



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 02:30 PM UTC

PDB ID : 4UEI / pdb_00004uei
Title : Solution structure of the sterol carrier protein domain 2 of Helicoverpa armigera
Authors : Liu, X.; Ma, H.; Yan, X.; Hong, H.; Peng, J.; Peng, R.
Deposited on : 2014-12-18

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

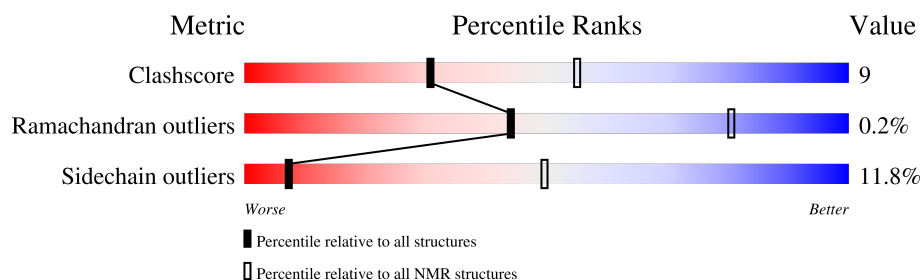
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 93%.

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	127	 65% 9% • 22%

2 Ensemble composition and analysis

This entry contains 20 models. Model 10 is the overall representative, medoid model (most similar to other models).

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:19-A:117 (99)	0.50	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 3 clusters. No single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1977 atoms, of which 990 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called STEROL CARRIER PROTEIN 2/3-OXOACYL-COA THIO-LASE.

Mol	Chain	Residues	Atoms						Trace
1	A	127	Total	C	H	N	O	S	0
			1977	623	990	168	192	4	

There are 3 discrepancies between the modelled and reference sequences:

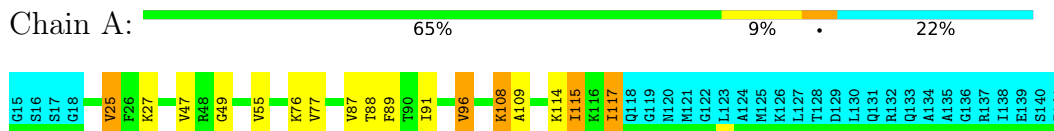
Chain	Residue	Modelled	Actual	Comment	Reference
A	15	GLY	-	expression tag	UNP K7NSY9
A	16	SER	-	expression tag	UNP K7NSY9
A	130	LEU	PRO	conflict	UNP K7NSY9

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: STEROL CARRIER PROTEIN 2/3-OXOACYL-COA THIOLASE

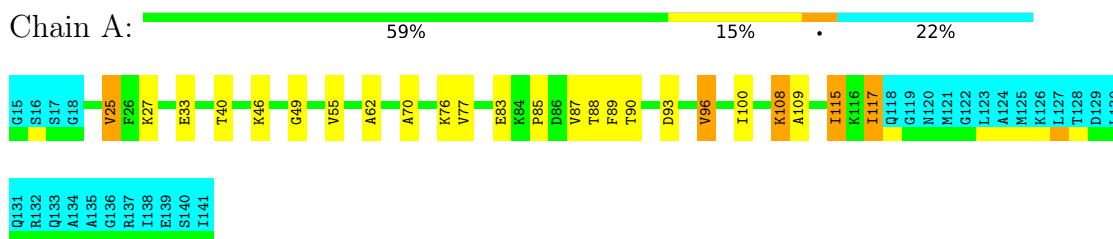


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

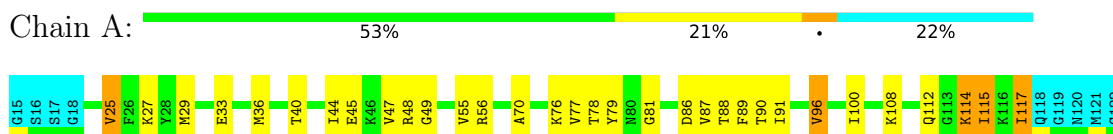
4.2.1 Score per residue for model 1

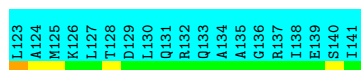
- Molecule 1: STEROL CARRIER PROTEIN 2/3-OXOACYL-COA THIOLASE



4.2.2 Score per residue for model 2

- Molecule 1: STEROL CARRIER PROTEIN 2/3-OXOACYL-COA THIOLASE

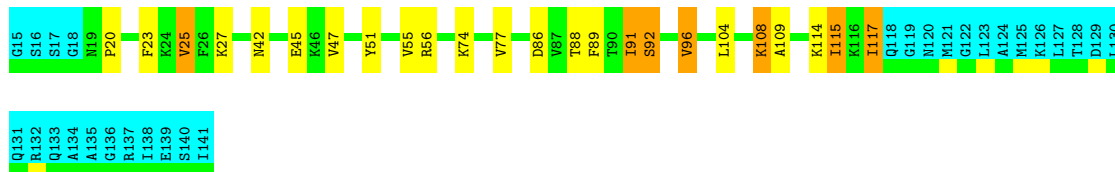




4.2.3 Score per residue for model 3

- Molecule 1: STEROL CARRIER PROTEIN 2/3-OXOACYL-COA THIOLASE

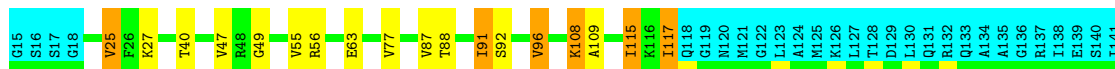
Chain A: 59% 13% 6% 22%



4.2.4 Score per residue for model 4

- Molecule 1: STEROL CARRIER PROTEIN 2/3-OXOACYL-COA THIOLASE

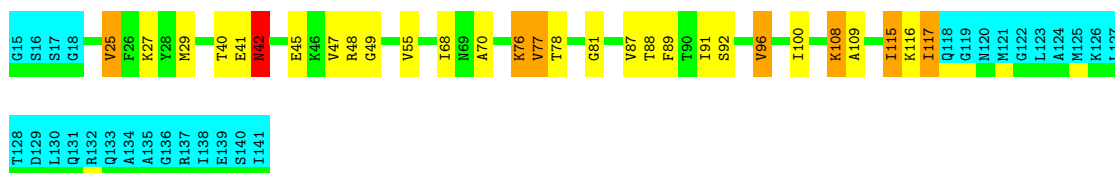
Chain A: 64% 9% 5% 22%



4.2.5 Score per residue for model 5

- Molecule 1: STEROL CARRIER PROTEIN 2/3-OXOACYL-COA THIOLASE

Chain A: 55% 17% 6% 22%



4.2.6 Score per residue for model 6

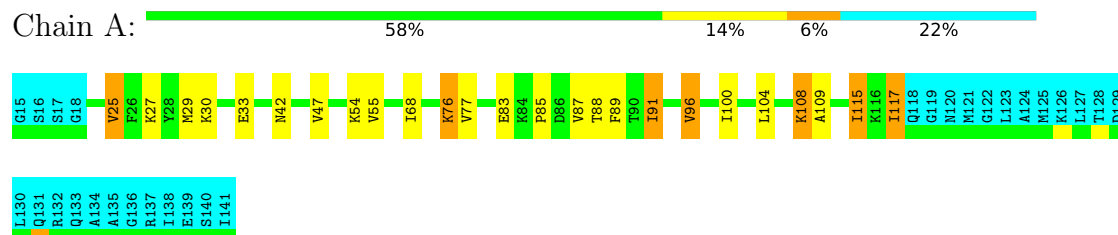
- Molecule 1: STEROL CARRIER PROTEIN 2/3-OXOACYL-COA THIOLASE

Chain A: 58% 14% 6% 22%



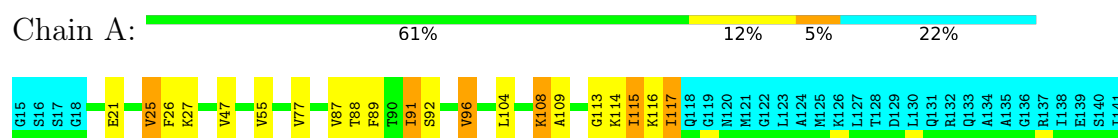
4.2.7 Score per residue for model 7

- Molecule 1: STEROL CARRIER PROTEIN 2/3-OXOACYL-COA THIOLASE



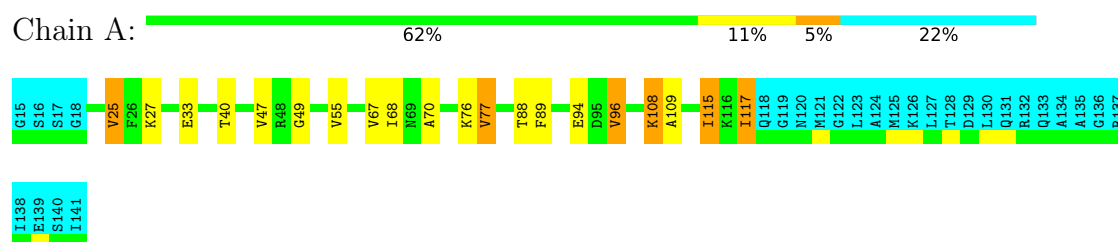
4.2.8 Score per residue for model 8

- Molecule 1: STEROL CARRIER PROTEIN 2/3-OXOACYL-COA THIOLASE



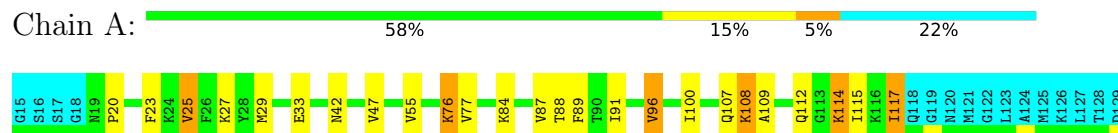
4.2.9 Score per residue for model 9

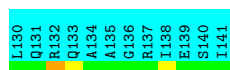
- Molecule 1: STEROL CARRIER PROTEIN 2/3-OXOACYL-COA THIOLASE



4.2.10 Score per residue for model 10 (medoid)

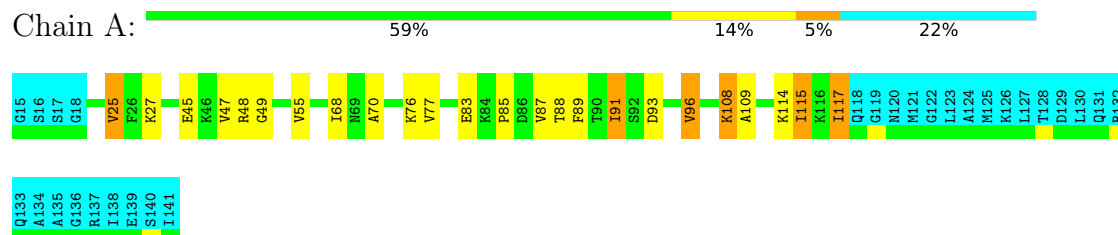
- Molecule 1: STEROL CARRIER PROTEIN 2/3-OXOACYL-COA THIOLASE





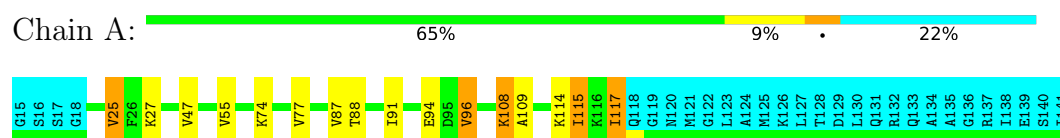
4.2.11 Score per residue for model 11

- Molecule 1: STEROL CARRIER PROTEIN 2/3-OXOACYL-COA THIOLASE



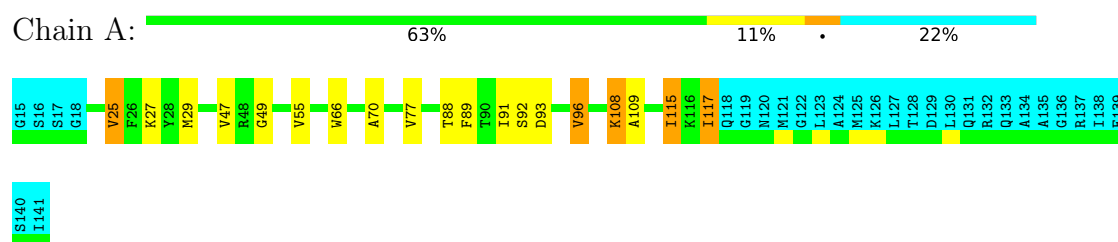
4.2.12 Score per residue for model 12

- Molecule 1: STEROL CARRIER PROTEIN 2/3-OXOACYL-COA THIOLASE



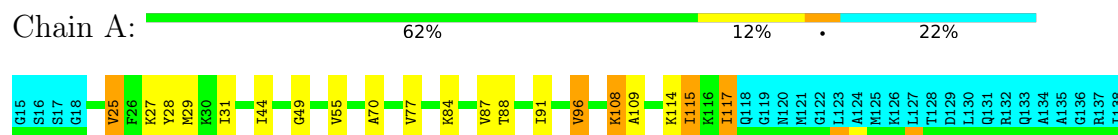
4.2.13 Score per residue for model 13

- Molecule 1: STEROL CARRIER PROTEIN 2/3-OXOACYL-COA THIOLASE



4.2.14 Score per residue for model 14

- Molecule 1: STEROL CARRIER PROTEIN 2/3-OXOACYL-COA THIOLASE



E139
S140
I141

4.2.15 Score per residue for model 15

- Molecule 1: STEROL CARRIER PROTEIN 2/3-OXOACYL-COA THIOLASE

Chain A: 65% 9% 5% 22%

G15 S16 S17 G18 V25 F26 K27 V47 V55 V77 K84 V87 T88 F89 T90 I91 S92 D93 V96 Q107 K108 A109 I115 K116 I117 Q118 G119 M120 M121 G122 L123 M124 M125 K126 L127 T128 D129 Q131 R132 Q133 A134 A135 G136 R137 I138 E139 S140 I141

4.2.16 Score per residue for model 16

- Molecule 1: STEROL CARRIER PROTEIN 2/3-OXOACYL-COA THIOLASE

Chain A: 64% 10% 22%

G15 S16 S17 G18 V25 F26 K27 E33 V47 V55 V77 E83 K84 P85 D86 T88 F89 T90 I91 V96 I100 K108 A109 I115 K116 I117 Q118 G119 M120 M121 G122 L123 M124 M125 K126 L127 T128 D129 Q131 R132 Q133 A134 A135 G136 R137 I138 S140

I141

4.2.17 Score per residue for model 17

- Molecule 1: STEROL CARRIER PROTEIN 2/3-OXOACYL-COA THIOLASE

Chain A: 62% 11% 5% 22%

G15 S16 S17 G18 V25 F26 K27 E33 G49 V55 I68 K76 V77 V87 T88 F89 T90 I91 S92 D93 V96 L104 K108 A109 I115 K114 I116 K117 Q118 G119 M120 M121 G122 L123 M124 M125 K126 L127 T128 D129 Q131 R132 Q133 A134 A135 G136 I138

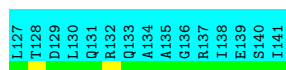
E139
S140
I141

4.2.18 Score per residue for model 18

- Molecule 1: STEROL CARRIER PROTEIN 2/3-OXOACYL-COA THIOLASE

Chain A: 57% 16% 5% 22%

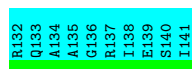
G15 S16 S17 G18 M19 P20 F23 K24 V25 F26 K27 V28 H29 E41 R42 E45 K46 V47 R48 C49 V55 T68 M69 A70 K76 V77 E83 K84 P85 D86 V87 T88 I91 V96 K108 A109 F110 I115 K116 I117 Q118 G119 M120 M121 G122 L123 M124 M125 K126



4.2.19 Score per residue for model 19

- Molecule 1: STEROL CARRIER PROTEIN 2/3-OXOACYL-COA THIOLASE

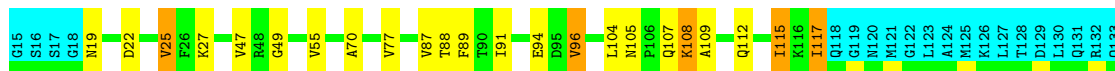
Chain A: 60% 14% 22%



4.2.20 Score per residue for model 20

- Molecule 1: STEROL CARRIER PROTEIN 2/3-OXOACYL-COA THIOLASE

Chain A: 60% 14% 22%



5 Refinement protocol and experimental data overview

The models were refined using the following method: *ARIA*.

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *LOWEST ENERGY*.

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

Software name	Classification	Version
CNS/ARIA	refinement	
CcpNmr Analysis	structure solution	2.3
PyRPF	structure solution	0.4
CcpNmr Analysis	structure solution	2.4
DANGLE	structure solution	1.1

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)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1557
Number of shifts mapped to atoms	1557
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	93%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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 [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	787	784	784	14±3
All	All	15740	15680	15680	279

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 9.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:VAL:HG12	1:A:96:VAL:HG11	0.89	1.45	3	20
1:A:88:THR:O	1:A:117:ILE:HA	0.64	1.92	18	20
1:A:25:VAL:HG11	1:A:55:VAL:HG11	0.64	1.69	19	19
1:A:104:LEU:HD11	1:A:108:LYS:NZ	0.62	2.09	6	6
1:A:47:VAL:HG22	1:A:51:TYR:OH	0.61	1.96	3	1
1:A:29:MET:HE1	1:A:66:TRP:CE2	0.59	2.32	13	1
1:A:110:PHE:HA	1:A:115:ILE:HG22	0.59	1.74	18	1
1:A:25:VAL:HG12	1:A:96:VAL:CG1	0.57	2.30	13	9
1:A:36:MET:HE2	1:A:36:MET:HA	0.56	1.76	2	1
1:A:29:MET:HB3	1:A:77:VAL:HG21	0.56	1.76	6	2
1:A:68:ILE:HA	1:A:76:LYS:O	0.55	2.02	19	8
1:A:49:GLY:O	1:A:70:ALA:HB3	0.55	2.01	20	10
1:A:89:PHE:CD2	1:A:117:ILE:HB	0.55	2.37	8	12
1:A:115:ILE:HG23	1:A:117:ILE:HG22	0.55	1.79	14	17

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:33:GLU:HG3	1:A:76:LYS:HA	0.54	1.80	7	5
1:A:114:LYS:CE	1:A:114:LYS:HA	0.54	2.32	6	1
1:A:105:ASN:OD1	1:A:107:GLN:HB2	0.53	2.04	20	1
1:A:25:VAL:HB	1:A:29:MET:SD	0.53	2.43	14	7
1:A:55:VAL:HA	1:A:91:ILE:O	0.52	2.04	16	18
1:A:21:GLU:HA	1:A:26:PHE:CG	0.52	2.40	8	1
1:A:104:LEU:HD11	1:A:108:LYS:HZ3	0.52	1.64	7	5
1:A:115:ILE:HG23	1:A:117:ILE:CG2	0.52	2.35	18	1
1:A:54:LYS:NZ	1:A:88:THR:HG21	0.51	2.21	7	1
1:A:91:ILE:CG1	1:A:115:ILE:HG13	0.50	2.36	3	7
1:A:56:ARG:NE	1:A:90:THR:HG22	0.50	2.21	2	1
1:A:87:VAL:HB	1:A:117:ILE:CD1	0.50	2.36	1	4
1:A:21:GLU:HA	1:A:26:PHE:CD1	0.49	2.42	8	1
1:A:41:GLU:C	1:A:42:ASN:HD22	0.49	2.15	5	2
1:A:89:PHE:CD1	1:A:117:ILE:HB	0.49	2.43	6	4
1:A:20:PRO:HA	1:A:23:PHE:CD1	0.49	2.42	10	3
1:A:68:ILE:HG13	1:A:77:VAL:HG12	0.48	1.84	17	1
1:A:114:LYS:NZ	1:A:114:LYS:HB3	0.48	2.23	10	1
1:A:114:LYS:HB3	1:A:114:LYS:HZ3	0.48	1.68	10	1
1:A:96:VAL:O	1:A:100:ILE:HG13	0.48	2.09	5	6
1:A:89:PHE:CE2	1:A:117:ILE:HD13	0.48	2.44	7	1
1:A:108:LYS:HE3	1:A:112:GLN:HG3	0.48	1.86	2	1
1:A:83:GLU:O	1:A:85:PRO:HD3	0.48	2.09	16	6
1:A:25:VAL:HG13	1:A:93:ASP:OD1	0.47	2.09	1	5
1:A:25:VAL:CG1	1:A:96:VAL:HG11	0.47	2.38	13	6
1:A:108:LYS:HG3	1:A:109:ALA:N	0.47	2.25	15	17
1:A:101:SER:OG	1:A:103:LYS:HD3	0.47	2.08	6	1
1:A:115:ILE:CG2	1:A:117:ILE:HG22	0.46	2.41	14	1
1:A:78:THR:HG23	1:A:81:GLY:HA2	0.46	1.88	2	2
1:A:54:LYS:HZ2	1:A:88:THR:HG21	0.46	1.71	7	1
1:A:114:LYS:HE3	1:A:114:LYS:HA	0.45	1.88	2	1
1:A:74:LYS:HE2	1:A:74:LYS:HA	0.45	1.87	3	1
1:A:108:LYS:O	1:A:112:GLN:HG2	0.45	2.12	2	1
1:A:56:ARG:CB	1:A:63:GLU:HG2	0.45	2.41	4	1
1:A:47:VAL:HG22	1:A:47:VAL:O	0.45	2.12	8	13
1:A:109:ALA:HB3	1:A:115:ILE:HD12	0.44	1.88	16	2
1:A:45:GLU:HA	1:A:48:ARG:HG3	0.44	1.88	2	3
1:A:108:LYS:HE2	1:A:108:LYS:C	0.43	2.37	20	2
1:A:42:ASN:O	1:A:45:GLU:HG2	0.43	2.14	18	2
1:A:113:GLY:O	1:A:116:LYS:HE3	0.43	2.13	8	1
1:A:91:ILE:HG22	1:A:92:SER:N	0.43	2.28	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:67:VAL:O	1:A:77:VAL:HA	0.42	2.14	9	1
1:A:96:VAL:O	1:A:100:ILE:HG12	0.42	2.14	6	1
1:A:33:GLU:CG	1:A:76:LYS:HA	0.42	2.43	7	2
1:A:47:VAL:O	1:A:47:VAL:HG22	0.42	2.15	7	1
1:A:76:LYS:HB2	1:A:76:LYS:NZ	0.42	2.29	7	1
1:A:84:LYS:HD2	1:A:84:LYS:N	0.42	2.29	15	1
1:A:28:TYR:O	1:A:31:ILE:HG12	0.42	2.15	14	1
1:A:25:VAL:HG23	1:A:29:MET:HE2	0.41	1.93	13	1
1:A:105:ASN:HB3	1:A:108:LYS:HG2	0.41	1.93	20	1
1:A:19:ASN:HB2	1:A:22:ASP:OD2	0.41	2.16	20	1
1:A:56:ARG:O	1:A:92:SER:HA	0.40	2.16	3	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	99/127 (78%)	92±1 (93±1%)	7±1 (7±1%)	0±0 (0±0%)	44	80
All	All	1980/2540 (78%)	1844 (93%)	133 (7%)	3 (0%)	44	80

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	42	ASN	3

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	84/104 (81%)	74±1 (88±2%)	10±1 (12±2%)	7	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1680/2080 (81%)	1482 (88%)	198 (12%)	7 49

All 26 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	25	VAL	20
1	A	27	LYS	20
1	A	77	VAL	20
1	A	96	VAL	20
1	A	115	ILE	20
1	A	117	ILE	20
1	A	108	LYS	19
1	A	114	LYS	9
1	A	91	ILE	9
1	A	40	THR	6
1	A	92	SER	6
1	A	42	ASN	3
1	A	76	LYS	3
1	A	74	LYS	3
1	A	94	GLU	3
1	A	33	GLU	3
1	A	44	ILE	2
1	A	84	LYS	2
1	A	107	GLN	2
1	A	112	GLN	2
1	A	90	THR	1
1	A	47	VAL	1
1	A	116	LYS	1
1	A	30	LYS	1
1	A	24	LYS	1
1	A	100	ILE	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

The completeness of assignment taking into account all chemical shift lists is 93% for the well-defined parts and 91% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list*

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	1557
Number of shifts mapped to atoms	1557
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	126	-0.24 ± 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	111	0.17 ± 0.15	None needed (< 0.5 ppm)
$^{13}\text{C}'$	120	-0.24 ± 0.15	None needed (< 0.5 ppm)
^{15}N	121	-0.16 ± 0.34	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 93%, i.e. 1255 atoms were assigned a chemical shift out of a possible 1352. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	494/498 (99%)	205/205 (100%)	194/198 (98%)	95/95 (100%)
Sidechain	667/746 (89%)	455/478 (95%)	202/239 (85%)	10/29 (34%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	94/108 (87%)	47/52 (90%)	46/55 (84%)	1/1 (100%)
Overall	1255/1352 (93%)	707/735 (96%)	442/492 (90%)	106/125 (85%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 91%, i.e. 1552 atoms were assigned a chemical shift out of a possible 1706. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	628/643 (98%)	261/266 (98%)	246/254 (97%)	121/123 (98%)
Sidechain	830/955 (87%)	569/614 (93%)	248/301 (82%)	13/40 (32%)
Aromatic	94/108 (87%)	47/52 (90%)	46/55 (84%)	1/1 (100%)
Overall	1552/1706 (91%)	877/932 (94%)	540/610 (89%)	135/164 (82%)

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.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	24	LYS	H	12.69	5.24 – 11.12	7.7

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. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:

