



Full wwPDB NMR Structure Validation Report ⓘ

Mar 1, 2026 – 05:19 PM UTC

PDB ID : 1MZI / pdb_00001mzi
Title : Solution ensemble structures of HIV-1 gp41 2F5 mAb epitope
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Deposited on : 2002-10-08

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

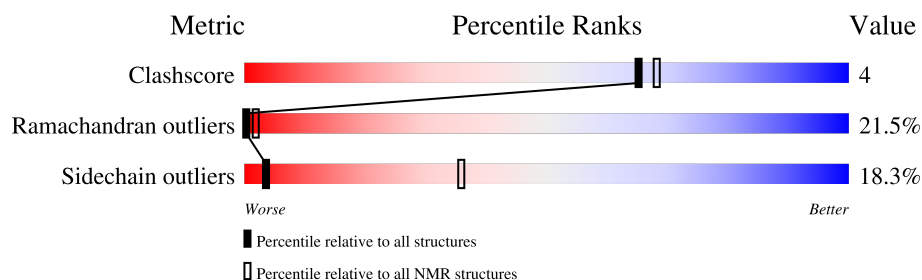
1 Overall quality at a glance

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	13	 15% 85%

2 Ensemble composition and analysis ⓘ

This entry contains 81 models. The atoms present in the NMR models are not consistent. Some calculations may have failed as a result. All residues are included in the validation scores.

Cyrange was unable to find well-defined residues.

Error message: Only domains with < 8 residues could be identified.

NmrClust was unable to cluster the ensemble.

Error message: Wrapper check: not enough residues in core to run NmrClust

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 225 atoms, of which 110 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called 2F5 epitope of HIV-1 gp41 fusion protein.

Mol	Chain	Residues	Atoms					Trace
1	A	13	Total	C	H	N	O	0
			225	76	110	17	22	

4 Residue-property plots [i](#)

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: 2F5 epitope of HIV-1 gp41 fusion protein

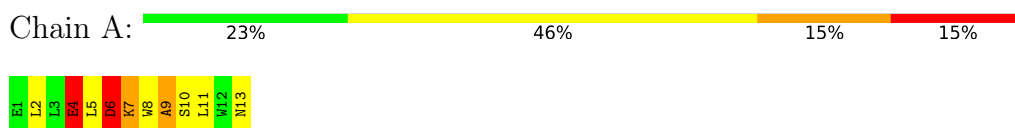


4.2 Scores per residue for each member of the ensemble

Colouring as in section [4.1](#) above.

4.2.1 Score per residue for model 1

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



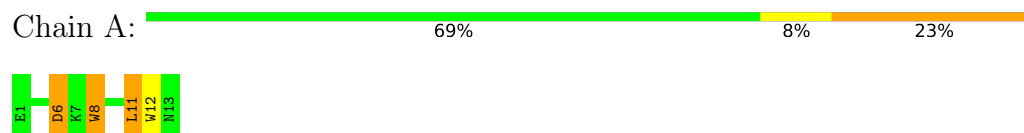
4.2.2 Score per residue for model 2

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



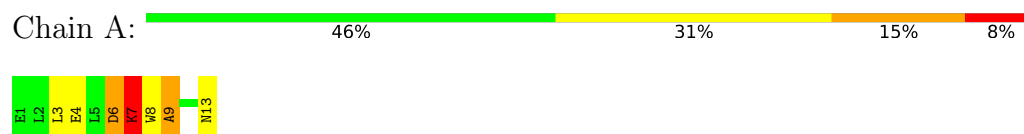
4.2.3 Score per residue for model 3

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



4.2.4 Score per residue for model 4

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



4.2.5 Score per residue for model 5

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



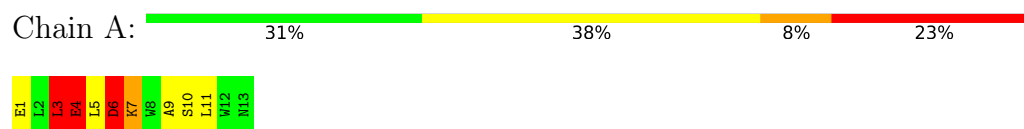
4.2.6 Score per residue for model 6

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



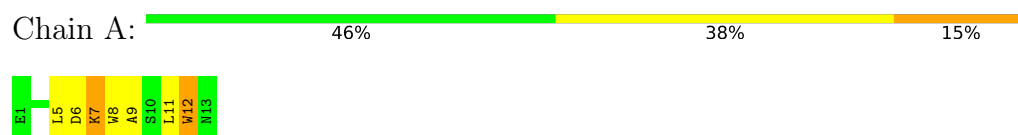
4.2.7 Score per residue for model 7

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



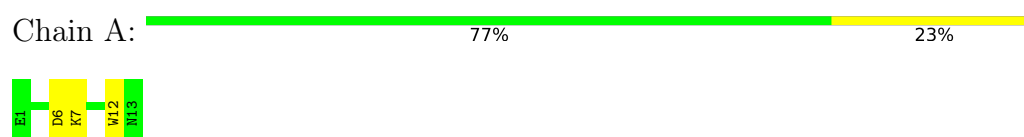
4.2.8 Score per residue for model 8

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



4.2.9 Score per residue for model 9

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



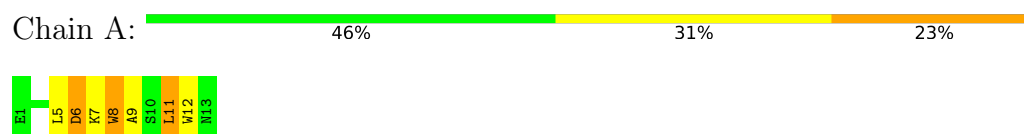
4.2.10 Score per residue for model 10

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



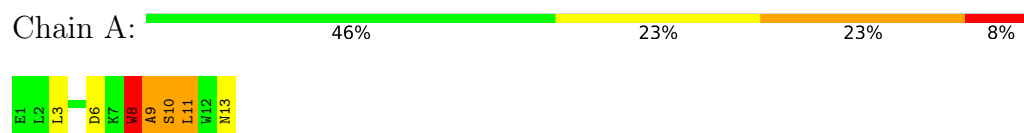
4.2.11 Score per residue for model 11

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



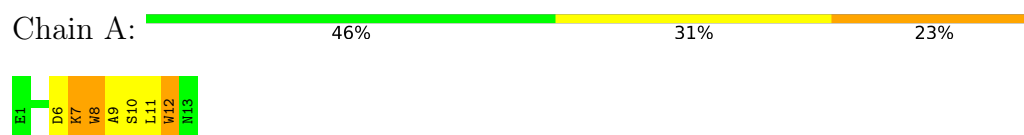
4.2.12 Score per residue for model 12

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



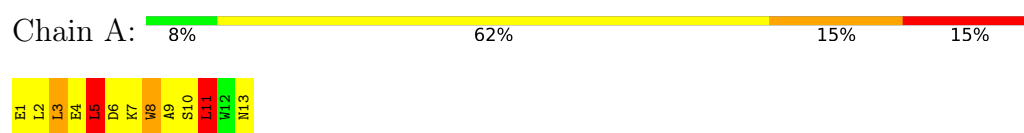
4.2.13 Score per residue for model 13

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



4.2.14 Score per residue for model 14

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



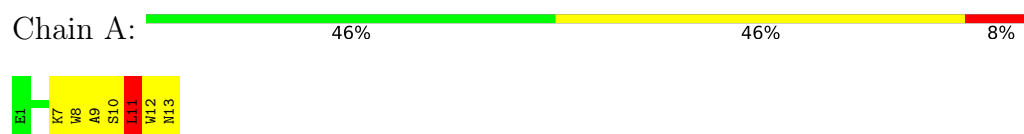
4.2.15 Score per residue for model 15

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



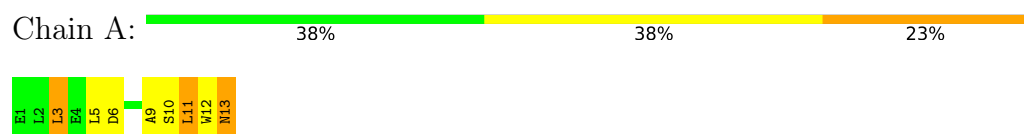
4.2.16 Score per residue for model 16

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



4.2.17 Score per residue for model 17

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



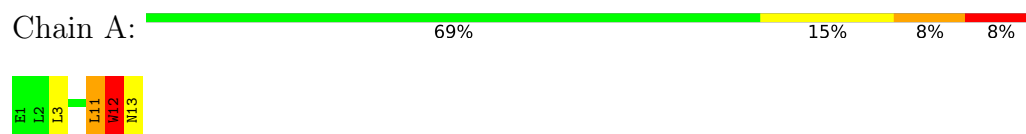
4.2.18 Score per residue for model 18

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



4.2.19 Score per residue for model 19

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



4.2.20 Score per residue for model 20

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



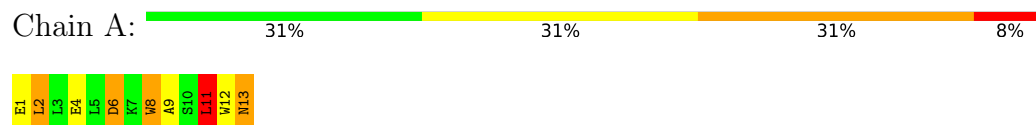
4.2.21 Score per residue for model 21

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



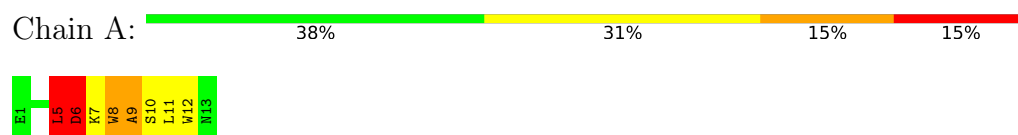
4.2.22 Score per residue for model 22

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



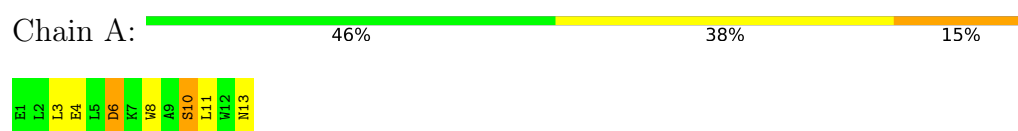
4.2.23 Score per residue for model 23

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



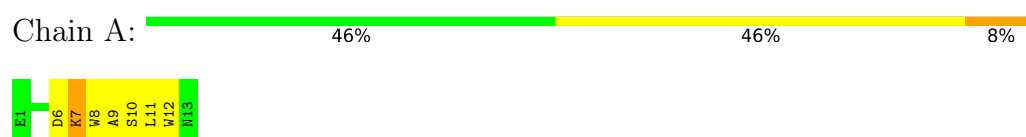
4.2.24 Score per residue for model 24

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



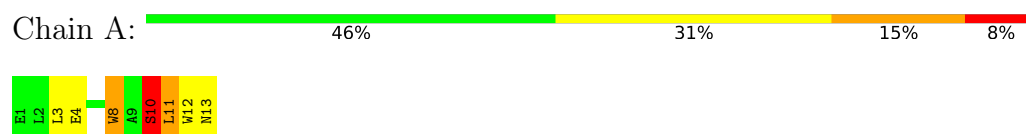
4.2.25 Score per residue for model 25

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



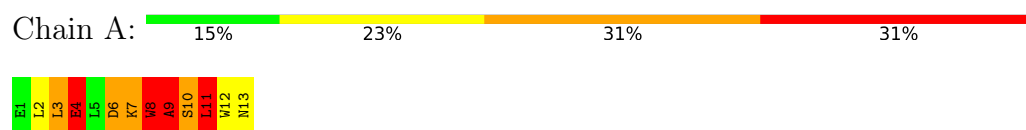
4.2.26 Score per residue for model 26

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



4.2.27 Score per residue for model 27

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



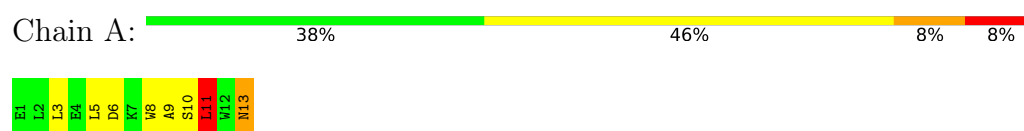
4.2.28 Score per residue for model 28

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



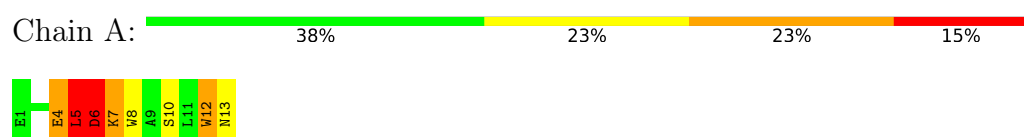
4.2.29 Score per residue for model 29

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



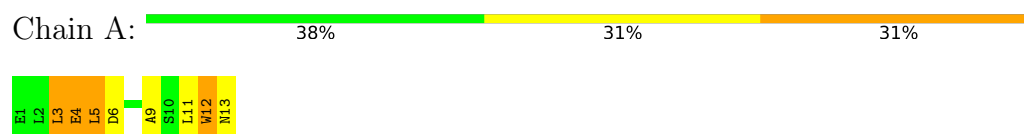
4.2.30 Score per residue for model 30

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



4.2.31 Score per residue for model 31

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



4.2.32 Score per residue for model 32

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



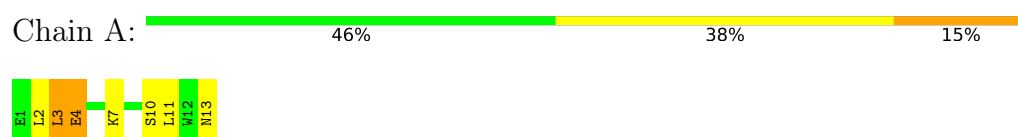
4.2.33 Score per residue for model 33

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



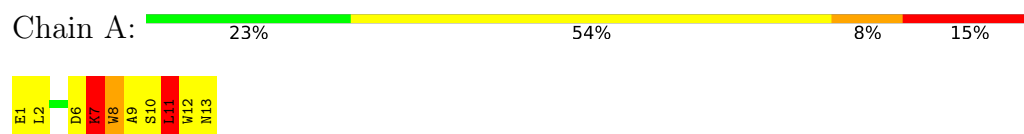
4.2.34 Score per residue for model 34

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



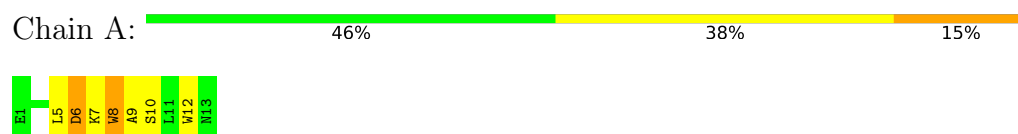
4.2.35 Score per residue for model 35

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



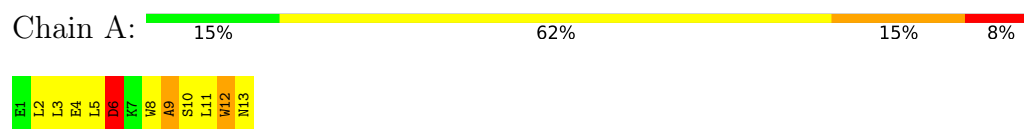
4.2.36 Score per residue for model 36

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



4.2.37 Score per residue for model 37

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



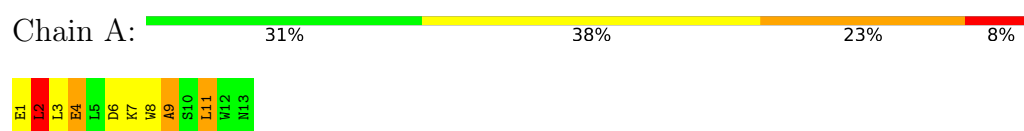
4.2.38 Score per residue for model 38

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



4.2.39 Score per residue for model 39

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



4.2.40 Score per residue for model 40

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



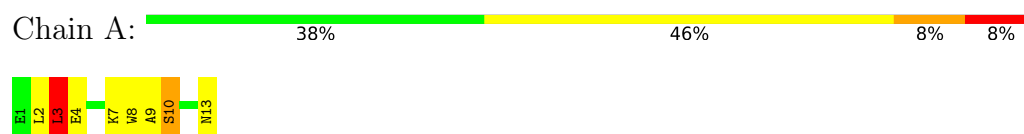
4.2.41 Score per residue for model 41

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



4.2.42 Score per residue for model 42

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



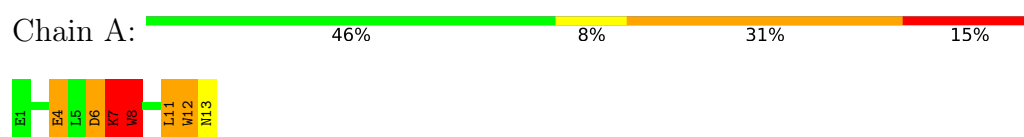
4.2.43 Score per residue for model 43

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



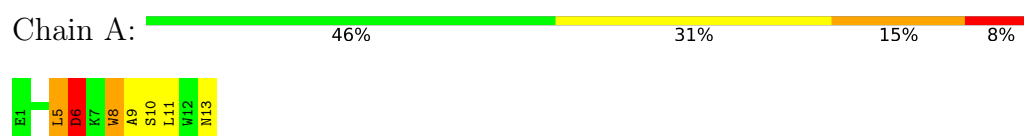
4.2.44 Score per residue for model 44

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



4.2.45 Score per residue for model 45

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



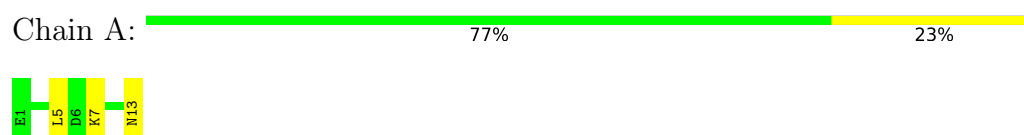
4.2.46 Score per residue for model 46

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



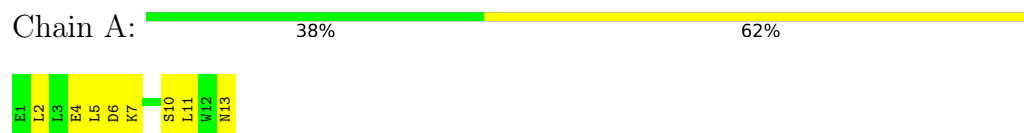
4.2.47 Score per residue for model 47

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



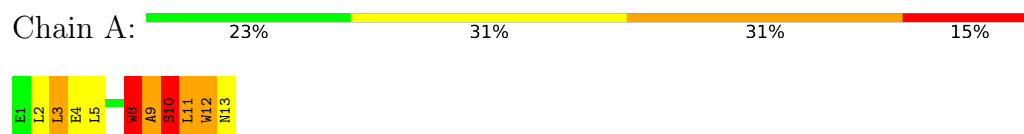
4.2.48 Score per residue for model 48

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



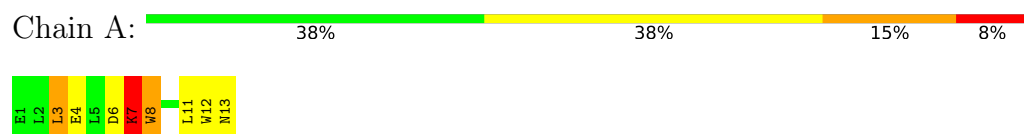
4.2.49 Score per residue for model 49

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



4.2.50 Score per residue for model 50

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



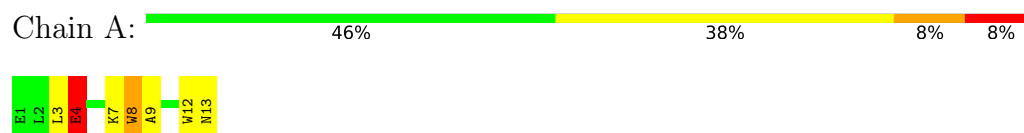
4.2.51 Score per residue for model 51

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



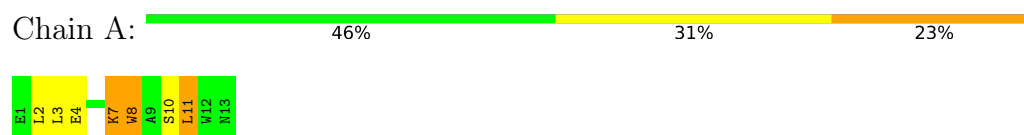
4.2.52 Score per residue for model 52

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



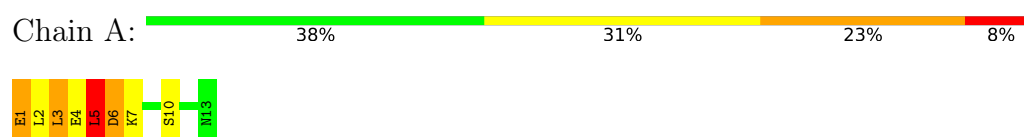
4.2.53 Score per residue for model 53

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



4.2.54 Score per residue for model 54

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



4.2.55 Score per residue for model 55

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



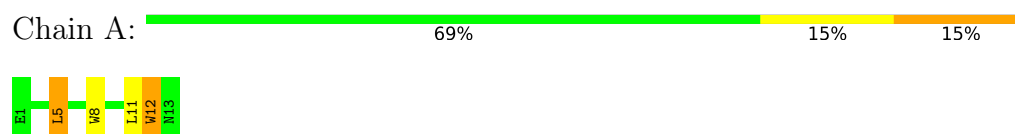
4.2.56 Score per residue for model 56

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



4.2.57 Score per residue for model 57

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



4.2.58 Score per residue for model 58

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein

Chain A:  85% 15%



4.2.59 Score per residue for model 59

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein

Chain A:  46% 46% 8%



4.2.60 Score per residue for model 60

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein

Chain A:  62% 31% 8%



4.2.61 Score per residue for model 61

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein

Chain A:  85% 15%



4.2.62 Score per residue for model 62

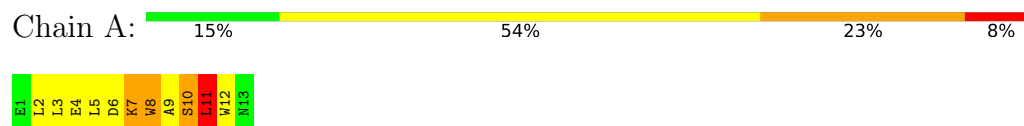
- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein

Chain A:  92% 8%



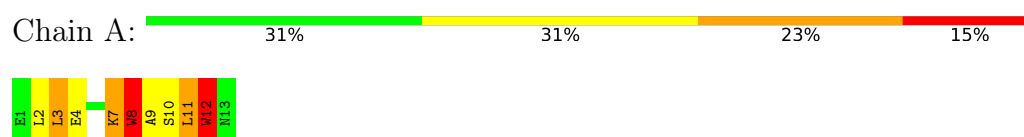
4.2.63 Score per residue for model 63

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



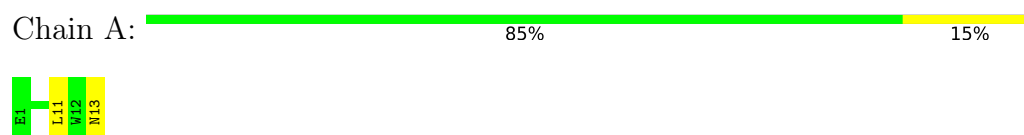
4.2.64 Score per residue for model 64

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



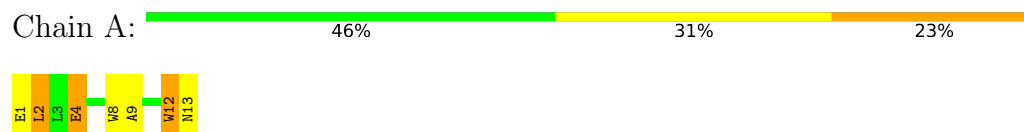
4.2.65 Score per residue for model 65

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



4.2.66 Score per residue for model 66

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



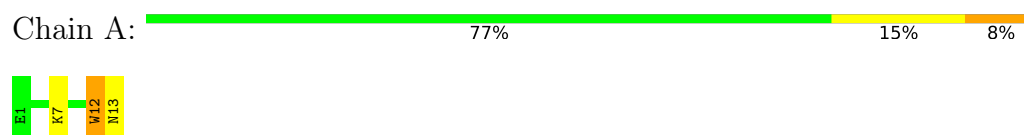
4.2.67 Score per residue for model 67

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



4.2.68 Score per residue for model 68

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



4.2.69 Score per residue for model 69

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



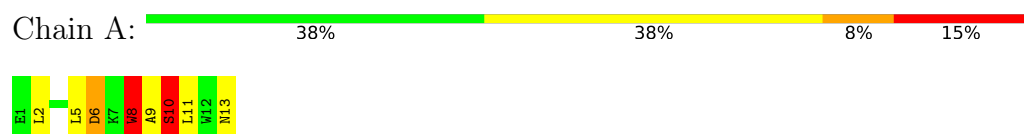
4.2.70 Score per residue for model 70

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



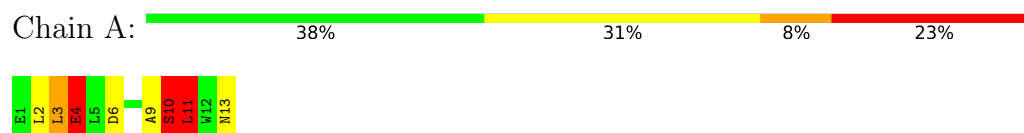
4.2.71 Score per residue for model 71

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



4.2.72 Score per residue for model 72

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



4.2.73 Score per residue for model 73

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



4.2.74 Score per residue for model 74

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



4.2.75 Score per residue for model 75

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



4.2.76 Score per residue for model 76

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



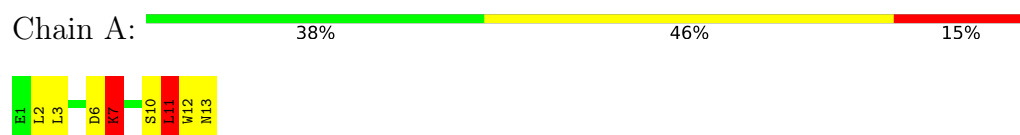
4.2.77 Score per residue for model 77

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



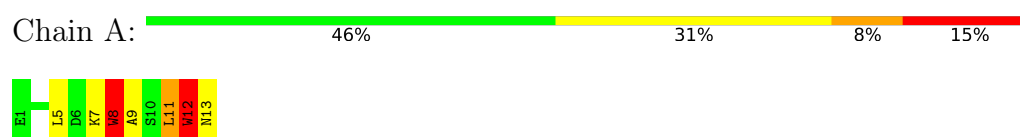
4.2.78 Score per residue for model 78

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



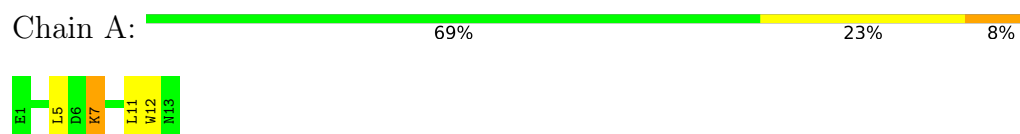
4.2.79 Score per residue for model 79

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



4.2.80 Score per residue for model 80

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



4.2.81 Score per residue for model 81

- Molecule 1: 2F5 epitope of HIV-1 gp41 fusion protein



5 Refinement protocol and experimental data overview

The models were refined using the following method: *Ensemble generation with MEDUSA, Clustering analysis with NMRCLUST, Statistical analysis of the ensemble with NAMFIS.*

Of the 6400 calculated structures, 81 were deposited, based on the following criterion: *Base set ensemble representative of the conformational space experimentally allowed.*

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

Software name	Classification	Version
DGII	refinement	MSI
NAMFIS	refinement	1.0
MEDUSA	refinement	in home
NMRCLUST	refinement	1.2

No chemical shift data was provided.

6 Model quality

6.1 Standard geometry

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	1.67±0.21	0±1/118 (0.4± 0.8%)	1.85±0.31	4±3/159 (2.4± 1.8%)
All	All	1.69	38/9558 (0.4%)	1.87	309/12879 (2.4%)

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	0.1±0.4	1.3±1.2
All	All	9	108

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	9	ALA	CA-CB	15.51	1.72	1.52	63	7
1	A	7	LYS	N-CA	10.57	1.59	1.46	1	2
1	A	6	ASP	CA-C	10.12	1.57	1.52	12	2
1	A	9	ALA	CA-C	8.64	1.64	1.52	27	1
1	A	4	GLU	N-CA	8.63	1.56	1.46	64	1
1	A	7	LYS	CA-C	8.07	1.63	1.52	27	3
1	A	4	GLU	CA-C	7.99	1.56	1.52	30	5
1	A	10	SER	CA-C	7.60	1.56	1.52	70	1
1	A	3	LEU	CA-C	7.59	1.56	1.52	50	4
1	A	10	SER	N-CA	6.19	1.50	1.46	24	1
1	A	5	LEU	CA-C	5.72	1.60	1.52	14	1
1	A	6	ASP	C-N	-5.60	1.26	1.33	11	2
1	A	11	LEU	CA-C	5.50	1.60	1.52	24	3
1	A	8	TRP	CA-C	5.46	1.59	1.53	29	1
1	A	12	TRP	CA-C	5.34	1.59	1.52	64	2
1	A	6	ASP	N-CA	5.11	1.52	1.46	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	8	TRP	N-CA	5.06	1.52	1.46	35	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	6	ASP	N-CA-CB	14.69	132.23	110.49	7	7
1	A	7	LYS	CB-CG-CD	14.61	144.91	111.30	73	1
1	A	8	TRP	CB-CA-C	13.78	130.62	111.74	22	12
1	A	11	LEU	O-C-N	-12.59	106.97	122.20	17	3
1	A	12	TRP	CB-CA-C	12.17	134.64	110.42	18	11
1	A	9	ALA	N-CA-CB	-11.14	93.40	110.44	64	16
1	A	3	LEU	N-CA-C	11.14	123.17	111.14	18	4
1	A	2	LEU	N-CA-CB	10.83	128.91	110.50	39	2
1	A	3	LEU	CB-CA-C	10.68	129.26	111.31	31	3
1	A	10	SER	CB-CA-C	10.11	131.63	117.07	24	6
1	A	6	ASP	CA-CB-CG	9.88	122.48	112.60	54	11
1	A	12	TRP	CA-CB-CG	9.77	132.17	113.60	49	9
1	A	11	LEU	N-CA-C	9.51	126.97	111.37	17	9
1	A	7	LYS	N-CA-C	9.11	130.19	110.80	35	7
1	A	7	LYS	N-CA-CB	8.93	125.59	110.49	44	8
1	A	4	GLU	O-C-N	-8.91	114.53	123.62	59	9
1	A	11	LEU	N-CA-CB	8.63	125.08	110.49	35	1
1	A	9	ALA	CB-CA-C	8.62	127.57	110.42	27	1
1	A	4	GLU	N-CA-CB	8.53	124.90	110.49	52	5
1	A	10	SER	N-CA-C	8.38	122.86	112.47	46	5
1	A	10	SER	N-CA-CB	8.27	124.46	110.49	42	3
1	A	12	TRP	O-C-N	-8.22	113.74	123.27	22	6
1	A	11	LEU	CB-CA-C	7.83	125.99	110.42	35	10
1	A	8	TRP	N-CA-CB	-7.74	101.45	110.35	23	4
1	A	6	ASP	N-CA-C	7.39	119.31	110.44	4	4
1	A	2	LEU	O-C-N	-7.18	111.52	123.00	14	9
1	A	13	ASN	OD1-CG-ND2	-7.17	115.42	122.60	22	9
1	A	8	TRP	CA-CB-CG	7.10	127.09	113.60	4	7
1	A	9	ALA	N-CA-C	7.07	121.93	113.16	64	4
1	A	13	ASN	CA-CB-CG	6.75	119.35	112.60	75	53
1	A	3	LEU	N-CA-CB	6.69	120.22	110.58	28	2
1	A	5	LEU	N-CA-CB	-6.61	102.10	112.08	23	2
1	A	5	LEU	O-C-N	-6.56	112.51	123.00	30	1
1	A	8	TRP	CB-CG-CD2	6.53	135.94	126.80	55	3
1	A	1	GLU	O-C-N	-6.48	112.63	123.00	39	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	5	LEU	CB-CA-C	6.38	123.12	110.42	63	2
1	A	6	ASP	CA-C-O	6.36	130.09	121.89	4	2
1	A	10	SER	O-C-N	-6.32	114.18	122.59	49	1
1	A	8	TRP	O-C-N	-6.23	114.89	123.12	5	1
1	A	6	ASP	O-C-N	-6.10	114.47	122.59	54	1
1	A	8	TRP	N-CA-C	6.10	120.09	111.92	27	8
1	A	7	LYS	CA-CB-CG	6.02	126.15	114.10	44	1
1	A	4	GLU	N-CA-C	6.00	123.59	110.80	7	3
1	A	12	TRP	CB-CG-CD2	6.00	135.19	126.80	79	6
1	A	7	LYS	O-C-N	5.97	130.53	122.59	63	1
1	A	12	TRP	N-CA-CB	-5.96	102.95	111.84	13	5
1	A	11	LEU	CA-C-N	5.78	132.10	121.70	77	2
1	A	11	LEU	C-N-CA	5.78	132.10	121.70	77	2
1	A	12	TRP	CB-CG-CD1	-5.64	118.43	126.90	27	2
1	A	1	GLU	CA-C-N	5.62	131.81	121.70	39	1
1	A	1	GLU	C-N-CA	5.62	131.81	121.70	39	1
1	A	5	LEU	CA-C-N	5.54	131.68	121.70	30	1
1	A	5	LEU	C-N-CA	5.54	131.68	121.70	30	1
1	A	12	TRP	N-CA-C	5.53	118.09	110.35	6	2
1	A	9	ALA	CA-C-O	5.42	128.27	120.51	4	1
1	A	8	TRP	CA-C-N	5.36	131.22	121.41	29	1
1	A	8	TRP	C-N-CA	5.36	131.22	121.41	29	1
1	A	8	TRP	CB-CG-CD1	-5.33	118.90	126.90	55	2
1	A	5	LEU	N-CA-C	5.29	122.06	110.80	31	2
1	A	10	SER	CA-C-O	-5.16	116.83	119.77	70	1
1	A	4	GLU	CB-CG-CD	5.14	121.34	112.60	7	1
1	A	2	LEU	CA-C-N	5.07	130.82	121.70	39	1
1	A	2	LEU	C-N-CA	5.07	130.82	121.70	39	1
1	A	7	LYS	CA-C-O	-5.04	113.30	120.51	35	1
1	A	1	GLU	CB-CA-C	5.01	119.61	110.10	66	1

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

Mol	Chain	Res	Type	Atoms	Models (Total)
1	A	11	LEU	CA	3
1	A	3	LEU	CA	3
1	A	10	SER	CA	1
1	A	12	TRP	CA	1
1	A	5	LEU	CA	1

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	4	GLU	Peptide	16
1	A	10	SER	Peptide	16
1	A	7	LYS	Peptide	13
1	A	8	TRP	Peptide	13
1	A	6	ASP	Peptide	12
1	A	9	ALA	Peptide	11
1	A	5	LEU	Peptide	8
1	A	11	LEU	Peptide	6
1	A	3	LEU	Peptide	5
1	A	13	ASN	Sidechain	3
1	A	12	TRP	Peptide	3
1	A	2	LEU	Peptide	2

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	115	111	111	1±2
All	All	9315	8911	8880	73

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 4.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:9:ALA:CA	1:A:9:ALA:CB	1.59	1.75	49	3
1:A:9:ALA:CB	1:A:9:ALA:C	0.71	2.61	49	2
1:A:6:ASP:CG	1:A:9:ALA:HB2	0.71	2.11	8	2
1:A:6:ASP:OD1	1:A:9:ALA:HB2	0.70	1.85	8	1
1:A:5:LEU:HD11	1:A:8:TRP:HB3	0.65	1.68	81	1
1:A:7:LYS:O	1:A:8:TRP:CG	0.65	2.49	13	1
1:A:9:ALA:CB	1:A:9:ALA:N	0.62	2.61	27	3
1:A:5:LEU:O	1:A:5:LEU:HD23	0.58	1.99	80	1
1:A:5:LEU:HD12	1:A:6:ASP:N	0.57	2.15	8	1
1:A:8:TRP:HA	1:A:11:LEU:HD12	0.57	1.75	3	2
1:A:5:LEU:HD11	1:A:8:TRP:CB	0.57	2.30	81	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:7:LYS:O	1:A:8:TRP:CD1	0.56	2.58	13	2
1:A:11:LEU:HD22	1:A:12:TRP:CZ3	0.55	2.36	11	3
1:A:6:ASP:O	1:A:8:TRP:N	0.52	2.42	8	1
1:A:6:ASP:O	1:A:7:LYS:C	0.52	2.52	13	1
1:A:8:TRP:CD2	1:A:8:TRP:N	0.52	2.77	33	2
1:A:11:LEU:HD22	1:A:12:TRP:H	0.51	1.65	35	1
1:A:11:LEU:H	1:A:11:LEU:HD13	0.51	1.65	22	1
1:A:9:ALA:CB	1:A:9:ALA:HA	0.51	2.16	27	1
1:A:6:ASP:HB3	1:A:9:ALA:HB2	0.50	1.84	25	1
1:A:5:LEU:HD23	1:A:5:LEU:C	0.50	2.31	11	1
1:A:5:LEU:O	1:A:6:ASP:CB	0.49	2.61	21	3
1:A:11:LEU:O	1:A:12:TRP:CD1	0.48	2.66	56	2
1:A:6:ASP:O	1:A:9:ALA:HB3	0.48	2.08	13	2
1:A:11:LEU:O	1:A:12:TRP:C	0.47	2.58	8	1
1:A:7:LYS:C	1:A:8:TRP:CE3	0.47	2.93	23	1
1:A:12:TRP:N	1:A:12:TRP:CE3	0.47	2.83	9	6
1:A:7:LYS:O	1:A:9:ALA:N	0.46	2.44	13	1
1:A:5:LEU:HD12	1:A:5:LEU:C	0.45	2.36	8	1
1:A:5:LEU:O	1:A:6:ASP:HB3	0.45	2.11	36	2
1:A:12:TRP:CD2	1:A:12:TRP:N	0.44	2.85	36	1
1:A:6:ASP:O	1:A:9:ALA:N	0.44	2.41	8	2
1:A:11:LEU:O	1:A:12:TRP:CE3	0.43	2.72	3	4
1:A:6:ASP:CB	1:A:9:ALA:HB2	0.43	2.43	11	1
1:A:8:TRP:CE3	1:A:8:TRP:C	0.43	2.96	13	2
1:A:7:LYS:O	1:A:8:TRP:CE3	0.42	2.72	23	1
1:A:8:TRP:O	1:A:11:LEU:HB2	0.42	2.14	11	1
1:A:12:TRP:N	1:A:12:TRP:CD2	0.42	2.87	9	4
1:A:5:LEU:O	1:A:5:LEU:CD2	0.41	2.68	23	2
1:A:8:TRP:CE3	1:A:9:ALA:N	0.41	2.88	21	1
1:A:7:LYS:C	1:A:9:ALA:H	0.41	2.24	13	1
1:A:6:ASP:OD1	1:A:8:TRP:CE2	0.40	2.74	25	1
1:A:12:TRP:CD1	1:A:12:TRP:N	0.40	2.87	13	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	11/13 (85%)	5±2 (47±21%)	3±2 (32±16%)	2±2 (22±14%)	0	2
All	All	891/1053 (85%)	417 (47%)	282 (32%)	192 (22%)	0	2

All 11 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	11	LEU	25
1	A	6	ASP	23
1	A	7	LYS	22
1	A	10	SER	18
1	A	3	LEU	18
1	A	12	TRP	18
1	A	5	LEU	17
1	A	2	LEU	15
1	A	4	GLU	15
1	A	8	TRP	12
1	A	9	ALA	9

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	12/12 (100%)	10±1 (82±10%)	2±1 (18±10%)	3	36
All	All	972/972 (100%)	794 (82%)	178 (18%)	3	36

All 11 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	11	LEU	46
1	A	8	TRP	35
1	A	3	LEU	24
1	A	12	TRP	17
1	A	10	SER	15
1	A	6	ASP	12
1	A	7	LYS	11

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Mol	Chain	Res	Type	Models (Total)
1	A	5	LEU	10
1	A	4	GLU	4
1	A	2	LEU	3
1	A	1	GLU	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 [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided