



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 11:30 PM UTC

PDB ID : 2V31 / pdb_00002v31
BMRB ID : 7053
Title : Structure of First Catalytic Cysteine Half-domain of mouse ubiquitin- activating enzyme
Authors : Jaremko, L.; Jaremko, M.; Wojciechowski, W.; Filipek, R.; Szczepanowski, R.H.; Bochtler, M.; Zhukov, I.
Deposited on : 2007-06-11

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

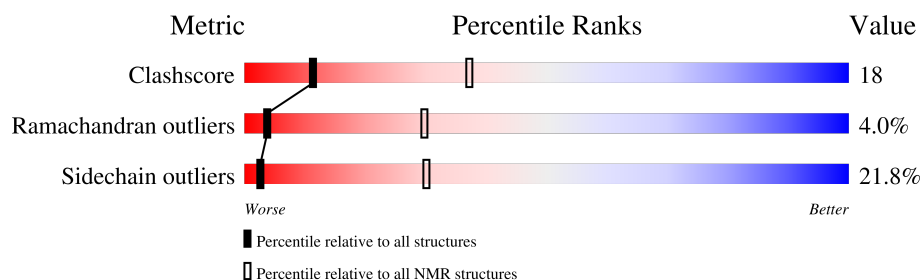
1 Overall quality at a glance

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	112	38% 30% . 30%

2 Ensemble composition and analysis

This entry contains 20 models. Model 15 is the overall representative, medoid model (most similar to other models). The authors have identified model 2 as representative.

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:217-A:294 (78)	0.52	15

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 2 clusters and 3 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1688 atoms, of which 837 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called UBIQUITIN-ACTIVATING ENZYME E1 X.

Mol	Chain	Residues	Atoms						Trace
1	A	112	Total	C	H	N	O	S	0
			1688	536	837	135	172	8	

There is a discrepancy between the modelled and reference sequences:

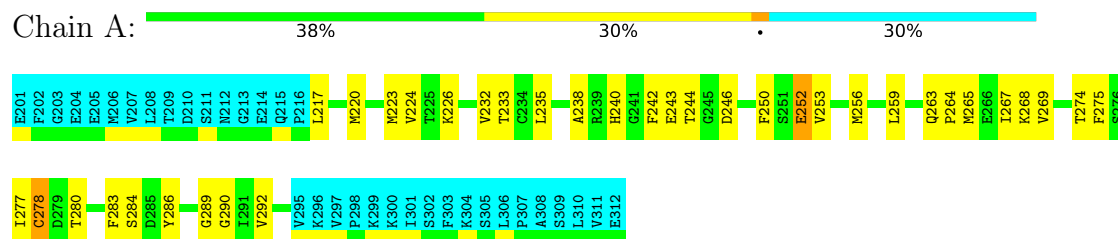
Chain	Residue	Modelled	Actual	Comment	Reference
A	201	GLU	-	expression tag	UNP Q02053

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: UBIQUITIN-ACTIVATING ENZYME E1 X

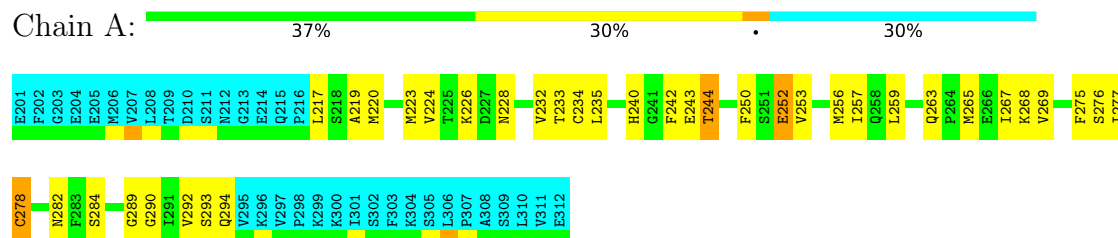


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: UBIQUITIN-ACTIVATING ENZYME E1 X



4.2.2 Score per residue for model 2

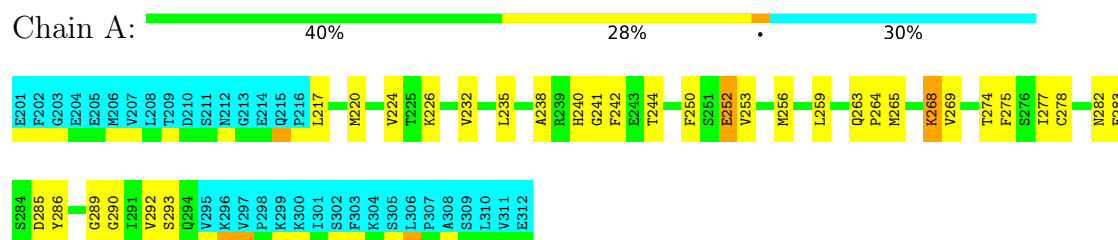
- Molecule 1: UBIQUITIN-ACTIVATING ENZYME E1 X





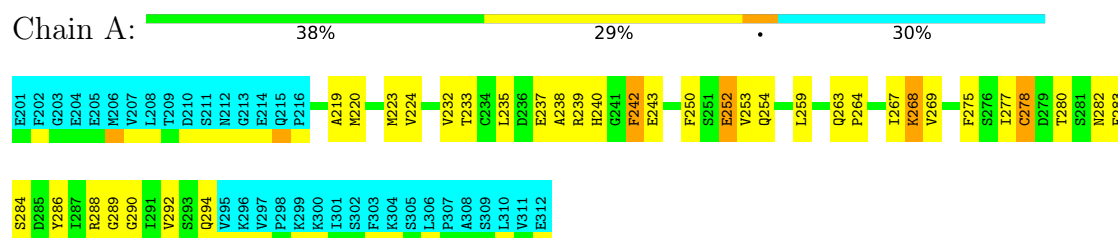
4.2.3 Score per residue for model 3

- Molecule 1: UBIQUITIN-ACTIVATING ENZYME E1 X



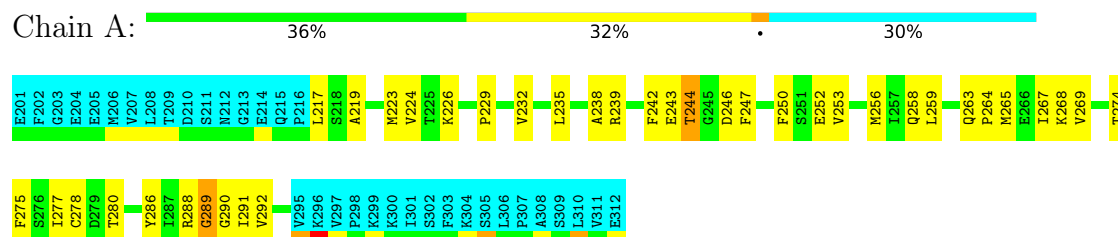
4.2.4 Score per residue for model 4

- Molecule 1: UBIQUITIN-ACTIVATING ENZYME E1 X



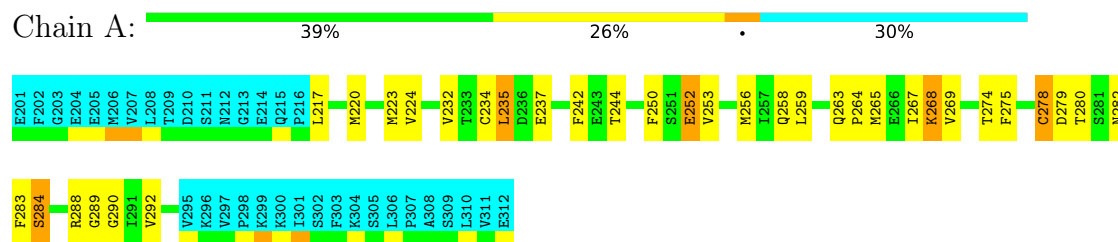
4.2.5 Score per residue for model 5

- Molecule 1: UBIQUITIN-ACTIVATING ENZYME E1 X



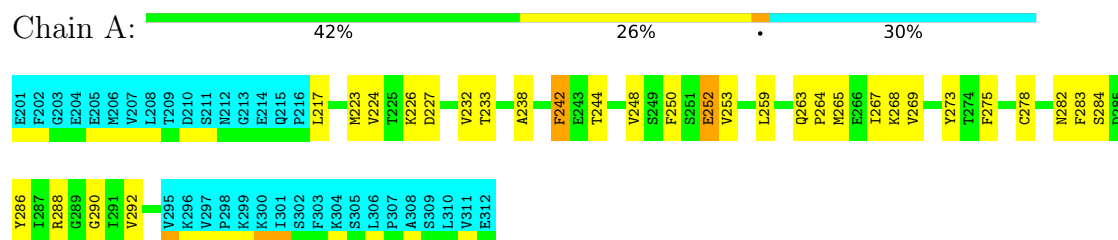
4.2.6 Score per residue for model 6

- Molecule 1: UBIQUITIN-ACTIVATING ENZYME E1 X



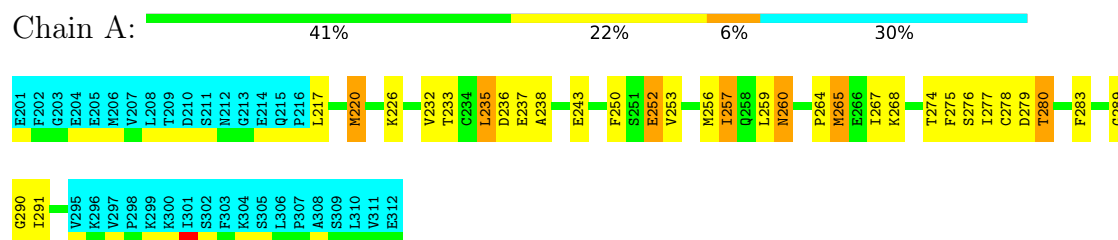
4.2.7 Score per residue for model 7

- Molecule 1: UBIQUITIN-ACTIVATING ENZYME E1 X



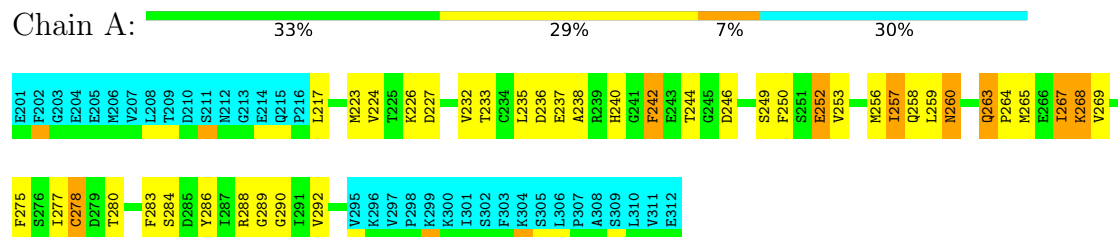
4.2.8 Score per residue for model 8

- Molecule 1: UBIQUITIN-ACTIVATING ENZYME E1 X



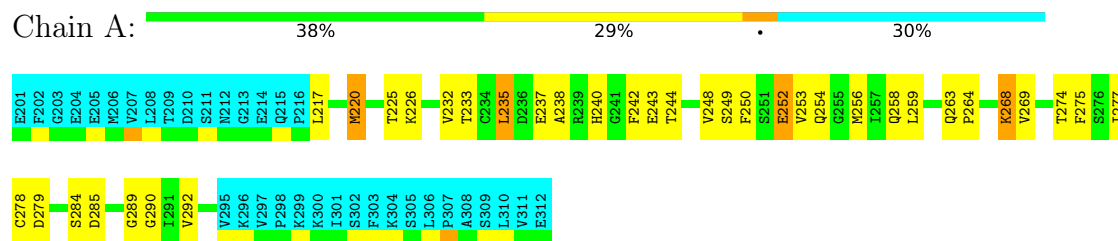
4.2.9 Score per residue for model 9

- Molecule 1: UBIQUITIN-ACTIVATING ENZYME E1 X



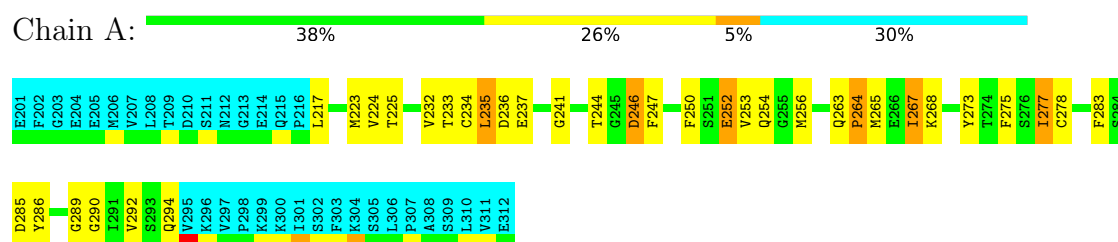
4.2.10 Score per residue for model 10

- Molecule 1: UBIQUITIN-ACTIVATING ENZYME E1 X



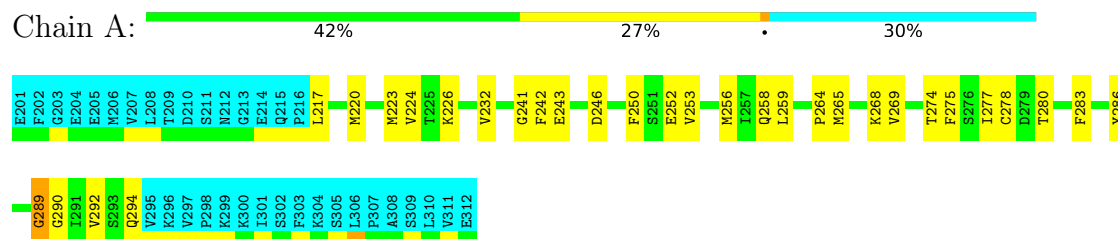
4.2.11 Score per residue for model 11

- Molecule 1: UBIQUITIN-ACTIVATING ENZYME E1 X



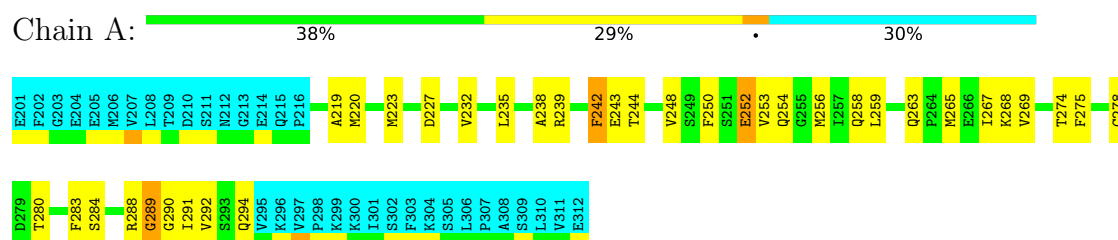
4.2.12 Score per residue for model 12

- Molecule 1: UBIQUITIN-ACTIVATING ENZYME E1 X



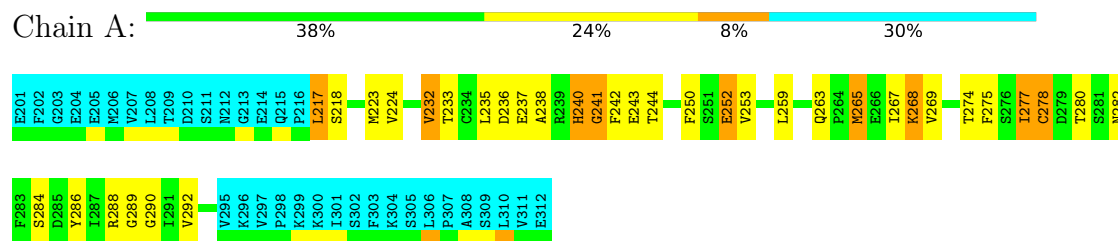
4.2.13 Score per residue for model 13

- Molecule 1: UBIQUITIN-ACTIVATING ENZYME E1 X



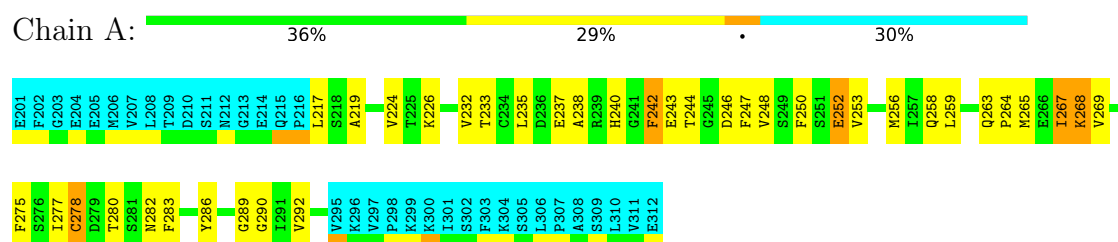
4.2.14 Score per residue for model 14

- Molecule 1: UBIQUITIN-ACTIVATING ENZYME E1 X



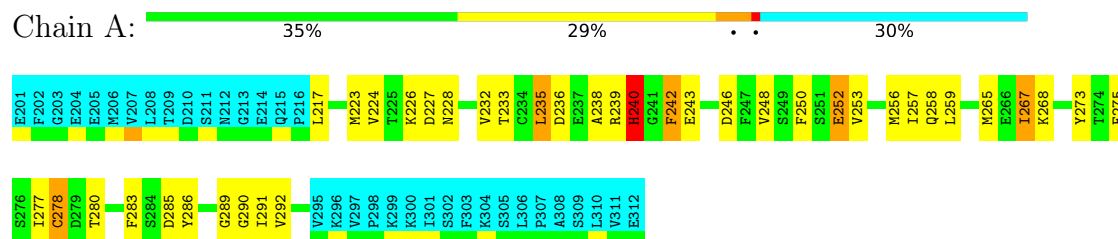
4.2.15 Score per residue for model 15 (medoid)

- Molecule 1: UBIQUITIN-ACTIVATING ENZYME E1 X



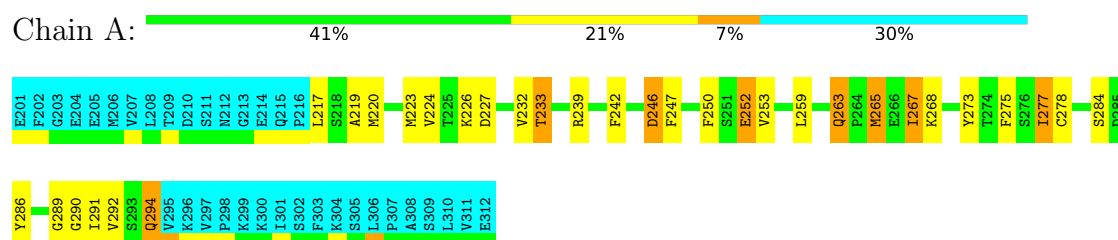
4.2.16 Score per residue for model 16

- Molecule 1: UBIQUITIN-ACTIVATING ENZYME E1 X



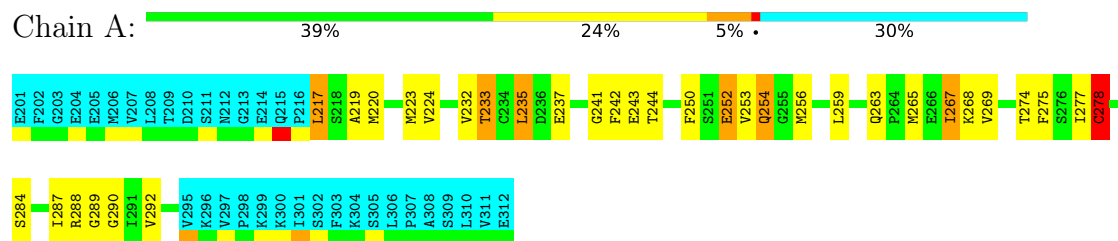
4.2.17 Score per residue for model 17

- Molecule 1: UBIQUITIN-ACTIVATING ENZYME E1 X



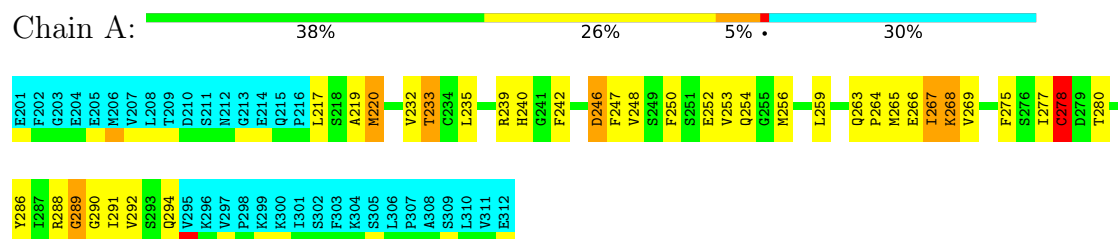
4.2.18 Score per residue for model 18

- Molecule 1: UBIQUITIN-ACTIVATING ENZYME E1 X



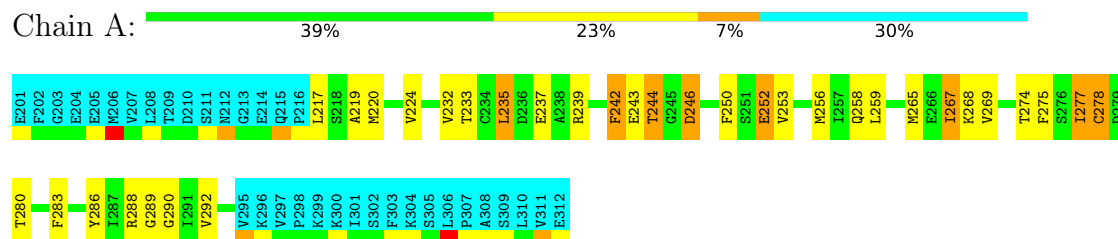
4.2.19 Score per residue for model 19

- Molecule 1: UBIQUITIN-ACTIVATING ENZYME E1 X



4.2.20 Score per residue for model 20

- Molecule 1: UBIQUITIN-ACTIVATING ENZYME E1 X



5 Refinement protocol and experimental data overview

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

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	refinement	
Sparky	structure solution	

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	589	569	568	21±4
All	All	11780	11380	11360	417

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 18.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:250:PHE:CD2	1:A:253:VAL:HG21	0.94	1.98	12	20
1:A:277:ILE:HD12	1:A:278:CYS:O	0.75	1.81	18	5
1:A:259:LEU:HD11	1:A:283:PHE:CE2	0.75	2.16	15	8
1:A:256:MET:HG2	1:A:259:LEU:HD23	0.75	1.58	16	12
1:A:233:THR:HG23	1:A:273:TYR:O	0.72	1.84	16	3
1:A:259:LEU:HD12	1:A:265:MET:SD	0.71	2.25	9	13
1:A:267:ILE:HG22	1:A:277:ILE:HG22	0.71	1.62	9	5
1:A:240:HIS:CE1	1:A:269:VAL:HG12	0.66	2.24	9	3
1:A:217:LEU:HD23	1:A:242:PHE:CE1	0.65	2.25	3	2
1:A:287:ILE:HG22	1:A:288:ARG:HD3	0.65	1.68	18	1
1:A:253:VAL:HG22	1:A:290:GLY:CA	0.64	2.23	2	4
1:A:217:LEU:HD21	1:A:241:GLY:C	0.64	2.17	14	1
1:A:253:VAL:HG13	1:A:286:TYR:CE2	0.64	2.28	2	2
1:A:217:LEU:HD21	1:A:241:GLY:O	0.64	1.93	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:256:MET:HE3	1:A:284:SER:O	0.64	1.92	6	1
1:A:219:ALA:HB3	1:A:292:VAL:CG1	0.63	2.22	5	4
1:A:242:PHE:O	1:A:269:VAL:HG11	0.63	1.94	5	9
1:A:220:MET:HE3	1:A:235:LEU:HD13	0.63	1.71	19	1
1:A:268:LYS:O	1:A:275:PHE:HB2	0.63	1.94	4	20
1:A:235:LEU:HB3	1:A:238:ALA:HB2	0.62	1.68	2	8
1:A:256:MET:SD	1:A:280:THR:HG21	0.62	2.35	19	1
1:A:232:VAL:HG13	1:A:275:PHE:CZ	0.61	2.30	16	19
1:A:252:GLU:CG	1:A:252:GLU:O	0.61	2.48	2	5
1:A:217:LEU:HD22	1:A:241:GLY:HA3	0.60	1.73	2	2
1:A:253:VAL:HG22	1:A:290:GLY:HA2	0.58	1.74	1	9
1:A:291:ILE:HD12	1:A:291:ILE:N	0.58	2.14	16	1
1:A:220:MET:HB3	1:A:235:LEU:HD13	0.58	1.75	10	2
1:A:277:ILE:HD11	1:A:280:THR:CG2	0.58	2.29	4	3
1:A:220:MET:SD	1:A:235:LEU:HD22	0.58	2.39	13	1
1:A:292:VAL:HG13	1:A:292:VAL:O	0.58	1.99	14	16
1:A:252:GLU:O	1:A:290:GLY:N	0.57	2.37	8	20
1:A:252:GLU:HG3	1:A:291:ILE:HD12	0.57	1.76	8	1
1:A:232:VAL:HG13	1:A:275:PHE:CE1	0.57	2.35	16	6
1:A:256:MET:CG	1:A:259:LEU:HD23	0.56	2.29	16	3
1:A:259:LEU:HD21	1:A:283:PHE:CD2	0.55	2.36	12	2
1:A:235:LEU:HB3	1:A:238:ALA:HB3	0.55	1.79	16	2
1:A:235:LEU:HD23	1:A:237:GLU:HG2	0.54	1.79	18	3
1:A:219:ALA:HB3	1:A:292:VAL:HG13	0.54	1.78	1	5
1:A:250:PHE:HD2	1:A:253:VAL:HG21	0.54	1.61	7	7
1:A:232:VAL:HG13	1:A:275:PHE:CE2	0.53	2.38	6	9
1:A:224:VAL:HG23	1:A:232:VAL:HB	0.53	1.81	6	6
1:A:278:CYS:O	1:A:280:THR:HG23	0.53	2.04	13	1
1:A:259:LEU:HB3	1:A:265:MET:HE1	0.52	1.81	6	5
1:A:235:LEU:HD23	1:A:237:GLU:H	0.52	1.65	11	2
1:A:259:LEU:HD22	1:A:259:LEU:N	0.51	2.20	13	15
1:A:253:VAL:O	1:A:257:ILE:HG22	0.51	2.05	16	1
1:A:220:MET:HE2	1:A:235:LEU:HD13	0.51	1.83	20	1
1:A:277:ILE:C	1:A:277:ILE:HD12	0.50	2.32	8	1
1:A:269:VAL:HG23	1:A:269:VAL:O	0.50	2.06	5	9
1:A:277:ILE:HD11	1:A:280:THR:HG21	0.50	1.83	9	1
1:A:224:VAL:HG13	1:A:224:VAL:O	0.50	2.06	5	4
1:A:224:VAL:HG12	1:A:286:TYR:CG	0.49	2.42	3	3
1:A:240:HIS:CE1	1:A:275:PHE:CD2	0.49	3.00	3	1
1:A:253:VAL:HG13	1:A:286:TYR:CE1	0.49	2.43	20	2
1:A:235:LEU:CB	1:A:238:ALA:HB2	0.49	2.38	8	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:292:VAL:O	1:A:292:VAL:HG13	0.48	2.07	11	2
1:A:256:MET:HE2	1:A:280:THR:OG1	0.48	2.08	16	1
1:A:248:VAL:HB	1:A:292:VAL:HG23	0.48	1.84	13	3
1:A:217:LEU:HD22	1:A:241:GLY:CA	0.47	2.38	2	1
1:A:259:LEU:HD11	1:A:283:PHE:CZ	0.47	2.44	20	1
1:A:247:PHE:HA	1:A:265:MET:O	0.47	2.09	19	5
1:A:256:MET:CE	1:A:280:THR:HG22	0.47	2.39	2	1
1:A:219:ALA:HB1	1:A:238:ALA:HB1	0.47	1.86	15	1
1:A:232:VAL:CG1	1:A:275:PHE:CE2	0.46	2.98	6	17
1:A:240:HIS:CE1	1:A:242:PHE:CD2	0.46	3.02	10	2
1:A:256:MET:HG3	1:A:259:LEU:HD23	0.46	1.87	12	2
1:A:232:VAL:CG1	1:A:275:PHE:CZ	0.46	2.99	14	7
1:A:248:VAL:HG21	1:A:292:VAL:CG2	0.45	2.41	10	2
1:A:224:VAL:CG1	1:A:286:TYR:CD2	0.45	2.99	12	1
1:A:240:HIS:CE1	1:A:242:PHE:CE2	0.45	3.04	3	1
1:A:224:VAL:HG12	1:A:286:TYR:CD1	0.45	2.46	4	1
1:A:235:LEU:HD23	1:A:237:GLU:CG	0.45	2.41	4	1
1:A:277:ILE:CD1	1:A:280:THR:HG21	0.45	2.42	5	1
1:A:224:VAL:CG1	1:A:286:TYR:CG	0.45	2.99	12	10
1:A:244:THR:HG23	1:A:269:VAL:HG22	0.45	1.88	9	1
1:A:242:PHE:CD1	1:A:242:PHE:N	0.45	2.82	15	3
1:A:259:LEU:CD1	1:A:283:PHE:CE2	0.45	3.00	4	3
1:A:253:VAL:HG23	1:A:260:ASN:ND2	0.45	2.26	9	1
1:A:232:VAL:HG22	1:A:233:THR:N	0.44	2.28	18	7
1:A:257:ILE:H	1:A:257:ILE:HD13	0.43	1.72	9	1
1:A:257:ILE:O	1:A:260:ASN:N	0.43	2.52	8	2
1:A:242:PHE:HB2	1:A:267:ILE:HD11	0.43	1.90	15	1
1:A:253:VAL:HG22	1:A:290:GLY:HA3	0.43	1.88	2	1
1:A:244:THR:CG2	1:A:269:VAL:HG22	0.43	2.44	15	1
1:A:269:VAL:O	1:A:269:VAL:HG23	0.42	2.14	13	1
1:A:248:VAL:CG2	1:A:292:VAL:CG2	0.42	2.98	7	1
1:A:268:LYS:O	1:A:276:SER:N	0.42	2.51	8	1
1:A:232:VAL:HG12	1:A:275:PHE:O	0.41	2.14	8	1
1:A:277:ILE:HD12	1:A:279:ASP:N	0.41	2.30	8	1
1:A:235:LEU:HD23	1:A:237:GLU:HB2	0.41	1.92	15	1
1:A:219:ALA:O	1:A:291:ILE:HG23	0.41	2.14	17	4
1:A:277:ILE:HD11	1:A:280:THR:HG23	0.41	1.92	8	1
1:A:259:LEU:HD12	1:A:265:MET:CE	0.41	2.45	16	1
1:A:258:GLN:CB	1:A:283:PHE:CD2	0.41	3.04	16	1
1:A:250:PHE:CD2	1:A:259:LEU:HB2	0.41	2.51	13	3
1:A:259:LEU:N	1:A:259:LEU:CD2	0.41	2.83	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:242:PHE:HB2	1:A:267:ILE:HD13	0.41	1.91	16	1
1:A:254:GLN:N	1:A:288:ARG:O	0.41	2.51	18	2
1:A:252:GLU:O	1:A:289:GLY:C	0.41	2.63	12	2
1:A:279:ASP:O	1:A:283:PHE:CE2	0.41	2.74	2	1
1:A:232:VAL:CG2	1:A:233:THR:N	0.41	2.84	7	3
1:A:286:TYR:CE2	1:A:289:GLY:O	0.41	2.74	19	2
1:A:282:ASN:OD1	1:A:283:PHE:CZ	0.41	2.74	6	1
1:A:282:ASN:O	1:A:283:PHE:CD1	0.41	2.74	3	3
1:A:238:ALA:O	1:A:273:TYR:CE2	0.41	2.74	7	1
1:A:248:VAL:HG22	1:A:267:ILE:CG2	0.41	2.46	19	1
1:A:239:ARG:O	1:A:240:HIS:CG	0.40	2.74	16	1
1:A:235:LEU:HB3	1:A:238:ALA:CB	0.40	2.46	14	1
1:A:241:GLY:C	1:A:242:PHE:CD1	0.40	3.00	12	1
1:A:248:VAL:HG22	1:A:267:ILE:HG23	0.40	1.93	7	1
1:A:290:GLY:C	1:A:291:ILE:HD12	0.40	2.40	16	1
1:A:240:HIS:NE2	1:A:242:PHE:CD2	0.40	2.90	15	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	78/112 (70%)	62±3 (80±4%)	13±3 (16±4%)	3±2 (4±2%)	4	30
All	All	1560/2240 (70%)	1242 (80%)	256 (16%)	62 (4%)	4	30

All 11 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	289	GLY	19
1	A	278	CYS	12
1	A	244	THR	8
1	A	263	GLN	7
1	A	246	ASP	5
1	A	241	GLY	3

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Mol	Chain	Res	Type	Models (Total)
1	A	283	PHE	2
1	A	264	PRO	2
1	A	240	HIS	2
1	A	229	PRO	1
1	A	294	GLN	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	68/99 (69%)	53±3 (78±4%)	15±3 (22±4%)	2	30
All	All	1360/1980 (69%)	1064 (78%)	296 (22%)	2	30

All 45 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	252	GLU	17
1	A	217	LEU	16
1	A	267	ILE	16
1	A	223	MET	14
1	A	278	CYS	14
1	A	243	GLU	13
1	A	226	LYS	11
1	A	274	THR	11
1	A	242	PHE	11
1	A	220	MET	10
1	A	263	GLN	10
1	A	284	SER	10
1	A	258	GLN	9
1	A	268	LYS	9
1	A	277	ILE	9
1	A	235	LEU	8
1	A	288	ARG	8
1	A	246	ASP	8
1	A	244	THR	7
1	A	233	THR	7

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Mol	Chain	Res	Type	Models (Total)
1	A	227	ASP	6
1	A	236	ASP	6
1	A	280	THR	6
1	A	239	ARG	6
1	A	294	GLN	5
1	A	254	GLN	5
1	A	240	HIS	4
1	A	285	ASP	4
1	A	265	MET	4
1	A	234	CYS	3
1	A	257	ILE	3
1	A	282	ASN	3
1	A	237	GLU	3
1	A	228	ASN	2
1	A	293	SER	2
1	A	266	GLU	2
1	A	279	ASP	2
1	A	260	ASN	2
1	A	249	SER	2
1	A	225	THR	2
1	A	256	MET	2
1	A	276	SER	1
1	A	251	SER	1
1	A	218	SER	1
1	A	232	VAL	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 ⓘ

There are no oligosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided