



Full wwPDB NMR Structure Validation Report ⓘ

Jul 26, 2021 – 06:08 pm BST

PDB ID : 7OVC
Title : Structure of the human UFC1 protein in complex with the UBA5 C-terminal UFC1-binding motif.
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Deposited on : 2021-06-14

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:

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	:	2.22
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.22

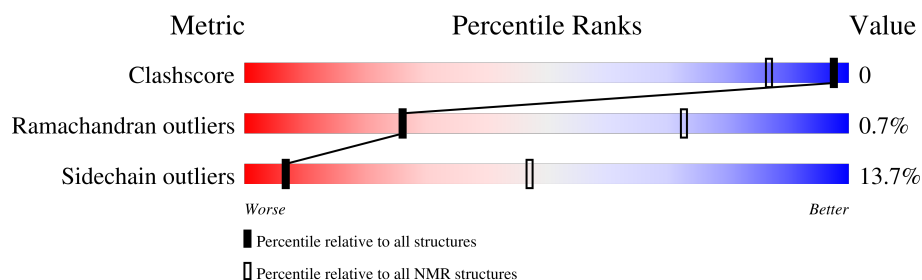
1 Overall quality at a glance

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	167	
2	B	27	

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 1 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:2-A:103, A:114-A:161, B:384-B:405 (172)	0.23	1

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 4 clusters and 2 single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3147 atoms, of which 1567 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Ubiquitin-fold modifier-conjugating enzyme 1.

Mol	Chain	Residues	Atoms						Trace
1	A	167	Total	C	H	N	O	S	0
			2739	884	1366	238	245	6	

- Molecule 2 is a protein called Ubiquitin-like modifier-activating enzyme 5.

Mol	Chain	Residues	Atoms						Trace
2	B	27	Total	C	H	N	O	S	0
			408	127	201	31	45	4	

There are 3 discrepancies between the modelled and reference sequences:

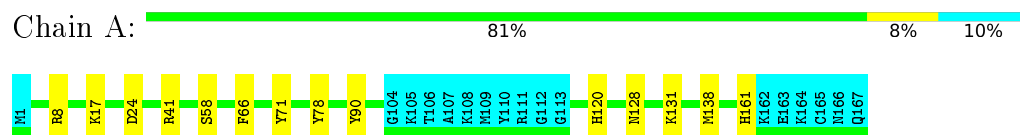
Chain	Residue	Modelled	Actual	Comment	Reference
B	379	GLY	-	expression tag	UNP Q9GZZ9
B	380	MET	-	expression tag	UNP Q9GZZ9
B	405	TRP	-	expression tag	UNP Q9GZZ9

4 Residue-property plots [i](#)

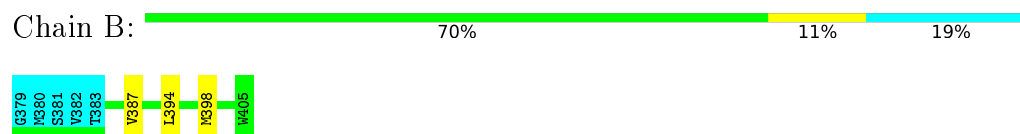
4.1 Average score per residue in the NMR ensemble

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: Ubiquitin-fold modifier-conjugating enzyme 1



- Molecule 2: Ubiquitin-like modifier-activating enzyme 5

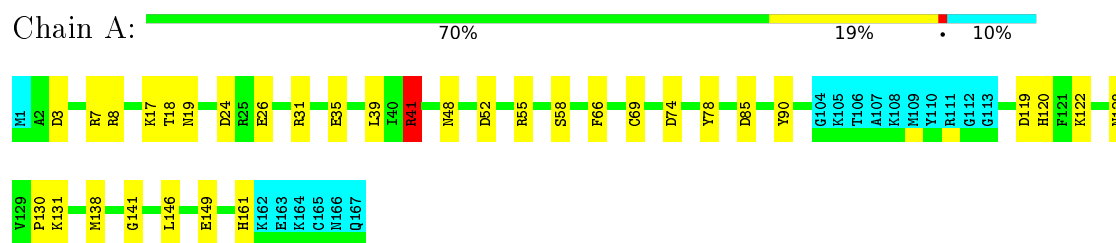


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Ubiquitin-fold modifier-conjugating enzyme 1



- Molecule 2: Ubiquitin-like modifier-activating enzyme 5





4.2.2 Score per residue for model 2

- Molecule 1: Ubiquitin-fold modifier-conjugating enzyme 1

Chain A: 78% 11% 10%



- Molecule 2: Ubiquitin-like modifier-activating enzyme 5

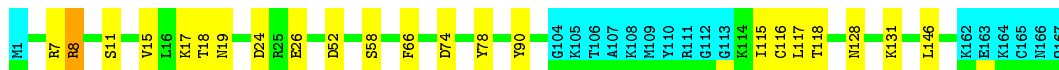
Chain B: 67% 15% 19%



4.2.3 Score per residue for model 3

- Molecule 1: Ubiquitin-fold modifier-conjugating enzyme 1

Chain A: 77% 13% 10%



- Molecule 2: Ubiquitin-like modifier-activating enzyme 5

Chain B: 52% 30% 19%



4.2.4 Score per residue for model 4

- Molecule 1: Ubiquitin-fold modifier-conjugating enzyme 1

Chain A: 77% 13% 10%

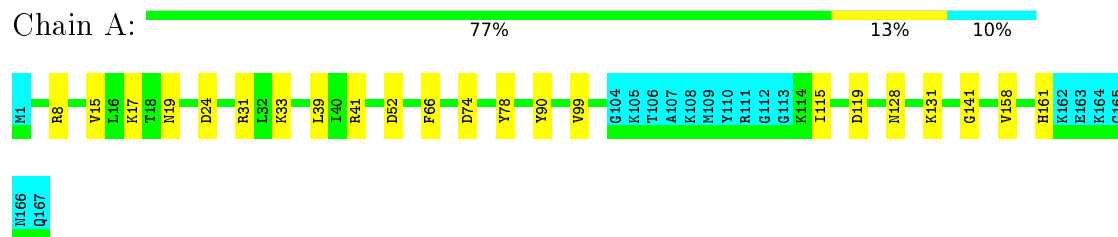


- Molecule 2: Ubiquitin-like modifier-activating enzyme 5

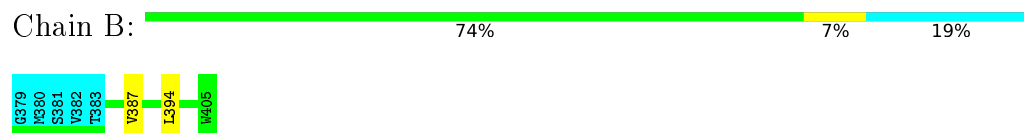


4.2.5 Score per residue for model 5

- Molecule 1: Ubiquitin-fold modifier-conjugating enzyme 1

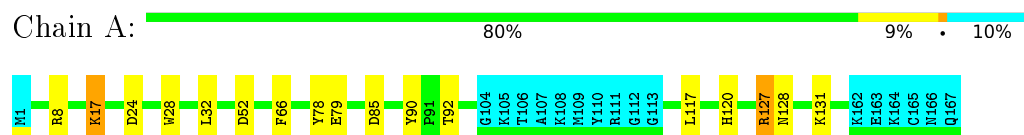


- Molecule 2: Ubiquitin-like modifier-activating enzyme 5

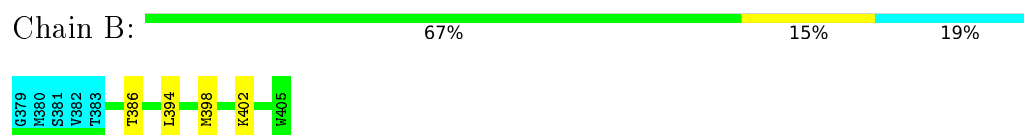


4.2.6 Score per residue for model 6

- Molecule 1: Ubiquitin-fold modifier-conjugating enzyme 1

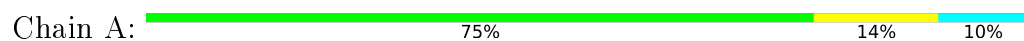


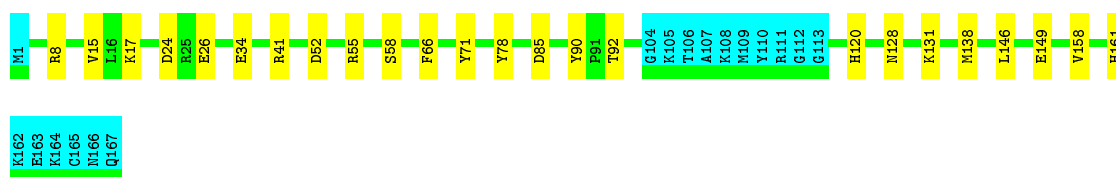
- Molecule 2: Ubiquitin-like modifier-activating enzyme 5



4.2.7 Score per residue for model 7

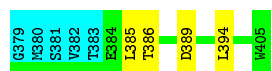
- Molecule 1: Ubiquitin-fold modifier-conjugating enzyme 1





- Molecule 2: Ubiquitin-like modifier-activating enzyme 5

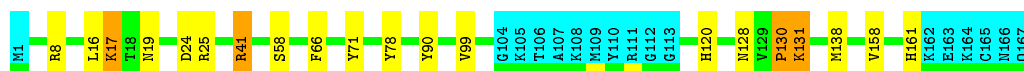
Chain B: 67% 15% 19%



4.2.8 Score per residue for model 8

- Molecule 1: Ubiquitin-fold modifier-conjugating enzyme 1

Chain A: 78% 10% 10%



- Molecule 2: Ubiquitin-like modifier-activating enzyme 5

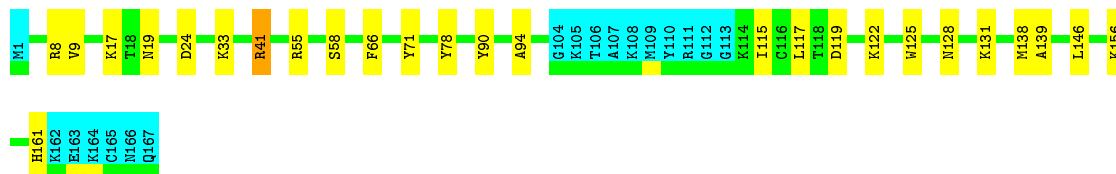
Chain B: 67% 15% 19%



4.2.9 Score per residue for model 9

- Molecule 1: Ubiquitin-fold modifier-conjugating enzyme 1

Chain A: 74% 15% 10%



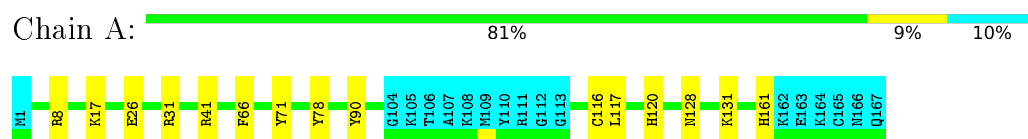
- Molecule 2: Ubiquitin-like modifier-activating enzyme 5

Chain B: 67% 15% 19%

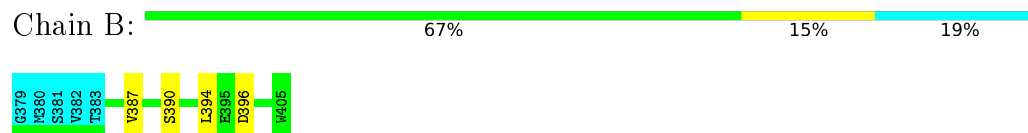


4.2.10 Score per residue for model 10

- Molecule 1: Ubiquitin-fold modifier-conjugating enzyme 1

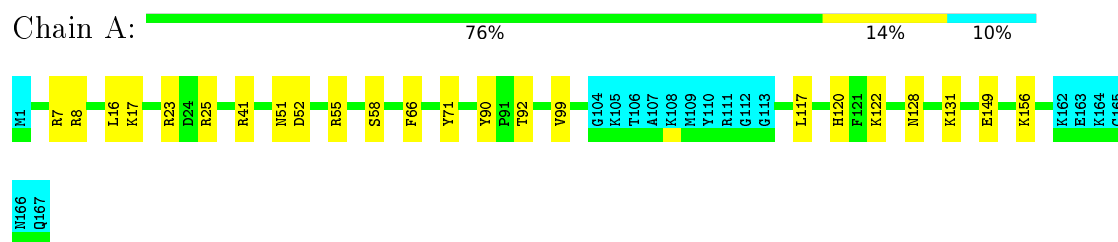


- Molecule 2: Ubiquitin-like modifier-activating enzyme 5

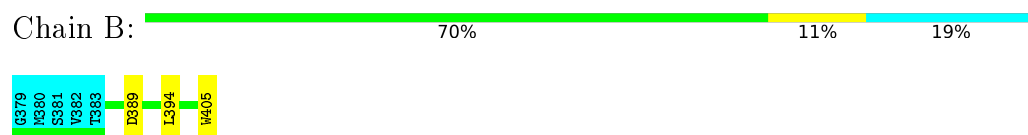


4.2.11 Score per residue for model 11

- Molecule 1: Ubiquitin-fold modifier-conjugating enzyme 1

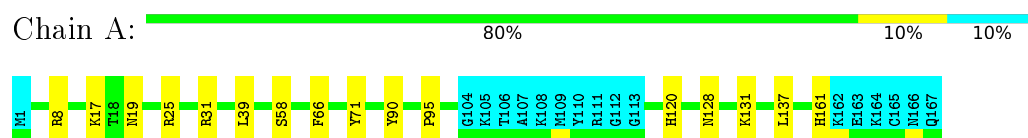


- Molecule 2: Ubiquitin-like modifier-activating enzyme 5



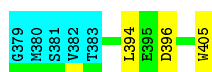
4.2.12 Score per residue for model 12

- Molecule 1: Ubiquitin-fold modifier-conjugating enzyme 1



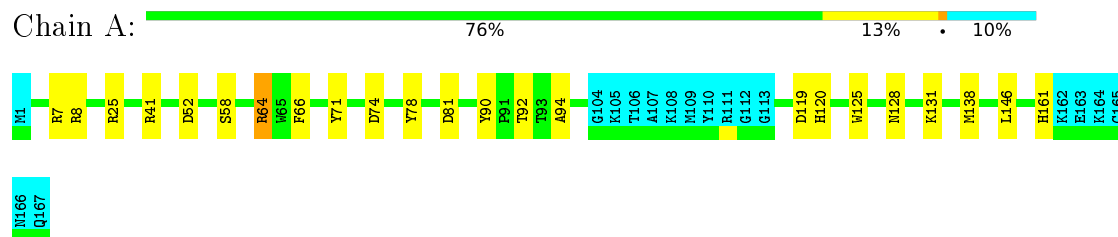
- Molecule 2: Ubiquitin-like modifier-activating enzyme 5





4.2.13 Score per residue for model 13

- Molecule 1: Ubiquitin-fold modifier-conjugating enzyme 1

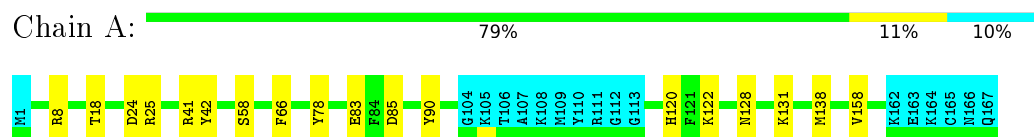


- Molecule 2: Ubiquitin-like modifier-activating enzyme 5

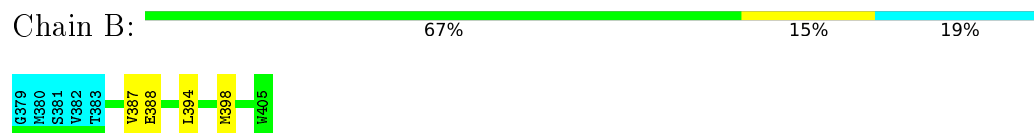


4.2.14 Score per residue for model 14

- Molecule 1: Ubiquitin-fold modifier-conjugating enzyme 1

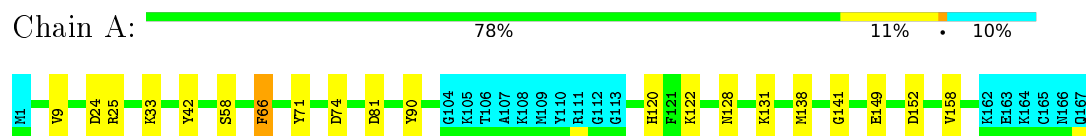


- Molecule 2: Ubiquitin-like modifier-activating enzyme 5

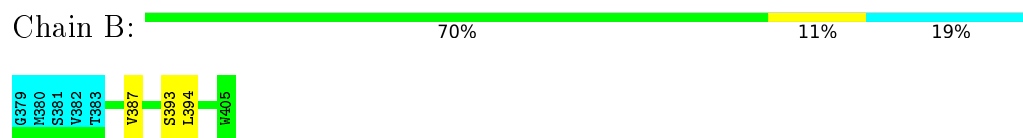


4.2.15 Score per residue for model 15

- Molecule 1: Ubiquitin-fold modifier-conjugating enzyme 1

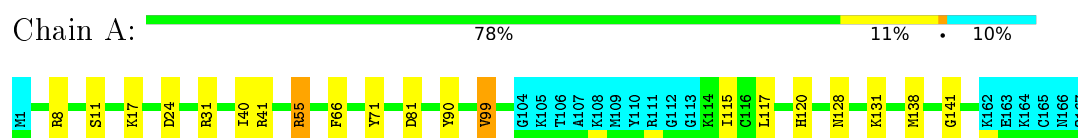


- Molecule 2: Ubiquitin-like modifier-activating enzyme 5



4.2.16 Score per residue for model 16

- Molecule 1: Ubiquitin-fold modifier-conjugating enzyme 1

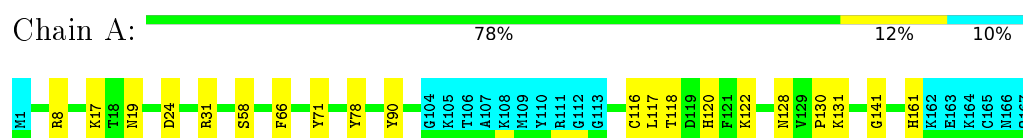


- Molecule 2: Ubiquitin-like modifier-activating enzyme 5



4.2.17 Score per residue for model 17

- Molecule 1: Ubiquitin-fold modifier-conjugating enzyme 1

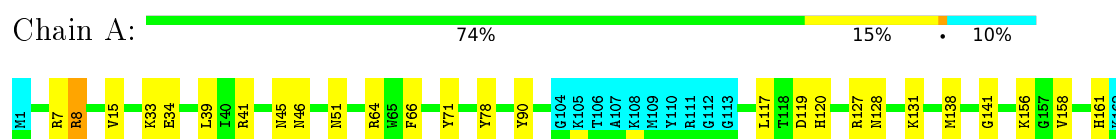


- Molecule 2: Ubiquitin-like modifier-activating enzyme 5



4.2.18 Score per residue for model 18

- Molecule 1: Ubiquitin-fold modifier-conjugating enzyme 1



E163
K164
C165
M166
Q167


- Molecule 2: Ubiquitin-like modifier-activating enzyme 5

Chain B:  67% 15% 19%

G379
K380
S381
V382
T383
E384
L385
T386
V387
L394
K398
W405

4.2.19 Score per residue for model 19

- Molecule 1: Ubiquitin-fold modifier-conjugating enzyme 1

Chain A:  80% 10% 10%

H1
T18
D24
R31
R41
F54
R55
S58
F66
Y71
Y78
Y90
G104
K105
T106
A107
K108
M109
Y110
R111
G112
G113
H120
M128
K131
M138
G141
V158
K162
E163
C164
M166
Q167

- Molecule 2: Ubiquitin-like modifier-activating enzyme 5

Chain B:  67% 15% 19%

G379
K380
S381
V382
T383
L394
E395
D396
L397
K398
W405

4.2.20 Score per residue for model 20

- Molecule 1: Ubiquitin-fold modifier-conjugating enzyme 1

Chain A:  75% 14% 10%

H1
R7
R8
K17
R23
D24
R25
R31
E34
R55
F66
Y71
D74
Y78
E79
D85
Y90
Y99
G104
K105
T106
A107
K108
M109
Y110
R111
G112
G113
K114
L115
C116
L117
H120
M128
K131
M138
H161
K162
E163
K164
C165

M166
Q167

- Molecule 2: Ubiquitin-like modifier-activating enzyme 5

Chain B:  67% 11% 19%

G379
K380
S381
V382
T383
V387
E388
D389
L394
M404
W405

5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 20 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 calculation	3.98
OPALp	refinement	1.4

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	2268
Number of shifts mapped to atoms	2268
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%

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	0.62±0.01	0±0/1279 (0.0± 0.0%)	1.06±0.02	1±1/1743 (0.1± 0.1%)
2	B	0.51±0.01	0±0/176 (0.0± 0.0%)	1.06±0.04	0±0/234 (0.0± 0.1%)
All	All	0.60	0/29100 (0.0%)	1.06	30/39540 (0.1%)

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	1.1±1.1
All	All	0	21

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(°)	Ideal(°)	Models	
								Worst	Total
1	A	64	ARG	NE-CZ-NH1	8.98	124.79	120.30	13	1
1	A	64	ARG	NE-CZ-NH2	-7.80	116.40	120.30	13	1
1	A	64	ARG	CD-NE-CZ	6.46	132.64	123.60	13	1
1	A	31	ARG	CD-NE-CZ	6.39	132.55	123.60	5	7
1	A	31	ARG	NE-CZ-NH1	6.08	123.34	120.30	16	4
1	A	31	ARG	NE-CZ-NH2	-5.83	117.38	120.30	5	4
1	A	25	ARG	NE-CZ-NH2	-5.64	117.48	120.30	20	1
1	A	41	ARG	NE-CZ-NH2	-5.55	117.53	120.30	1	2
1	A	55	ARG	NE-CZ-NH2	-5.42	117.59	120.30	9	2
2	B	389	ASP	CB-CG-OD2	5.36	123.12	118.30	8	1
1	A	85	ASP	CB-CG-OD1	5.36	123.12	118.30	7	1
1	A	55	ARG	NE-CZ-NH1	5.35	122.98	120.30	19	2
1	A	127	ARG	NE-CZ-NH2	-5.30	117.65	120.30	18	2
1	A	23	ARG	NE-CZ-NH2	-5.03	117.78	120.30	11	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	7	ARG	Sidechain	6
1	A	41	ARG	Sidechain	3
1	A	55	ARG	Sidechain	3
1	A	8	ARG	Sidechain	2
1	A	42	TYR	Sidechain	2
1	A	31	ARG	Sidechain	1
1	A	127	ARG	Sidechain	1
1	A	66	PHE	Sidechain	1
1	A	64	ARG	Sidechain	1
1	A	23	ARG	Sidechain	1

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	1242	1228	1228	1±1
2	B	175	168	168	1±1
All	All	28340	27920	27920	27

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 0.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:17:LYS:HE2	2:B:386:THR:HG23	0.55	1.77	7	6
1:A:28:TRP:CZ2	1:A:32:LEU:HD13	0.51	2.39	6	1
1:A:94:ALA:HB2	1:A:125:TRP:CD2	0.50	2.41	13	2
1:A:99:VAL:CG1	1:A:115:ILE:HG21	0.48	2.39	16	1
1:A:94:ALA:HB2	1:A:125:TRP:CE2	0.47	2.45	13	2
1:A:95:PRO:HG2	1:A:137:LEU:HD22	0.46	1.88	12	3
1:A:15:VAL:HG22	2:B:385:LEU:O	0.46	2.10	3	3
1:A:16:LEU:N	1:A:16:LEU:HD12	0.44	2.26	11	3
1:A:40:ILE:HD13	2:B:400:LYS:HE3	0.43	1.88	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:SER:O	2:B:385:LEU:HD11	0.43	2.14	16	2
1:A:130:PRO:CG	1:A:131:LYS:HE3	0.42	2.45	8	1
1:A:17:LYS:HE3	2:B:386:THR:HG23	0.41	1.93	6	1
1:A:9:VAL:CG1	1:A:139:ALA:HB1	0.40	2.47	9	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	150/167 (90%)	140±2 (93±1%)	10±2 (6±1%)	1±1 (1±1%)	29	74
2	B	21/27 (78%)	17±1 (82±6%)	3±1 (16±6%)	0±0 (1±2%)	15	61
All	All	3420/3880 (88%)	3138 (92%)	259 (8%)	23 (1%)	26	73

All 8 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	141	GLY	7
2	B	389	ASP	5
1	A	119	ASP	4
1	A	130	PRO	3
1	A	52	ASP	1
1	A	116	CYS	1
2	B	387	VAL	1
1	A	25	ARG	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	133/146 (91%)	116±3 (87±3%)	18±3 (13±3%)	7	48
2	B	20/24 (83%)	17±1 (83±5%)	3±1 (17±5%)	5	40
All	All	3060/3400 (90%)	2642 (86%)	418 (14%)	7	47

All 66 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	66	PHE	20
1	A	90	TYR	20
1	A	128	ASN	20
1	A	131	LYS	20
2	B	394	LEU	20
1	A	8	ARG	18
1	A	120	HIS	17
1	A	24	ASP	15
1	A	78	TYR	15
1	A	71	TYR	15
1	A	41	ARG	13
1	A	58	SER	12
1	A	138	MET	12
1	A	161	HIS	12
2	B	387	VAL	11
2	B	398	MET	11
1	A	17	LYS	10
2	B	396	ASP	9
1	A	117	LEU	9
1	A	122	LYS	8
1	A	19	ASN	7
1	A	52	ASP	7
1	A	25	ARG	7
1	A	158	VAL	7
1	A	18	THR	6
1	A	74	ASP	6
1	A	99	VAL	6
1	A	85	ASP	5
1	A	146	LEU	5
2	B	405	TRP	5
1	A	26	GLU	4
1	A	39	LEU	4
1	A	149	GLU	4
1	A	115	ILE	4

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Mol	Chain	Res	Type	Models (Total)
1	A	33	LYS	4
1	A	92	THR	4
2	B	393	SER	3
2	B	390	SER	3
1	A	34	GLU	3
1	A	156	LYS	3
1	A	81	ASP	3
1	A	55	ARG	3
1	A	116	CYS	2
1	A	118	THR	2
1	A	79	GLU	2
1	A	51	ASN	2
1	A	3	ASP	1
1	A	35	GLU	1
1	A	48	ASN	1
1	A	69	CYS	1
1	A	119	ASP	1
2	B	385	LEU	1
1	A	15	VAL	1
2	B	402	LYS	1
1	A	7	ARG	1
1	A	64	ARG	1
2	B	386	THR	1
1	A	83	GLU	1
2	B	388	GLU	1
1	A	9	VAL	1
1	A	152	ASP	1
1	A	45	ASN	1
1	A	46	ASN	1
1	A	54	PHE	1
2	B	389	ASP	1
2	B	404	MET	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 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

The completeness of assignment taking into account all chemical shift lists is 83% for the well-defined parts and 81% for the entire structure.

7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: *starch_output*

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	2268
Number of shifts mapped to atoms	2268
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	13

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	190	-0.47 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	179	0.03 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	175	0.43 ± 0.23	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 83%, i.e. 1844 atoms were assigned a chemical shift out of a possible 2220. 29 out of 29 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	663/840 (79%)	331/334 (99%)	172/344 (50%)	160/162 (99%)
Sidechain	1023/1174 (87%)	635/688 (92%)	376/435 (86%)	12/51 (24%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	158/206 (77%)	91/108 (84%)	60/87 (69%)	7/11 (64%)
Overall	1844/2220 (83%)	1057/1130 (94%)	608/866 (70%)	179/224 (80%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 81%, i.e. 2011 atoms were assigned a chemical shift out of a possible 2481. 30 out of 30 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	727/950 (77%)	362/378 (96%)	190/388 (49%)	175/184 (95%)
Sidechain	1120/1317 (85%)	697/774 (90%)	409/483 (85%)	14/60 (23%)
Aromatic	164/214 (77%)	95/112 (85%)	62/91 (68%)	7/11 (64%)
Overall	2011/2481 (81%)	1154/1264 (91%)	661/962 (69%)	196/255 (77%)

7.1.4 Statistically unusual chemical shifts ⓘ

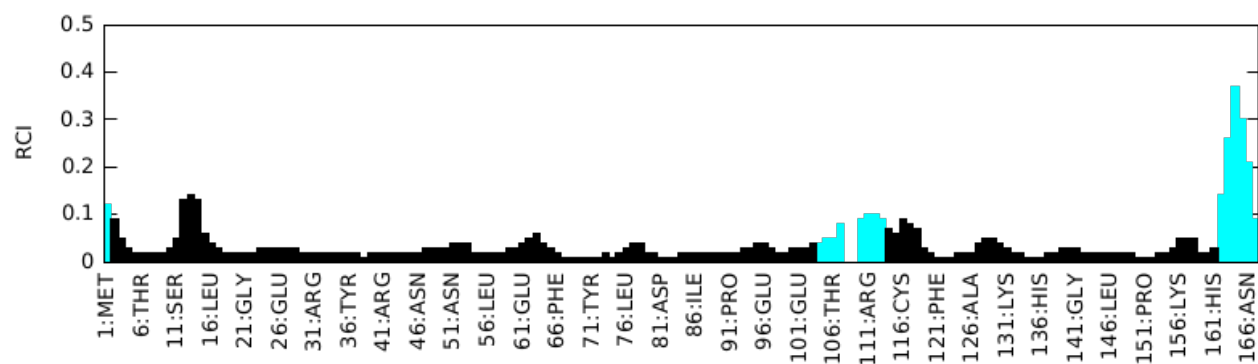
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	58	SER	HB2	0.81	5.18 – 2.58	-11.8
1	A	149	GLU	HB2	0.28	3.08 – 0.98	-8.3
1	A	149	GLU	HG2	0.84	3.33 – 1.23	-6.9
1	A	65	TRP	HB2	1.03	4.94 – 1.44	-6.2
1	A	128	ASN	HB2	0.94	4.36 – 1.26	-6.0
1	A	22	PRO	HA	2.44	6.05 – 2.75	-5.9
1	A	46	ASN	HD21	4.58	9.74 – 4.94	-5.8
1	A	54	PHE	HD1	5.40	8.56 – 5.56	-5.5
1	A	54	PHE	HD2	5.40	8.56 – 5.56	-5.5
1	A	94	ALA	HB1	0.03	2.61 – 0.11	-5.3
1	A	94	ALA	HB2	0.03	2.61 – 0.11	-5.3
1	A	94	ALA	HB3	0.03	2.61 – 0.11	-5.3
1	A	115	ILE	HB	0.29	3.24 – 0.34	-5.2

7.1.5 Random Coil Index (RCI) plots ⓘ

The images below report *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:



Random coil index (RCI) for chain B:

