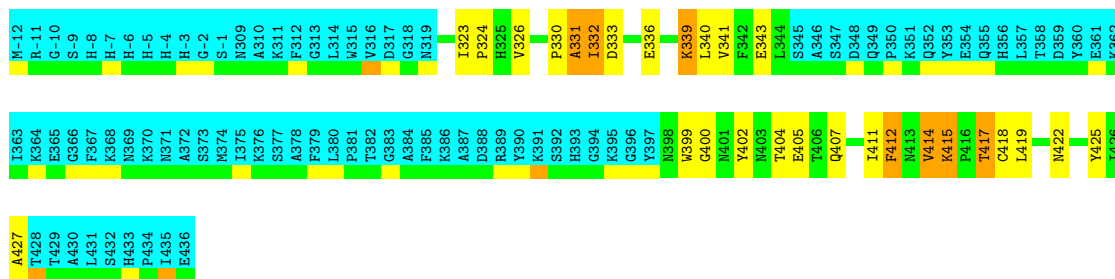
- Molecule 1: apical membrane antigen 1



4.2.2 Score per residue for model 2

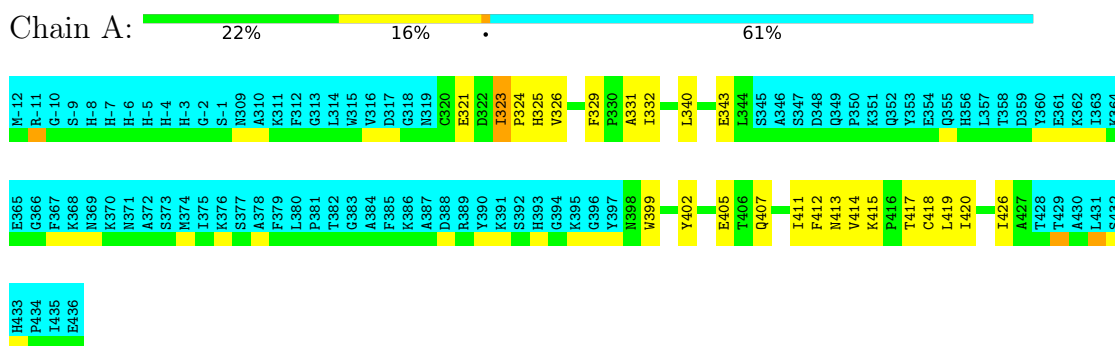
- Molecule 1: apical membrane antigen 1





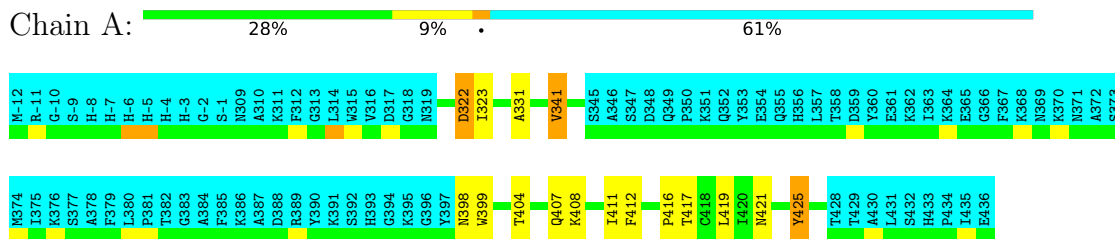
4.2.3 Score per residue for model 3

- Molecule 1: apical membrane antigen 1



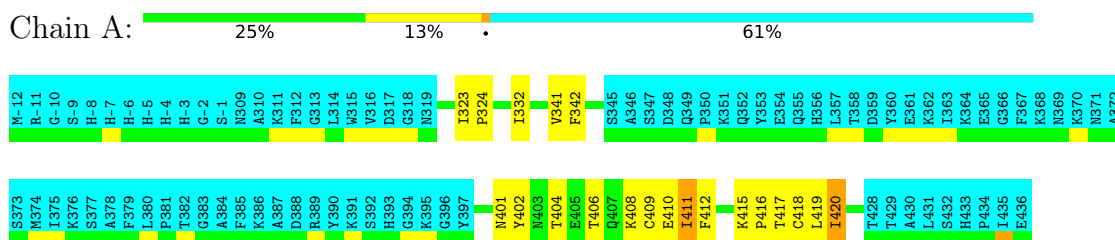
4.2.4 Score per residue for model 4

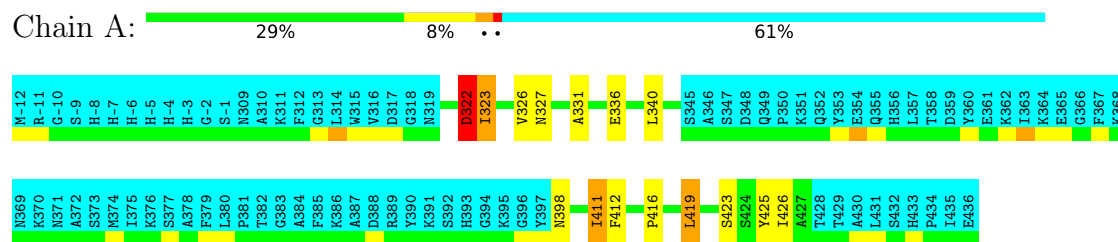
- Molecule 1: apical membrane antigen 1



4.2.5 Score per residue for model 5

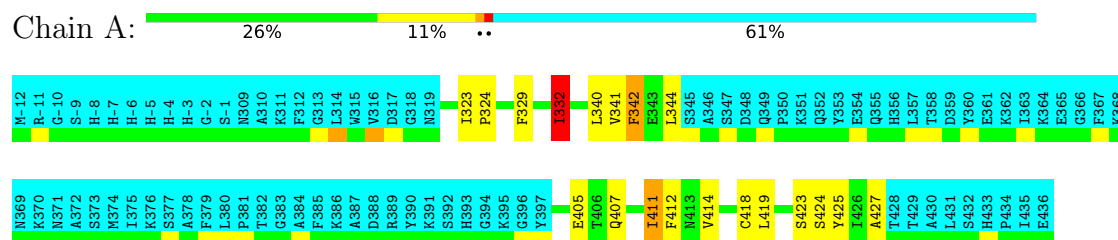
- Molecule 1: apical membrane antigen 1





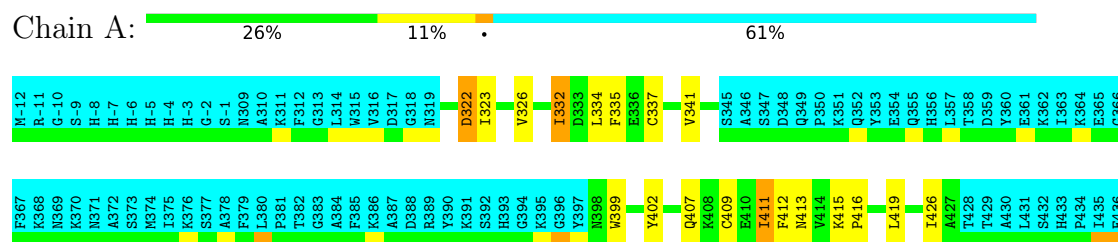
4.2.10 Score per residue for model 10

- Molecule 1: apical membrane antigen 1



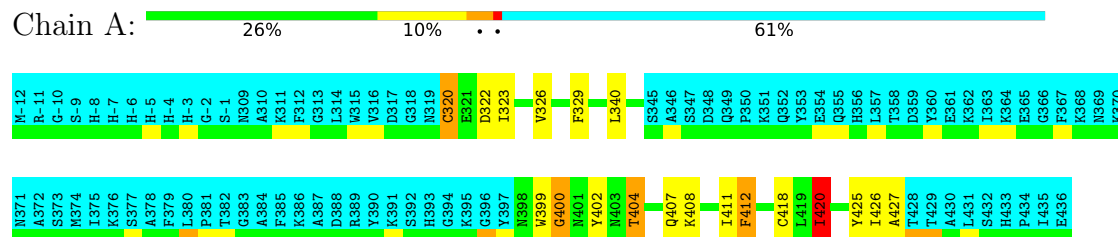
4.2.11 Score per residue for model 11 (medoid)

- Molecule 1: apical membrane antigen 1



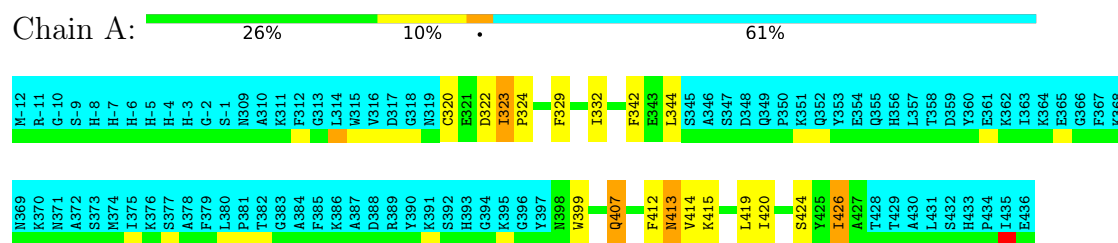
4.2.12 Score per residue for model 12

- Molecule 1: apical membrane antigen 1



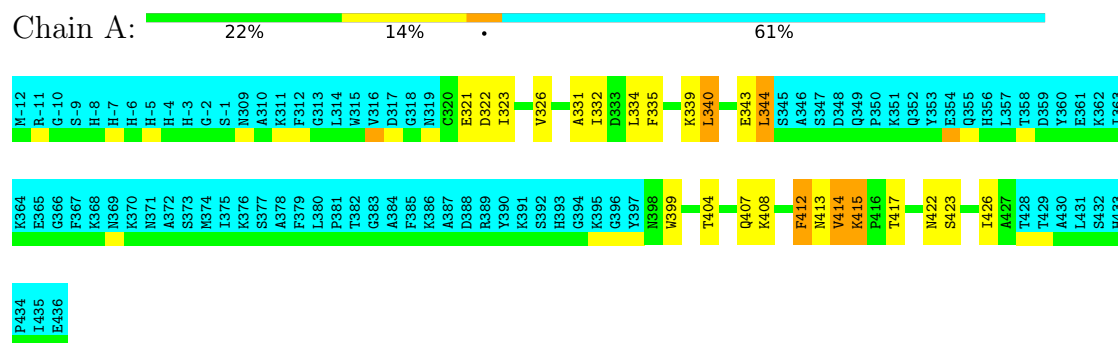
4.2.13 Score per residue for model 13

- Molecule 1: apical membrane antigen 1



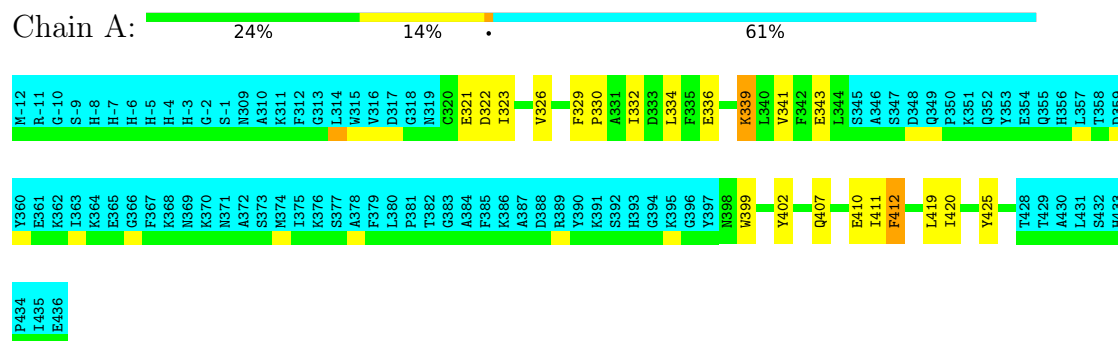
4.2.14 Score per residue for model 14

- Molecule 1: apical membrane antigen 1



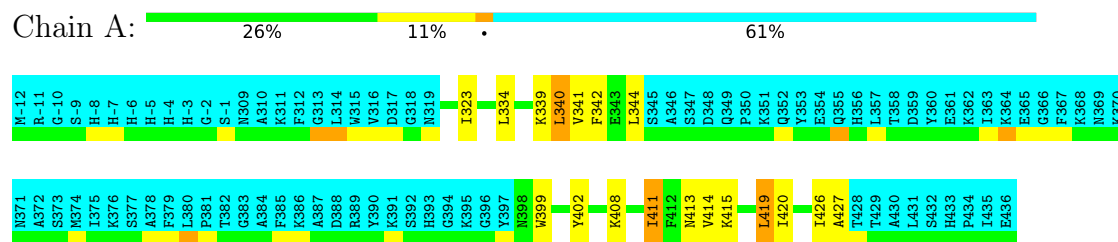
4.2.15 Score per residue for model 15

- Molecule 1: apical membrane antigen 1



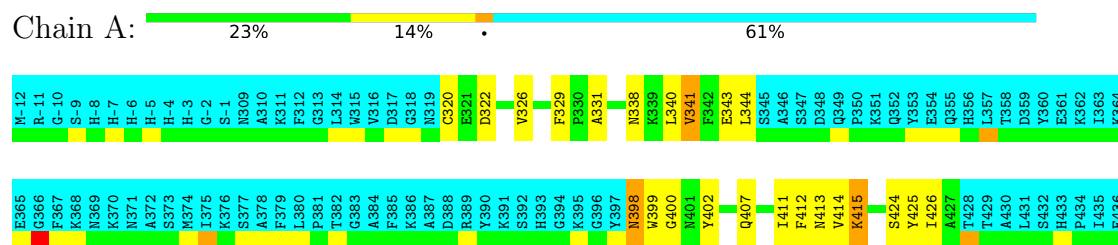
4.2.16 Score per residue for model 16

- Molecule 1: apical membrane antigen 1



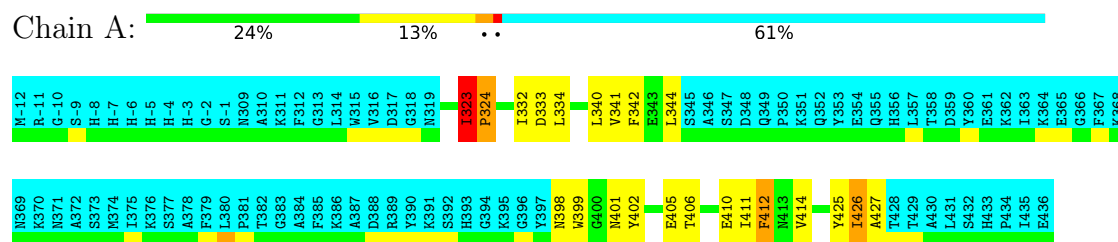
4.2.17 Score per residue for model 17

- Molecule 1: apical membrane antigen 1



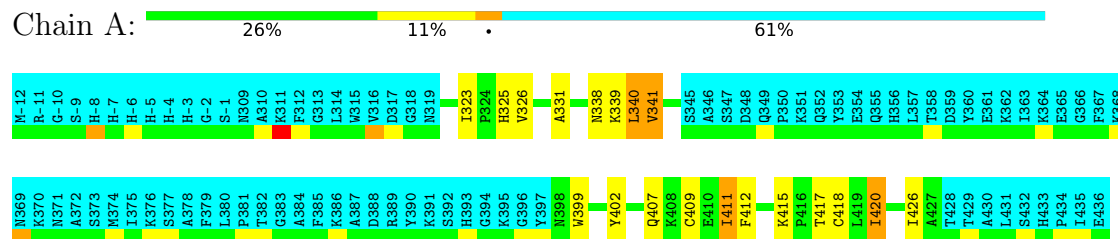
4.2.18 Score per residue for model 18

- Molecule 1: apical membrane antigen 1



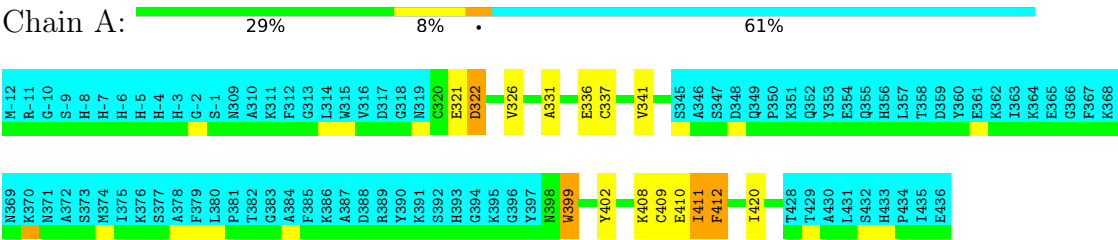
4.2.19 Score per residue for model 19

- 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

No chemical shift data was provided.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.40±0.02	0±1/459 (0.1± 0.1%)	1.51±0.02	1±1/627 (0.1± 0.1%)
All	All	1.40	5/9180 (0.1%)	1.51	17/12540 (0.1%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	400	GLY	N-CA	5.91	1.49	1.44	6	3
1	A	415	LYS	N-CA	5.14	1.50	1.45	5	1
1	A	407	GLN	N-CA	5.03	1.52	1.46	6	1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	341	VAL	N-CA-CB	-7.10	105.18	112.28	15	3
1	A	414	VAL	N-CA-CB	-7.04	105.23	112.06	10	1
1	A	426	ILE	N-CA-CB	-5.78	105.07	111.66	12	5
1	A	323	ILE	N-CA-CB	-5.71	103.21	111.21	18	2
1	A	427	ALA	N-CA-CB	-5.69	104.96	111.79	16	1
1	A	425	TYR	N-CA-CB	-5.69	104.96	111.79	6	2
1	A	417	THR	N-CA-CB	-5.59	105.08	111.79	4	1
1	A	332	ILE	N-CA-CB	-5.20	105.11	112.12	14	2

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	12±4
All	All	8940	8340	8340	238

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 14.

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	1.94	9	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:HD13	1:A:419:LEU:N	0.67	2.04	1	2
1:A:419:LEU:HD12	1:A:419:LEU:O	0.67	1.90	13	4
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
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:HD22	1:A:344:LEU:CD1	0.63	2.24	8	1
1:A:340:LEU:HD13	1:A:340:LEU:N	0.63	2.08	19	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:339:LYS:C	1:A:340:LEU:HD13	0.62	2.19	19	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	3
1:A:344:LEU:O	1:A:344:LEU:HD23	0.60	1.97	14	1
1:A:404:THR:HG21	1:A:408:LYS:CB	0.59	2.27	5	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:412:PHE:CE1	1:A:414:VAL:HG21	0.58	2.34	8	1
1:A:332:ILE:O	1:A:332:ILE:HD13	0.57	2.00	10	1
1:A:399:TRP:HA	1:A:426:ILE:HD13	0.57	1.75	13	1
1:A:344:LEU:HD22	1:A:344:LEU:N	0.57	2.14	17	1
1:A:411:ILE:HD13	1:A:411:ILE:C	0.56	2.25	20	5
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:O	1:A:323:ILE:HG23	0.56	2.01	15	6
1:A:323:ILE:HG23	1:A:323:ILE:O	0.56	2.01	16	3
1:A:420:ILE:O	1:A:420:ILE:HG22	0.55	2.02	16	3
1:A:404:THR:O	1:A:404:THR:HG23	0.55	2.02	4	3
1:A:341:VAL:O	1:A:341:VAL:HG22	0.55	2.02	4	2
1:A:411:ILE:HD13	1:A:411:ILE:H	0.55	1.62	16	2
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:334:LEU:C	1:A:334:LEU:HD12	0.54	2.28	14	1
1:A:410:GLU:C	1:A:411:ILE:HD12	0.54	2.27	15	2
1:A:341:VAL:O	1:A:341:VAL:HG23	0.54	2.01	19	1
1:A:404:THR:HG23	1:A:404:THR:O	0.54	2.03	2	1
1:A:321:GLU:O	1:A:420:ILE:HD11	0.54	2.03	3	1
1:A:323:ILE:HD13	1:A:323:ILE:C	0.53	2.29	18	1
1:A:406:THR:O	1:A:406:THR:HG23	0.53	2.04	6	1
1:A:340:LEU:HD22	1:A:340:LEU:N	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:426:ILE:HD12	1:A:426:ILE:C	0.52	2.30	18	1
1:A:419:LEU:H	1:A:419:LEU:HD13	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:HG12	1:A:341:VAL:O	0.51	2.05	2	1
1:A:341:VAL:HG22	1:A:341:VAL:O	0.51	2.04	8	1
1:A:332:ILE:HD13	1:A:332:ILE:C	0.50	2.31	10	1
1:A:342:PHE:O	1:A:342:PHE:CD2	0.49	2.66	18	2
1:A:417:THR:O	1:A:417:THR:HG23	0.49	2.08	19	1
1:A:326:VAL:HG11	1:A:417:THR:HG21	0.48	1.83	2	1
1:A:406:THR:O	1:A:407:GLN:C	0.48	2.56	6	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:332:ILE:HG21	1:A:407:GLN:HG3	0.48	1.85	13	1
1:A:340:LEU:CD1	1:A:344:LEU:HD23	0.48	2.38	1	1
1:A:339:LYS:O	1:A:340:LEU:HD22	0.48	2.07	2	2
1:A:411:ILE:HD12	1:A:411:ILE:N	0.48	2.23	15	2
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:402:TYR:CD1	1:A:402:TYR:N	0.47	2.83	2	11
1:A:334:LEU:HD12	1:A:335:PHE:N	0.47	2.24	14	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: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:419:LEU:N	1:A:419:LEU:CD1	0.45	2.75	1	1
1:A:341:VAL:HG23	1:A:343:GLU:H	0.45	1.70	17	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:HD23	1:A:340:LEU:N	0.45	2.27	16	1
1:A:402:TYR:CD2	1:A:409:CYS:CB	0.45	3.00	20	2
1:A:413:ASN:C	1:A:414:VAL:HG13	0.45	2.37	13	2
1:A:411:ILE:N	1:A:411:ILE:CD1	0.45	2.79	16	3
1:A:402:TYR:CE1	1:A:425:TYR:CE1	0.45	3.04	15	1
1:A:332:ILE:O	1:A:332:ILE:HG23	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	2
1:A:339:LYS:C	1:A:340:LEU:HD23	0.44	2.38	16	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: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:323:ILE:N	1:A:324:PRO:CD	0.43	2.81	2	1
1:A:399:TRP:CH2	1:A:411:ILE:HD11	0.43	2.49	11	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:425:TYR:C	1:A:426:ILE:HG23	0.43	2.38	18	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:HG22	1:A:426:ILE:O	0.43	2.14	3	2
1:A:417:THR:HG23	1:A:417:THR:O	0.43	2.14	3	1
1:A:411:ILE:N	1:A:411:ILE:HD12	0.42	2.29	3	2
1:A:325:HIS:O	1:A:325:HIS:CG	0.42	2.72	1	2
1:A:419:LEU:HD22	1:A:419:LEU:N	0.42	2.29	3	1
1:A:323:ILE:HB	1:A:324:PRO:CD	0.42	2.45	3	1
1:A:419:LEU:N	1:A:419:LEU:CD2	0.42	2.82	3	1
1:A:341:VAL:HG12	1:A:342:PHE:N	0.42	2.29	18	1
1:A:410:GLU:C	1:A:411:ILE:HG23	0.42	2.40	5	1
1:A:329:PHE:CE1	1:A:331:ALA:HB3	0.42	2.50	8	1
1:A:426:ILE:O	1:A:426:ILE:HG22	0.42	2.15	11	1
1:A:412:PHE:CE2	1:A:413:ASN:ND2	0.42	2.87	14	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:412:PHE:CZ	1:A:415:LYS:O	0.42	2.73	2	1
1:A:413:ASN:C	1:A:414:VAL:HG23	0.42	2.40	3	1
1:A:414:VAL:HG12	1:A:415:LYS:N	0.42	2.29	8	2
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:411:ILE:C	1:A:411:ILE:CD1	0.41	2.93	20	2
1:A:341:VAL:HG13	1:A:342:PHE:N	0.41	2.30	10	1
1:A:412:PHE:CD2	1:A:413:ASN:OD1	0.41	2.74	17	1
1:A:340:LEU:N	1:A:340:LEU:CD1	0.41	2.79	19	1
1:A:340:LEU:CD2	1:A:340:LEU:C	0.41	2.93	19	1
1:A:412:PHE:CD1	1:A:412:PHE:C	0.41	2.98	5	1
1:A:414:VAL:HG12	1:A:426:ILE:HG21	0.41	1.91	7	1
1:A:344:LEU:C	1:A:344:LEU:HD23	0.41	2.41	16	1
1:A:420:ILE:HG23	1:A:420:ILE:O	0.41	2.16	19	1
1:A:399:TRP:CD1	1:A:399:TRP:O	0.41	2.73	12	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:401:ASN:C	1:A:402:TYR:CD1	0.41	2.99	5	2
1:A:329:PHE:CD1	1:A:331:ALA:O	0.41	2.74	17	1
1:A:334:LEU:O	1:A:335:PHE:CD2	0.41	2.74	1	1
1:A:425:TYR:O	1:A:425:TYR:CD2	0.41	2.74	9	1
1:A:335:PHE:O	1:A:335:PHE:CD1	0.40	2.74	11	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:325:HIS:O	1:A:412:PHE:CE1	0.40	2.74	19	1
1:A:335:PHE:CD1	1:A:335:PHE:O	0.40	2.74	8	1
1:A:338:ASN:OD1	1:A:402:TYR:CE2	0.40	2.74	17	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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%)	4±2 (8±3%)	1	13
All	All	1100/2800 (39%)	700 (64%)	310 (28%)	90 (8%)	1	13

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	416	PRO	6
1	A	331	ALA	6
1	A	322	ASP	6
1	A	417	THR	4
1	A	341	VAL	4
1	A	324	PRO	4
1	A	342	PHE	4
1	A	343	GLU	3
1	A	420	ILE	3
1	A	399	TRP	3
1	A	426	ILE	3
1	A	332	ILE	3
1	A	330	PRO	2
1	A	414	VAL	2
1	A	336	GLU	2
1	A	398	ASN	2
1	A	413	ASN	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	335	PHE	1
1	A	422	ASN	1
1	A	323	ILE	1
1	A	423	SER	1
1	A	427	ALA	1
1	A	339	LYS	1
1	A	340	LEU	1

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	52/122 (43%)	47±1 (90±2%)	5±1 (10±2%)	9	53
All	All	1040/2440 (43%)	933 (90%)	107 (10%)	9	53

All 36 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	411	ILE	9
1	A	340	LEU	7
1	A	415	LYS	7
1	A	329	PHE	6
1	A	334	LEU	6
1	A	408	LYS	5
1	A	344	LEU	5
1	A	419	LEU	4
1	A	339	LYS	4
1	A	405	GLU	4
1	A	332	ILE	3
1	A	336	GLU	3
1	A	322	ASP	3
1	A	323	ILE	3
1	A	423	SER	3
1	A	424	SER	3
1	A	320	CYS	3
1	A	321	GLU	3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	422	ASN	2
1	A	333	ASP	2
1	A	425	TYR	2
1	A	406	THR	2
1	A	418	CYS	2
1	A	410	GLU	2
1	A	337	CYS	2
1	A	420	ILE	2
1	A	399	TRP	1
1	A	398	ASN	1
1	A	421	ASN	1
1	A	413	ASN	1
1	A	342	PHE	1
1	A	403	ASN	1
1	A	327	ASN	1
1	A	404	THR	1
1	A	343	GLU	1
1	A	409	CYS	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 oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided