



Full wwPDB NMR Structure Validation Report ⓘ

Apr 27, 2016 – 02:02 AM BST

PDB ID : 2LZN
Title : Solution structure of S. aureus primase C-terminal domain
Authors : Shortridge, M.D.; Griep, M.A.; Powers, R.
Deposited on : 2012-10-04

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

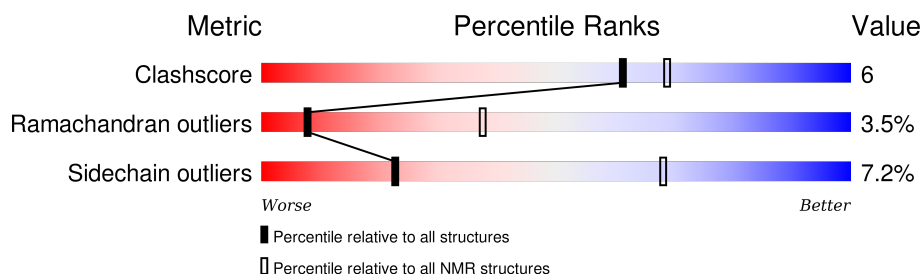
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 72%.

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	143	<div> <div></div> <div>59%</div> <div>11%</div> <div>29%</div> </div>

2 Ensemble composition and analysis

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:466-A:566 (101)	1.20	1

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

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

The models can be grouped into 3 clusters and 4 single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2374 atoms, of which 1152 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called DNA primase.

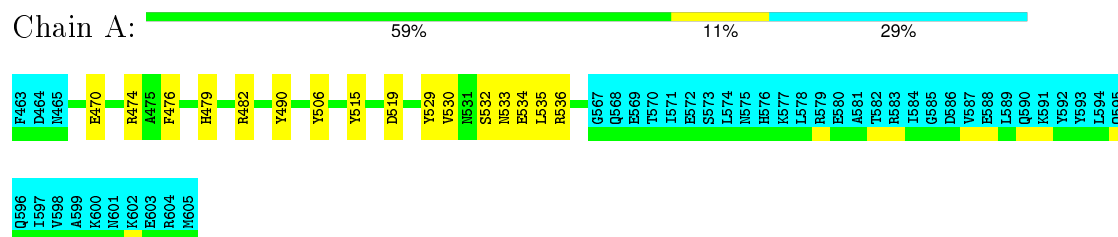
Mol	Chain	Residues	Atoms						Trace
1	A	143	Total	C	H	N	O	S	0
			2374	766	1152	206	248	2	

4 Residue-property plots [i](#)

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: DNA primase

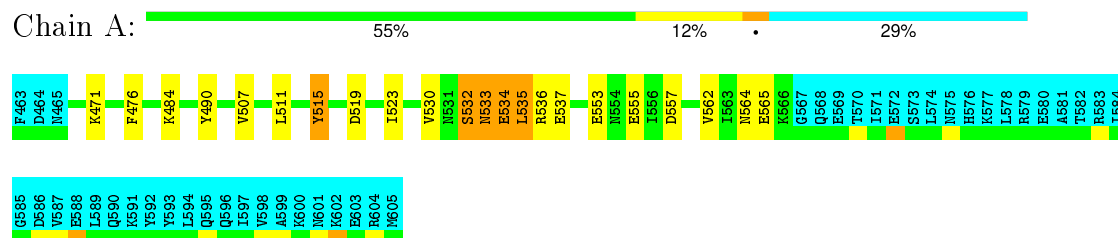


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: DNA primase



4.2.2 Score per residue for model 2

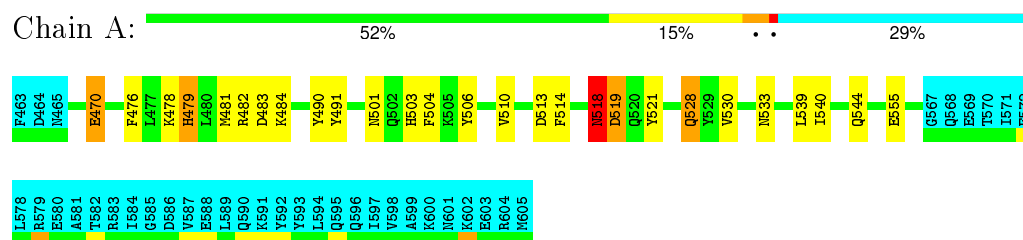
- Molecule 1: DNA primase





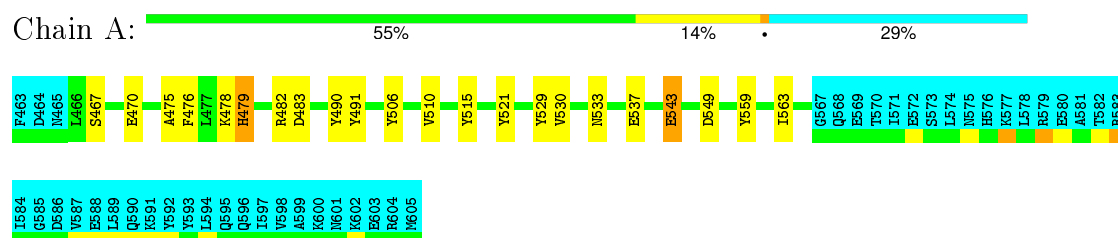
4.2.3 Score per residue for model 3

- Molecule 1: DNA primase



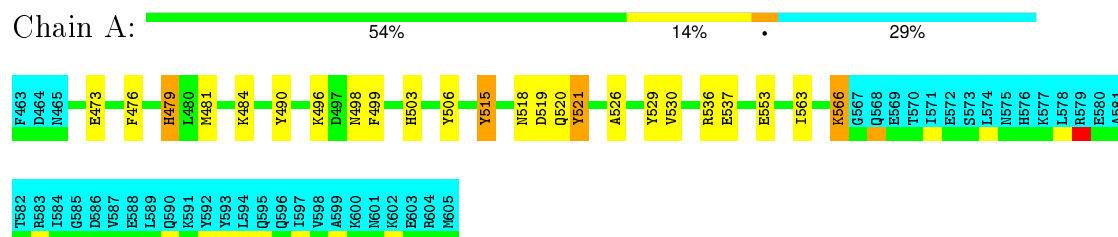
4.2.4 Score per residue for model 4

- Molecule 1: DNA primase



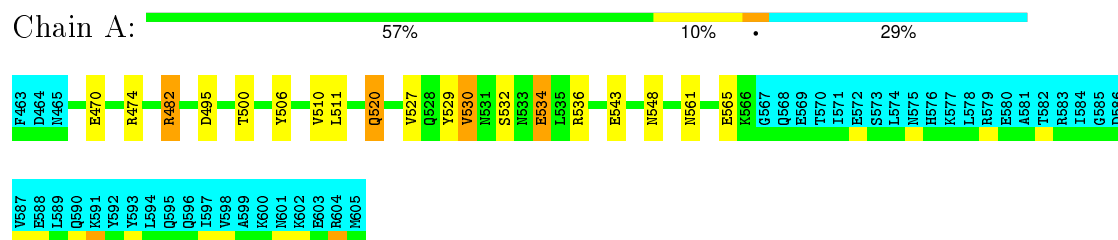
4.2.5 Score per residue for model 5

- Molecule 1: DNA primase



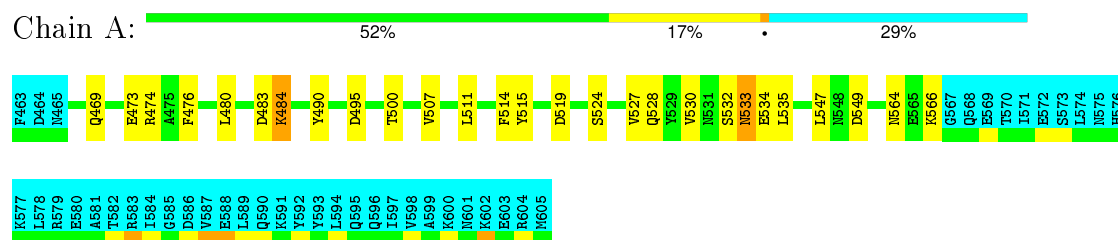
4.2.6 Score per residue for model 6

- Molecule 1: DNA primase



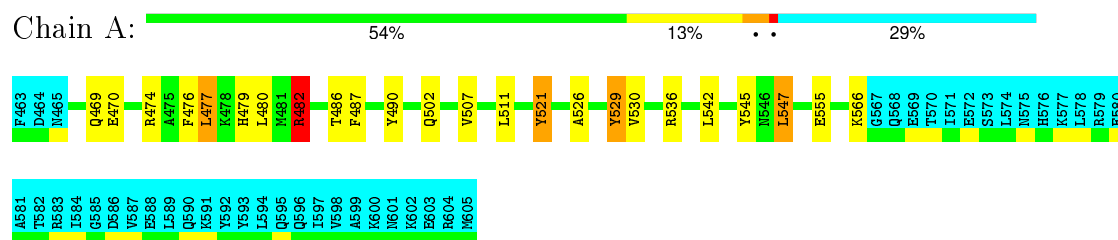
4.2.7 Score per residue for model 7

- Molecule 1: DNA primase



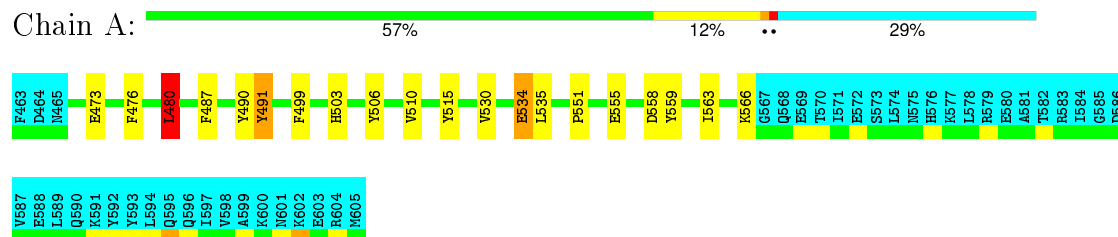
4.2.8 Score per residue for model 8

- Molecule 1: DNA primase



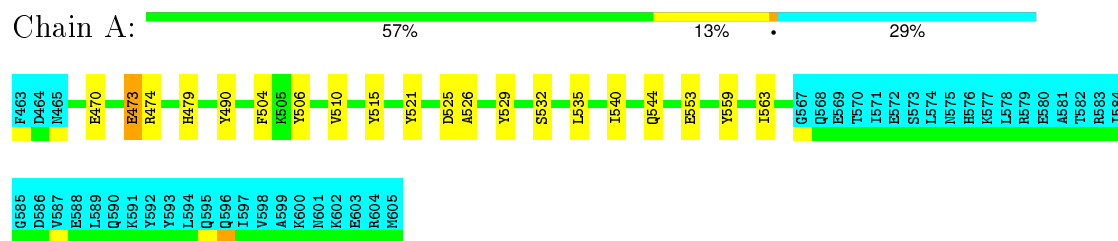
4.2.9 Score per residue for model 9

- Molecule 1: DNA primase



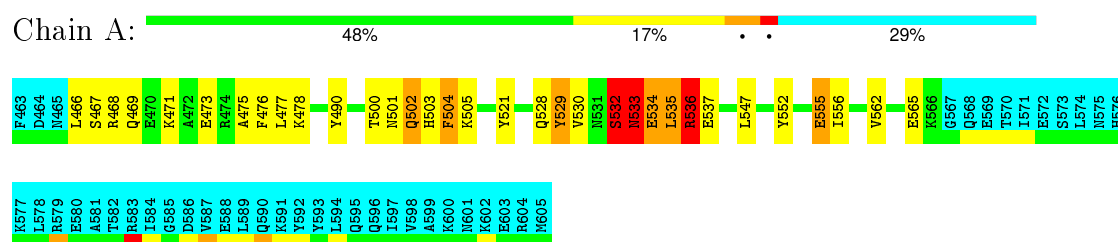
4.2.10 Score per residue for model 10

- Molecule 1: DNA primase



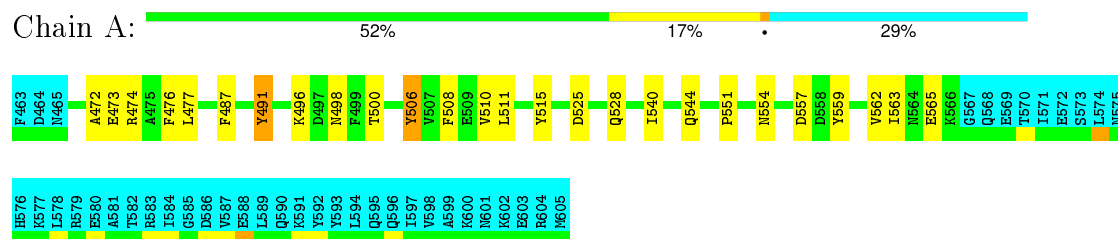
4.2.11 Score per residue for model 11

- Molecule 1: DNA primase



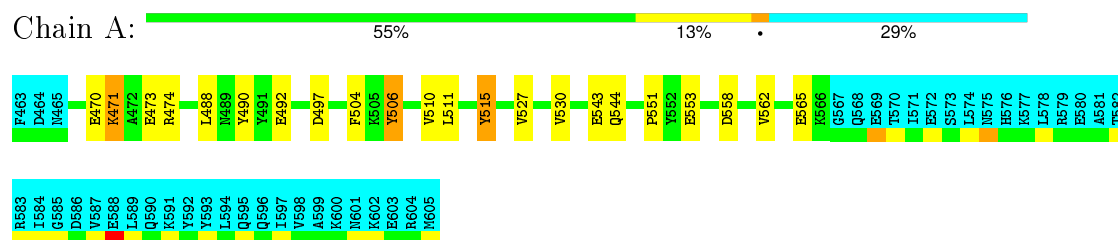
4.2.12 Score per residue for model 12

- Molecule 1: DNA primase



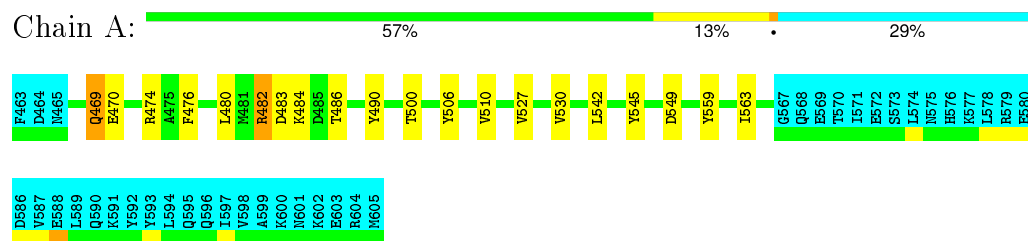
4.2.13 Score per residue for model 13

- Molecule 1: DNA primase

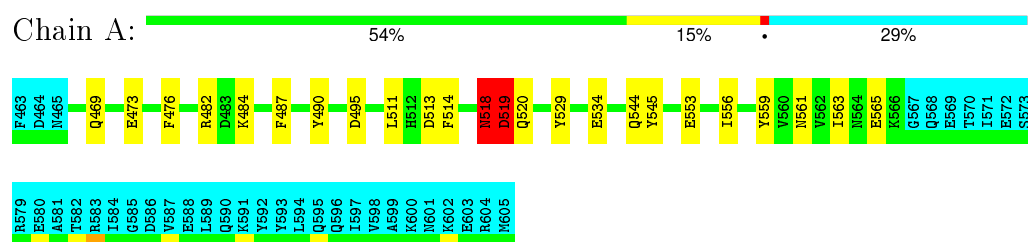


4.2.14 Score per residue for model 14

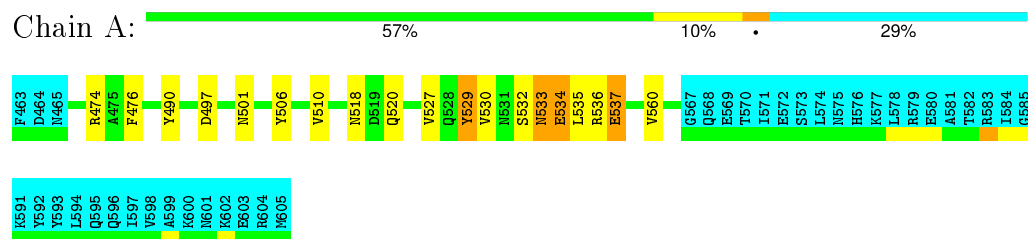
- Molecule 1: DNA primase



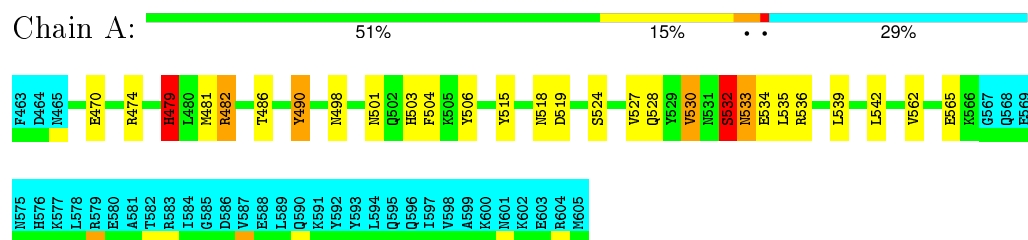
- Molecule 1: DNA primase



- Molecule 1: DNA primase

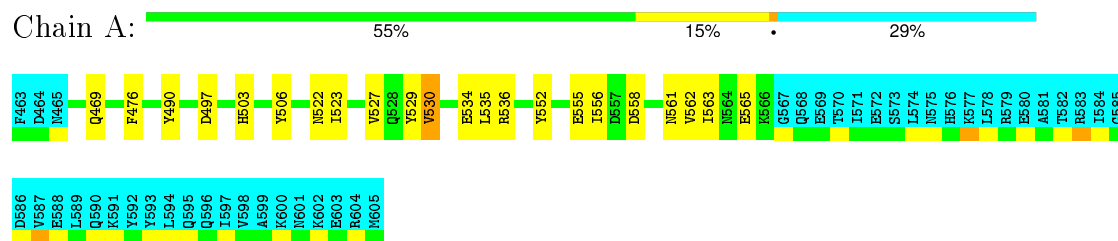


- Molecule 1: DNA primase



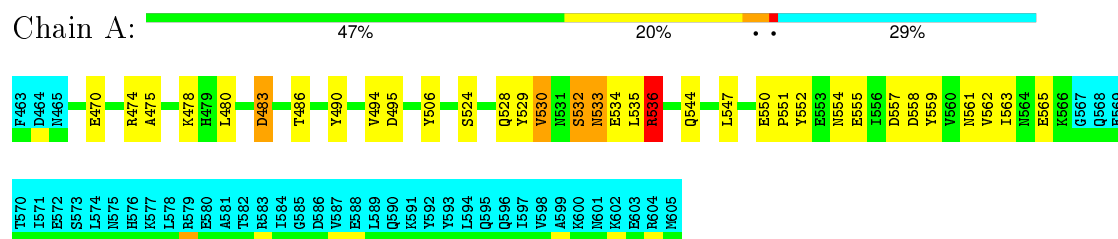
4.2.18 Score per residue for model 18

- Molecule 1: DNA primase



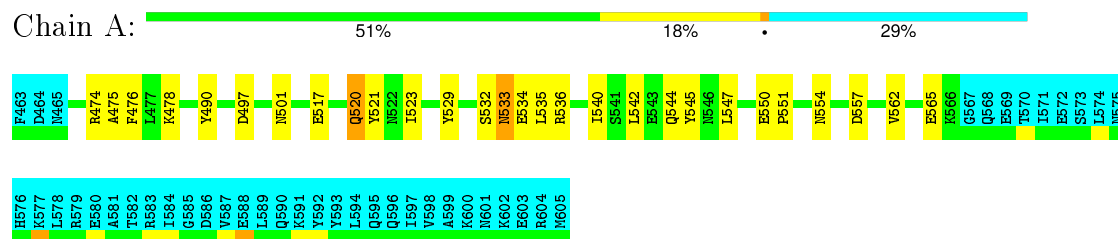
4.2.19 Score per residue for model 19

- Molecule 1: DNA primase



4.2.20 Score per residue for model 20

- Molecule 1: DNA primase



5 Refinement protocol and experimental data overview

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

Of the 2000 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
XPLOR-NIH	refinement	

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)	2lzn_cs.str
Number of chemical shift lists	1
Total number of shifts	1550
Number of shifts mapped to atoms	1550
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	72%

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

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	0.81±0.04	0±1/889 (0.0±0.1%)	0.80±0.04	1±1/1204 (0.0±0.1%)
All	All	0.81	4/17780 (0.0%)	0.80	10/24080 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.6±0.7
All	All	0	12

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	490	TYR	CD1-CE1	-6.44	1.29	1.39	17	1
1	A	521	TYR	CD1-CE1	-5.31	1.31	1.39	11	2
1	A	521	TYR	CB-CG	-5.06	1.44	1.51	20	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	532	SER	C-N-CA	6.92	138.99	121.70	1	6
1	A	521	TYR	CB-CG-CD1	-5.83	117.50	121.00	11	2
1	A	490	TYR	CB-CG-CD1	-5.55	117.67	121.00	17	1
1	A	532	SER	N-CA-CB	-5.50	102.25	110.50	17	1

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the

ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	536	ARG	Sidechain	3
1	A	474	ARG	Sidechain	2
1	A	519	ASP	Peptide	2
1	A	518	ASN	Peptide	2
1	A	482	ARG	Sidechain	1
1	A	498	ASN	Peptide	1
1	A	533	ASN	Mainchain	1

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	870	798	798	9±3
All	All	17400	15960	15960	187

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 6.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:514:PHE:O	1:A:518:ASN:HA	0.78	1.78	15	2
1:A:479:HIS:HA	1:A:486:THR:HG21	0.72	1.61	17	1
1:A:530:VAL:HA	1:A:536:ARG:NH2	0.65	2.06	19	1
1:A:497:ASP:O	1:A:501:ASN:HB3	0.63	1.94	20	1
1:A:503:HIS:HA	1:A:506:TYR:CE2	0.62	2.29	5	3
1:A:534:GLU:HA	1:A:536:ARG:HD3	0.61	1.73	11	1
1:A:501:ASN:OD1	1:A:503:HIS:HB2	0.61	1.96	17	1
1:A:534:GLU:O	1:A:537:GLU:HG3	0.60	1.95	16	1
1:A:511:LEU:HA	1:A:514:PHE:HB3	0.59	1.73	15	1
1:A:527:VAL:O	1:A:530:VAL:HG12	0.58	1.98	18	3
1:A:477:LEU:O	1:A:480:LEU:HG	0.58	1.98	8	1
1:A:503:HIS:CE1	1:A:535:LEU:HG	0.58	2.34	18	1
1:A:553:GLU:O	1:A:557:ASP:HB3	0.58	1.99	1	1
1:A:469:GLN:N	1:A:469:GLN:HE21	0.57	1.97	14	1
1:A:469:GLN:NE2	1:A:566:LYS:HB3	0.56	2.15	8	1
1:A:534:GLU:HA	1:A:536:ARG:CD	0.56	2.29	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:559:TYR:CE1	1:A:563:ILE:HD12	0.55	2.37	10	1
1:A:482:ARG:HG3	1:A:483:ASP:N	0.55	2.17	3	1
1:A:470:GLU:O	1:A:474:ARG:HG2	0.54	2.02	17	2
1:A:475:ALA:O	1:A:478:LYS:HG2	0.54	2.03	19	3
1:A:475:ALA:O	1:A:478:LYS:HG3	0.54	2.03	4	1
1:A:482:ARG:O	1:A:520:GLN:HG2	0.53	2.04	6	1
1:A:483:ASP:OD2	1:A:484:LYS:HG3	0.53	2.03	14	1
1:A:519:ASP:OD2	1:A:520:GLN:HG3	0.53	2.03	15	1
1:A:530:VAL:HA	1:A:536:ARG:NH1	0.53	2.18	17	1
1:A:561:ASN:O	1:A:565:GLU:HG3	0.53	2.03	19	3
1:A:470:GLU:O	1:A:474:ARG:HG3	0.53	2.04	8	6
1:A:482:ARG:HB2	1:A:486:THR:OG1	0.53	2.04	14	1
1:A:482:ARG:HA	1:A:520:GLN:NE2	0.53	2.18	15	1
1:A:530:VAL:HA	1:A:536:ARG:CZ	0.52	2.34	1	2
1:A:536:ARG:HD2	1:A:537:GLU:N	0.52	2.19	1	1
1:A:559:TYR:CE1	1:A:563:ILE:HG13	0.52	2.39	15	1
1:A:536:ARG:C	1:A:536:ARG:HD2	0.52	2.24	19	1
1:A:526:ALA:HA	1:A:529:TYR:CD2	0.52	2.40	10	1
1:A:480:LEU:HD13	1:A:480:LEU:H	0.51	1.65	9	1
1:A:559:TYR:CZ	1:A:563:ILE:HG13	0.51	2.41	15	1
1:A:558:ASP:O	1:A:562:VAL:HG23	0.51	2.06	2	4
1:A:552:TYR:O	1:A:555:GLU:HG3	0.51	2.04	19	1
1:A:559:TYR:O	1:A:563:ILE:HG12	0.51	2.05	12	4
1:A:515:TYR:HA	1:A:519:ASP:HB3	0.51	1.83	7	1
1:A:524:SER:O	1:A:528:GLN:HG3	0.50	2.05	7	2
1:A:542:LEU:O	1:A:545:TYR:HB3	0.50	2.07	8	2
1:A:547:LEU:O	1:A:550:GLU:HG3	0.50	2.07	19	1
1:A:506:TYR:O	1:A:510:VAL:HG23	0.50	2.07	13	9
1:A:554:ASN:HA	1:A:557:ASP:OD2	0.49	2.06	12	1
1:A:480:LEU:HA	1:A:483:ASP:HB2	0.49	1.85	19	1
1:A:482:ARG:HB3	1:A:519:ASP:O	0.49	2.07	17	1
1:A:533:ASN:O	1:A:535:LEU:N	0.49	2.45	7	7
1:A:482:ARG:HB3	1:A:486:THR:OG1	0.49	2.07	8	1
1:A:530:VAL:HA	1:A:536:ARG:NE	0.49	2.23	1	1
1:A:529:TYR:O	1:A:536:ARG:HG2	0.49	2.07	6	1
1:A:562:VAL:O	1:A:565:GLU:HG2	0.48	2.08	12	3
1:A:532:SER:O	1:A:534:GLU:HG3	0.48	2.09	11	1
1:A:553:GLU:O	1:A:556:ILE:HG12	0.48	2.08	15	1
1:A:540:ILE:O	1:A:544:GLN:HG3	0.48	2.08	3	3
1:A:552:TYR:O	1:A:556:ILE:HG13	0.48	2.09	18	1
1:A:484:LYS:HD2	1:A:515:TYR:CD2	0.48	2.44	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:473:GLU:O	1:A:477:LEU:HG	0.47	2.08	11	2
1:A:544:GLN:HG2	1:A:544:GLN:O	0.47	2.09	13	2
1:A:536:ARG:NH1	1:A:537:GLU:HB2	0.47	2.25	1	1
1:A:521:TYR:CE2	1:A:526:ALA:HB2	0.47	2.44	8	1
1:A:478:LYS:HD2	1:A:542:LEU:O	0.47	2.10	2	1
1:A:469:GLN:O	1:A:473:GLU:HG2	0.47	2.10	15	1
1:A:529:TYR:HB3	1:A:536:ARG:HG3	0.47	1.86	8	2
1:A:511:LEU:O	1:A:514:PHE:HB3	0.47	2.09	15	1
1:A:484:LYS:HD3	1:A:519:ASP:OD2	0.46	2.10	7	1
1:A:552:TYR:O	1:A:555:GLU:HG2	0.46	2.10	11	1
1:A:507:VAL:O	1:A:511:LEU:HG	0.46	2.11	8	2
1:A:471:LYS:HD3	1:A:471:LYS:O	0.46	2.11	13	1
1:A:481:MET:HG3	1:A:521:TYR:O	0.46	2.11	5	1
1:A:479:HIS:CD2	1:A:487:PHE:HA	0.46	2.45	8	1
1:A:540:ILE:O	1:A:544:GLN:HG2	0.46	2.10	20	1
1:A:552:TYR:HB2	1:A:555:GLU:HB3	0.46	1.87	18	1
1:A:554:ASN:O	1:A:557:ASP:HB3	0.46	2.11	20	2
1:A:539:LEU:O	1:A:542:LEU:HB2	0.46	2.10	17	1
1:A:563:ILE:O	1:A:566:LYS:HG3	0.46	2.11	5	1
1:A:529:TYR:HB3	1:A:536:ARG:HD2	0.45	1.86	20	1
1:A:547:LEU:HD13	1:A:547:LEU:H	0.45	1.71	8	1
1:A:474:ARG:HG3	1:A:542:LEU:CD2	0.45	2.42	20	1
1:A:518:ASN:CG	1:A:519:ASP:H	0.45	2.15	5	1
1:A:484:LYS:HE3	1:A:511:LEU:HD23	0.45	1.89	1	1
1:A:473:GLU:HB3	1:A:504:PHE:CD2	0.45	2.47	13	1
1:A:468:ARG:O	1:A:471:LYS:HB2	0.45	2.12	11	1
1:A:503:HIS:CD2	1:A:535:LEU:HD11	0.45	2.47	9	1
1:A:527:VAL:O	1:A:530:VAL:HG22	0.44	2.11	16	4
1:A:470:GLU:OE2	1:A:501:ASN:HB2	0.44	2.11	3	1
1:A:496:LYS:HA	1:A:500:THR:OG1	0.44	2.12	12	1
1:A:487:PHE:O	1:A:491:TYR:HB2	0.44	2.12	9	2
1:A:480:LEU:HB3	1:A:483:ASP:HB2	0.44	1.90	7	1
1:A:524:SER:O	1:A:528:GLN:HG2	0.44	2.13	19	1
1:A:469:GLN:NE2	1:A:563:ILE:HA	0.44	2.27	18	1
1:A:559:TYR:O	1:A:563:ILE:HD13	0.43	2.13	2	2
1:A:476:PHE:O	1:A:479:HIS:HB2	0.43	2.13	5	1
1:A:529:TYR:CG	1:A:536:ARG:HD3	0.43	2.49	16	1
1:A:532:SER:OG	1:A:535:LEU:HB2	0.43	2.13	10	1
1:A:466:LEU:O	1:A:466:LEU:HD12	0.43	2.13	11	1
1:A:467:SER:O	1:A:470:GLU:HG2	0.43	2.13	4	1
1:A:490:TYR:CE1	1:A:504:PHE:CE1	0.43	3.06	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:533:ASN:O	1:A:537:GLU:HG2	0.43	2.13	4	1
1:A:478:LYS:HG3	1:A:479:HIS:N	0.43	2.29	3	1
1:A:515:TYR:HA	1:A:519:ASP:HB2	0.43	1.90	1	1
1:A:525:ASP:O	1:A:528:GLN:HB3	0.43	2.14	12	1
1:A:562:VAL:O	1:A:565:GLU:HB3	0.43	2.13	20	2
1:A:534:GLU:HA	1:A:536:ARG:NE	0.42	2.29	1	1
1:A:511:LEU:O	1:A:515:TYR:HB2	0.42	2.13	13	2
1:A:472:ALA:HB3	1:A:563:ILE:HD11	0.42	1.90	12	1
1:A:520:GLN:H	1:A:520:GLN:NE2	0.42	2.13	20	1
1:A:481:MET:SD	1:A:481:MET:N	0.42	2.92	2	1
1:A:469:GLN:O	1:A:473:GLU:HG3	0.42	2.15	7	1
1:A:528:GLN:HE21	1:A:528:GLN:HA	0.42	1.74	3	1
1:A:526:ALA:O	1:A:529:TYR:HB2	0.42	2.15	5	1
1:A:561:ASN:O	1:A:565:GLU:HB2	0.42	2.15	6	1
1:A:469:GLN:NE2	1:A:566:LYS:HB2	0.42	2.29	7	1
1:A:529:TYR:CB	1:A:536:ARG:HD2	0.42	2.45	20	1
1:A:527:VAL:HA	1:A:530:VAL:HG13	0.42	1.92	17	1
1:A:479:HIS:CG	1:A:543:GLU:HA	0.42	2.50	4	1
1:A:502:GLN:O	1:A:505:LYS:HB3	0.41	2.15	11	1
1:A:488:LEU:O	1:A:492:GLU:HG2	0.41	2.15	13	1
1:A:473:GLU:HB3	1:A:504:PHE:CZ	0.41	2.51	10	1
1:A:536:ARG:HD3	1:A:537:GLU:N	0.41	2.31	11	1
1:A:495:ASP:OD2	1:A:500:THR:HA	0.41	2.16	7	1
1:A:501:ASN:C	1:A:503:HIS:H	0.41	2.19	11	1
1:A:530:VAL:HA	1:A:536:ARG:CB	0.41	2.46	5	1
1:A:500:THR:HB	1:A:504:PHE:CE2	0.41	2.51	11	1
1:A:484:LYS:O	1:A:487:PHE:HB3	0.41	2.16	15	1
1:A:507:VAL:O	1:A:511:LEU:HD13	0.41	2.16	1	1
1:A:529:TYR:CB	1:A:536:ARG:HG3	0.41	2.46	19	1
1:A:467:SER:HB2	1:A:469:GLN:OE1	0.41	2.16	11	1
1:A:483:ASP:HB3	1:A:486:THR:HB	0.40	1.93	19	1
1:A:484:LYS:HE3	1:A:520:GLN:HA	0.40	1.92	5	1
1:A:542:LEU:O	1:A:545:TYR:HB2	0.40	2.17	14	1
1:A:529:TYR:CB	1:A:536:ARG:HD3	0.40	2.47	16	1
1:A:484:LYS:NZ	1:A:519:ASP:OD1	0.40	2.53	1	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	101/143 (71%)	86±4 (85±4%)	11±4 (11±4%)	4±2 (3±2%)	8	37
All	All	2020/2860 (71%)	1724 (85%)	226 (11%)	70 (3%)	8	37

All 22 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	530	VAL	9
1	A	534	GLU	9
1	A	533	ASN	8
1	A	551	PRO	5
1	A	532	SER	5
1	A	479	HIS	4
1	A	555	GLU	4
1	A	482	ARG	4
1	A	549	ASP	3
1	A	499	PHE	2
1	A	547	LEU	2
1	A	519	ASP	2
1	A	495	ASP	2
1	A	553	GLU	2
1	A	518	ASN	2
1	A	483	ASP	1
1	A	502	GLN	1
1	A	480	LEU	1
1	A	500	THR	1
1	A	548	ASN	1
1	A	497	ASP	1
1	A	544	GLN	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	97/135 (72%)	90±2 (93±2%)	7±2 (7±2%)	23	68
All	All	1940/2700 (72%)	1800 (93%)	140 (7%)	23	68

All 57 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	490	TYR	17
1	A	476	PHE	13
1	A	529	TYR	7
1	A	515	TYR	7
1	A	521	TYR	5
1	A	506	TYR	5
1	A	491	TYR	4
1	A	534	GLU	4
1	A	520	GLN	3
1	A	523	ILE	3
1	A	473	GLU	3
1	A	543	GLU	3
1	A	481	MET	3
1	A	547	LEU	2
1	A	535	LEU	2
1	A	496	LYS	2
1	A	528	GLN	2
1	A	469	GLN	2
1	A	566	LYS	2
1	A	479	HIS	2
1	A	480	LEU	2
1	A	504	PHE	2
1	A	484	LYS	2
1	A	536	ARG	2
1	A	513	ASP	2
1	A	471	LYS	2
1	A	498	ASN	2
1	A	537	GLU	2
1	A	539	LEU	2
1	A	518	ASN	2
1	A	532	SER	2
1	A	497	ASP	2
1	A	483	ASP	1

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Mol	Chain	Res	Type	Models (Total)
1	A	556	ILE	1
1	A	501	ASN	1
1	A	550	GLU	1
1	A	517	GLU	1
1	A	519	ASP	1
1	A	502	GLN	1
1	A	545	TYR	1
1	A	514	PHE	1
1	A	500	THR	1
1	A	494	VAL	1
1	A	495	ASP	1
1	A	522	ASN	1
1	A	474	ARG	1
1	A	477	LEU	1
1	A	553	GLU	1
1	A	508	PHE	1
1	A	565	GLU	1
1	A	511	LEU	1
1	A	531	ASN	1
1	A	470	GLU	1
1	A	525	ASP	1
1	A	564	ASN	1
1	A	555	GLU	1
1	A	482	ARG	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 ⓘ

There are no carbohydrates in this entry.

6.6 Ligand geometry ⓘ

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 72% for the well-defined parts and 75% for the entire structure.

7.1 Chemical shift list 1

File name: 2lzn_cs.str

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	1550
Number of shifts mapped to atoms	1550
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	139	-0.53 ± 0.14	Should be applied
$^{13}\text{C}_\beta$	136	0.02 ± 0.06	None needed (< 0.5 ppm)
$^{13}\text{C}'$	131	2.32 ± 0.14	Should be applied
^{15}N	135	0.06 ± 0.21	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 72%, i.e. 950 atoms were assigned a chemical shift out of a possible 1323. 13 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	466/503 (93%)	186/201 (93%)	187/202 (93%)	93/100 (93%)
Sidechain	444/673 (66%)	271/391 (69%)	173/247 (70%)	0/35 (0%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	40/147 (27%)	23/78 (29%)	17/66 (26%)	0/3 (0%)
Overall	950/1323 (72%)	480/670 (72%)	377/515 (73%)	93/138 (67%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 75%, i.e. 1411 atoms were assigned a chemical shift out of a possible 1885. 19 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	674/713 (95%)	269/285 (94%)	270/286 (94%)	135/142 (95%)
Sidechain	684/993 (69%)	418/578 (72%)	266/360 (74%)	0/55 (0%)
Aromatic	53/179 (30%)	30/95 (32%)	23/80 (29%)	0/4 (0%)
Overall	1411/1885 (75%)	717/958 (75%)	559/726 (77%)	135/201 (67%)

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	512	HIS	CD2	0.00	137.40 – 103.40	-35.4
1	A	555	GLU	CB	39.34	38.65 – 21.35	5.4
1	A	484	LYS	HB2	3.06	3.03 – 0.53	5.1

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:

