Full wwPDB NMR Structure Validation Report (i)

Dec 13, 2023 – 10:39 PM EST

PDB ID	:	2JO0
Title	:	The solution structure of the monomeric species of the C terminal domain of the CA protein of HIV-1
Authors	:	Alcaraz, L.A.; del Alamo, M.; Barrera, F.N.; Mateu, M.G.; Neira, J.L.
Deposited on	:	2007-02-17

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 (i) 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 (i)) were used in the production of this report:

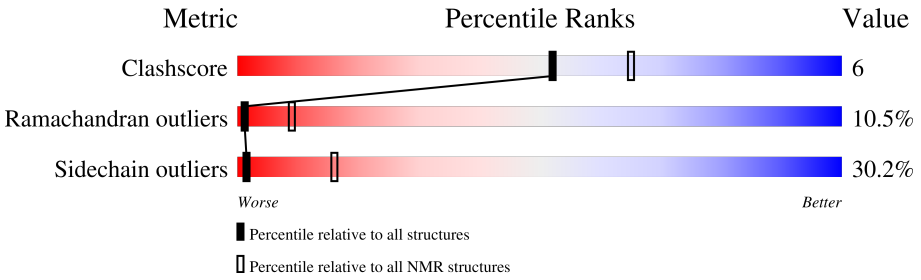
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	87	51% 26% • 20%

2 Ensemble composition and analysis (i)

This entry contains 30 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. Model 14 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:6-A:75 (70)	1.45	14

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 4 single-model clusters were found.

Cluster number	Models
1	7, 12, 14, 16, 20, 21, 22, 27, 28
2	2, 3, 4, 8, 9, 25
3	1, 10, 13, 17, 24, 26
4	6, 15, 29
5	5, 11
Single-model clusters	18; 19; 23; 30

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1343 atoms, of which 677 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Gag-Pol polyprotein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	87	1343	414	677	118	128	6	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP P35963
A	40	ALA	TRP	engineered mutation	UNP P35963

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: Gag-Pol polyprotein

Chain A: 51% 26% • 20%

M1 S2 P3 T4 S5 I6 L7 R10 E15 P16 F17 R18 V21 D22 R23 F24 Y25 K26 T27 L28 R29 A33 S34 Q35 K38 N39 T42 E43 T44 L45 L46 C54 L58 K59 A60 L61 L67 M70 G76 V77 G78 G79 P80 G81 H82 K83 A84 R85 V86

L87

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: Gag-Pol polyprotein

Chain A: 43% 33% • • 20%

M1 S2 P3 T4 S5 I6 R10 Q11 G12 P13 K14 E15 P16 F17 R18 V21 D22 R23 F24 Y25 K26 T27 L28 R29 S34 V37 K38 N39 T42 E43 T44 L45 L46 N49 A50 C54 K55 L58 K59 L67 M70 M71 T72 Q75 G76 V77 G78 G79 P80

G81 H82 K83 A84 R85 V86 L87

4.2.2 Score per residue for model 2

• Molecule 1: Gag-Pol polyprotein

Chain A: 43% 32% 5% • 20%

4.2.3 Score per residue for model 3

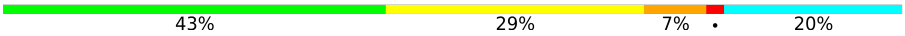
- Molecule 1: Gag-Pol polyprotein

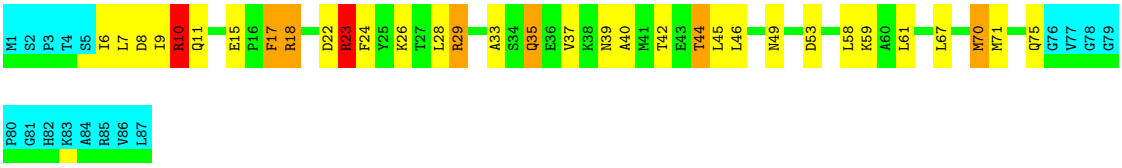
Chain A:

4.2.4 Score per residue for model 4

- Molecule 1: Gag-Pol polyprotein

Chain A:

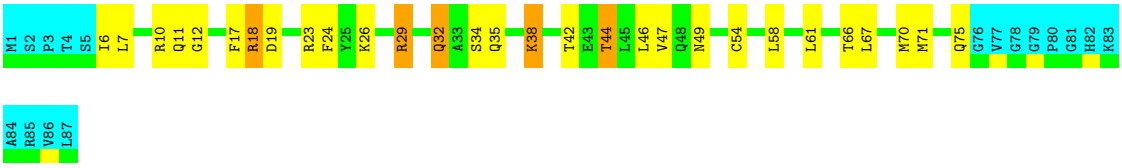




4.2.5 Score per residue for model 5

- Molecule 1: Gag-Pol polyprotein

Chain A:



4.2.6 Score per residue for model 6

- Molecule 1: Gag-Pol polyprotein

Chain A: 49% 21% 8% • 20%

M1 S2 P3 T4 S5 I6 L7 R10 F17 R18 D19 Y20 V21 D22 R23 F24 Y25 K26 R29 Q32 A33 N39 T44 L45 L46 V47 Q48 N49 A50 N51 C54 K55 L58 L61 L67 M70 M71 G76 V77 G78 G79 P80 G81 H82 K83 A84 R85 V86

L87

4.2.7 Score per residue for model 7

- Molecule 1: Gag-Pol polyprotein

Chain A: 45% 28% 8% 20%

M1 S2 P3 T4 S5 I6 R10 Q11 E15 R18 R23 F24 Y25 K26 T27 L28 R29 A30 E31 Q32 A33 K38 N39 A40 M41 T42 E43 T44 L45 L46 V47 Q48 N51 C54 L58 K59 T66 L67 M70 M71 T72 Q75 G76 V77 G78 G79 P80 G81 H82

K83 A84 R85 V86 L87

4.2.8 Score per residue for model 8

- Molecule 1: Gag-Pol polyprotein

Chain A: 48% 25% 6% • 20%

M1 S2 P3 T4 S5 I6 G12 P13 K14 E15 P16 F17 R18 V21 D22 R23 K26 T27 L28 R29 A33 S34 Q35 K38 N39 A40 M41 T42 L46 D53 C54 L58 K59 A60 L61 T66 L67 M70 G76 V77 G78 G79 P80 G81 H82 K83 A84 R85 V86

L87

4.2.9 Score per residue for model 9

- Molecule 1: Gag-Pol polyprotein

Chain A: 45% 30% 6% 20%

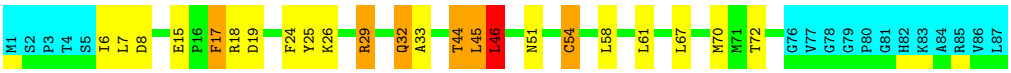
M1 S2 P3 T4 S5 I6 L7 R10 Q11 G12 E15 P16 F17 R18 V21 D22 R23 K26 R29 A33 S34 Q35 N39 A40 M41 T42 E43 T44 L45 L46 V47 Q48 N49 A50 N51 C54 L58 K59 T66 L67 M70 M71 T72 Q75 G76 V77 G78 G79

P80 G81 H82 K83 A84 R85 V86 L87

4.2.10 Score per residue for model 10

- Molecule 1: Gag-Pol polyprotein

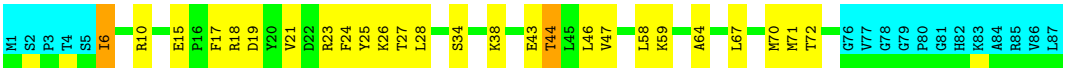
Chain A: 54% 18% 7% • 20%



4.2.11 Score per residue for model 11

- Molecule 1: Gag-Pol polyprotein

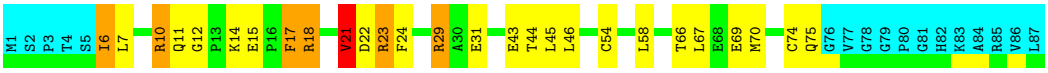
Chain A: 51% 28% • 20%



4.2.12 Score per residue for model 12

- Molecule 1: Gag-Pol polyprotein

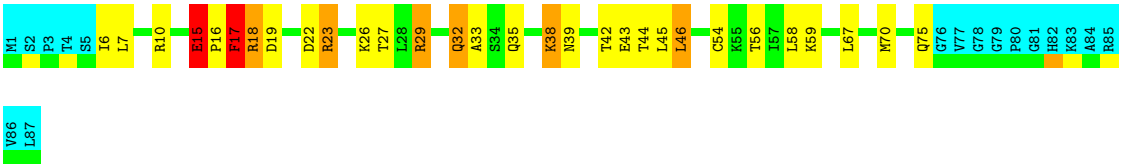
Chain A: 49% 23% 7% • 20%



4.2.13 Score per residue for model 13

- Molecule 1: Gag-Pol polyprotein

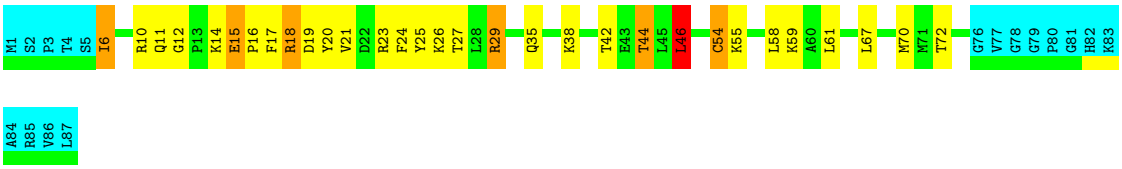
Chain A: 46% 25% 7% • 20%



4.2.14 Score per residue for model 14 (medoid)

- Molecule 1: Gag-Pol polyprotein

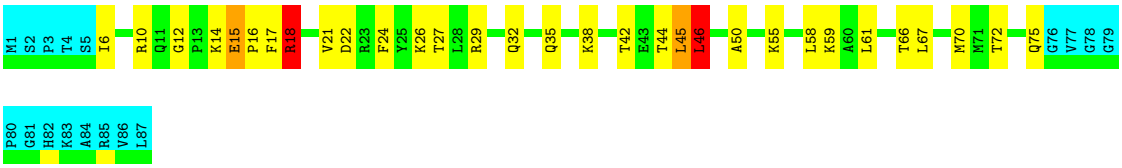
Chain A: 45% 28% 7% • 20%



4.2.15 Score per residue for model 15

- Molecule 1: Gag-Pol polyprotein

Chain A: 45% 31% • • 20%



4.2.16 Score per residue for model 16

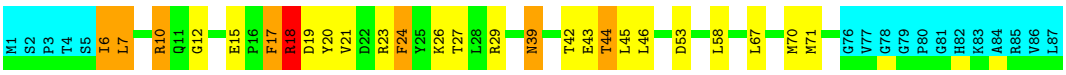
- Molecule 1: Gag-Pol polyprotein

Chain A: 46% 25% 7% • 20%

4.2.17 Score per residue for model 17

- Molecule 1: Gag-Pol polyprotein

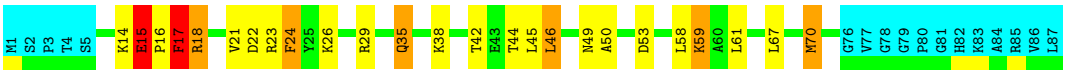
Chain A: 51% 21% 8% • 20%



4.2.18 Score per residue for model 18

- Molecule 1: Gag-Pol polyprotein

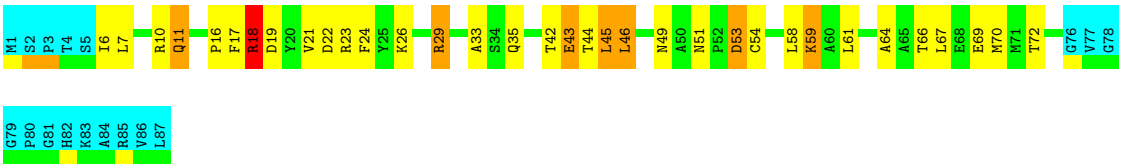
Chain A: 52% 20% 7% • 20%



4.2.19 Score per residue for model 19

- Molecule 1: Gag-Pol polyprotein

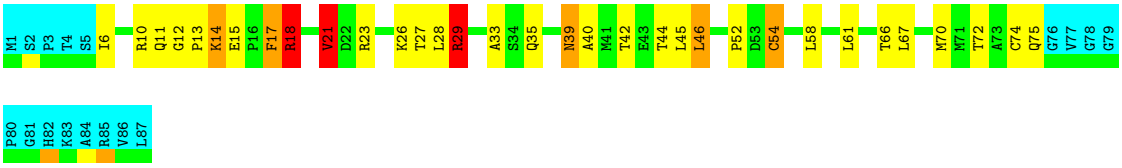
Chain A: 41% 30% 8% • 20%



4.2.20 Score per residue for model 20

- Molecule 1: Gag-Pol polyprotein

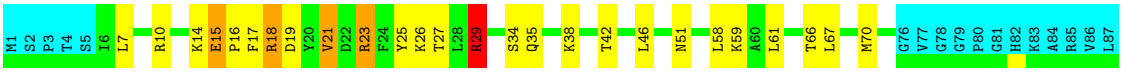
Chain A: 43% 29% 6% • 20%



4.2.21 Score per residue for model 21

- Molecule 1: Gag-Pol polyprotein

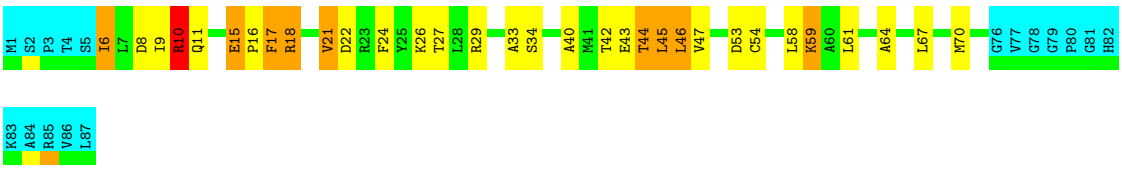
Chain A: 51% 24% 5% • 20%



4.2.22 Score per residue for model 22

- Molecule 1: Gag-Pol polyprotein

Chain A: 44% 25% 10% • 20%



4.2.23 Score per residue for model 23

- Molecule 1: Gag-Pol polyprotein

Chain A: 47% 24% 8% • 20%

M1 S2 P3 T4 S5 I6 I9 R10 Q11 K14 E15 P16 F17 R18 D19 Y20 V21 D22 R23 K26 T27 L28 R29 Q35 K38 N39 T42 E43 T44 L45 L46 C54 L58 L61 T66 L67 M70 M71 G76 V77 G78 G79 P80 G81 H82 K83 A84 R85 V86 L87

4.2.24 Score per residue for model 24

- Molecule 1: Gag-Pol polyprotein

Chain A: 47% 28% 6% 20%

M1 S2 P3 T4 S5 I6 L7 D8 I9 R10 Q11 G12 E15 P16 F17 R18 V21 F24 T27 L28 R29 T44 L45 L46 N49 A50 N51 P52 D53 C54 K55 L58 K59 A60 L61 A64 A65 T66 L67 M70 M71 T72 G76 V77 G78 G79 P80 G81 H82 K83 A84 R85 V86 L87

4.2.25 Score per residue for model 25

- Molecule 1: Gag-Pol polyprotein

Chain A: 53% 22% 6% 20%

M1 S2 P3 T4 S5 I6 L7 R10 F17 R18 R23 K26 T27 Q32 A33 S34 K38 N39 A40 M41 L45 L46 N51 T56 I57 L58 L61 T66 L67 M70 G76 V77 G78 G79 P80 G81 H82 K83 A84 R85 V86 L87

4.2.26 Score per residue for model 26

- Molecule 1: Gag-Pol polyprotein

Chain A: 57% 17% 6% 20%

M1 S2 P3 T4 S5 I6 I9 K14 F17 R18 V21 F24 L28 R29 Q35 N39 T44 L45 L46 V47 Q48 N49 L58 K59 A60 L61 L67 M70 G76 V77 G78 G79 P80 G81 H82 K83 A84 R85 V86 L87

4.2.27 Score per residue for model 27

- Molecule 1: Gag-Pol polyprotein

Chain A: 47% 24% 9% 20%

M1 S2 P3 T4 S5 I6 L7 R10 Q11 G12 E15 P16 F17 R18 D19 Y20 R23 F24 Y25 K26 T27 L28 R29 A33 S34 K38 N39 T44 L45 L46 N51 C54 K55 L58 L61 L67 M70 Q75 G76 V77 G78 G79 P80 G81 H82 K83 A84 R85 V86 L87

4.2.28 Score per residue for model 28

- Molecule 1: Gag-Pol polyprotein

Chain A: 49% 22% 9% 20%

M1 S2 P3 T4 S5 I6 L7 D8 I9 R10 Q11 G12 F17 R18 D19 Y20 V21 D22 T27 L28 R29 A33 K38 M41 T42 E43 T44 L45 L46 C54 L58 L61 L67 E68 E69 M70 M71 T72 Q75 G76 V77 G78 G79 P80 G81 H82 K83 A84 R85 V86 L87

4.2.29 Score per residue for model 29

- Molecule 1: Gag-Pol polyprotein

Chain A: 46% 28% 6% • 20%

M1 S2 P3 T4 S5 I6 L7 D8 I9 R10 F17 R18 V21 D22 R23 F24 Y25 K26 T27 L28 R29 A33 N39 T44 L45 L46 V47 C54 K55 T56 I57 L58 K59 T66 L67 M70 M71 C74 Q75 G76 V77 G78 G79 P80 G81 H82 K83 A84 R85 V86 L87

4.2.30 Score per residue for model 30

- Molecule 1: Gag-Pol polyprotein

Chain A: 51% 21% 6% • 20%

M1 S2 P3 T4 S5 I6 L7 R10 Q11 G12 F17 R18 V21 D22 R23 F24 L28 R29 Q32 T42 E43 T44 L45 L46 D53 L58 K59 A60 L61 A64 A65 T66 L67 M70 M71 G76 V77 G78 G79 P80 G81 H82 K83 A84 R85 V86 L87

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *molecular dynamics*.

Of the 50 calculated structures, 30 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
CYANA	structure solution	2.1
Amber	refinement	8

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	0.70±0.01	0±0/559 (0.0± 0.0%)	1.33±0.05	3±2/756 (0.4± 0.2%)
All	All	0.70	0/16770 (0.0%)	1.33	89/22680 (0.4%)

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	0.0±0.0	0.9±0.7
All	All	0	27

There are no bond-length outliers.

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(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	23	ARG	NE-CZ-NH1	11.93	126.26	120.30	20	6
1	A	10	ARG	NE-CZ-NH1	10.28	125.44	120.30	4	10
1	A	18	ARG	NE-CZ-NH1	10.04	125.32	120.30	6	20
1	A	18	ARG	NE-CZ-NH2	-7.39	116.61	120.30	19	3
1	A	29	ARG	NE-CZ-NH1	7.13	123.87	120.30	21	8
1	A	21	VAL	CA-CB-CG1	6.84	121.15	110.90	20	4
1	A	18	ARG	CD-NE-CZ	6.49	132.68	123.60	19	2
1	A	10	ARG	NE-CZ-NH2	5.85	123.22	120.30	11	2
1	A	22	ASP	CB-CG-OD2	-5.83	113.05	118.30	12	2
1	A	46	LEU	CB-CG-CD2	5.82	120.89	111.00	3	10
1	A	24	PHE	CB-CG-CD2	-5.74	116.78	120.80	16	2
1	A	24	PHE	CB-CG-CD1	5.70	124.79	120.80	16	1
1	A	10	ARG	NH1-CZ-NH2	-5.56	113.29	119.40	16	2
1	A	7	LEU	C-N-CA	5.53	135.52	121.70	10	1
1	A	45	LEU	CB-CG-CD2	5.44	120.25	111.00	4	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	29	ARG	NE-CZ-NH2	-5.39	117.60	120.30	6	1
1	A	20	TYR	CB-CG-CD2	-5.38	117.77	121.00	6	2
1	A	9	ILE	C-N-CA	5.28	134.89	121.70	4	1
1	A	21	VAL	CA-CB-CG2	5.27	118.81	110.90	30	1
1	A	10	ARG	CD-NE-CZ	5.22	130.91	123.60	4	1
1	A	23	ARG	NE-CZ-NH2	-5.21	117.69	120.30	8	2
1	A	43	GLU	C-N-CA	5.21	134.72	121.70	22	3
1	A	50	ALA	CB-CA-C	5.14	117.81	110.10	24	1
1	A	46	LEU	CA-CB-CG	5.07	126.97	115.30	30	1
1	A	44	THR	CA-CB-CG2	5.02	119.43	112.40	26	1
1	A	10	ARG	N-CA-C	5.02	124.56	111.00	4	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	25	TYR	Sidechain	10
1	A	18	ARG	Sidechain	4
1	A	10	ARG	Sidechain	4
1	A	24	PHE	Sidechain	4
1	A	23	ARG	Sidechain	2
1	A	20	TYR	Sidechain	2
1	A	29	ARG	Sidechain	1

6.2 Too-close contacts (i)

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	551	558	558	6±2
All	All	16530	16740	16740	189

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:58:LEU:HD21	1:A:70:MET:HB2	0.78	1.54	16	27
1:A:58:LEU:HD21	1:A:70:MET:CB	0.70	2.15	10	27
1:A:21:VAL:HG23	1:A:46:LEU:HD23	0.64	1.68	8	3
1:A:21:VAL:HG12	1:A:46:LEU:HB2	0.63	1.71	24	1
1:A:24:PHE:CE1	1:A:44:THR:HG23	0.60	2.31	14	2
1:A:21:VAL:HG23	1:A:46:LEU:CD2	0.60	2.25	8	1
1:A:18:ARG:HA	1:A:21:VAL:HG12	0.60	1.74	9	11
1:A:21:VAL:HG13	1:A:46:LEU:HB2	0.59	1.74	30	1
1:A:47:VAL:HG22	1:A:71:MET:HA	0.58	1.74	29	1
1:A:17:PHE:CZ	1:A:58:LEU:HD22	0.57	2.33	12	11
1:A:39:ASN:ND2	1:A:44:THR:HG22	0.57	2.15	2	2
1:A:58:LEU:HD21	1:A:70:MET:HB3	0.57	1.76	17	7
1:A:39:ASN:HD21	1:A:44:THR:CG2	0.56	2.14	27	1
1:A:17:PHE:O	1:A:21:VAL:HG13	0.56	2.01	24	1
1:A:24:PHE:CZ	1:A:28:LEU:HD13	0.55	2.36	26	1
1:A:24:PHE:CZ	1:A:44:THR:HA	0.55	2.36	18	14
1:A:6:ILE:HD12	1:A:6:ILE:O	0.54	2.02	25	5
1:A:54:CYS:O	1:A:58:LEU:HD12	0.52	2.05	20	11
1:A:6:ILE:C	1:A:6:ILE:HD12	0.51	2.24	22	3
1:A:15:GLU:H	1:A:16:PRO:CD	0.51	2.18	13	2
1:A:39:ASN:HD22	1:A:44:THR:HG21	0.51	1.66	20	1
1:A:39:ASN:HD21	1:A:44:THR:HG22	0.51	1.66	27	1
1:A:54:CYS:SG	1:A:58:LEU:HD13	0.50	2.46	9	1
1:A:15:GLU:H	1:A:16:PRO:HD2	0.50	1.67	18	7
1:A:36:GLU:CD	1:A:38:LYS:HE2	0.50	2.27	3	1
1:A:47:VAL:HG23	1:A:71:MET:HG2	0.50	1.82	5	1
1:A:58:LEU:HD23	1:A:67:LEU:HG	0.49	1.84	16	1
1:A:16:PRO:HA	1:A:59:LYS:HE3	0.48	1.85	19	1
1:A:24:PHE:CZ	1:A:28:LEU:HD12	0.48	2.44	30	1
1:A:21:VAL:HG21	1:A:47:VAL:C	0.47	2.31	26	3
1:A:20:TYR:CD2	1:A:46:LEU:HD11	0.46	2.45	6	1
1:A:58:LEU:HD12	1:A:58:LEU:H	0.46	1.70	9	3
1:A:17:PHE:O	1:A:21:VAL:HG23	0.46	2.11	18	2
1:A:21:VAL:HG22	1:A:46:LEU:HG	0.46	1.88	18	1
1:A:21:VAL:HG23	1:A:46:LEU:HG	0.46	1.88	14	1
1:A:18:ARG:HA	1:A:21:VAL:HG22	0.45	1.87	2	1
1:A:28:LEU:C	1:A:28:LEU:HD13	0.45	2.31	11	1
1:A:39:ASN:HD22	1:A:44:THR:HG22	0.45	1.71	17	1
1:A:7:LEU:H	1:A:7:LEU:HD23	0.45	1.71	9	1
1:A:6:ILE:HG21	1:A:24:PHE:CE1	0.45	2.47	12	1
1:A:18:ARG:CD	1:A:18:ARG:C	0.45	2.85	20	1
1:A:24:PHE:CE1	1:A:44:THR:HA	0.45	2.47	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:VAL:HG23	1:A:46:LEU:HD13	0.44	1.88	23	1
1:A:58:LEU:HD11	1:A:70:MET:HB2	0.44	1.87	8	1
1:A:58:LEU:CD2	1:A:70:MET:HB2	0.44	2.42	30	1
1:A:55:LYS:HA	1:A:55:LYS:HE3	0.43	1.88	6	1
1:A:6:ILE:HG13	1:A:24:PHE:CD1	0.43	2.48	16	1
1:A:14:LYS:HE2	1:A:14:LYS:O	0.43	2.13	8	1
1:A:21:VAL:HG23	1:A:46:LEU:CG	0.43	2.44	8	1
1:A:18:ARG:HD2	1:A:18:ARG:C	0.43	2.34	28	1
1:A:39:ASN:HD21	1:A:47:VAL:HG22	0.43	1.74	9	1
1:A:15:GLU:N	1:A:16:PRO:CD	0.43	2.82	13	1
1:A:18:ARG:C	1:A:18:ARG:HD3	0.42	2.34	20	1
1:A:17:PHE:C	1:A:21:VAL:HG23	0.42	2.35	18	1
1:A:13:PRO:CD	1:A:45:LEU:HD13	0.42	2.45	20	1
1:A:18:ARG:HD3	1:A:19:ASP:N	0.42	2.30	17	1
1:A:39:ASN:ND2	1:A:47:VAL:HG22	0.41	2.30	9	1
1:A:16:PRO:HA	1:A:59:LYS:CE	0.41	2.45	19	1
1:A:28:LEU:HD11	1:A:32:GLN:HE21	0.41	1.75	30	1
1:A:21:VAL:HG22	1:A:46:LEU:CG	0.41	2.46	18	1
1:A:58:LEU:H	1:A:58:LEU:HD12	0.41	1.74	6	1
1:A:6:ILE:HG23	1:A:31:GLU:OE2	0.41	2.16	12	1
1:A:46:LEU:HD22	1:A:46:LEU:N	0.41	2.31	15	1
1:A:54:CYS:HB2	1:A:74:CYS:CB	0.41	2.45	29	1
1:A:46:LEU:N	1:A:46:LEU:HD22	0.40	2.32	10	1
1:A:18:ARG:HA	1:A:21:VAL:CG1	0.40	2.47	21	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	70/87 (80%)	43±3 (62±4%)	20±3 (28±5%)	7±2 (10±3%)	1 9
All	All	2100/2610 (80%)	1292 (62%)	588 (28%)	220 (10%)	1 9

All 35 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	15	GLU	20
1	A	44	THR	19
1	A	29	ARG	16
1	A	33	ALA	16
1	A	12	GLY	15
1	A	7	LEU	13
1	A	11	GLN	11
1	A	45	LEU	11
1	A	38	LYS	10
1	A	40	ALA	8
1	A	34	SER	7
1	A	49	ASN	7
1	A	39	ASN	6
1	A	10	ARG	6
1	A	14	LYS	6
1	A	64	ALA	6
1	A	59	LYS	5
1	A	6	ILE	4
1	A	17	PHE	4
1	A	50	ALA	3
1	A	35	GLN	3
1	A	32	GLN	3
1	A	51	ASN	3
1	A	43	GLU	3
1	A	75	GLN	2
1	A	41	MET	2
1	A	18	ARG	2
1	A	53	ASP	2
1	A	13	PRO	1
1	A	48	GLN	1
1	A	8	ASP	1
1	A	16	PRO	1
1	A	66	THR	1
1	A	52	PRO	1
1	A	9	ILE	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	60/72 (83%)	42±3 (70±6%)	18±3 (30±6%)	1 16
All	All	1800/2160 (83%)	1256 (70%)	544 (30%)	1 16

All 51 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	46	LEU	30
1	A	67	LEU	30
1	A	18	ARG	28
1	A	6	ILE	27
1	A	17	PHE	25
1	A	29	ARG	24
1	A	26	LYS	23
1	A	10	ARG	22
1	A	45	LEU	21
1	A	61	LEU	21
1	A	27	THR	19
1	A	42	THR	19
1	A	23	ARG	18
1	A	59	LYS	16
1	A	54	CYS	15
1	A	66	THR	14
1	A	75	GLN	13
1	A	35	GLN	13
1	A	72	THR	12
1	A	22	ASP	10
1	A	39	ASN	10
1	A	55	LYS	8
1	A	28	LEU	8
1	A	32	GLN	8
1	A	19	ASP	8
1	A	38	LYS	7
1	A	71	MET	7
1	A	8	ASP	7
1	A	53	ASP	7
1	A	44	THR	6
1	A	51	ASN	6
1	A	43	GLU	5
1	A	15	GLU	5
1	A	70	MET	5
1	A	14	LYS	5
1	A	7	LEU	4

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Mol	Chain	Res	Type	Models (Total)
1	A	56	THR	4
1	A	69	GLU	4
1	A	11	GLN	4
1	A	21	VAL	4
1	A	24	PHE	3
1	A	20	TYR	3
1	A	9	ILE	3
1	A	37	VAL	2
1	A	49	ASN	2
1	A	74	CYS	2
1	A	47	VAL	2
1	A	41	MET	2
1	A	31	GLU	1
1	A	48	GLN	1
1	A	34	SER	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 monosaccharides 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 (i)

No chemical shift data were provided