



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 09:41 AM UTC

PDB ID : 1Z66 / pdb_00001z66
Title : NMR solution structure of domain III of E-protein of tick-borne Langat flavivirus (no RDC restraints)
Authors : Mukherjee, M.; Dutta, K.; White, M.A.; Cowburn, D.; Fox, R.O.
Deposited on : 2005-03-21

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

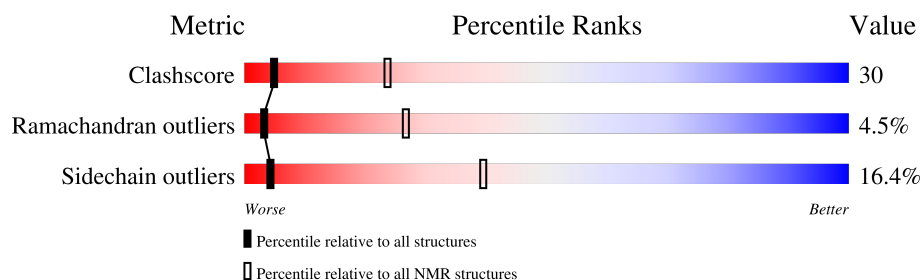
1 Overall quality at a glance

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	96	47% 41% 8% ..

2 Ensemble composition and analysis

This entry contains 20 models. Model 15 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:303-A:395 (93)	0.55	15

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 5 clusters and 6 single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1427 atoms, of which 704 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Major envelope protein E.

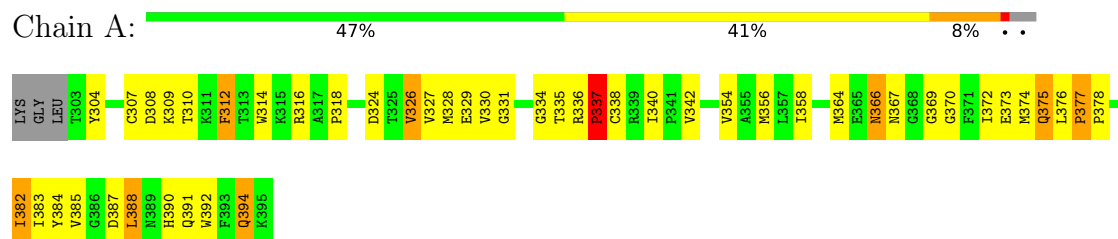
Mol	Chain	Residues	Atoms						Trace
1	A	93	Total	C	H	N	O	S	0
			1427	457	704	126	134	6	

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: Major envelope protein E

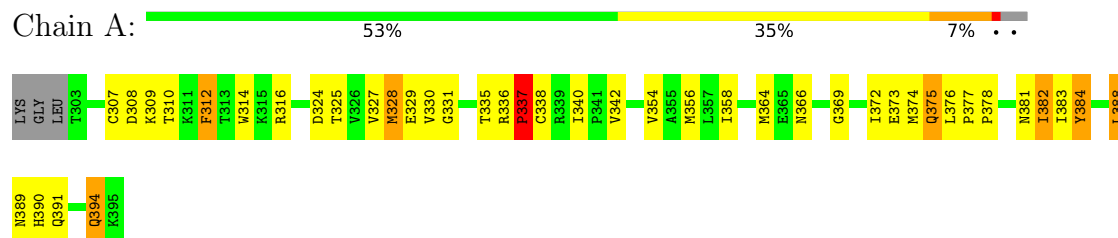


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

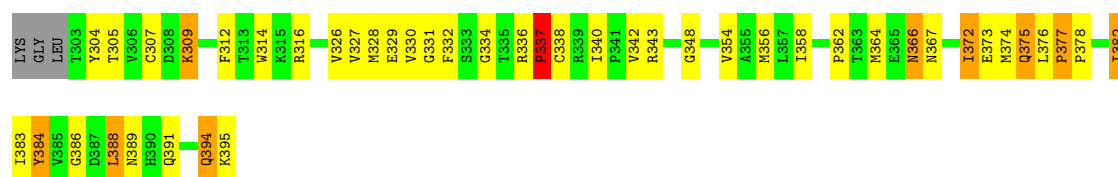
- Molecule 1: Major envelope protein E



4.2.2 Score per residue for model 2

- Molecule 1: Major envelope protein E

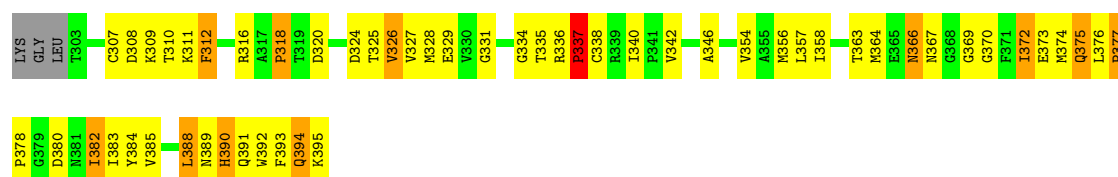




4.2.3 Score per residue for model 3

- Molecule 1: Major envelope protein E

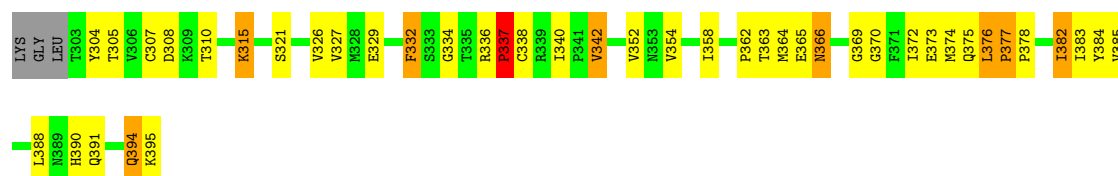
Chain A: 41% 44% 11% ..



4.2.4 Score per residue for model 4

- Molecule 1: Major envelope protein E

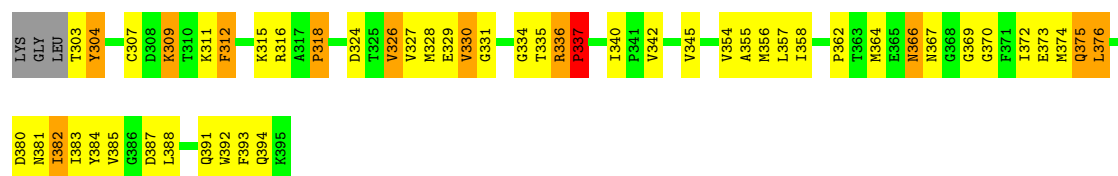
Chain A: 52% 35% 8% ..



4.2.5 Score per residue for model 5

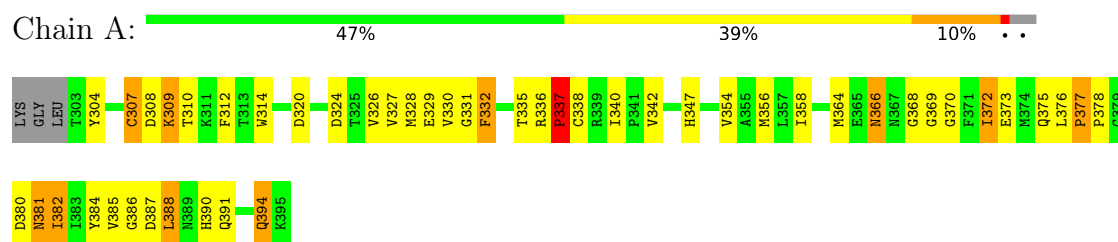
- Molecule 1: Major envelope protein E

Chain A: 44% 41% 11% ..



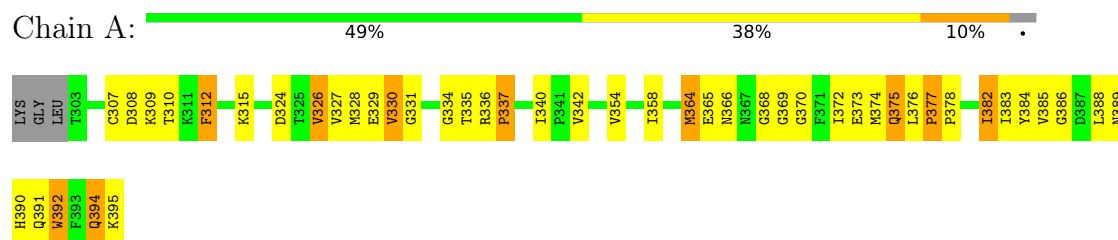
4.2.6 Score per residue for model 6

- Molecule 1: Major envelope protein E



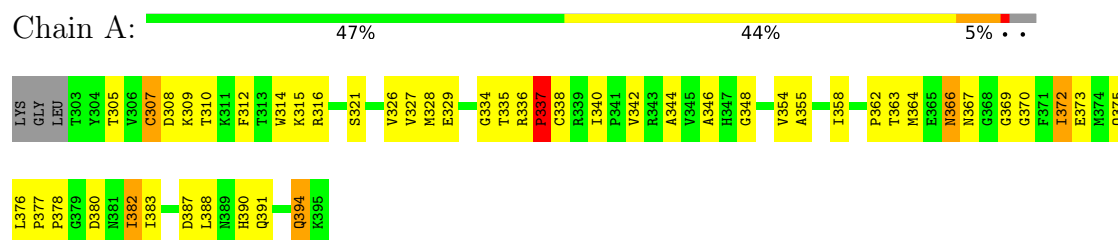
4.2.7 Score per residue for model 7

- Molecule 1: Major envelope protein E



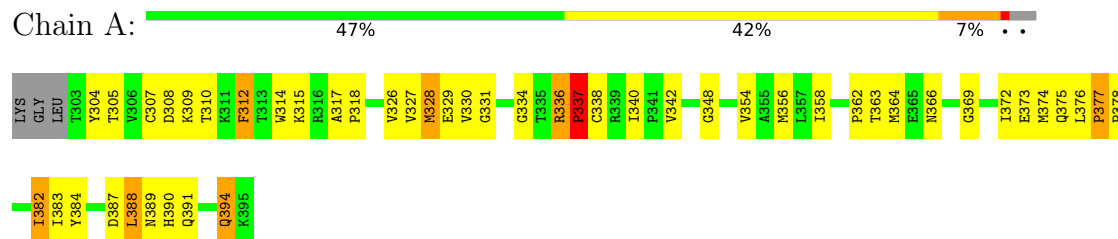
4.2.8 Score per residue for model 8

- Molecule 1: Major envelope protein E



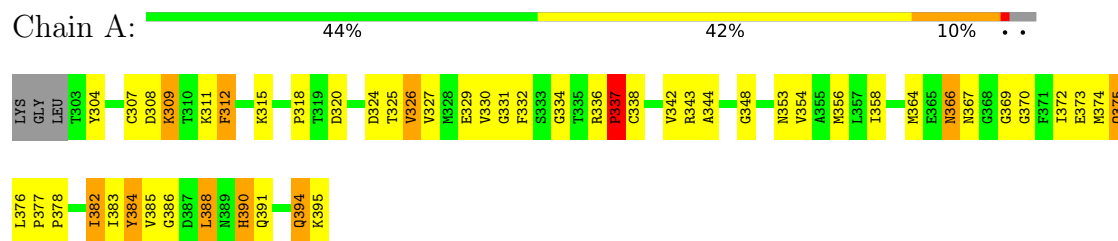
4.2.9 Score per residue for model 9

- Molecule 1: Major envelope protein E



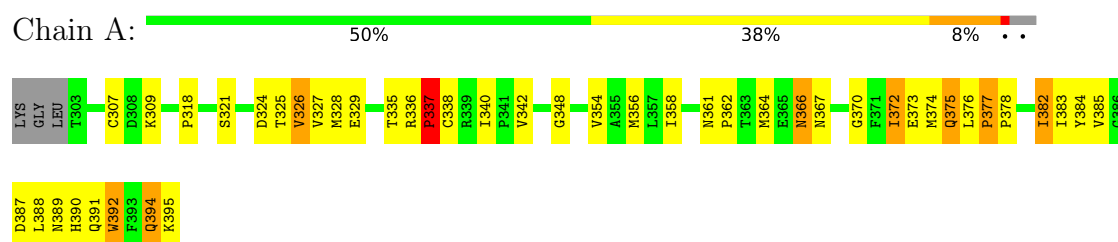
4.2.10 Score per residue for model 10

- Molecule 1: Major envelope protein E



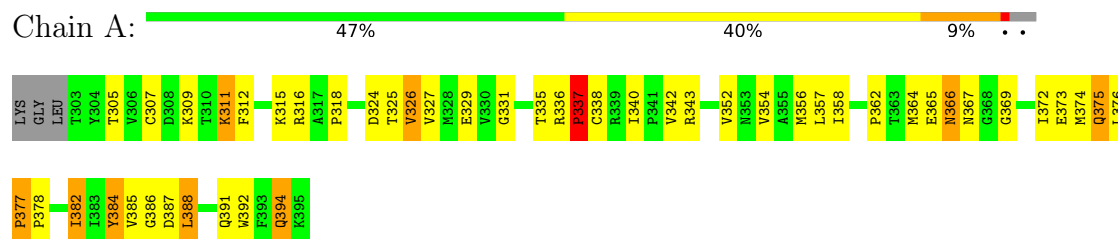
4.2.11 Score per residue for model 11

- Molecule 1: Major envelope protein E



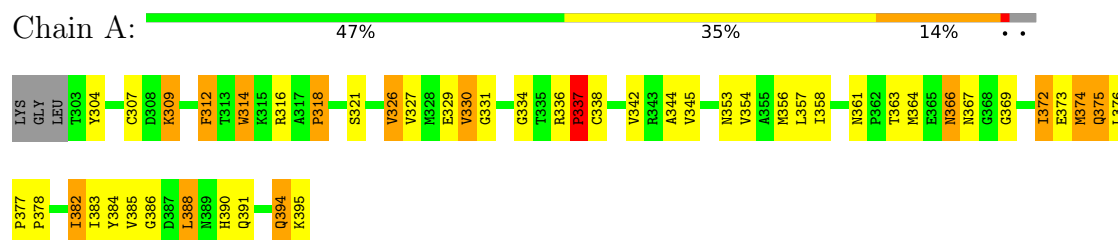
4.2.12 Score per residue for model 12

- Molecule 1: Major envelope protein E



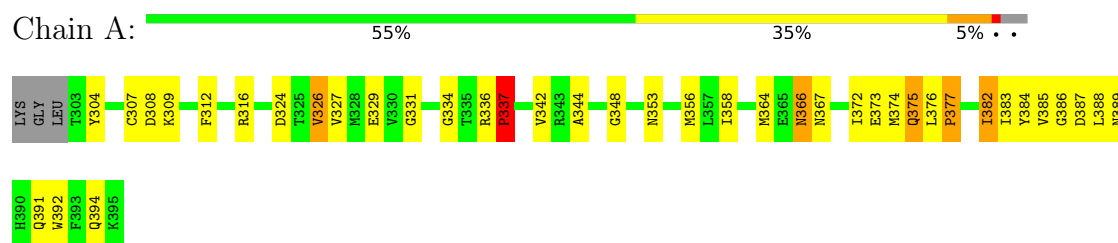
4.2.13 Score per residue for model 13

- Molecule 1: Major envelope protein E



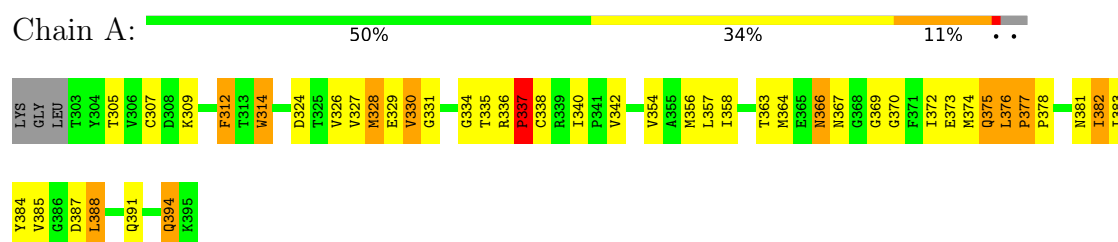
4.2.14 Score per residue for model 14

- Molecule 1: Major envelope protein E



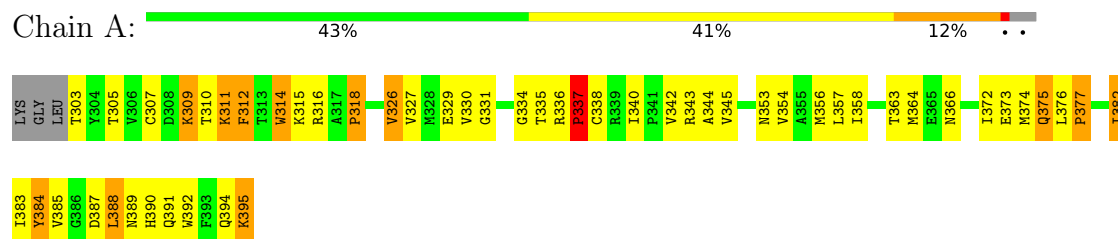
4.2.15 Score per residue for model 15 (medoid)

- Molecule 1: Major envelope protein E



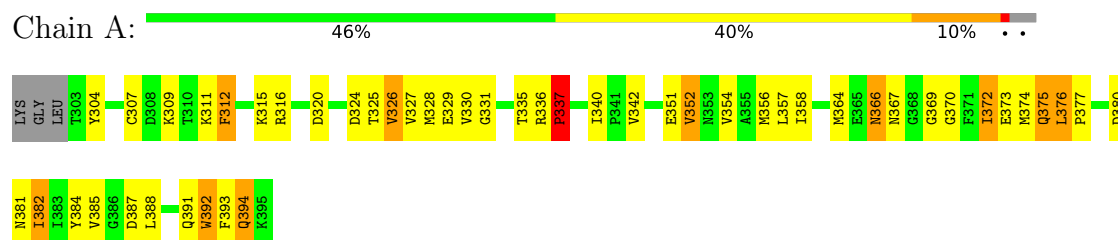
4.2.16 Score per residue for model 16

- Molecule 1: Major envelope protein E



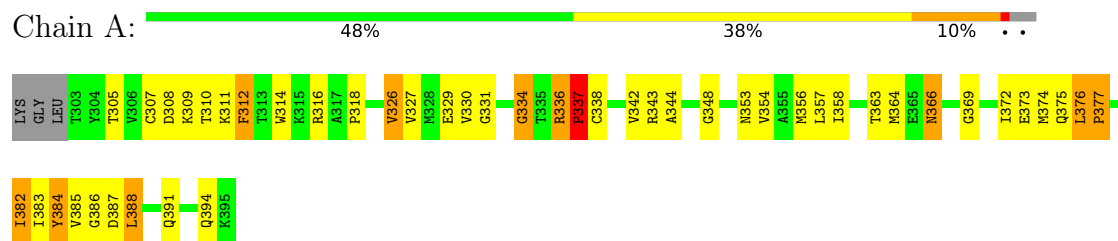
4.2.17 Score per residue for model 17

- Molecule 1: Major envelope protein E



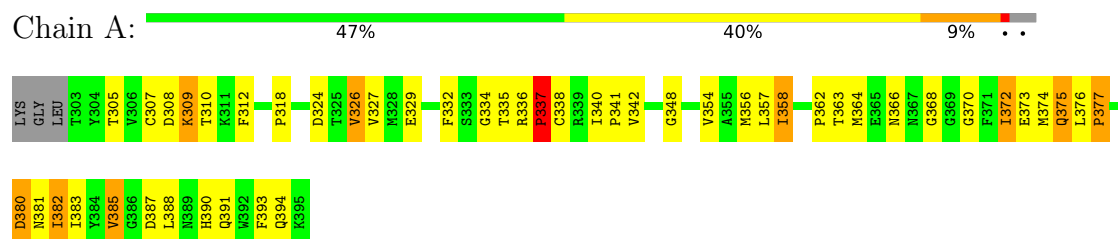
4.2.18 Score per residue for model 18

- Molecule 1: Major envelope protein E



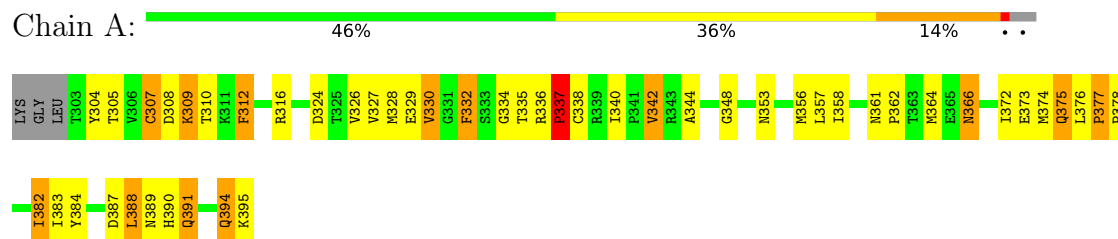
4.2.19 Score per residue for model 19

- Molecule 1: Major envelope protein E



4.2.20 Score per residue for model 20

- Molecule 1: Major envelope protein E



5 Refinement protocol and experimental data overview

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

Of the 500 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
ARIA	structure solution	2.0
CNS	structure solution	1.1
CNS	refinement	1.1

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	723	704	700	42±6
All	All	14460	14080	14000	845

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 30.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:382:ILE:HB	1:A:391:GLN:HA	1.08	1.24	4	20
1:A:354:VAL:HB	1:A:376:LEU:HG	1.02	1.24	17	2
1:A:376:LEU:HG	1:A:377:PRO:HD2	1.00	1.34	8	13
1:A:375:GLN:HE21	1:A:375:GLN:HA	0.84	1.32	11	10
1:A:354:VAL:HB	1:A:376:LEU:HB3	0.84	1.48	5	1
1:A:374:MET:HE2	1:A:383:ILE:HD11	0.83	1.47	13	1
1:A:364:MET:HA	1:A:369:GLY:HA2	0.83	1.51	4	12
1:A:327:VAL:HG12	1:A:373:GLU:HG2	0.82	1.51	12	16
1:A:342:VAL:HG21	1:A:362:PRO:HG2	0.81	1.52	20	1
1:A:316:ARG:HB3	1:A:329:GLU:HB2	0.79	1.52	17	4
1:A:382:ILE:HB	1:A:391:GLN:CA	0.79	2.07	5	20
1:A:315:LYS:HD3	1:A:329:GLU:HG2	0.79	1.55	10	6
1:A:316:ARG:HB2	1:A:329:GLU:HB2	0.76	1.57	20	1
1:A:374:MET:HG2	1:A:383:ILE:HD11	0.75	1.58	19	6

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:326:VAL:HG23	1:A:375:GLN:HG2	0.75	1.55	10	5
1:A:338:CYS:SG	1:A:364:MET:HG2	0.75	2.20	11	3
1:A:354:VAL:HA	1:A:376:LEU:HD22	0.75	1.57	6	9
1:A:335:THR:HB	1:A:364:MET:SD	0.73	2.24	11	1
1:A:338:CYS:SG	1:A:364:MET:HG3	0.72	2.25	2	2
1:A:354:VAL:HG12	1:A:376:LEU:HD22	0.72	1.60	1	2
1:A:312:PHE:CE1	1:A:330:VAL:HB	0.71	2.20	20	1
1:A:342:VAL:HG13	1:A:385:VAL:HG13	0.71	1.62	4	1
1:A:325:THR:HA	1:A:375:GLN:HG3	0.70	1.61	10	4
1:A:356:MET:HB3	1:A:375:GLN:O	0.70	1.85	2	8
1:A:316:ARG:HB3	1:A:329:GLU:HB3	0.69	1.65	14	6
1:A:311:LYS:O	1:A:332:PHE:HA	0.69	1.87	10	1
1:A:357:LEU:HD22	1:A:374:MET:HE2	0.69	1.63	20	1
1:A:312:PHE:CE2	1:A:385:VAL:HG12	0.69	2.22	19	1
1:A:337:PRO:HA	1:A:364:MET:O	0.69	1.86	7	20
1:A:376:LEU:HD22	1:A:377:PRO:HD2	0.69	1.64	12	5
1:A:318:PRO:HG3	1:A:383:ILE:HD12	0.68	1.63	5	4
1:A:378:PRO:HB3	1:A:395:LYS:HA	0.68	1.65	13	2
1:A:375:GLN:HE22	1:A:394:GLN:HG3	0.68	1.48	17	3
1:A:340:ILE:HD12	1:A:362:PRO:HB2	0.68	1.63	9	2
1:A:326:VAL:HB	1:A:374:MET:SD	0.68	2.29	13	1
1:A:309:LYS:HA	1:A:312:PHE:CZ	0.67	2.24	6	12
1:A:376:LEU:HG	1:A:377:PRO:CD	0.67	2.17	3	7
1:A:340:ILE:HD11	1:A:364:MET:HB3	0.67	1.66	2	1
1:A:326:VAL:HG13	1:A:394:GLN:HE22	0.67	1.49	16	2
1:A:336:ARG:HB2	1:A:337:PRO:HD2	0.67	1.66	16	18
1:A:378:PRO:HA	1:A:394:GLN:HE22	0.67	1.47	4	8
1:A:304:TYR:HB3	1:A:336:ARG:HG3	0.67	1.66	14	6
1:A:362:PRO:HB3	1:A:372:ILE:HG23	0.66	1.67	9	4
1:A:326:VAL:HG21	1:A:392:TRP:HZ2	0.65	1.49	12	2
1:A:378:PRO:HB3	1:A:395:LYS:HB2	0.65	1.67	3	1
1:A:372:ILE:HB	1:A:374:MET:HE1	0.65	1.66	9	7
1:A:312:PHE:HA	1:A:331:GLY:O	0.65	1.92	12	15
1:A:348:GLY:H	1:A:382:ILE:HG21	0.64	1.52	2	9
1:A:380:ASP:HA	1:A:393:PHE:HA	0.64	1.68	5	4
1:A:358:ILE:HB	1:A:373:GLU:CB	0.64	2.23	19	18
1:A:358:ILE:HB	1:A:373:GLU:HB3	0.64	1.69	10	20
1:A:382:ILE:CB	1:A:391:GLN:HA	0.64	2.16	8	13
1:A:376:LEU:CG	1:A:377:PRO:HD2	0.63	2.22	3	12
1:A:312:PHE:HD1	1:A:388:LEU:HD13	0.63	1.52	2	3
1:A:327:VAL:HA	1:A:372:ILE:O	0.63	1.94	19	17

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:328:MET:SD	1:A:330:VAL:HG13	0.63	2.34	15	2
1:A:375:GLN:HE21	1:A:375:GLN:CA	0.61	2.08	12	10
1:A:375:GLN:HA	1:A:375:GLN:NE2	0.61	2.09	12	4
1:A:340:ILE:HG13	1:A:342:VAL:HG22	0.61	1.71	4	1
1:A:375:GLN:NE2	1:A:376:LEU:H	0.61	1.92	5	4
1:A:329:GLU:HA	1:A:370:GLY:O	0.61	1.96	6	8
1:A:356:MET:HB2	1:A:375:GLN:O	0.61	1.95	13	5
1:A:309:LYS:HB2	1:A:387:ASP:HB2	0.61	1.72	5	6
1:A:340:ILE:HG22	1:A:342:VAL:HG13	0.61	1.73	11	4
1:A:332:PHE:HB3	1:A:364:MET:SD	0.60	2.35	4	1
1:A:342:VAL:HG11	1:A:372:ILE:HD13	0.60	1.73	14	12
1:A:328:MET:HE3	1:A:372:ILE:HD12	0.60	1.71	3	3
1:A:312:PHE:CD1	1:A:388:LEU:HD13	0.60	2.31	2	1
1:A:340:ILE:HD12	1:A:364:MET:HE3	0.60	1.71	16	2
1:A:378:PRO:HA	1:A:394:GLN:NE2	0.60	2.11	4	13
1:A:311:LYS:HE3	1:A:334:GLY:HA3	0.59	1.73	18	1
1:A:385:VAL:HB	1:A:388:LEU:HB2	0.59	1.73	17	8
1:A:312:PHE:HE2	1:A:385:VAL:HG12	0.59	1.55	19	1
1:A:340:ILE:CG2	1:A:364:MET:HG3	0.59	2.28	4	1
1:A:384:TYR:HA	1:A:388:LEU:O	0.58	1.98	3	8
1:A:338:CYS:SG	1:A:364:MET:HB2	0.58	2.38	6	3
1:A:375:GLN:HE22	1:A:394:GLN:HG2	0.57	1.58	7	2
1:A:354:VAL:HA	1:A:376:LEU:HG	0.57	1.77	4	3
1:A:311:LYS:HE3	1:A:335:THR:CB	0.57	2.30	12	2
1:A:340:ILE:HG21	1:A:364:MET:HG3	0.56	1.78	3	4
1:A:308:ASP:OD2	1:A:310:THR:HG22	0.56	2.00	4	2
1:A:307:CYS:HB2	1:A:311:LYS:HD3	0.56	1.77	16	1
1:A:328:MET:SD	1:A:372:ILE:HB	0.56	2.40	2	1
1:A:338:CYS:O	1:A:363:THR:HA	0.56	2.01	19	8
1:A:318:PRO:HG2	1:A:390:HIS:O	0.56	2.01	16	3
1:A:335:THR:HB	1:A:364:MET:HE3	0.55	1.76	15	1
1:A:354:VAL:HB	1:A:381:ASN:OD1	0.55	2.02	19	1
1:A:309:LYS:HA	1:A:312:PHE:CE2	0.55	2.35	9	6
1:A:327:VAL:HG12	1:A:373:GLU:HG3	0.55	1.77	10	2
1:A:316:ARG:HB3	1:A:329:GLU:CB	0.55	2.31	14	7
1:A:315:LYS:HA	1:A:315:LYS:HE3	0.55	1.78	4	1
1:A:338:CYS:SG	1:A:364:MET:HE3	0.55	2.41	19	1
1:A:326:VAL:HB	1:A:374:MET:HG2	0.54	1.80	16	1
1:A:366:ASN:HD22	1:A:366:ASN:C	0.54	2.11	3	6
1:A:326:VAL:HG21	1:A:392:TRP:CZ2	0.54	2.35	12	2
1:A:305:THR:O	1:A:338:CYS:HB2	0.54	2.03	19	10

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:312:PHE:HD1	1:A:364:MET:SD	0.54	2.26	18	1
1:A:376:LEU:HB2	1:A:377:PRO:HD2	0.54	1.78	17	1
1:A:308:ASP:OD1	1:A:310:THR:HG22	0.53	2.03	7	8
1:A:309:LYS:HD2	1:A:387:ASP:HB2	0.53	1.79	15	1
1:A:356:MET:HE2	1:A:376:LEU:HD12	0.53	1.81	1	1
1:A:326:VAL:HG23	1:A:374:MET:O	0.53	2.03	18	4
1:A:343:ARG:HG2	1:A:384:TYR:O	0.53	2.03	12	5
1:A:366:ASN:HD22	1:A:367:ASN:N	0.53	2.01	11	11
1:A:358:ILE:HD11	1:A:375:GLN:HB2	0.53	1.80	10	4
1:A:376:LEU:HD13	1:A:377:PRO:HD2	0.53	1.80	15	1
1:A:376:LEU:HD13	1:A:377:PRO:CD	0.53	2.33	15	3
1:A:309:LYS:HD2	1:A:310:THR:N	0.53	2.19	19	2
1:A:340:ILE:HD11	1:A:362:PRO:HB2	0.53	1.79	8	3
1:A:376:LEU:HD23	1:A:394:GLN:HG3	0.53	1.79	5	1
1:A:331:GLY:HA2	1:A:368:GLY:HA3	0.52	1.81	6	2
1:A:328:MET:HE3	1:A:383:ILE:HB	0.52	1.81	1	1
1:A:342:VAL:HG12	1:A:385:VAL:HG13	0.52	1.81	19	9
1:A:375:GLN:HE21	1:A:376:LEU:H	0.52	1.47	4	4
1:A:354:VAL:CB	1:A:376:LEU:HG	0.52	2.16	17	3
1:A:374:MET:HE1	1:A:381:ASN:HB3	0.52	1.79	1	2
1:A:383:ILE:HB	1:A:390:HIS:CE1	0.52	2.40	7	1
1:A:354:VAL:HB	1:A:376:LEU:CG	0.52	2.16	17	1
1:A:311:LYS:HE3	1:A:335:THR:HB	0.51	1.81	16	2
1:A:328:MET:HE1	1:A:385:VAL:HG22	0.51	1.81	11	3
1:A:340:ILE:HG12	1:A:364:MET:HG3	0.51	1.81	9	1
1:A:307:CYS:HB3	1:A:335:THR:HG21	0.51	1.82	8	1
1:A:309:LYS:HD3	1:A:387:ASP:CB	0.51	2.34	9	1
1:A:378:PRO:HB3	1:A:395:LYS:HD2	0.51	1.81	11	1
1:A:335:THR:HG22	1:A:336:ARG:O	0.51	2.05	1	5
1:A:342:VAL:HG12	1:A:385:VAL:HG22	0.51	1.82	4	1
1:A:309:LYS:HB2	1:A:387:ASP:N	0.51	2.21	8	1
1:A:375:GLN:C	1:A:376:LEU:HD13	0.51	2.31	5	1
1:A:309:LYS:HD3	1:A:387:ASP:HB2	0.51	1.82	11	3
1:A:361:ASN:N	1:A:362:PRO:HD3	0.50	2.20	20	2
1:A:335:THR:HB	1:A:364:MET:CE	0.50	2.37	8	3
1:A:312:PHE:HB3	1:A:364:MET:HE1	0.50	1.82	7	2
1:A:354:VAL:HG12	1:A:376:LEU:CD2	0.50	2.37	3	1
1:A:395:LYS:HA	1:A:395:LYS:NZ	0.50	2.21	16	1
1:A:314:TRP:CE2	1:A:388:LEU:HG	0.49	2.42	9	7
1:A:311:LYS:HE3	1:A:335:THR:OG1	0.49	2.07	12	1
1:A:336:ARG:HB2	1:A:337:PRO:CD	0.49	2.36	16	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:374:MET:SD	1:A:392:TRP:CH2	0.49	3.05	7	1
1:A:326:VAL:HG13	1:A:394:GLN:NE2	0.49	2.19	16	1
1:A:340:ILE:HD11	1:A:364:MET:HG3	0.49	1.85	17	1
1:A:375:GLN:NE2	1:A:394:GLN:HG3	0.49	2.22	17	2
1:A:383:ILE:O	1:A:389:ASN:HA	0.49	2.07	20	7
1:A:338:CYS:SG	1:A:364:MET:HE2	0.49	2.47	20	2
1:A:376:LEU:HD11	1:A:381:ASN:CG	0.49	2.33	17	1
1:A:328:MET:CE	1:A:372:ILE:HD12	0.49	2.38	11	3
1:A:327:VAL:CG1	1:A:373:GLU:HG2	0.48	2.33	1	2
1:A:316:ARG:CB	1:A:329:GLU:HB2	0.48	2.34	17	2
1:A:380:ASP:HB3	1:A:391:GLN:HE21	0.48	1.69	17	1
1:A:321:SER:HB3	1:A:327:VAL:HG13	0.48	1.84	8	4
1:A:342:VAL:CG1	1:A:385:VAL:HG22	0.48	2.38	4	1
1:A:344:ALA:O	1:A:353:ASN:HA	0.48	2.08	18	6
1:A:308:ASP:OD1	1:A:309:LYS:HG2	0.48	2.09	14	1
1:A:374:MET:CE	1:A:383:ILE:HD11	0.48	2.29	13	1
1:A:374:MET:SD	1:A:383:ILE:HD13	0.48	2.48	20	1
1:A:332:PHE:HB3	1:A:364:MET:HE2	0.48	1.85	10	1
1:A:374:MET:HG2	1:A:383:ILE:CD1	0.48	2.37	19	4
1:A:338:CYS:SG	1:A:364:MET:CG	0.48	3.01	2	1
1:A:394:GLN:NE2	1:A:395:LYS:HG2	0.47	2.24	3	1
1:A:311:LYS:HE2	1:A:335:THR:OG1	0.47	2.09	3	3
1:A:357:LEU:HA	1:A:374:MET:HA	0.47	1.84	16	8
1:A:328:MET:SD	1:A:330:VAL:HG22	0.47	2.49	5	1
1:A:376:LEU:N	1:A:376:LEU:HD22	0.47	2.24	5	1
1:A:312:PHE:HD2	1:A:332:PHE:CE1	0.47	2.28	2	1
1:A:382:ILE:HD13	1:A:382:ILE:C	0.47	2.34	5	9
1:A:347:HIS:HA	1:A:380:ASP:OD2	0.47	2.08	6	1
1:A:392:TRP:CD1	1:A:394:GLN:NE2	0.47	2.82	17	1
1:A:326:VAL:O	1:A:373:GLU:HA	0.47	2.10	19	1
1:A:342:VAL:CG2	1:A:362:PRO:HG2	0.47	2.33	20	1
1:A:364:MET:HG2	1:A:369:GLY:CA	0.47	2.39	1	5
1:A:378:PRO:HB3	1:A:395:LYS:HD3	0.47	1.86	10	1
1:A:340:ILE:CD1	1:A:364:MET:HG3	0.47	2.40	17	1
1:A:381:ASN:HD22	1:A:394:GLN:HG2	0.47	1.70	19	1
1:A:315:LYS:HB3	1:A:329:GLU:C	0.46	2.35	7	1
1:A:385:VAL:HB	1:A:388:LEU:CB	0.46	2.39	14	2
1:A:392:TRP:NE1	1:A:394:GLN:HB3	0.46	2.24	12	2
1:A:356:MET:HE2	1:A:376:LEU:HA	0.46	1.87	1	1
1:A:346:ALA:HA	1:A:380:ASP:O	0.46	2.10	8	1
1:A:309:LYS:CD	1:A:387:ASP:HB2	0.46	2.40	11	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:317:ALA:HB1	1:A:318:PRO:HD2	0.46	1.88	9	1
1:A:366:ASN:N	1:A:366:ASN:HD22	0.46	2.07	4	3
1:A:329:GLU:HG2	1:A:370:GLY:O	0.46	2.11	17	1
1:A:307:CYS:SG	1:A:335:THR:HB	0.46	2.51	6	1
1:A:312:PHE:CD1	1:A:364:MET:SD	0.46	3.09	18	1
1:A:318:PRO:HG3	1:A:383:ILE:CD1	0.45	2.41	3	1
1:A:307:CYS:SG	1:A:340:ILE:HD13	0.45	2.51	20	1
1:A:395:LYS:HD3	1:A:395:LYS:C	0.45	2.37	7	1
1:A:320:ASP:HB2	1:A:392:TRP:CZ2	0.45	2.47	3	1
1:A:345:VAL:HG22	1:A:382:ILE:HD12	0.45	1.88	16	3
1:A:357:LEU:CD2	1:A:374:MET:HB3	0.45	2.42	20	2
1:A:392:TRP:HD1	1:A:394:GLN:OE1	0.45	1.95	14	1
1:A:304:TYR:HB3	1:A:336:ARG:HE	0.44	1.73	9	1
1:A:324:ASP:HB2	1:A:395:LYS:NZ	0.44	2.28	3	1
1:A:332:PHE:HD1	1:A:368:GLY:HA2	0.44	1.72	19	1
1:A:340:ILE:CG2	1:A:342:VAL:HG13	0.44	2.41	20	1
1:A:354:VAL:O	1:A:376:LEU:HB2	0.43	2.13	18	2
1:A:312:PHE:CD1	1:A:330:VAL:HB	0.43	2.47	20	1
1:A:358:ILE:CB	1:A:373:GLU:HB3	0.43	2.41	19	2
1:A:315:LYS:HE3	1:A:329:GLU:OE1	0.43	2.13	17	1
1:A:335:THR:CG2	1:A:338:CYS:HB3	0.43	2.44	1	1
1:A:346:ALA:HB2	1:A:354:VAL:CG1	0.43	2.43	3	1
1:A:375:GLN:NE2	1:A:375:GLN:CA	0.43	2.79	12	1
1:A:304:TYR:HB3	1:A:336:ARG:HD3	0.43	1.90	20	1
1:A:380:ASP:HB3	1:A:391:GLN:NE2	0.43	2.27	17	1
1:A:303:THR:HG23	1:A:335:THR:HG23	0.43	1.91	5	1
1:A:318:PRO:HD3	1:A:390:HIS:CD2	0.43	2.48	10	1
1:A:337:PRO:HG3	1:A:365:GLU:HA	0.43	1.91	12	1
1:A:374:MET:HE2	1:A:383:ILE:CD1	0.43	2.32	13	1
1:A:354:VAL:C	1:A:376:LEU:HD12	0.43	2.38	5	1
1:A:382:ILE:HB	1:A:391:GLN:CB	0.43	2.43	18	1
1:A:336:ARG:O	1:A:337:PRO:C	0.43	2.62	7	16
1:A:309:LYS:HB2	1:A:387:ASP:CB	0.43	2.44	17	1
1:A:304:TYR:HB3	1:A:336:ARG:HD2	0.42	1.90	5	1
1:A:326:VAL:HG11	1:A:392:TRP:CE2	0.42	2.49	11	1
1:A:392:TRP:HD1	1:A:394:GLN:NE2	0.42	2.12	17	1
1:A:383:ILE:HB	1:A:390:HIS:HE1	0.42	1.74	7	1
1:A:388:LEU:HD23	1:A:390:HIS:CE1	0.42	2.49	10	1
1:A:384:TYR:CE1	1:A:389:ASN:HB3	0.42	2.49	1	2
1:A:326:VAL:HG11	1:A:394:GLN:HE22	0.42	1.75	5	1
1:A:330:VAL:HG23	1:A:369:GLY:HA3	0.42	1.92	15	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:304:TYR:HB3	1:A:336:ARG:CG	0.42	2.45	4	2
1:A:344:ALA:N	1:A:355:ALA:HB2	0.42	2.30	8	1
1:A:329:GLU:HG3	1:A:370:GLY:O	0.42	2.15	8	2
1:A:376:LEU:HB2	1:A:381:ASN:CG	0.42	2.40	5	1
1:A:326:VAL:HG11	1:A:394:GLN:NE2	0.41	2.30	5	1
1:A:342:VAL:HG23	1:A:357:LEU:HD11	0.41	1.90	18	1
1:A:325:THR:HA	1:A:375:GLN:CG	0.41	2.45	17	1
1:A:328:MET:CE	1:A:372:ILE:HB	0.41	2.46	2	1
1:A:340:ILE:HD11	1:A:385:VAL:HG11	0.41	1.92	6	2
1:A:328:MET:CE	1:A:330:VAL:HG13	0.41	2.45	7	1
1:A:375:GLN:HE22	1:A:394:GLN:CG	0.41	2.28	7	1
1:A:332:PHE:HD2	1:A:335:THR:H	0.41	1.58	20	1
1:A:318:PRO:HD2	1:A:390:HIS:HB3	0.41	1.92	13	2
1:A:374:MET:O	1:A:375:GLN:HB2	0.41	2.16	16	2
1:A:340:ILE:HB	1:A:364:MET:HG3	0.41	1.93	6	1
1:A:328:MET:HB3	1:A:383:ILE:HD12	0.41	1.92	8	1
1:A:332:PHE:H	1:A:332:PHE:HD2	0.41	1.56	6	1
1:A:312:PHE:CE1	1:A:385:VAL:O	0.41	2.74	14	2
1:A:326:VAL:CG2	1:A:375:GLN:HE21	0.41	2.27	19	1
1:A:382:ILE:C	1:A:382:ILE:HD13	0.41	2.41	8	2
1:A:354:VAL:CG1	1:A:376:LEU:HD22	0.41	2.44	13	1
1:A:358:ILE:HD11	1:A:375:GLN:HB3	0.41	1.92	20	1
1:A:321:SER:CB	1:A:327:VAL:HG13	0.41	2.46	13	1
1:A:351:GLU:HG2	1:A:352:VAL:HG12	0.41	1.93	17	1
1:A:354:VAL:HB	1:A:376:LEU:CB	0.40	2.46	4	2
1:A:342:VAL:HG21	1:A:362:PRO:HG3	0.40	1.93	8	1
1:A:344:ALA:CB	1:A:355:ALA:HB2	0.40	2.46	8	1
1:A:382:ILE:HG12	1:A:390:HIS:C	0.40	2.41	9	2
1:A:315:LYS:CD	1:A:329:GLU:HG2	0.40	2.38	10	1
1:A:303:THR:O	1:A:335:THR:HG23	0.40	2.16	16	1
1:A:376:LEU:HD22	1:A:377:PRO:O	0.40	2.15	17	1
1:A:312:PHE:HB3	1:A:364:MET:SD	0.40	2.57	5	1
1:A:308:ASP:HB3	1:A:311:LYS:HD2	0.40	1.93	10	1
1:A:340:ILE:HG22	1:A:362:PRO:O	0.40	2.16	12	1
1:A:312:PHE:CE2	1:A:332:PHE:HE2	0.40	2.34	19	1
1:A:312:PHE:HZ	1:A:341:PRO:HD2	0.40	1.76	19	1
1:A:381:ASN:N	1:A:381:ASN:HD22	0.40	2.15	6	1
1:A:315:LYS:HD3	1:A:329:GLU:CG	0.40	2.38	10	1
1:A:325:THR:HB	1:A:358:ILE:HG13	0.40	1.92	12	1
1:A:366:ASN:HD22	1:A:366:ASN:N	0.40	2.15	18	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	91/96 (95%)	72±2 (79±3%)	15±3 (16±3%)	4±1 (5±1%)	3	27
All	All	1820/1920 (95%)	1445 (79%)	293 (16%)	82 (5%)	3	27

All 8 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	337	PRO	20
1	A	334	GLY	15
1	A	377	PRO	14
1	A	324	ASP	11
1	A	386	GLY	8
1	A	318	PRO	8
1	A	314	TRP	5
1	A	355	ALA	1

6.3.2 Protein sidechains [i](#)

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	80/82 (98%)	67±3 (84±3%)	13±3 (16±3%)	4	39
All	All	1600/1640 (98%)	1338 (84%)	262 (16%)	4	39

All 40 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	366	ASN	20
1	A	382	ILE	20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	307	CYS	19
1	A	337	PRO	19
1	A	326	VAL	19
1	A	388	LEU	17
1	A	375	GLN	15
1	A	394	GLN	15
1	A	312	PHE	13
1	A	330	VAL	12
1	A	384	TYR	12
1	A	390	HIS	9
1	A	372	ILE	9
1	A	309	LYS	8
1	A	328	MET	5
1	A	376	LEU	5
1	A	392	TRP	5
1	A	395	LYS	4
1	A	356	MET	4
1	A	332	PHE	3
1	A	352	VAL	3
1	A	336	ARG	3
1	A	320	ASP	3
1	A	342	VAL	2
1	A	365	GLU	2
1	A	311	LYS	2
1	A	315	LYS	1
1	A	304	TYR	1
1	A	381	ASN	1
1	A	364	MET	1
1	A	325	THR	1
1	A	361	ASN	1
1	A	363	THR	1
1	A	374	MET	1
1	A	387	ASP	1
1	A	324	ASP	1
1	A	358	ILE	1
1	A	380	ASP	1
1	A	385	VAL	1
1	A	391	GLN	1

6.3.3 RNA ⓘ

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 [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided