



Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 02:42 PM UTC

PDB ID : 2OUT / pdb_00002out
Title : Solution Structure of HI1506, a Novel Two Domain Protein from Haemophilus influenzae
Authors : Sari, N.; He, Y.; Doseeva, V.; Surabian, K.; Schwarz, F.; Herzberg, O.; Orban, J.; Structure 2 Function Project (S2F)
Deposited on : 2007-02-12

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

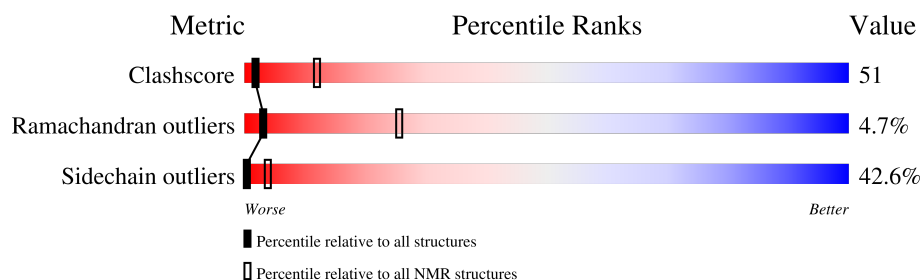
1 Overall quality at a glance

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	131	15% 26% 10% 49%

2 Ensemble composition and analysis

This entry contains 20 models. Model 12 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:7-A:14, A:31-A:56 (34)	0.48	12
2	A:89-A:121 (33)	0.84	10

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 6 clusters. No single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1975 atoms, of which 982 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Mu-like prophage FluMu protein gp35, Protein HI1507 in Mu-like prophage FluMu region.

Mol	Chain	Residues	Atoms						Trace
1	A	131	Total	C	H	N	O	S	0
			1975	612	982	175	204	2	

There are 27 discrepancies between the modelled and reference sequences:

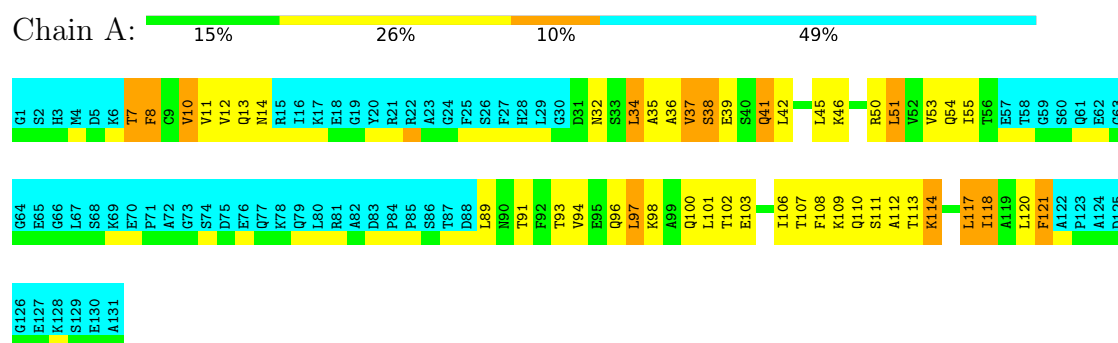
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P44228
A	2	SER	-	expression tag	UNP P44228
A	3	HIS	-	expression tag	UNP P44228
A	71	PRO	-	SEE REMARK 999	UNP P44229
A	72	ALA	-	SEE REMARK 999	UNP P44229
A	73	GLY	-	SEE REMARK 999	UNP P44229
A	74	SER	-	SEE REMARK 999	UNP P44229
A	75	ASP	-	SEE REMARK 999	UNP P44229
A	76	GLU	-	SEE REMARK 999	UNP P44229
A	77	GLN	-	SEE REMARK 999	UNP P44229
A	78	LYS	-	SEE REMARK 999	UNP P44229
A	79	GLN	-	SEE REMARK 999	UNP P44229
A	80	LEU	-	SEE REMARK 999	UNP P44229
A	81	ARG	-	SEE REMARK 999	UNP P44229
A	82	ALA	-	SEE REMARK 999	UNP P44229
A	83	ASP	-	SEE REMARK 999	UNP P44229
A	84	PRO	-	SEE REMARK 999	UNP P44229
A	85	PRO	-	SEE REMARK 999	UNP P44229
A	86	SER	-	SEE REMARK 999	UNP P44229
A	87	THR	-	SEE REMARK 999	UNP P44229
A	88	ASP	-	SEE REMARK 999	UNP P44229
A	89	LEU	-	SEE REMARK 999	UNP P44229
A	90	ASN	-	SEE REMARK 999	UNP P44229
A	91	THR	-	SEE REMARK 999	UNP P44229
A	92	PHE	-	SEE REMARK 999	UNP P44229
A	93	THR	-	SEE REMARK 999	UNP P44229
A	94	VAL	-	SEE REMARK 999	UNP P44229

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: Mu-like prophage FluMu protein gp35, Protein HI1507 in Mu-like prophage FluMu region

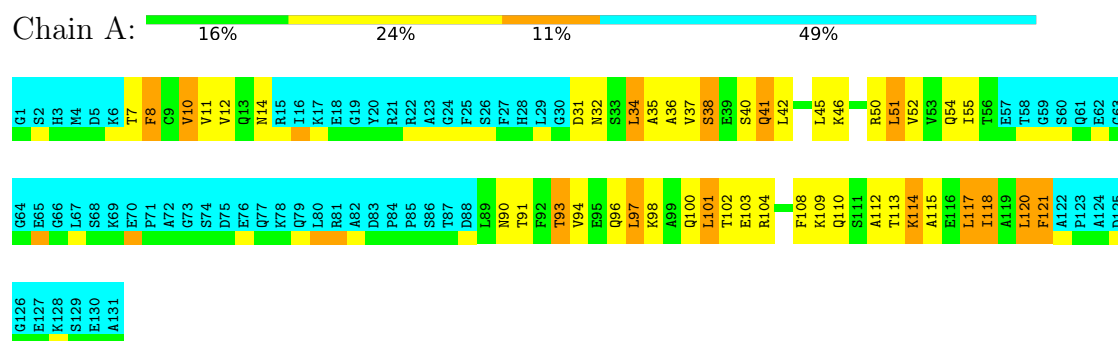


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

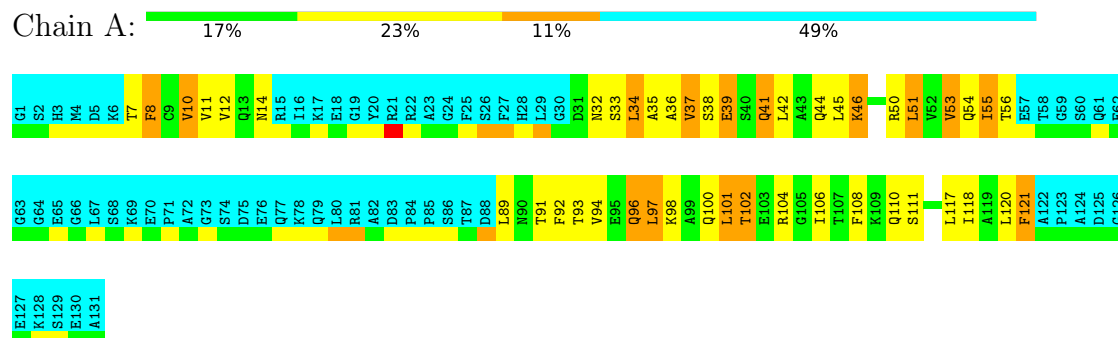
4.2.1 Score per residue for model 1

- Molecule 1: Mu-like prophage FluMu protein gp35, Protein HI1507 in Mu-like prophage FluMu region



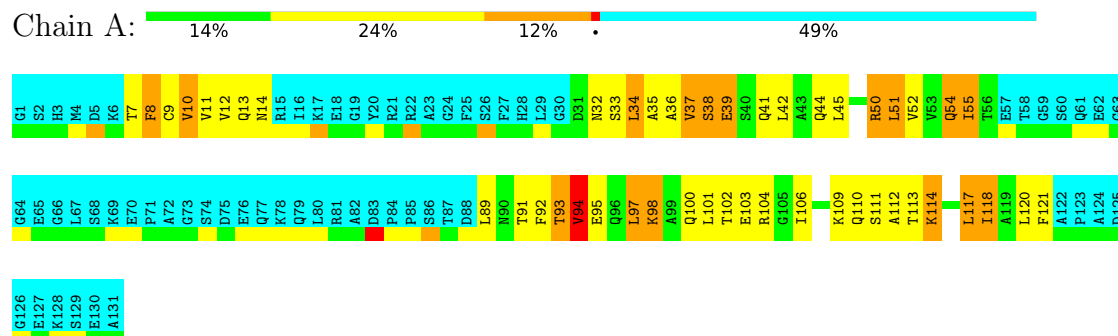
4.2.2 Score per residue for model 2

- Molecule 1: Mu-like prophage FluMu protein gp35, Protein HI1507 in Mu-like prophage FluMu region



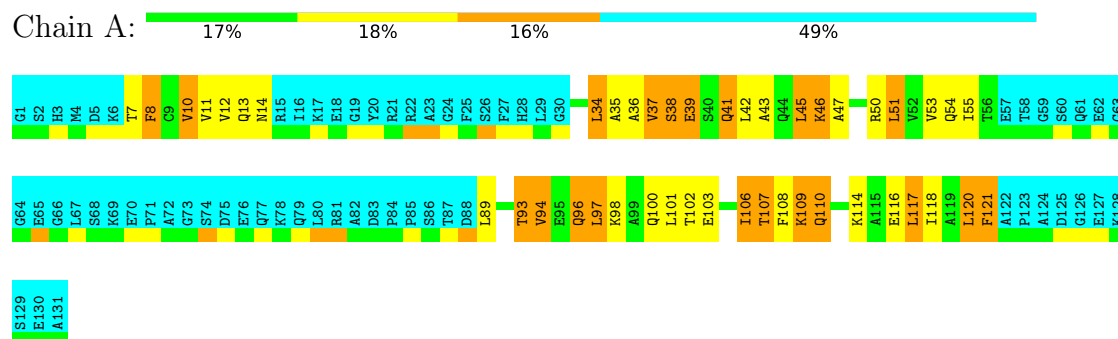
4.2.5 Score per residue for model 5

- Molecule 1: Mu-like prophage FluMu protein gp35, Protein HI1507 in Mu-like prophage FluMu region



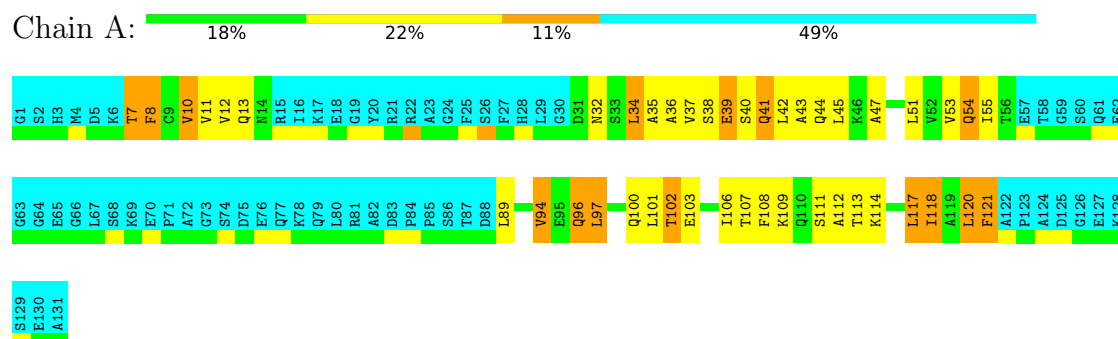
4.2.6 Score per residue for model 6

- Molecule 1: Mu-like prophage FluMu protein gp35, Protein HI1507 in Mu-like prophage FluMu region



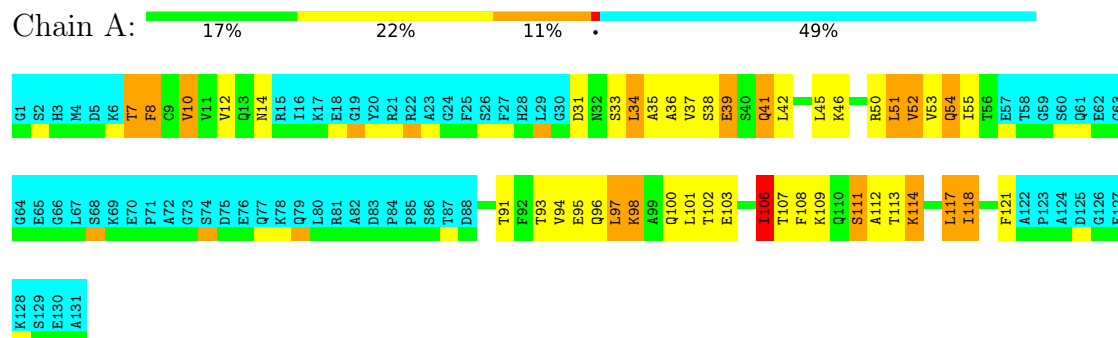
4.2.7 Score per residue for model 7

- Molecule 1: Mu-like prophage FluMu protein gp35, Protein HI1507 in Mu-like prophage FluMu region



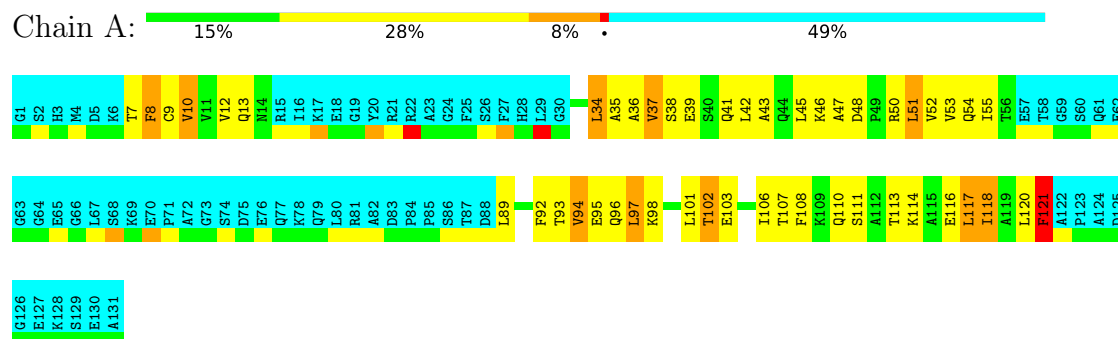
4.2.8 Score per residue for model 8

- Molecule 1: Mu-like prophage FluMu protein gp35, Protein HI1507 in Mu-like prophage FluMu region



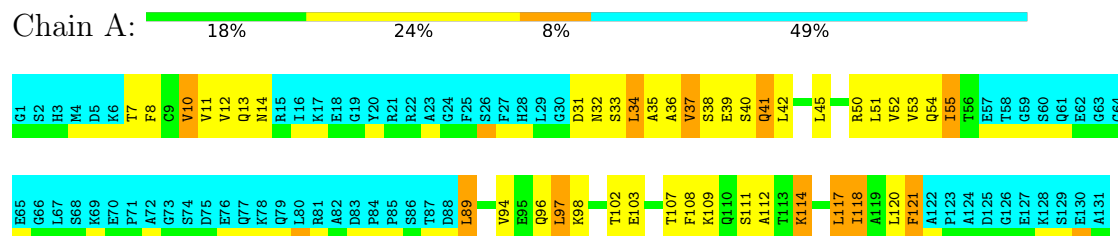
4.2.9 Score per residue for model 9

- Molecule 1: Mu-like prophage FluMu protein gp35, Protein HI1507 in Mu-like prophage FluMu region



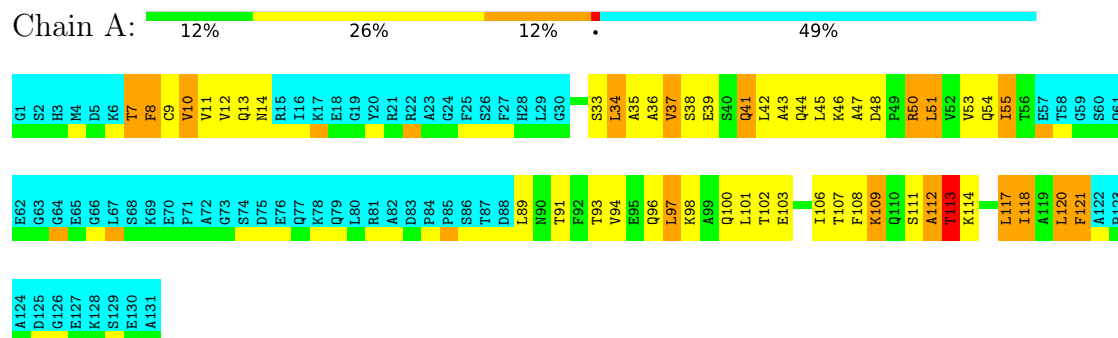
4.2.10 Score per residue for model 10

- Molecule 1: Mu-like prophage FluMu protein gp35, Protein HI1507 in Mu-like prophage FluMu region



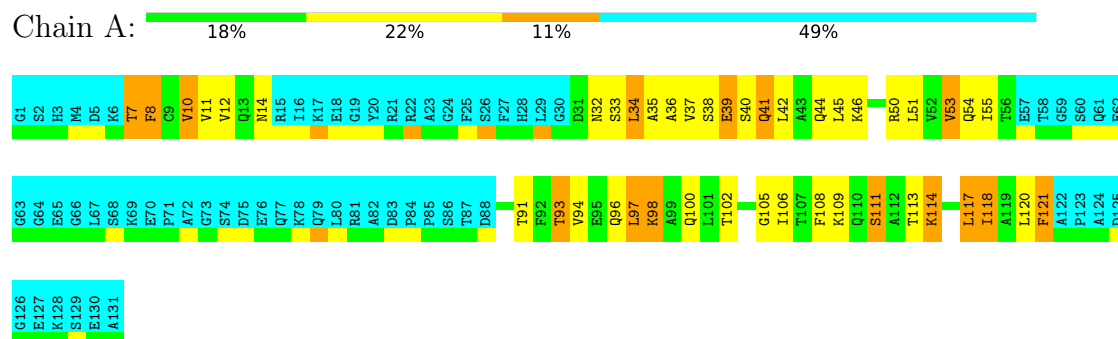
4.2.11 Score per residue for model 11

- Molecule 1: Mu-like prophage FluMu protein gp35, Protein HI1507 in Mu-like prophage FluMu region



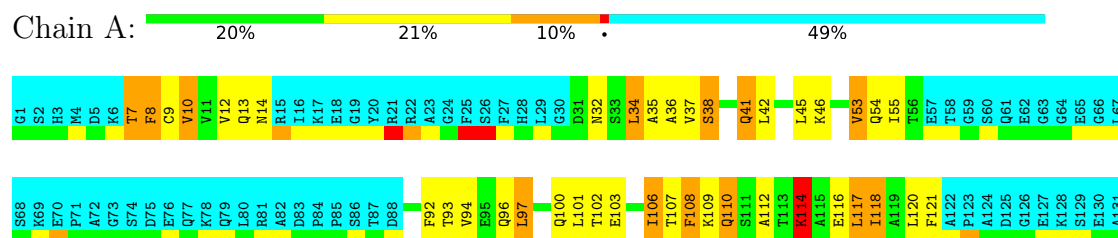
4.2.12 Score per residue for model 12 (medoid)

- Molecule 1: Mu-like prophage FluMu protein gp35, Protein HI1507 in Mu-like prophage FluMu region



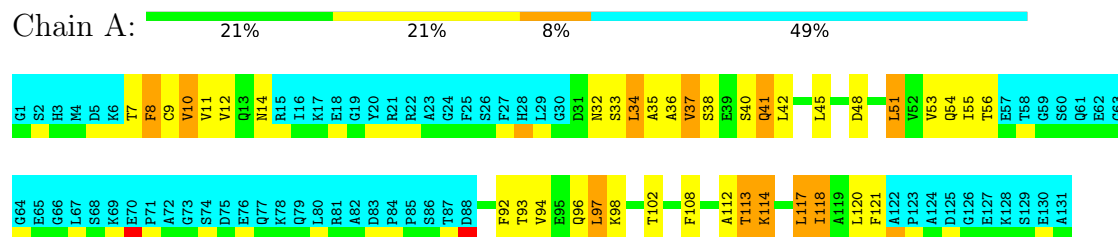
4.2.13 Score per residue for model 13

- Molecule 1: Mu-like prophage FluMu protein gp35, Protein HI1507 in Mu-like prophage FluMu region



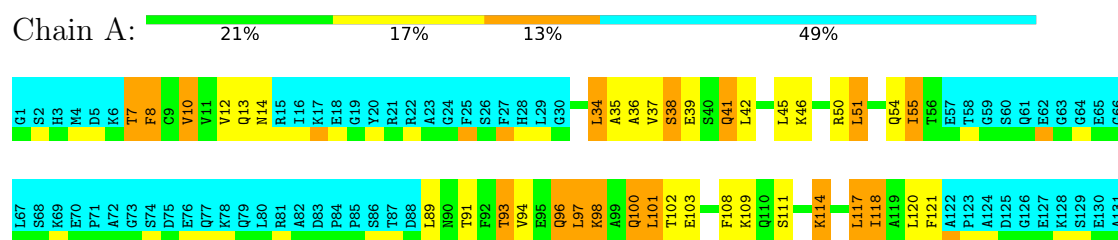
4.2.14 Score per residue for model 14

- Molecule 1: Mu-like prophage FluMu protein gp35, Protein HI1507 in Mu-like prophage FluMu region



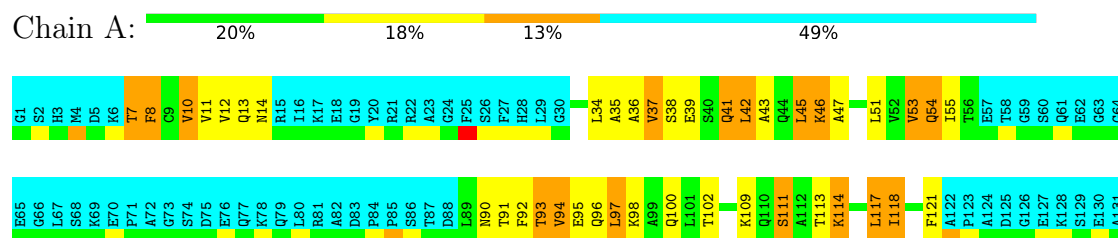
4.2.15 Score per residue for model 15

- Molecule 1: Mu-like prophage FluMu protein gp35, Protein HI1507 in Mu-like prophage FluMu region



4.2.16 Score per residue for model 16

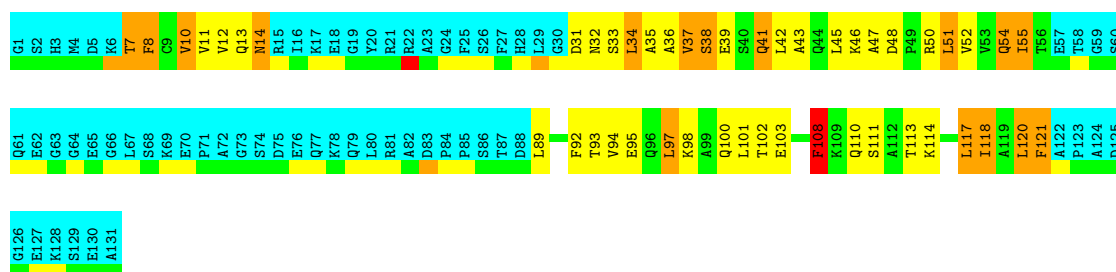
- Molecule 1: Mu-like prophage FluMu protein gp35, Protein HI1507 in Mu-like prophage FluMu region



4.2.17 Score per residue for model 17

- Molecule 1: Mu-like prophage FluMu protein gp35, Protein HI1507 in Mu-like prophage FluMu region

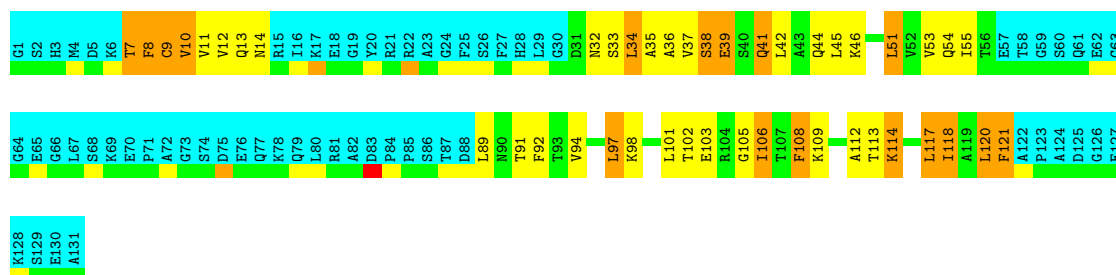




4.2.18 Score per residue for model 18

- Molecule 1: Mu-like prophage FluMu protein gp35, Protein HI1507 in Mu-like prophage FluMu region

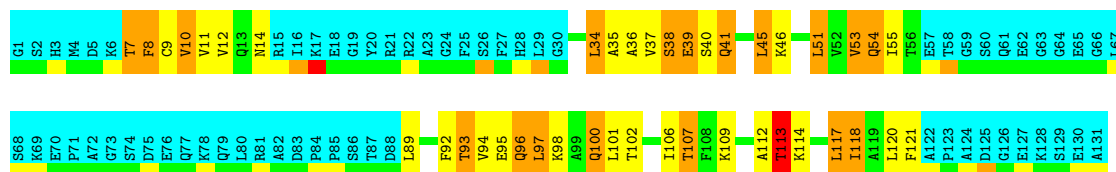
Chain A: 17% 21% 13% 49%



4.2.19 Score per residue for model 19

- Molecule 1: Mu-like prophage FluMu protein gp35, Protein HI1507 in Mu-like prophage FluMu region

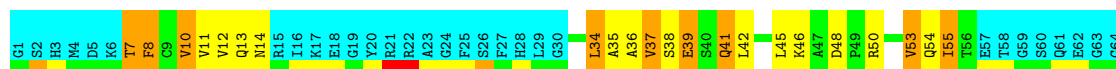
Chain A: 19% 18% 14% 49%



4.2.20 Score per residue for model 20

- Molecule 1: Mu-like prophage FluMu protein gp35, Protein HI1507 in Mu-like prophage FluMu region

Chain A: 21% 18% 11% 49%





5 Refinement protocol and experimental data overview

The models were refined using the following method: *structures were calculated using standard simulated annealing and torsion angle dynamics protocols in CNS version 1.1.*

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with acceptable covalent geometry.*

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

Software name	Classification	Version
CNS	structure solution	1.1
CNS	refinement	1.1

No chemical shift data was provided.

6 Model quality

6.1 Standard geometry

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	516	538	539	54±6
All	All	10320	10760	10780	1082

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 51.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:VAL:HG13	1:A:45:LEU:HD13	1.03	1.28	3	11
1:A:12:VAL:HG13	1:A:45:LEU:HD23	0.98	1.35	7	1
1:A:12:VAL:HG21	1:A:45:LEU:HD22	0.93	1.40	11	5
1:A:10:VAL:HG23	1:A:55:ILE:HG22	0.89	1.41	16	4
1:A:117:LEU:HD23	1:A:118:ILE:N	0.87	1.83	16	14
1:A:45:LEU:HD12	1:A:53:VAL:HG23	0.87	1.46	14	4
1:A:114:LYS:O	1:A:118:ILE:HG23	0.87	1.70	6	2
1:A:34:LEU:HD22	1:A:35:ALA:N	0.86	1.86	15	19
1:A:97:LEU:HD22	1:A:118:ILE:HA	0.85	1.48	6	7
1:A:101:LEU:HD22	1:A:106:ILE:HG21	0.85	1.49	13	6
1:A:106:ILE:HD11	1:A:108:PHE:CD2	0.83	2.08	18	1
1:A:97:LEU:H	1:A:97:LEU:HD13	0.82	1.31	19	6
1:A:97:LEU:HD13	1:A:97:LEU:N	0.82	1.89	19	5
1:A:12:VAL:CG1	1:A:45:LEU:HD13	0.82	2.04	3	12

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:117:LEU:HD12	1:A:118:ILE:N	0.82	1.90	2	1
1:A:12:VAL:HG22	1:A:45:LEU:HD13	0.82	1.51	20	1
1:A:97:LEU:HD11	1:A:118:ILE:HD12	0.81	1.52	2	1
1:A:14:ASN:CB	1:A:51:LEU:HD22	0.81	2.05	10	1
1:A:106:ILE:HD11	1:A:108:PHE:CE2	0.80	2.11	20	2
1:A:12:VAL:CG2	1:A:45:LEU:HD13	0.79	2.08	20	5
1:A:7:THR:OG1	1:A:36:ALA:HB1	0.79	1.76	2	9
1:A:34:LEU:HD13	1:A:35:ALA:O	0.78	1.77	16	20
1:A:7:THR:HG22	1:A:36:ALA:C	0.78	2.03	19	10
1:A:97:LEU:HD23	1:A:117:LEU:HD21	0.78	1.54	5	2
1:A:97:LEU:N	1:A:97:LEU:HD13	0.77	1.94	12	4
1:A:50:ARG:C	1:A:51:LEU:HD13	0.77	2.05	17	9
1:A:118:ILE:HD13	1:A:118:ILE:O	0.77	1.80	17	12
1:A:34:LEU:HD22	1:A:35:ALA:H	0.77	1.40	2	20
1:A:45:LEU:HD12	1:A:53:VAL:CG2	0.77	2.08	14	4
1:A:106:ILE:HD11	1:A:108:PHE:CZ	0.76	2.14	20	1
1:A:12:VAL:CG1	1:A:45:LEU:HD23	0.76	2.10	7	1
1:A:94:VAL:HA	1:A:97:LEU:HD21	0.76	1.58	8	7
1:A:98:LYS:O	1:A:102:THR:HG23	0.75	1.80	10	1
1:A:94:VAL:HG12	1:A:98:LYS:NZ	0.74	1.97	16	7
1:A:101:LEU:HD21	1:A:120:LEU:HD11	0.74	1.60	9	1
1:A:34:LEU:CD1	1:A:35:ALA:O	0.73	2.36	16	20
1:A:14:ASN:HB3	1:A:51:LEU:HD22	0.73	1.57	10	1
1:A:7:THR:HB	1:A:36:ALA:HB1	0.73	1.60	13	11
1:A:89:LEU:HD21	1:A:118:ILE:HG12	0.72	1.59	2	1
1:A:101:LEU:HD21	1:A:120:LEU:HD12	0.72	1.59	17	1
1:A:101:LEU:HD22	1:A:106:ILE:HA	0.72	1.61	20	2
1:A:12:VAL:HG21	1:A:45:LEU:HD13	0.71	1.59	19	3
1:A:34:LEU:HD13	1:A:35:ALA:N	0.71	2.00	16	2
1:A:108:PHE:HB2	1:A:112:ALA:HB3	0.71	1.60	11	5
1:A:98:LYS:HE2	1:A:117:LEU:HD11	0.71	1.63	12	3
1:A:39:GLU:OE1	1:A:42:LEU:HD23	0.71	1.86	2	1
1:A:11:VAL:HA	1:A:32:ASN:O	0.70	1.85	3	10
1:A:93:THR:O	1:A:97:LEU:HD21	0.70	1.85	16	3
1:A:12:VAL:HG21	1:A:45:LEU:CD2	0.70	2.15	11	4
1:A:101:LEU:HD12	1:A:117:LEU:CD1	0.70	2.16	19	2
1:A:10:VAL:HG23	1:A:55:ILE:HA	0.70	1.64	10	9
1:A:10:VAL:HG11	1:A:45:LEU:HD11	0.69	1.65	20	1
1:A:108:PHE:HB3	1:A:112:ALA:HB3	0.69	1.64	13	2
1:A:97:LEU:CD1	1:A:97:LEU:N	0.69	2.56	18	5
1:A:101:LEU:HD13	1:A:106:ILE:CD1	0.69	2.18	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:120:LEU:HD22	1:A:120:LEU:O	0.68	1.88	6	1
1:A:94:VAL:O	1:A:97:LEU:CD2	0.68	2.42	5	4
1:A:101:LEU:O	1:A:106:ILE:HG22	0.68	1.88	13	1
1:A:97:LEU:HD23	1:A:118:ILE:HD13	0.67	1.67	3	1
1:A:11:VAL:HG23	1:A:32:ASN:C	0.67	2.15	5	2
1:A:118:ILE:HD12	1:A:118:ILE:O	0.67	1.90	10	1
1:A:89:LEU:HD11	1:A:118:ILE:O	0.66	1.90	17	3
1:A:93:THR:N	1:A:97:LEU:HD11	0.66	2.04	16	2
1:A:10:VAL:HG22	1:A:54:GLN:O	0.66	1.90	6	19
1:A:108:PHE:CB	1:A:112:ALA:HB3	0.66	2.20	18	2
1:A:43:ALA:O	1:A:47:ALA:HB2	0.66	1.91	11	6
1:A:97:LEU:CG	1:A:118:ILE:HG22	0.66	2.20	5	1
1:A:101:LEU:HD21	1:A:120:LEU:CD1	0.66	2.21	9	2
1:A:10:VAL:O	1:A:34:LEU:N	0.65	2.29	9	20
1:A:114:LYS:O	1:A:118:ILE:HG22	0.65	1.91	3	7
1:A:101:LEU:HD22	1:A:106:ILE:HB	0.65	1.66	9	2
1:A:10:VAL:HG12	1:A:34:LEU:HB3	0.65	1.67	20	5
1:A:114:LYS:HA	1:A:117:LEU:HD22	0.65	1.66	18	12
1:A:10:VAL:CG1	1:A:45:LEU:HD12	0.65	2.22	18	6
1:A:93:THR:O	1:A:97:LEU:HD11	0.64	1.92	19	3
1:A:97:LEU:CD1	1:A:118:ILE:HG22	0.64	2.22	6	2
1:A:97:LEU:HD13	1:A:97:LEU:H	0.64	1.52	12	2
1:A:106:ILE:HG23	1:A:107:THR:N	0.64	2.07	6	2
1:A:37:VAL:HG23	1:A:38:SER:N	0.64	2.08	17	10
1:A:97:LEU:HD21	1:A:118:ILE:HD13	0.63	1.70	10	1
1:A:97:LEU:CD2	1:A:118:ILE:HD13	0.63	2.23	3	2
1:A:12:VAL:HG21	1:A:45:LEU:CD1	0.63	2.23	19	2
1:A:10:VAL:HG11	1:A:45:LEU:HD12	0.63	1.69	2	7
1:A:94:VAL:O	1:A:97:LEU:HD22	0.63	1.93	19	6
1:A:41:GLN:O	1:A:45:LEU:HG	0.62	1.93	13	4
1:A:94:VAL:HA	1:A:97:LEU:HD22	0.62	1.71	14	5
1:A:106:ILE:HD11	1:A:108:PHE:CG	0.62	2.28	18	1
1:A:117:LEU:HD23	1:A:117:LEU:C	0.62	2.20	13	12
1:A:12:VAL:HG22	1:A:53:VAL:HA	0.62	1.70	11	1
1:A:52:VAL:O	1:A:52:VAL:HG23	0.62	1.95	5	2
1:A:101:LEU:HD12	1:A:117:LEU:HB2	0.61	1.72	13	1
1:A:105:GLY:O	1:A:106:ILE:HG22	0.61	1.95	18	1
1:A:97:LEU:HD13	1:A:117:LEU:HG	0.61	1.72	6	1
1:A:89:LEU:HD12	1:A:118:ILE:O	0.61	1.95	19	3
1:A:97:LEU:N	1:A:97:LEU:CD1	0.61	2.62	19	6
1:A:120:LEU:HD12	1:A:120:LEU:C	0.61	2.21	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:98:LYS:CE	1:A:117:LEU:HD11	0.61	2.25	12	1
1:A:114:LYS:HA	1:A:117:LEU:CD2	0.61	2.26	7	9
1:A:93:THR:C	1:A:97:LEU:HD21	0.61	2.20	16	1
1:A:97:LEU:HG	1:A:118:ILE:HG22	0.61	1.72	5	1
1:A:7:THR:HA	1:A:37:VAL:O	0.61	1.94	2	3
1:A:10:VAL:H	1:A:34:LEU:HB3	0.60	1.56	16	2
1:A:42:LEU:HD13	1:A:55:ILE:CG2	0.60	2.27	5	4
1:A:97:LEU:CD1	1:A:118:ILE:HD12	0.60	2.26	2	1
1:A:34:LEU:HD11	1:A:41:GLN:HG2	0.59	1.74	10	10
1:A:93:THR:O	1:A:94:VAL:HG13	0.59	1.97	6	1
1:A:97:LEU:CD1	1:A:117:LEU:HD21	0.59	2.27	6	1
1:A:7:THR:HG22	1:A:37:VAL:C	0.59	2.22	18	1
1:A:101:LEU:HB3	1:A:106:ILE:HD13	0.59	1.74	18	1
1:A:12:VAL:HG11	1:A:45:LEU:HD22	0.59	1.72	19	5
1:A:10:VAL:HG11	1:A:45:LEU:CD1	0.59	2.27	20	3
1:A:34:LEU:HD13	1:A:34:LEU:C	0.58	2.22	16	11
1:A:116:GLU:O	1:A:120:LEU:HD13	0.58	1.98	13	1
1:A:50:ARG:O	1:A:51:LEU:HD13	0.58	1.97	17	1
1:A:14:ASN:CG	1:A:51:LEU:HD12	0.58	2.23	5	2
1:A:12:VAL:CG2	1:A:45:LEU:HD22	0.58	2.24	11	1
1:A:14:ASN:HD21	1:A:52:VAL:HG13	0.58	1.59	17	2
1:A:97:LEU:HD13	1:A:117:LEU:CD2	0.58	2.29	3	2
1:A:12:VAL:HG12	1:A:52:VAL:O	0.58	1.99	9	4
1:A:93:THR:HG22	1:A:94:VAL:HG22	0.58	1.74	11	1
1:A:97:LEU:HD22	1:A:118:ILE:CA	0.58	2.29	3	1
1:A:106:ILE:O	1:A:106:ILE:HG23	0.58	1.99	7	3
1:A:51:LEU:HD22	1:A:51:LEU:N	0.57	2.14	5	8
1:A:94:VAL:HG12	1:A:98:LYS:HZ1	0.57	1.56	16	4
1:A:97:LEU:HD11	1:A:118:ILE:HG22	0.57	1.74	6	1
1:A:108:PHE:CD1	1:A:108:PHE:N	0.57	2.72	3	9
1:A:97:LEU:HD13	1:A:117:LEU:CG	0.57	2.30	6	1
1:A:120:LEU:C	1:A:120:LEU:HD13	0.57	2.25	6	2
1:A:14:ASN:ND2	1:A:51:LEU:HD12	0.57	2.15	15	3
1:A:51:LEU:HD13	1:A:51:LEU:N	0.57	2.15	4	8
1:A:101:LEU:HD12	1:A:117:LEU:HD12	0.56	1.77	19	2
1:A:101:LEU:CD2	1:A:120:LEU:HD11	0.56	2.29	9	1
1:A:112:ALA:HB1	1:A:117:LEU:HB3	0.56	1.77	18	2
1:A:12:VAL:HG23	1:A:12:VAL:O	0.56	2.01	14	9
1:A:120:LEU:O	1:A:121:PHE:C	0.56	2.49	9	1
1:A:14:ASN:ND2	1:A:52:VAL:HG13	0.56	2.15	17	1
1:A:118:ILE:HD13	1:A:118:ILE:C	0.55	2.26	7	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:101:LEU:HD11	1:A:120:LEU:HD11	0.55	1.78	9	1
1:A:51:LEU:H	1:A:51:LEU:HD22	0.55	1.61	8	7
1:A:97:LEU:HB2	1:A:117:LEU:HD13	0.55	1.78	2	1
1:A:101:LEU:HD23	1:A:121:PHE:CZ	0.55	2.37	4	3
1:A:112:ALA:HB1	1:A:117:LEU:HB2	0.55	1.78	4	1
1:A:114:LYS:HA	1:A:117:LEU:HD23	0.55	1.78	5	1
1:A:41:GLN:CD	1:A:42:LEU:N	0.55	2.65	7	12
1:A:94:VAL:CA	1:A:97:LEU:HD21	0.55	2.32	16	4
1:A:97:LEU:CD2	1:A:117:LEU:HD21	0.55	2.32	8	1
1:A:94:VAL:HA	1:A:97:LEU:HD11	0.54	1.78	17	4
1:A:39:GLU:CD	1:A:42:LEU:HD23	0.54	2.26	2	1
1:A:46:LYS:N	1:A:53:VAL:HG11	0.54	2.18	19	4
1:A:89:LEU:HD22	1:A:89:LEU:N	0.54	2.17	15	3
1:A:37:VAL:HG12	1:A:38:SER:H	0.54	1.62	18	3
1:A:51:LEU:HD22	1:A:51:LEU:H	0.54	1.63	5	4
1:A:92:PHE:CD1	1:A:121:PHE:CE2	0.53	2.96	9	1
1:A:10:VAL:HG12	1:A:34:LEU:CB	0.53	2.32	6	7
1:A:8:PHE:CE2	1:A:41:GLN:NE2	0.53	2.76	18	2
1:A:106:ILE:N	1:A:106:ILE:HD12	0.53	2.19	2	1
1:A:97:LEU:HA	1:A:121:PHE:CE2	0.53	2.39	9	10
1:A:37:VAL:HG22	1:A:41:GLN:HG3	0.52	1.82	17	3
1:A:114:LYS:HA	1:A:117:LEU:HD21	0.52	1.79	7	2
1:A:45:LEU:HD12	1:A:53:VAL:HG21	0.52	1.80	13	1
1:A:97:LEU:N	1:A:97:LEU:HD12	0.52	2.19	9	2
1:A:94:VAL:HA	1:A:97:LEU:CD2	0.52	2.35	18	4
1:A:114:LYS:CA	1:A:117:LEU:HD22	0.52	2.34	9	10
1:A:10:VAL:CG2	1:A:55:ILE:HG22	0.52	2.32	2	3
1:A:8:PHE:CD1	1:A:8:PHE:N	0.52	2.78	18	12
1:A:7:THR:OG1	1:A:36:ALA:CB	0.52	2.58	14	5
1:A:101:LEU:HD13	1:A:106:ILE:HG21	0.51	1.82	6	3
1:A:51:LEU:N	1:A:51:LEU:HD22	0.51	2.19	6	2
1:A:34:LEU:HG	1:A:41:GLN:HB2	0.51	1.81	6	8
1:A:105:GLY:O	1:A:106:ILE:CG2	0.51	2.58	18	1
1:A:10:VAL:HG23	1:A:55:ILE:CG2	0.51	2.34	2	1
1:A:51:LEU:N	1:A:51:LEU:HD12	0.51	2.20	7	1
1:A:101:LEU:HG	1:A:121:PHE:CE2	0.51	2.41	11	6
1:A:101:LEU:HG	1:A:121:PHE:CZ	0.51	2.41	3	5
1:A:114:LYS:HE3	1:A:115:ALA:HB2	0.51	1.83	1	1
1:A:34:LEU:CD1	1:A:41:GLN:CB	0.51	2.89	18	6
1:A:114:LYS:CE	1:A:115:ALA:HB2	0.51	2.35	1	1
1:A:14:ASN:HB2	1:A:51:LEU:HD22	0.51	1.81	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:51:LEU:N	1:A:51:LEU:CD1	0.51	2.74	7	1
1:A:34:LEU:CD1	1:A:41:GLN:HG2	0.51	2.36	18	8
1:A:41:GLN:OE1	1:A:42:LEU:N	0.51	2.44	17	3
1:A:41:GLN:HE22	1:A:55:ILE:HG22	0.50	1.65	11	1
1:A:113:THR:O	1:A:117:LEU:HD13	0.50	2.05	11	2
1:A:8:PHE:CD1	1:A:41:GLN:OE1	0.50	2.64	19	2
1:A:35:ALA:O	1:A:37:VAL:HG23	0.50	2.06	16	10
1:A:97:LEU:CD1	1:A:117:LEU:CD2	0.50	2.90	3	4
1:A:97:LEU:HB3	1:A:121:PHE:CE2	0.49	2.42	4	2
1:A:112:ALA:HB1	1:A:117:LEU:CB	0.49	2.37	18	3
1:A:46:LYS:HB2	1:A:53:VAL:HG11	0.49	1.83	9	1
1:A:97:LEU:HD23	1:A:118:ILE:HB	0.49	1.84	10	2
1:A:114:LYS:O	1:A:117:LEU:CD2	0.49	2.60	1	9
1:A:101:LEU:CD2	1:A:121:PHE:CZ	0.49	2.95	3	3
1:A:10:VAL:HB	1:A:41:GLN:OE1	0.49	2.07	2	1
1:A:97:LEU:CD2	1:A:118:ILE:HB	0.49	2.37	10	2
1:A:10:VAL:CG1	1:A:45:LEU:HD11	0.49	2.38	4	2
1:A:101:LEU:HD22	1:A:106:ILE:CG2	0.49	2.37	7	2
1:A:39:GLU:HA	1:A:41:GLN:NE2	0.49	2.23	18	1
1:A:97:LEU:H	1:A:97:LEU:HD22	0.49	1.68	16	1
1:A:106:ILE:HG22	1:A:107:THR:HG22	0.49	1.83	19	1
1:A:34:LEU:HG	1:A:41:GLN:CB	0.49	2.37	5	9
1:A:97:LEU:HD23	1:A:117:LEU:CD2	0.49	2.37	8	2
1:A:7:THR:HG22	1:A:37:VAL:N	0.49	2.23	17	9
1:A:9:CYS:HB3	1:A:34:LEU:O	0.48	2.07	18	2
1:A:105:GLY:O	1:A:106:ILE:O	0.48	2.32	18	1
1:A:112:ALA:O	1:A:113:THR:HG23	0.48	2.08	19	1
1:A:89:LEU:HD12	1:A:92:PHE:HB2	0.48	1.85	2	1
1:A:10:VAL:O	1:A:34:LEU:HB3	0.48	2.08	18	3
1:A:93:THR:C	1:A:97:LEU:HD11	0.48	2.34	8	2
1:A:8:PHE:CE1	1:A:41:GLN:OE1	0.48	2.67	7	6
1:A:97:LEU:HD21	1:A:118:ILE:CG1	0.48	2.39	9	3
1:A:94:VAL:HG13	1:A:114:LYS:HG3	0.48	1.85	7	1
1:A:97:LEU:HD22	1:A:98:LYS:H	0.48	1.69	8	1
1:A:101:LEU:CD1	1:A:117:LEU:HD12	0.47	2.39	5	1
1:A:105:GLY:O	1:A:106:ILE:HD13	0.47	2.09	12	1
1:A:37:VAL:HG12	1:A:38:SER:N	0.47	2.24	19	9
1:A:97:LEU:CB	1:A:121:PHE:CE1	0.47	2.97	15	2
1:A:7:THR:HG22	1:A:37:VAL:CA	0.47	2.38	18	1
1:A:94:VAL:HG12	1:A:98:LYS:HZ2	0.47	1.69	9	4
1:A:101:LEU:HG	1:A:121:PHE:CE1	0.47	2.44	15	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:34:LEU:CD1	1:A:41:GLN:HB3	0.47	2.39	2	1
1:A:97:LEU:HD21	1:A:118:ILE:HG12	0.47	1.86	4	1
1:A:102:THR:HG23	1:A:108:PHE:CE1	0.47	2.45	4	1
1:A:45:LEU:N	1:A:45:LEU:CD1	0.47	2.77	7	1
1:A:34:LEU:HG	1:A:41:GLN:HB3	0.47	1.85	11	2
1:A:94:VAL:CA	1:A:97:LEU:CD2	0.47	2.93	16	1
1:A:97:LEU:HB3	1:A:121:PHE:CD2	0.47	2.45	19	2
1:A:96:GLN:O	1:A:100:GLN:N	0.47	2.47	7	5
1:A:37:VAL:CG2	1:A:38:SER:N	0.47	2.78	10	6
1:A:94:VAL:O	1:A:98:LYS:CD	0.47	2.62	5	1
1:A:102:THR:HG23	1:A:108:PHE:HE1	0.46	1.69	9	2
1:A:11:VAL:HG23	1:A:32:ASN:O	0.46	2.10	5	1
1:A:94:VAL:O	1:A:98:LYS:CE	0.46	2.63	5	2
1:A:97:LEU:CA	1:A:121:PHE:CE2	0.46	2.99	11	4
1:A:46:LYS:CA	1:A:53:VAL:HG11	0.46	2.41	2	3
1:A:14:ASN:OD1	1:A:51:LEU:HD12	0.46	2.11	5	1
1:A:93:THR:HG22	1:A:94:VAL:N	0.46	2.26	17	3
1:A:97:LEU:HG	1:A:118:ILE:HA	0.46	1.87	19	5
1:A:111:SER:O	1:A:112:ALA:HB2	0.46	2.09	3	1
1:A:101:LEU:HB3	1:A:106:ILE:HD12	0.46	1.88	20	1
1:A:97:LEU:HD13	1:A:117:LEU:CD1	0.45	2.41	2	1
1:A:52:VAL:O	1:A:52:VAL:CG2	0.45	2.64	5	2
1:A:97:LEU:CB	1:A:121:PHE:CE2	0.45	2.99	11	1
1:A:97:LEU:HA	1:A:121:PHE:CE1	0.45	2.46	1	3
1:A:94:VAL:HA	1:A:97:LEU:CD1	0.45	2.40	17	2
1:A:100:GLN:HB3	1:A:121:PHE:CZ	0.45	2.46	13	2
1:A:12:VAL:CG1	1:A:45:LEU:HG	0.45	2.42	9	1
1:A:38:SER:O	1:A:39:GLU:CB	0.45	2.65	16	1
1:A:97:LEU:CD1	1:A:97:LEU:H	0.45	2.25	9	1
1:A:8:PHE:CE2	1:A:55:ILE:HB	0.45	2.46	2	1
1:A:92:PHE:N	1:A:92:PHE:CD1	0.45	2.85	5	3
1:A:92:PHE:CD1	1:A:121:PHE:CZ	0.45	3.04	9	1
1:A:8:PHE:CE2	1:A:55:ILE:HD13	0.45	2.47	16	1
1:A:106:ILE:O	1:A:107:THR:HG22	0.45	2.12	4	1
1:A:8:PHE:CD1	1:A:8:PHE:O	0.45	2.70	20	1
1:A:10:VAL:HG21	1:A:41:GLN:HE22	0.45	1.72	20	1
1:A:98:LYS:CE	1:A:117:LEU:HD21	0.44	2.42	4	1
1:A:101:LEU:HD23	1:A:104:ARG:HD3	0.44	1.89	5	1
1:A:10:VAL:HG11	1:A:45:LEU:HD22	0.44	1.87	7	1
1:A:35:ALA:O	1:A:37:VAL:HG13	0.44	2.13	5	5
1:A:8:PHE:CE1	1:A:41:GLN:CD	0.44	2.96	17	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:8:PHE:CD2	1:A:41:GLN:NE2	0.44	2.86	9	2
1:A:97:LEU:CD2	1:A:118:ILE:HA	0.44	2.40	3	1
1:A:97:LEU:HD23	1:A:118:ILE:CB	0.44	2.43	9	1
1:A:10:VAL:HG11	1:A:41:GLN:NE2	0.44	2.28	12	1
1:A:97:LEU:HD12	1:A:117:LEU:HG	0.44	1.90	7	2
1:A:34:LEU:HD11	1:A:41:GLN:CG	0.44	2.43	18	3
1:A:106:ILE:CG2	1:A:107:THR:N	0.44	2.77	6	1
1:A:114:LYS:CA	1:A:117:LEU:CD2	0.44	2.95	7	1
1:A:55:ILE:HD12	1:A:55:ILE:O	0.44	2.12	12	3
1:A:97:LEU:HD23	1:A:117:LEU:HD23	0.44	1.89	19	1
1:A:97:LEU:CA	1:A:121:PHE:CE1	0.43	3.01	15	3
1:A:97:LEU:HD13	1:A:117:LEU:HD23	0.43	1.88	3	1
1:A:12:VAL:HG13	1:A:45:LEU:CD2	0.43	2.24	7	1
1:A:102:THR:HG23	1:A:108:PHE:CD1	0.43	2.48	2	1
1:A:8:PHE:N	1:A:37:VAL:O	0.43	2.52	2	1
1:A:97:LEU:HD23	1:A:118:ILE:HA	0.43	1.88	10	2
1:A:45:LEU:CD1	1:A:53:VAL:HG23	0.43	2.37	4	1
1:A:93:THR:O	1:A:118:ILE:HG21	0.43	2.12	5	1
1:A:108:PHE:O	1:A:112:ALA:HB3	0.43	2.13	7	1
1:A:108:PHE:O	1:A:108:PHE:CD2	0.43	2.72	12	2
1:A:92:PHE:HB3	1:A:97:LEU:HD23	0.43	1.90	17	1
1:A:101:LEU:HD13	1:A:106:ILE:HD13	0.43	1.87	18	1
1:A:93:THR:O	1:A:118:ILE:CG1	0.43	2.66	19	1
1:A:10:VAL:CG1	1:A:45:LEU:CD1	0.43	2.96	4	3
1:A:100:GLN:O	1:A:104:ARG:N	0.43	2.52	2	1
1:A:42:LEU:HD13	1:A:55:ILE:HG23	0.43	1.89	11	4
1:A:100:GLN:CB	1:A:121:PHE:CZ	0.43	3.02	2	4
1:A:97:LEU:HD23	1:A:118:ILE:CA	0.43	2.43	10	2
1:A:97:LEU:HD23	1:A:118:ILE:CD1	0.43	2.41	3	1
1:A:55:ILE:C	1:A:55:ILE:HD12	0.43	2.38	7	2
1:A:8:PHE:O	1:A:36:ALA:HA	0.42	2.14	9	3
1:A:94:VAL:O	1:A:98:LYS:HE3	0.42	2.14	12	1
1:A:120:LEU:HD13	1:A:121:PHE:N	0.42	2.29	17	1
1:A:41:GLN:NE2	1:A:42:LEU:N	0.42	2.67	13	1
1:A:92:PHE:CE1	1:A:100:GLN:OE1	0.42	2.72	17	1
1:A:10:VAL:N	1:A:41:GLN:OE1	0.42	2.52	2	1
1:A:9:CYS:HA	1:A:34:LEU:O	0.42	2.15	19	4
1:A:93:THR:OG1	1:A:94:VAL:HG22	0.42	2.15	5	1
1:A:34:LEU:HD11	1:A:37:VAL:CG2	0.42	2.43	16	1
1:A:34:LEU:HD11	1:A:41:GLN:CB	0.42	2.44	18	1
1:A:101:LEU:O	1:A:106:ILE:N	0.42	2.53	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:113:THR:OG1	1:A:114:LYS:N	0.42	2.52	4	2
1:A:117:LEU:C	1:A:117:LEU:CD2	0.42	2.91	13	1
1:A:93:THR:HG22	1:A:94:VAL:HG23	0.42	1.90	17	1
1:A:97:LEU:CD1	1:A:117:LEU:CD1	0.42	2.98	2	1
1:A:34:LEU:HD22	1:A:34:LEU:C	0.42	2.39	20	2
1:A:41:GLN:CG	1:A:42:LEU:N	0.42	2.82	1	1
1:A:8:PHE:O	1:A:8:PHE:HD1	0.42	1.98	20	2
1:A:108:PHE:CD1	1:A:108:PHE:O	0.42	2.73	18	1
1:A:31:ASP:OD1	1:A:31:ASP:N	0.41	2.52	1	1
1:A:12:VAL:HG11	1:A:45:LEU:HB3	0.41	1.92	10	1
1:A:10:VAL:HG12	1:A:34:LEU:HB2	0.41	1.91	16	1
1:A:108:PHE:C	1:A:108:PHE:CD1	0.41	2.98	20	1
1:A:97:LEU:O	1:A:121:PHE:CZ	0.41	2.73	3	1
1:A:96:GLN:O	1:A:100:GLN:CB	0.41	2.69	13	2
1:A:10:VAL:HB	1:A:41:GLN:NE2	0.41	2.30	16	1
1:A:101:LEU:HD23	1:A:121:PHE:CE1	0.41	2.50	3	1
1:A:94:VAL:C	1:A:97:LEU:HD22	0.41	2.40	16	1
1:A:101:LEU:CD1	1:A:120:LEU:HD11	0.41	2.43	9	1
1:A:96:GLN:O	1:A:100:GLN:CG	0.41	2.68	12	1
1:A:98:LYS:HG3	1:A:108:PHE:CE2	0.41	2.49	15	1
1:A:120:LEU:O	1:A:120:LEU:HD22	0.41	2.15	17	1
1:A:92:PHE:O	1:A:97:LEU:CD1	0.41	2.69	19	1
1:A:89:LEU:N	1:A:89:LEU:CD2	0.41	2.84	9	1
1:A:120:LEU:CD1	1:A:120:LEU:C	0.41	2.92	9	1
1:A:12:VAL:HG13	1:A:45:LEU:HG	0.41	1.91	15	1
1:A:106:ILE:HG12	1:A:108:PHE:CZ	0.41	2.50	18	1
1:A:41:GLN:HG2	1:A:42:LEU:N	0.41	2.30	6	1
1:A:37:VAL:HG11	1:A:40:SER:OG	0.41	2.16	7	1
1:A:101:LEU:HD11	1:A:120:LEU:HD23	0.41	1.93	15	1
1:A:101:LEU:CD2	1:A:106:ILE:HD12	0.41	2.45	9	1
1:A:12:VAL:O	1:A:12:VAL:HG23	0.41	2.16	12	1
1:A:8:PHE:CZ	1:A:38:SER:O	0.41	2.74	1	2
1:A:97:LEU:HB3	1:A:121:PHE:CE1	0.41	2.51	15	2
1:A:10:VAL:N	1:A:34:LEU:HB3	0.41	2.29	2	1
1:A:118:ILE:C	1:A:118:ILE:HD12	0.41	2.40	6	1
1:A:92:PHE:CD1	1:A:92:PHE:N	0.41	2.88	13	1
1:A:93:THR:OG1	1:A:94:VAL:N	0.41	2.54	15	1
1:A:8:PHE:CZ	1:A:41:GLN:OE1	0.41	2.74	20	1
1:A:97:LEU:HD22	1:A:118:ILE:HG12	0.40	1.93	7	1
1:A:100:GLN:CD	1:A:121:PHE:CE1	0.40	2.99	13	1
1:A:8:PHE:O	1:A:35:ALA:O	0.40	2.39	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:100:GLN:HG2	1:A:121:PHE:CE1	0.40	2.52	19	1
1:A:113:THR:O	1:A:117:LEU:HD22	0.40	2.16	19	1
1:A:92:PHE:HB3	1:A:118:ILE:CD1	0.40	2.47	3	1
1:A:108:PHE:O	1:A:108:PHE:CG	0.40	2.73	8	1
1:A:42:LEU:O	1:A:46:LYS:CB	0.40	2.69	17	1
1:A:101:LEU:HD12	1:A:117:LEU:HD11	0.40	1.90	19	1
1:A:118:ILE:O	1:A:118:ILE:CD1	0.40	2.69	19	1
1:A:97:LEU:CD2	1:A:118:ILE:CB	0.40	3.00	9	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	67/131 (51%)	54±2 (80±4%)	10±2 (15±3%)	3±2 (5±2%)	3	25
All	All	1340/2620 (51%)	1071 (80%)	206 (15%)	63 (5%)	3	25

All 15 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	121	PHE	13
1	A	39	GLU	10
1	A	94	VAL	6
1	A	111	SER	6
1	A	109	LYS	5
1	A	110	GLN	4
1	A	93	THR	3
1	A	112	ALA	3
1	A	106	ILE	3
1	A	113	THR	3
1	A	38	SER	2
1	A	50	ARG	2
1	A	114	LYS	1
1	A	108	PHE	1

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Mol	Chain	Res	Type	Models (Total)
1	A	107	THR	1

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	58/106 (55%)	33±3 (57±5%)	25±3 (43±5%)	0 4
All	All	1160/2120 (55%)	666 (57%)	494 (43%)	0 4

All 55 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	8	PHE	20
1	A	10	VAL	20
1	A	97	LEU	20
1	A	34	LEU	19
1	A	102	THR	19
1	A	117	LEU	18
1	A	41	GLN	17
1	A	118	ILE	17
1	A	96	GLN	15
1	A	51	LEU	14
1	A	103	GLU	13
1	A	109	LYS	13
1	A	114	LYS	13
1	A	55	ILE	13
1	A	13	GLN	13
1	A	120	LEU	12
1	A	39	GLU	12
1	A	7	THR	12
1	A	46	LYS	11
1	A	113	THR	11
1	A	37	VAL	11
1	A	53	VAL	11
1	A	91	THR	10
1	A	14	ASN	10

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Mol	Chain	Res	Type	Models (Total)
1	A	33	SER	10
1	A	111	SER	10
1	A	93	THR	10
1	A	98	LYS	9
1	A	54	GLN	9
1	A	110	GLN	8
1	A	38	SER	8
1	A	95	GLU	8
1	A	107	THR	7
1	A	100	GLN	6
1	A	44	GLN	6
1	A	48	ASP	6
1	A	40	SER	5
1	A	108	PHE	5
1	A	11	VAL	5
1	A	50	ARG	4
1	A	106	ILE	4
1	A	90	ASN	3
1	A	101	LEU	3
1	A	45	LEU	3
1	A	31	ASP	3
1	A	89	LEU	3
1	A	9	CYS	3
1	A	56	THR	2
1	A	52	VAL	2
1	A	94	VAL	2
1	A	116	GLU	2
1	A	104	ARG	1
1	A	121	PHE	1
1	A	32	ASN	1
1	A	42	LEU	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 [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