



Full wwPDB NMR Structure Validation Report ⓘ

May 28, 2020 – 11:12 pm BST

PDB ID : 2LF4
Title : Structure of a monomeric mutant of the HIV-1 capsid protein
Authors : Shin, R.S.; Tzou, Y.; Krishna, N.
Deposited on : 2011-06-28

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 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
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : 2.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

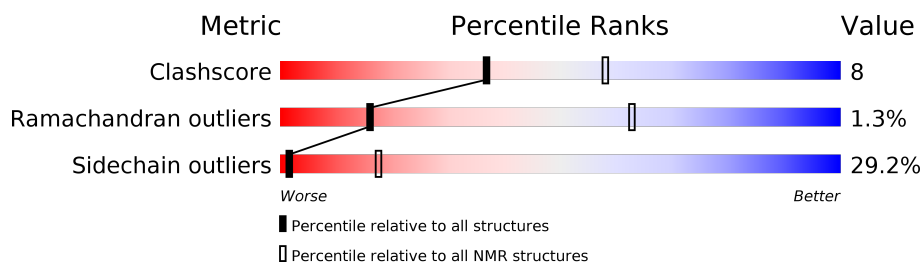
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 83%.

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	240	

2 Ensemble composition and analysis

This entry contains 20 models. Model 16 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:12-A:84, A:100-A:145 (119)	0.57	16
2	A:150-A:175, A:184-A:221 (64)	0.45	11

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

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

The models can be grouped into 5 clusters. No single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3589 atoms, of which 1799 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Gag polyprotein.

Mol	Chain	Residues	Atoms						Trace
1	A	232	Total	C	H	N	O	S	0
			3589	1126	1799	317	334	13	

There are 11 discrepancies between the modelled and reference sequences:

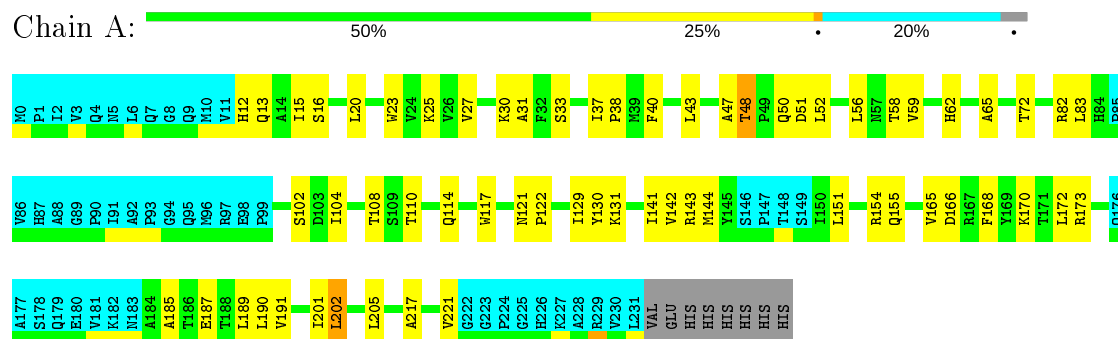
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	INITIATING METHIONINE	UNP Q72497
A	184	ALA	TRP	ENGINEERED MUTATION	UNP Q72497
A	185	ALA	MET	ENGINEERED MUTATION	UNP Q72497
A	232	VAL	-	EXPRESSION TAG	UNP Q72497
A	233	GLU	-	EXPRESSION TAG	UNP Q72497
A	234	HIS	-	EXPRESSION TAG	UNP Q72497
A	235	HIS	-	EXPRESSION TAG	UNP Q72497
A	236	HIS	-	EXPRESSION TAG	UNP Q72497
A	237	HIS	-	EXPRESSION TAG	UNP Q72497
A	238	HIS	-	EXPRESSION TAG	UNP Q72497
A	239	HIS	-	EXPRESSION TAG	UNP Q72497

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: Gag polyprotein

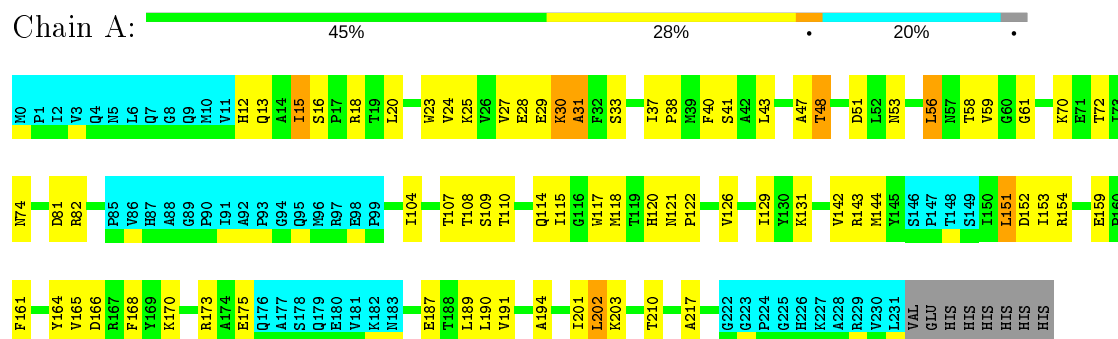


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

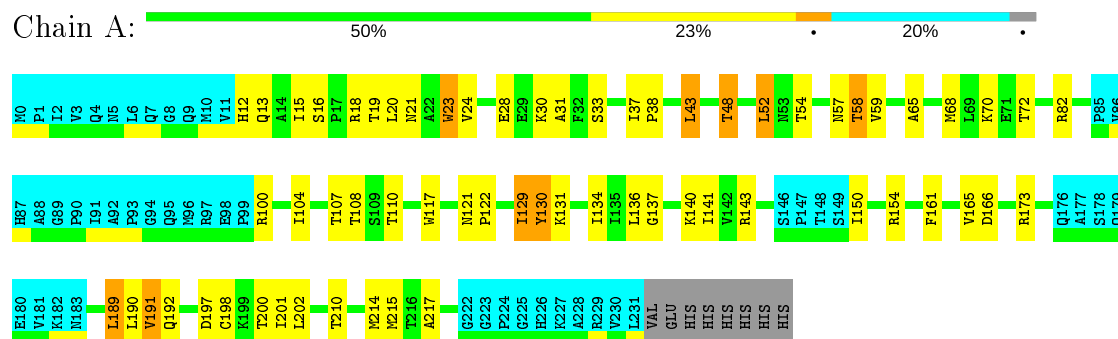
4.2.1 Score per residue for model 1

- Molecule 1: Gag polyprotein



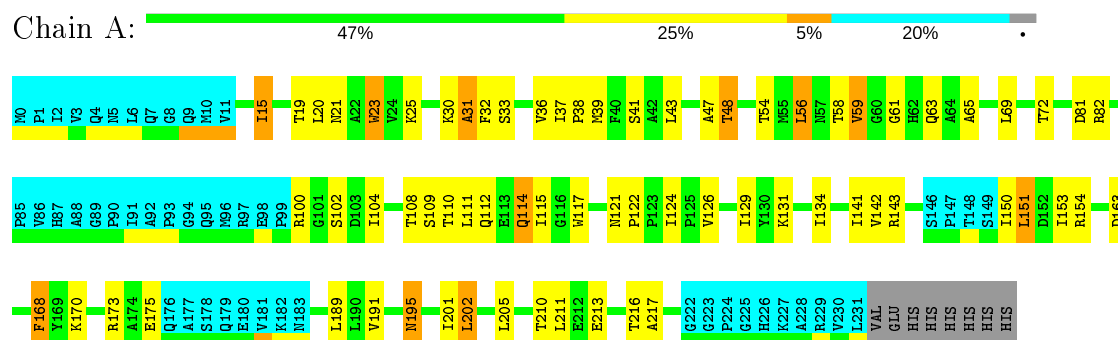
4.2.2 Score per residue for model 2

• Molecule 1: Gag polyprotein



4.2.3 Score per residue for model 3

• Molecule 1: Gag polyprotein



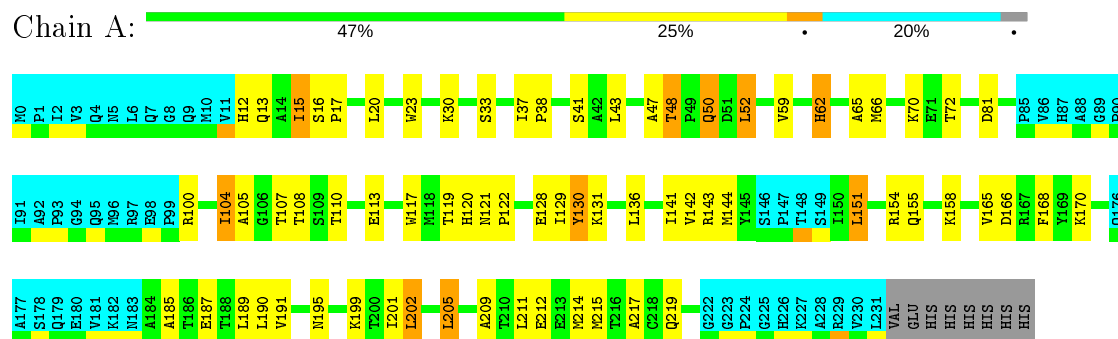
4.2.4 Score per residue for model 4

• Molecule 1: Gag polyprotein



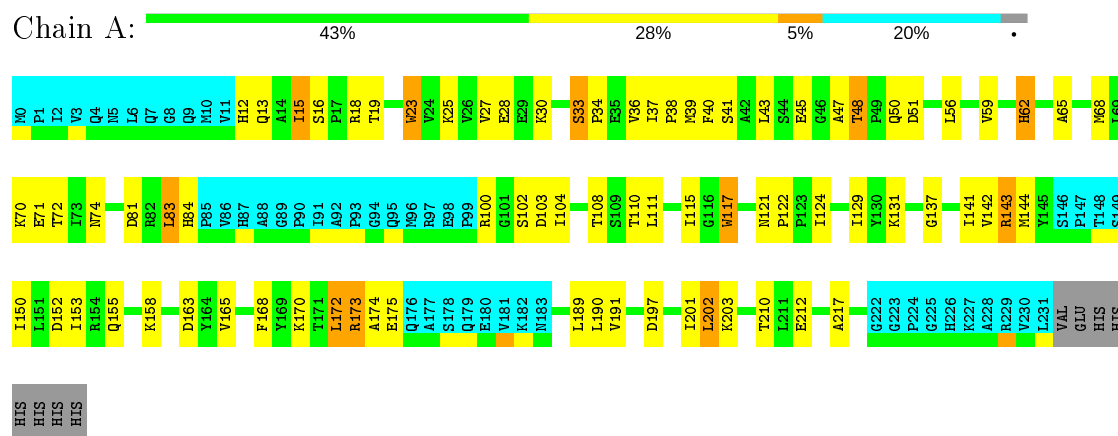
4.2.8 Score per residue for model 8

- Molecule 1: Gag polyprotein



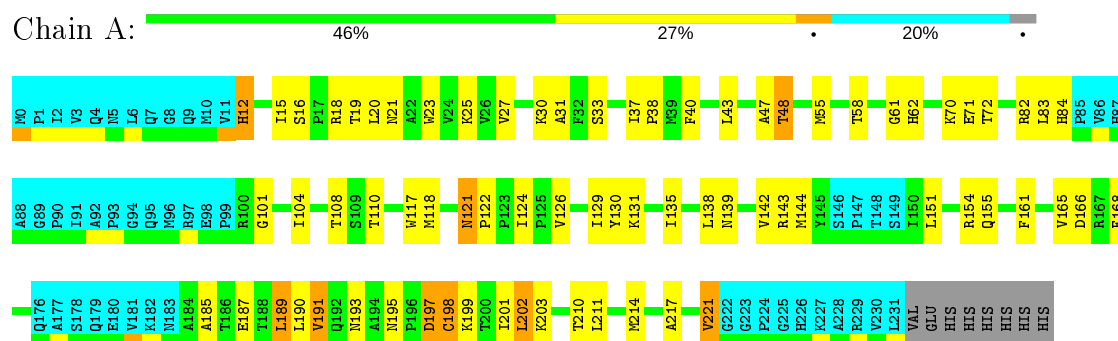
4.2.9 Score per residue for model 9

- Molecule 1: Gag polyprotein



4.2.10 Score per residue for model 10

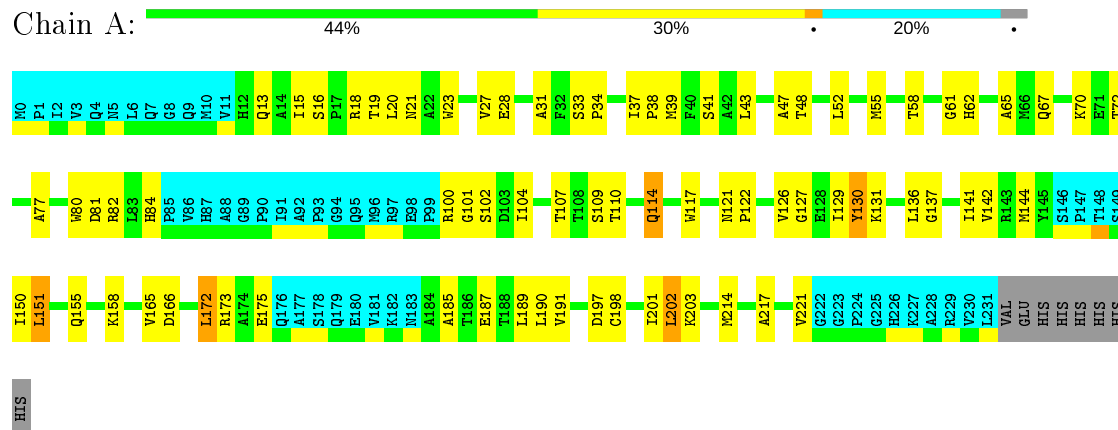
- Molecule 1: Gag polyprotein



4.2.11 Score per residue for model 11

- Molecule 1: Gag polyprotein

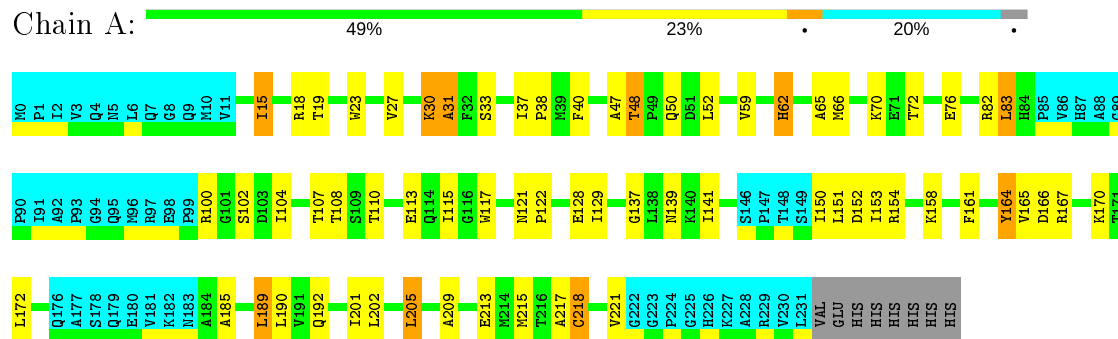
Chain A:



4.2.12 Score per residue for model 12

- Molecule 1: Gag polyprotein

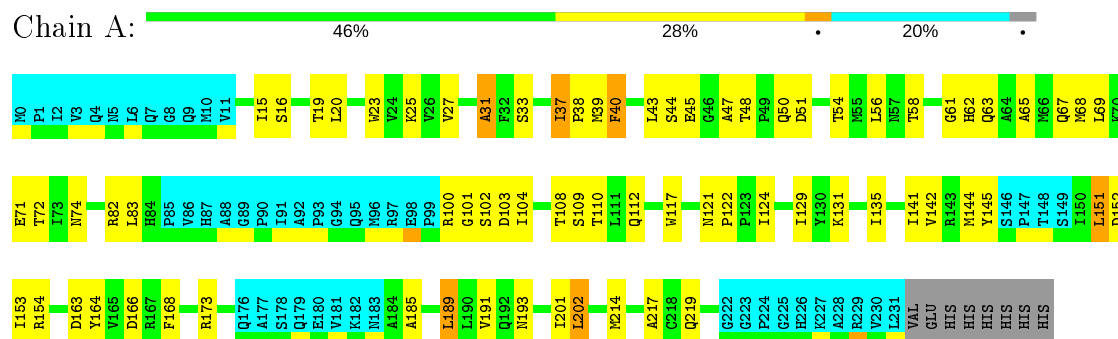
Chain A:



4.2.13 Score per residue for model 13

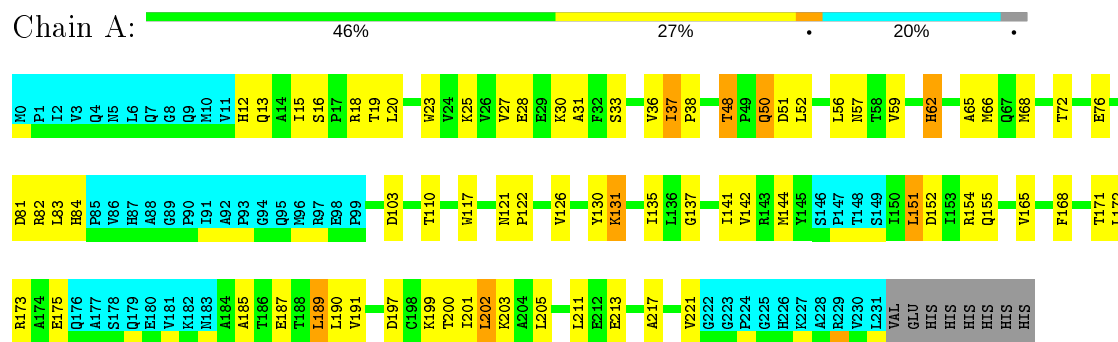
- Molecule 1: Gag polyprotein

Chain A:



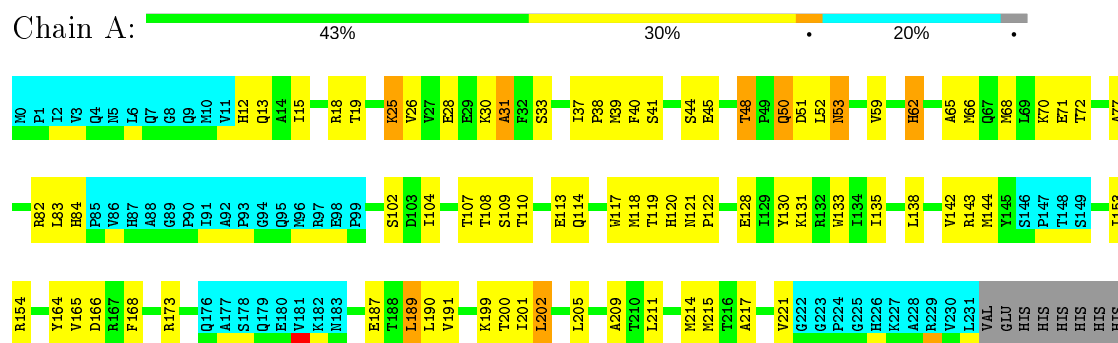
4.2.14 Score per residue for model 14

- Molecule 1: Gag polyprotein



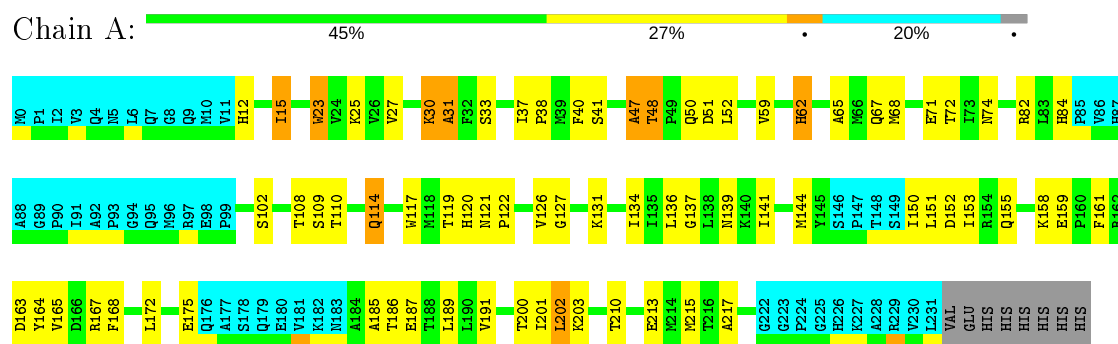
4.2.15 Score per residue for model 15

- Molecule 1: Gag polyprotein



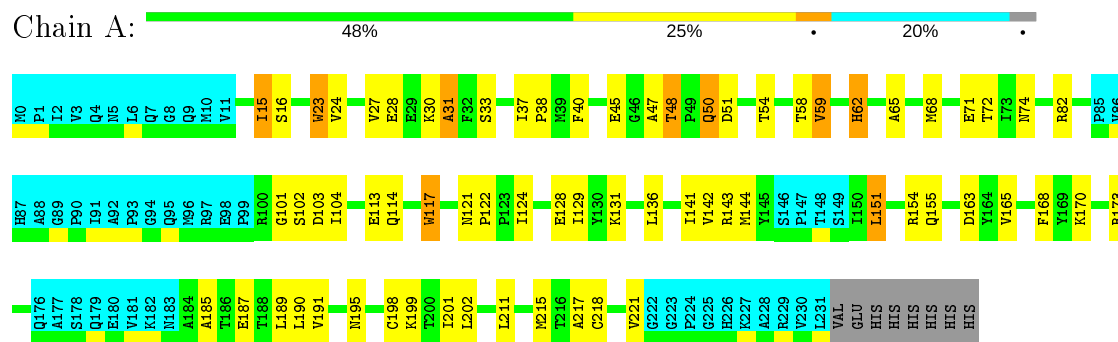
4.2.16 Score per residue for model 16 (medoid)

- Molecule 1: Gag polyprotein



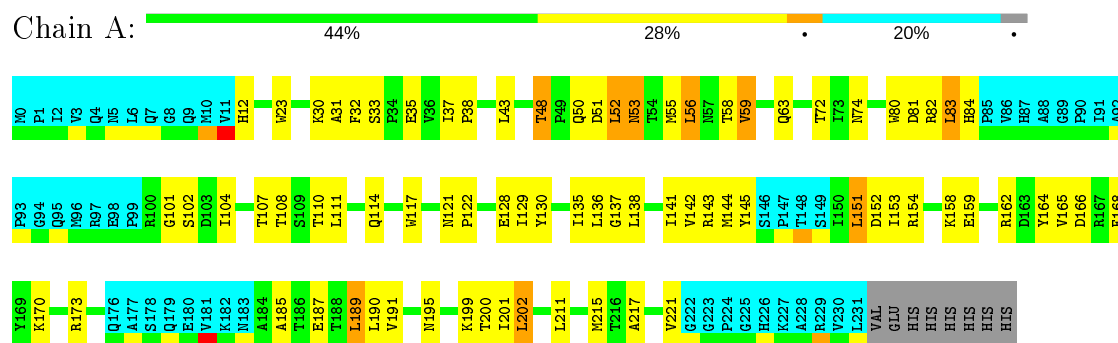
4.2.17 Score per residue for model 17

- Molecule 1: Gag polyprotein



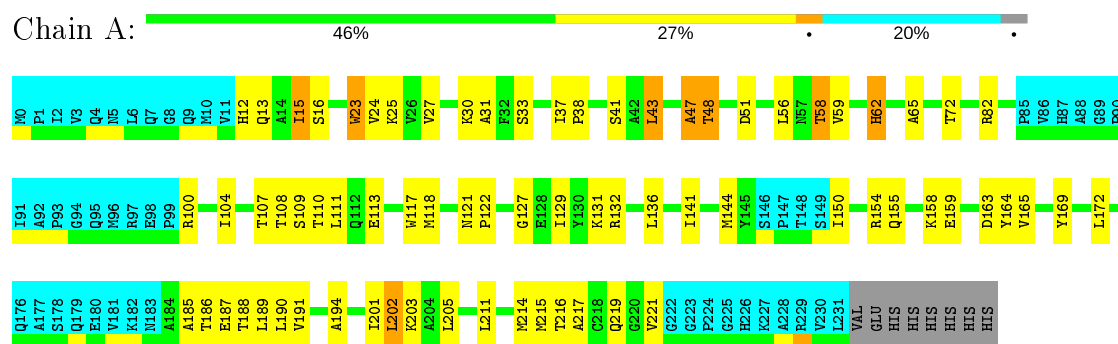
4.2.18 Score per residue for model 18

- Molecule 1: Gag polyprotein



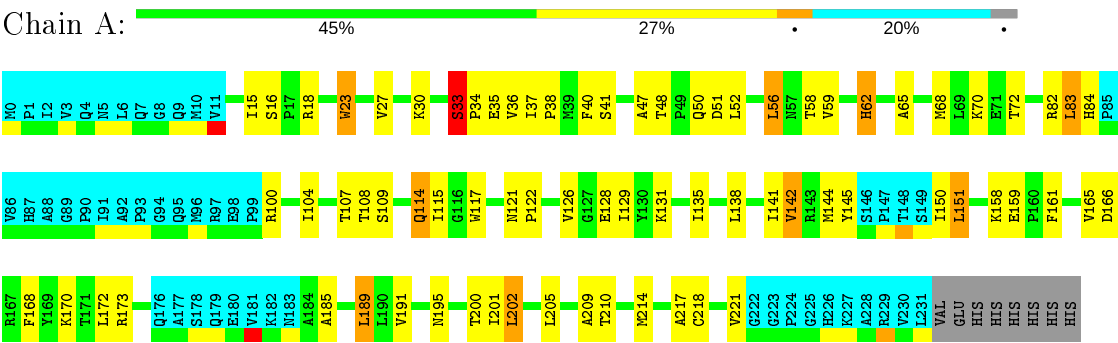
4.2.19 Score per residue for model 19

- Molecule 1: Gag polyprotein



4.2.20 Score per residue for model 20

● Molecule 1: Gag polyprotein



5 Refinement protocol and experimental data overview

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

Of the 500 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CYANA	structure solution	2.1
CYANA	refinement	2.1

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)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	2600
Number of shifts mapped to atoms	2600
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	83%

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

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	1433	1436	1436	24±4
All	All	28660	28720	28720	474

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 8.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:165:VAL:HG22	1:A:190:LEU:HD11	1.03	1.30	9	10
1:A:191:VAL:HG23	1:A:202:LEU:HD23	0.94	1.37	7	4
1:A:20:LEU:HD22	1:A:54:THR:HG21	0.92	1.40	2	1
1:A:201:ILE:HG21	1:A:217:ALA:HB1	0.82	1.49	6	20
1:A:191:VAL:HG22	1:A:202:LEU:HD23	0.82	1.50	20	11
1:A:201:ILE:HD11	1:A:221:VAL:HG11	0.74	1.59	15	1
1:A:201:ILE:HD11	1:A:221:VAL:HG21	0.71	1.60	10	2
1:A:65:ALA:HB2	1:A:141:ILE:HG21	0.70	1.63	6	3
1:A:23:TRP:CH2	1:A:27:VAL:HG21	0.69	2.23	13	5
1:A:59:VAL:HG11	1:A:62:HIS:CE1	0.68	2.24	15	5
1:A:12:HIS:CG	1:A:48:THR:HG21	0.67	2.23	16	7
1:A:24:VAL:HG23	1:A:58:THR:HG22	0.66	1.68	2	2
1:A:62:HIS:CG	1:A:65:ALA:HB3	0.65	2.26	20	10
1:A:59:VAL:HG21	1:A:62:HIS:CE1	0.64	2.28	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:HIS:CE1	1:A:48:THR:HG21	0.63	2.28	2	2
1:A:191:VAL:HG23	1:A:202:LEU:CD2	0.63	2.23	2	3
1:A:145:TYR:CD1	1:A:189:LEU:HD11	0.63	2.29	18	1
1:A:40:PHE:CZ	1:A:59:VAL:HG23	0.62	2.30	17	1
1:A:165:VAL:HG22	1:A:190:LEU:CD1	0.61	2.24	8	6
1:A:23:TRP:O	1:A:27:VAL:HG23	0.61	1.94	5	6
1:A:135:ILE:HA	1:A:138:LEU:HD12	0.61	1.72	18	5
1:A:47:ALA:HB2	1:A:131:LYS:CE	0.61	2.25	19	1
1:A:191:VAL:HG22	1:A:202:LEU:CD2	0.61	2.25	16	12
1:A:23:TRP:CZ2	1:A:27:VAL:HG21	0.61	2.30	7	6
1:A:191:VAL:HG22	1:A:202:LEU:HD12	0.61	1.72	3	2
1:A:77:ALA:HB1	1:A:101:GLY:CA	0.61	2.24	11	1
1:A:104:ILE:HD13	1:A:129:ILE:HD12	0.61	1.73	9	13
1:A:105:ALA:HB2	1:A:130:TYR:CZ	0.61	2.30	8	1
1:A:168:PHE:CZ	1:A:189:LEU:HD23	0.61	2.31	15	3
1:A:25:LYS:HD2	1:A:26:VAL:HG23	0.61	1.72	15	1
1:A:12:HIS:CD2	1:A:48:THR:HG21	0.61	2.30	18	3
1:A:137:GLY:O	1:A:141:ILE:HD12	0.60	1.96	14	8
1:A:12:HIS:CE1	1:A:111:LEU:HD11	0.60	2.31	5	1
1:A:24:VAL:CG2	1:A:58:THR:HG22	0.60	2.26	19	2
1:A:59:VAL:HG11	1:A:62:HIS:NE2	0.60	2.12	9	5
1:A:24:VAL:HG23	1:A:58:THR:OG1	0.60	1.97	17	1
1:A:201:ILE:HD11	1:A:221:VAL:HG23	0.59	1.73	11	2
1:A:205:LEU:HD21	1:A:209:ALA:CB	0.59	2.28	12	3
1:A:114:GLN:HG3	1:A:126:VAL:HG21	0.59	1.75	3	2
1:A:15:ILE:HD12	1:A:51:ASP:OD2	0.58	1.98	7	6
1:A:104:ILE:HD12	1:A:129:ILE:HD11	0.58	1.74	11	1
1:A:27:VAL:HG11	1:A:59:VAL:O	0.58	1.99	17	2
1:A:48:THR:O	1:A:52:LEU:HD23	0.57	2.00	18	3
1:A:150:ILE:HG21	1:A:189:LEU:CD2	0.57	2.28	12	2
1:A:153:ILE:HG21	1:A:168:PHE:HA	0.57	1.75	1	8
1:A:101:GLY:HA2	1:A:104:ILE:HD12	0.57	1.77	17	6
1:A:105:ALA:HB2	1:A:130:TYR:OH	0.57	1.99	8	1
1:A:48:THR:O	1:A:52:LEU:HD22	0.57	2.00	4	1
1:A:153:ILE:HG22	1:A:164:TYR:CE1	0.56	2.34	12	1
1:A:145:TYR:CB	1:A:189:LEU:HD11	0.56	2.30	20	1
1:A:65:ALA:HA	1:A:141:ILE:HG21	0.56	1.77	17	5
1:A:15:ILE:HD13	1:A:20:LEU:HD21	0.56	1.76	13	1
1:A:65:ALA:HA	1:A:141:ILE:HD13	0.56	1.75	5	7
1:A:15:ILE:HG21	1:A:20:LEU:HD21	0.56	1.77	8	2
1:A:23:TRP:CH2	1:A:43:LEU:HD22	0.56	2.36	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:TRP:CZ2	1:A:43:LEU:HD22	0.56	2.35	19	1
1:A:59:VAL:HG11	1:A:62:HIS:CD2	0.56	2.36	16	1
1:A:15:ILE:HD12	1:A:51:ASP:CG	0.55	2.22	20	2
1:A:161:PHE:O	1:A:165:VAL:HG12	0.55	2.02	20	6
1:A:65:ALA:CB	1:A:141:ILE:HG21	0.55	2.32	6	2
1:A:165:VAL:HG23	1:A:190:LEU:CD1	0.54	2.32	10	4
1:A:169:TYR:HB3	1:A:186:THR:HG21	0.54	1.79	19	2
1:A:83:LEU:O	1:A:83:LEU:HD12	0.54	2.03	12	4
1:A:114:GLN:CG	1:A:126:VAL:HG21	0.54	2.32	20	3
1:A:83:LEU:HD12	1:A:83:LEU:O	0.54	2.03	6	3
1:A:104:ILE:HD12	1:A:129:ILE:CD1	0.54	2.33	11	1
1:A:202:LEU:HD11	1:A:214:MET:HB3	0.53	1.80	10	3
1:A:47:ALA:HB3	1:A:127:GLY:HA3	0.53	1.79	6	3
1:A:150:ILE:HD11	1:A:172:LEU:HA	0.53	1.79	11	2
1:A:117:TRP:CH2	1:A:124:ILE:HG21	0.53	2.38	13	7
1:A:77:ALA:HB1	1:A:101:GLY:HA3	0.53	1.79	11	2
1:A:53:ASN:HA	1:A:56:LEU:HD23	0.53	1.78	18	2
1:A:107:THR:HG22	1:A:108:THR:HG23	0.52	1.80	20	2
1:A:20:LEU:HD22	1:A:54:THR:CG2	0.52	2.27	2	1
1:A:27:VAL:HG22	1:A:36:VAL:HG21	0.52	1.80	14	1
1:A:145:TYR:HB2	1:A:189:LEU:HD11	0.52	1.81	20	1
1:A:172:LEU:HD23	1:A:173:ARG:N	0.52	2.18	9	1
1:A:77:ALA:HB2	1:A:133:TRP:CZ3	0.52	2.40	15	1
1:A:65:ALA:CA	1:A:141:ILE:HG21	0.52	2.35	2	1
1:A:23:TRP:CZ3	1:A:27:VAL:HG21	0.51	2.40	1	1
1:A:150:ILE:HG21	1:A:189:LEU:HD23	0.51	1.80	12	2
1:A:56:LEU:O	1:A:56:LEU:HD12	0.51	2.04	20	3
1:A:114:GLN:CD	1:A:126:VAL:HG21	0.51	2.26	11	1
1:A:191:VAL:HG22	1:A:202:LEU:HD21	0.50	1.82	6	1
1:A:191:VAL:CG2	1:A:202:LEU:HD12	0.50	2.37	11	2
1:A:32:PHE:CZ	1:A:59:VAL:HG22	0.50	2.41	18	2
1:A:104:ILE:CD1	1:A:129:ILE:HD12	0.50	2.37	8	2
1:A:23:TRP:CH2	1:A:59:VAL:HG23	0.50	2.42	1	1
1:A:202:LEU:HD11	1:A:214:MET:HE3	0.49	1.82	11	1
1:A:24:VAL:HG22	1:A:58:THR:O	0.49	2.07	1	1
1:A:33:SER:CB	1:A:34:PRO:CD	0.49	2.90	20	1
1:A:150:ILE:CD1	1:A:172:LEU:HD12	0.49	2.37	5	2
1:A:47:ALA:HB3	1:A:127:GLY:CA	0.49	2.37	6	1
1:A:50:GLN:NE2	1:A:111:LEU:HD21	0.49	2.23	18	1
1:A:210:THR:HG23	1:A:213:GLU:H	0.49	1.67	16	1
1:A:37:ILE:N	1:A:38:PRO:HD2	0.49	2.23	1	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:30:LYS:O	1:A:31:ALA:HB2	0.49	2.07	15	8
1:A:201:ILE:CG2	1:A:217:ALA:HB1	0.48	2.34	19	5
1:A:40:PHE:HB3	1:A:135:ILE:HD11	0.48	1.84	15	2
1:A:68:MET:HB3	1:A:141:ILE:HD11	0.48	1.85	2	2
1:A:19:THR:HG22	1:A:23:TRP:CE3	0.48	2.44	3	1
1:A:165:VAL:HG23	1:A:190:LEU:HD11	0.48	1.86	10	1
1:A:33:SER:HB2	1:A:142:VAL:HG22	0.48	1.84	20	1
1:A:52:LEU:HD23	1:A:53:ASN:N	0.48	2.24	4	2
1:A:191:VAL:HG13	1:A:202:LEU:HD23	0.47	1.85	9	3
1:A:83:LEU:HD12	1:A:84:HIS:CG	0.47	2.44	15	2
1:A:143:ARG:NE	1:A:174:ALA:HB2	0.47	2.24	9	1
1:A:23:TRP:CE2	1:A:27:VAL:HG21	0.47	2.44	10	1
1:A:195:ASN:ND2	1:A:198:CYS:H	0.47	2.07	7	2
1:A:52:LEU:O	1:A:52:LEU:HD12	0.47	2.08	2	1
1:A:56:LEU:HD13	1:A:69:LEU:HD21	0.47	1.87	13	1
1:A:185:ALA:O	1:A:189:LEU:HD23	0.47	2.10	16	2
1:A:58:THR:HG22	1:A:58:THR:O	0.47	2.10	18	1
1:A:191:VAL:CG2	1:A:202:LEU:HD23	0.47	2.33	20	1
1:A:201:ILE:HD11	1:A:221:VAL:CG2	0.47	2.39	18	3
1:A:121:ASN:HA	1:A:122:PRO:C	0.47	2.31	3	19
1:A:20:LEU:CD2	1:A:54:THR:HG21	0.47	2.28	2	2
1:A:73:ILE:HD11	1:A:134:ILE:HG13	0.47	1.87	5	1
1:A:31:ALA:HB2	1:A:193:ASN:CG	0.46	2.31	13	1
1:A:12:HIS:NE2	1:A:111:LEU:HD21	0.46	2.25	5	1
1:A:20:LEU:HD22	1:A:58:THR:HG21	0.46	1.87	7	1
1:A:17:PRO:HA	1:A:20:LEU:HD12	0.46	1.87	8	1
1:A:47:ALA:HB1	1:A:52:LEU:HD11	0.46	1.88	11	2
1:A:54:THR:O	1:A:58:THR:HG22	0.46	2.10	13	2
1:A:52:LEU:HD13	1:A:130:TYR:CD2	0.46	2.45	11	1
1:A:205:LEU:HD11	1:A:213:GLU:CG	0.46	2.41	12	1
1:A:187:GLU:O	1:A:191:VAL:HG23	0.46	2.11	17	1
1:A:39:MET:O	1:A:43:LEU:HD13	0.46	2.11	3	1
1:A:47:ALA:HB1	1:A:127:GLY:HA3	0.45	1.87	19	1
1:A:150:ILE:HD11	1:A:172:LEU:CA	0.45	2.41	11	2
1:A:20:LEU:HB3	1:A:58:THR:HG21	0.45	1.89	10	2
1:A:150:ILE:HG13	1:A:172:LEU:HD12	0.45	1.88	16	1
1:A:59:VAL:HG21	1:A:62:HIS:NE2	0.45	2.26	12	2
1:A:119:THR:HG23	1:A:120:HIS:ND1	0.45	2.27	8	2
1:A:197:ASP:O	1:A:201:ILE:HD12	0.45	2.12	10	1
1:A:68:MET:CB	1:A:141:ILE:HD11	0.44	2.42	14	1
1:A:119:THR:HG23	1:A:120:HIS:CD2	0.44	2.47	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:151:LEU:O	1:A:151:LEU:HD12	0.44	2.13	11	2
1:A:145:TYR:CG	1:A:189:LEU:HD21	0.44	2.48	13	1
1:A:218:CYS:O	1:A:221:VAL:HG12	0.44	2.12	12	3
1:A:205:LEU:HD23	1:A:209:ALA:CB	0.44	2.42	4	2
1:A:56:LEU:HD12	1:A:56:LEU:O	0.44	2.13	1	1
1:A:168:PHE:CE1	1:A:189:LEU:HD23	0.44	2.48	14	1
1:A:59:VAL:HG21	1:A:66:MET:HE2	0.44	1.87	5	1
1:A:151:LEU:HD12	1:A:151:LEU:O	0.44	2.12	20	3
1:A:205:LEU:HD21	1:A:213:GLU:HG2	0.44	1.90	14	2
1:A:172:LEU:HD12	1:A:172:LEU:O	0.44	2.13	12	1
1:A:12:HIS:CE1	1:A:111:LEU:HD21	0.44	2.47	5	1
1:A:34:PRO:HG3	1:A:151:LEU:HD22	0.44	1.90	11	1
1:A:69:LEU:HD21	1:A:134:ILE:HD13	0.44	1.90	3	1
1:A:23:TRP:CZ2	1:A:43:LEU:HD13	0.44	2.48	19	1
1:A:130:TYR:CD2	1:A:134:ILE:HD11	0.43	2.49	5	1
1:A:104:ILE:HD13	1:A:129:ILE:CD1	0.43	2.43	18	2
1:A:36:VAL:HG22	1:A:39:MET:CE	0.43	2.43	9	1
1:A:37:ILE:HG22	1:A:38:PRO:N	0.43	2.29	13	2
1:A:50:GLN:HE21	1:A:111:LEU:HD21	0.43	1.72	18	1
1:A:15:ILE:HG23	1:A:20:LEU:HD11	0.43	1.89	14	1
1:A:205:LEU:HD21	1:A:209:ALA:HB2	0.42	1.90	6	1
1:A:130:TYR:O	1:A:134:ILE:HD12	0.42	2.14	2	1
1:A:27:VAL:HG13	1:A:32:PHE:CE2	0.42	2.49	5	1
1:A:83:LEU:HD12	1:A:84:HIS:N	0.42	2.29	15	1
1:A:150:ILE:HA	1:A:153:ILE:HD12	0.42	1.90	3	1
1:A:20:LEU:O	1:A:24:VAL:HG23	0.42	2.14	1	2
1:A:115:ILE:HD13	1:A:118:MET:SD	0.42	2.54	1	1
1:A:33:SER:CB	1:A:34:PRO:HD2	0.42	2.45	9	1
1:A:190:LEU:O	1:A:194:ALA:HB2	0.42	2.14	1	3
1:A:150:ILE:HD12	1:A:172:LEU:HB2	0.42	1.91	16	1
1:A:205:LEU:HD11	1:A:213:GLU:HG2	0.42	1.92	12	1
1:A:12:HIS:CB	1:A:48:THR:HG21	0.41	2.44	14	1
1:A:131:LYS:O	1:A:135:ILE:HD12	0.41	2.15	14	1
1:A:83:LEU:HD11	1:A:84:HIS:CD2	0.41	2.50	14	1
1:A:161:PHE:O	1:A:165:VAL:HG23	0.41	2.15	12	1
1:A:47:ALA:HB2	1:A:131:LYS:HE3	0.41	1.92	19	1
1:A:40:PHE:CE1	1:A:59:VAL:HG23	0.41	2.50	20	1
1:A:195:ASN:ND2	1:A:195:ASN:H	0.41	2.14	3	1
1:A:205:LEU:HD23	1:A:209:ALA:HB2	0.41	1.93	15	2
1:A:37:ILE:CB	1:A:38:PRO:CD	0.41	2.99	12	11
1:A:15:ILE:HD13	1:A:51:ASP:OD1	0.41	2.16	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:52:LEU:HD23	1:A:53:ASN:H	0.40	1.77	15	1
1:A:201:ILE:HG21	1:A:217:ALA:CB	0.40	2.45	16	1
1:A:37:ILE:O	1:A:135:ILE:HD12	0.40	2.17	13	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	183/240 (76%)	168±2 (92±1%)	13±2 (7±1%)	2±1 (1±0%)	16	63
All	All	3660/4800 (76%)	3360 (92%)	252 (7%)	48 (1%)	16	63

All 6 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	31	ALA	16
1	A	47	ALA	13
1	A	50	GLN	10
1	A	61	GLY	7
1	A	120	HIS	1
1	A	33	SER	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	154/201 (77%)	109±4 (71±3%)	45±4 (29±3%)	1	17
All	All	3080/4020 (77%)	2180 (71%)	900 (29%)	1	17

All 123 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	72	THR	20
1	A	33	SER	20
1	A	48	THR	20
1	A	202	LEU	19
1	A	189	LEU	18
1	A	82	ARG	18
1	A	110	THR	18
1	A	144	MET	17
1	A	117	TRP	16
1	A	62	HIS	15
1	A	173	ARG	15
1	A	151	LEU	15
1	A	142	VAL	15
1	A	15	ILE	15
1	A	131	LYS	15
1	A	30	LYS	14
1	A	154	ARG	14
1	A	43	LEU	12
1	A	102	SER	12
1	A	25	LYS	12
1	A	143	ARG	12
1	A	170	LYS	12
1	A	16	SER	12
1	A	108	THR	12
1	A	166	ASP	11
1	A	155	GLN	11
1	A	23	TRP	11
1	A	187	GLU	11
1	A	13	GLN	11
1	A	136	LEU	10
1	A	114	GLN	10
1	A	41	SER	10
1	A	109	SER	10
1	A	100	ARG	10
1	A	158	LYS	10
1	A	70	LYS	10
1	A	203	LYS	9
1	A	28	GLU	9
1	A	18	ARG	9
1	A	71	GLU	9
1	A	152	ASP	9

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Mol	Chain	Res	Type	Models (Total)
1	A	56	LEU	9
1	A	164	TYR	8
1	A	211	LEU	8
1	A	83	LEU	8
1	A	19	THR	8
1	A	215	MET	8
1	A	40	PHE	8
1	A	68	MET	8
1	A	163	ASP	8
1	A	199	LYS	8
1	A	130	TYR	8
1	A	107	THR	8
1	A	50	GLN	8
1	A	74	ASN	8
1	A	81	ASP	7
1	A	59	VAL	7
1	A	84	HIS	7
1	A	113	GLU	7
1	A	200	THR	7
1	A	51	ASP	7
1	A	195	ASN	7
1	A	52	LEU	7
1	A	197	ASP	7
1	A	210	THR	7
1	A	175	GLU	6
1	A	45	GLU	6
1	A	128	GLU	6
1	A	159	GLU	6
1	A	214	MET	6
1	A	66	MET	6
1	A	21	ASN	6
1	A	103	ASP	5
1	A	205	LEU	5
1	A	198	CYS	5
1	A	121	ASN	5
1	A	63	GLN	5
1	A	139	ASN	4
1	A	111	LEU	4
1	A	39	MET	4
1	A	168	PHE	4
1	A	172	LEU	4
1	A	191	VAL	4

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Mol	Chain	Res	Type	Models (Total)
1	A	58	THR	4
1	A	219	GLN	4
1	A	55	MET	4
1	A	57	ASN	4
1	A	140	LYS	4
1	A	126	VAL	3
1	A	44	SER	3
1	A	67	GLN	3
1	A	221	VAL	3
1	A	120	HIS	3
1	A	132	ARG	3
1	A	118	MET	3
1	A	192	GLN	3
1	A	104	ILE	3
1	A	53	ASN	3
1	A	212	GLU	2
1	A	186	THR	2
1	A	79	GLU	2
1	A	112	GLN	2
1	A	29	GLU	2
1	A	76	GLU	2
1	A	36	VAL	2
1	A	162	ARG	2
1	A	37	ILE	2
1	A	167	ARG	2
1	A	35	GLU	2
1	A	115	ILE	2
1	A	80	TRP	2
1	A	26	VAL	1
1	A	141	ILE	1
1	A	218	CYS	1
1	A	12	HIS	1
1	A	216	THR	1
1	A	27	VAL	1
1	A	129	ILE	1
1	A	188	THR	1
1	A	193	ASN	1
1	A	119	THR	1
1	A	134	ILE	1
1	A	150	ILE	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 carbohydrates 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

The completeness of assignment taking into account all chemical shift lists is 83% for the well-defined parts and 83% for the entire structure.

7.1 Chemical shift list 1

File name: input_cs.cif

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	2600
Number of shifts mapped to atoms	2600
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	4

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	225	0.22 ± 0.15	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	206	0.85 ± 0.11	Should be applied
$^{13}\text{C}'$	206	-0.08 ± 0.14	None needed (< 0.5 ppm)
^{15}N	212	0.51 ± 0.16	Should be applied

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 83%, i.e. 1871 atoms were assigned a chemical shift out of a possible 2245. 0 out of 26 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	866/893 (97%)	353/355 (99%)	341/366 (93%)	172/172 (100%)
Sidechain	963/1208 (80%)	602/707 (85%)	361/448 (81%)	0/53 (0%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	42/144 (29%)	40/76 (53%)	0/60 (0%)	2/8 (25%)
Overall	1871/2245 (83%)	995/1138 (87%)	702/874 (80%)	174/233 (75%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 83%, i.e. 2353 atoms were assigned a chemical shift out of a possible 2820. 0 out of 33 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	1084/1124 (96%)	441/446 (99%)	431/464 (93%)	212/214 (99%)
Sidechain	1224/1538 (80%)	768/905 (85%)	456/564 (81%)	0/69 (0%)
Aromatic	45/158 (28%)	43/84 (51%)	0/64 (0%)	2/10 (20%)
Overall	2353/2820 (83%)	1252/1435 (87%)	887/1092 (81%)	214/293 (73%)

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	80	TRP	NE1	116.99	139.19 – 119.59	-6.3
1	A	104	ILE	HD11	-0.96	2.13 – -0.77	-5.7
1	A	104	ILE	HD13	-0.96	2.13 – -0.77	-5.7
1	A	104	ILE	HD12	-0.96	2.13 – -0.77	-5.7

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:

