



Full wwPDB NMR Structure Validation Report ⓘ

May 29, 2020 – 01:29 am BST

PDB ID : 2V31
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : 2.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

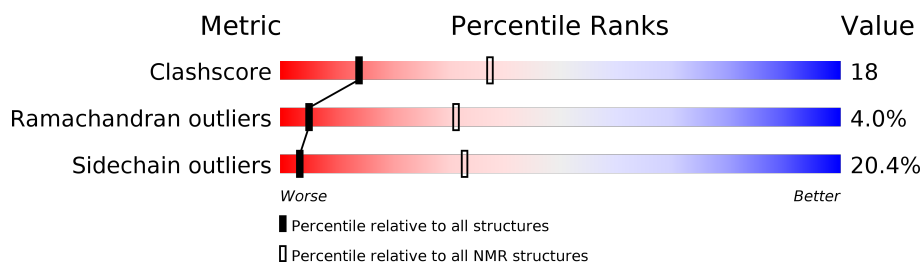
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment 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	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	112	

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)	0.30	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 [i](#)

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
			Total	C	H	N	O	S	
1	A	112	1688	536	837	135	172	8	0

There is a discrepancy between the modelled and reference sequences:

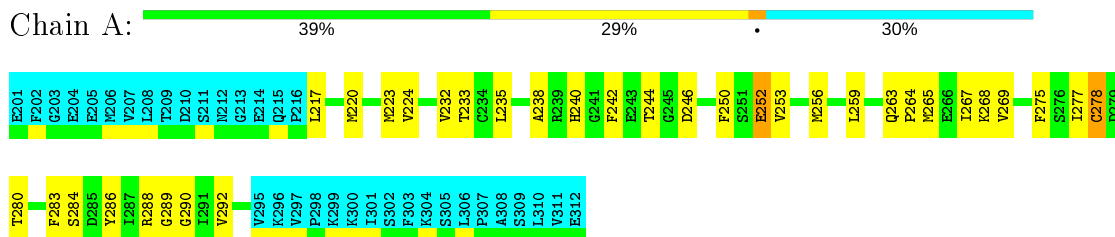
Chain	Residue	Modelled	Actual	Comment	Reference
A	201	GLU	-	expression tag	UNP Q02053

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: UBIQUITIN-ACTIVATING ENZYME E1 X

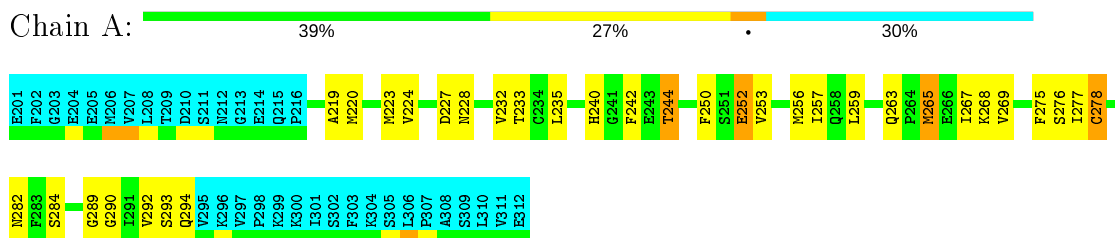


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

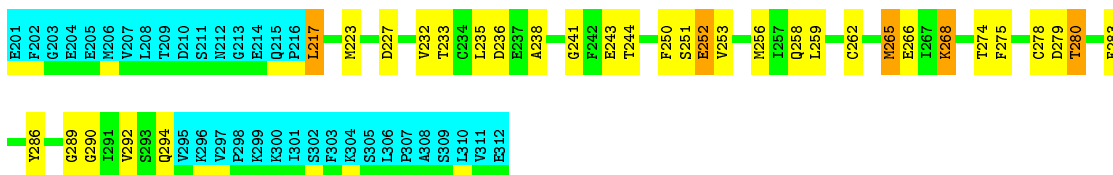
- Molecule 1: UBIQUITIN-ACTIVATING ENZYME E1 X



4.2.2 Score per residue for model 2

- Molecule 1: UBIQUITIN-ACTIVATING ENZYME E1 X

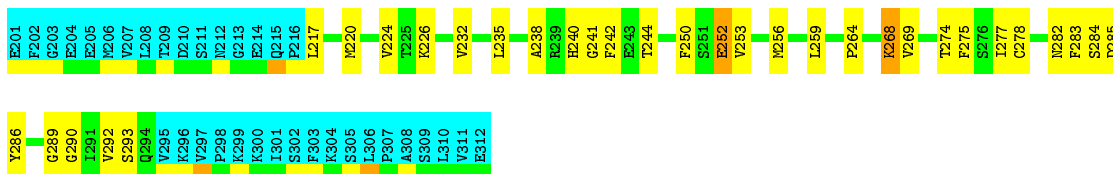




4.2.3 Score per residue for model 3

- Molecule 1: UBIQUITIN-ACTIVATING ENZYME E1 X

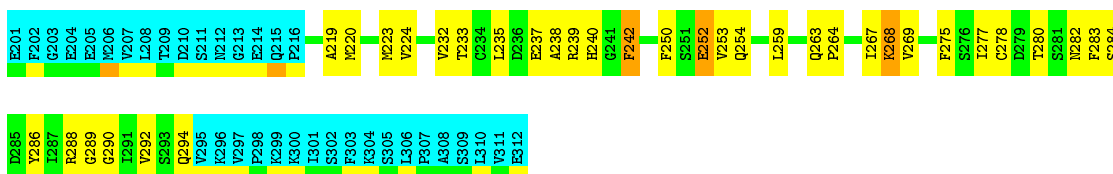
Chain A: 41% 27% 30%



4.2.4 Score per residue for model 4

- Molecule 1: UBIQUITIN-ACTIVATING ENZYME E1 X

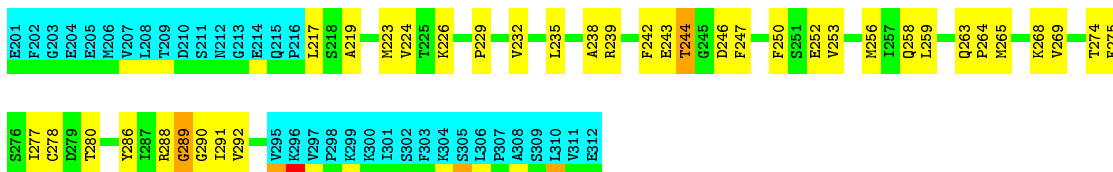
Chain A: 38% 29% 30%



4.2.5 Score per residue for model 5

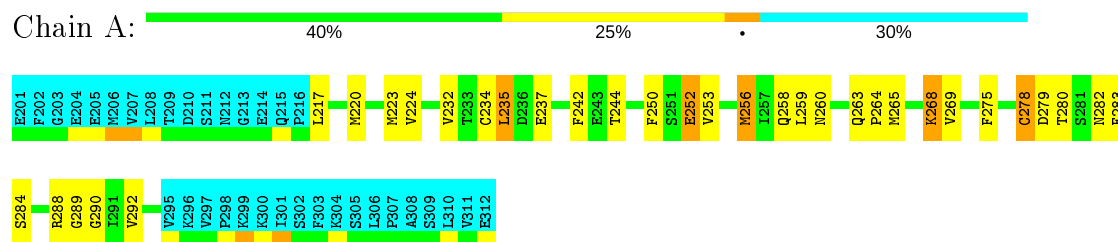
- Molecule 1: UBIQUITIN-ACTIVATING ENZYME E1 X

Chain A: 37% 31% 30%



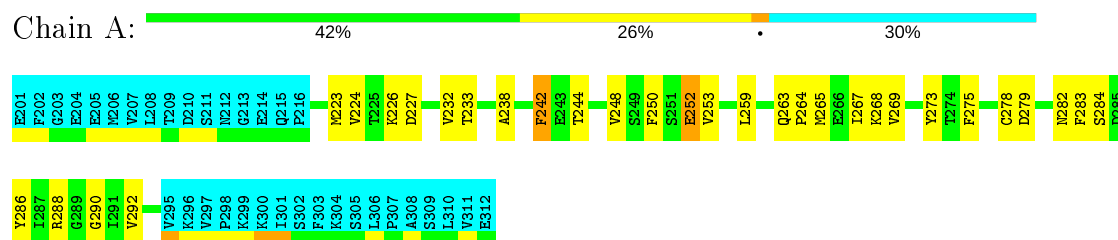
4.2.6 Score per residue for model 6

- Molecule 1: UBIQUITIN-ACTIVATING ENZYME E1 X



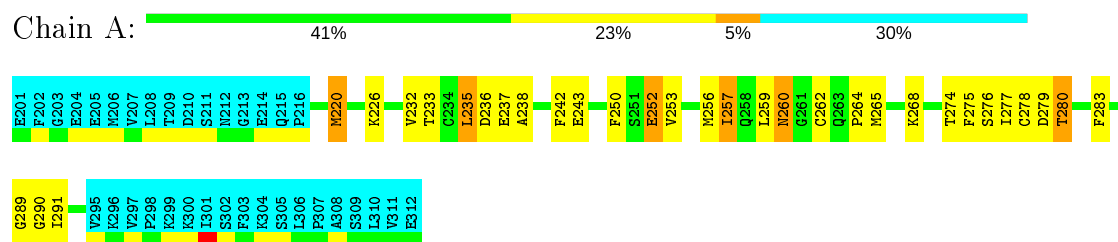
4.2.7 Score per residue for model 7

- Molecule 1: UBIQUITIN-ACTIVATING ENZYME E1 X



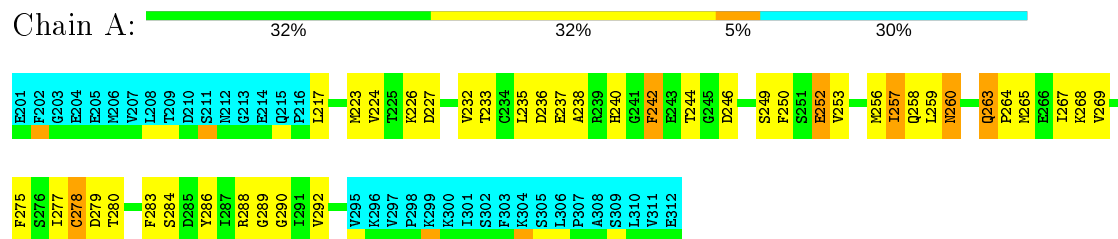
4.2.8 Score per residue for model 8

- Molecule 1: UBIQUITIN-ACTIVATING ENZYME E1 X



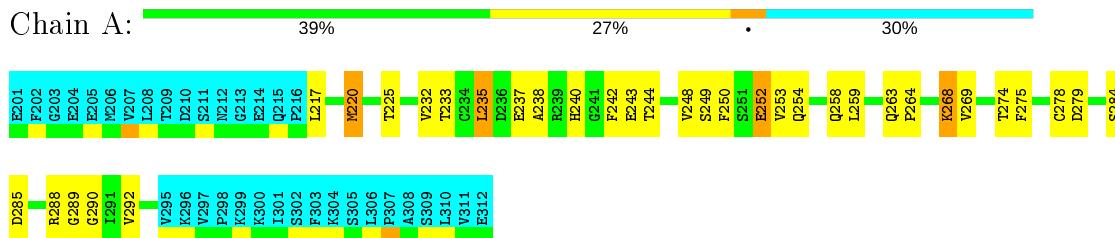
4.2.9 Score per residue for model 9

- Molecule 1: UBIQUITIN-ACTIVATING ENZYME E1 X



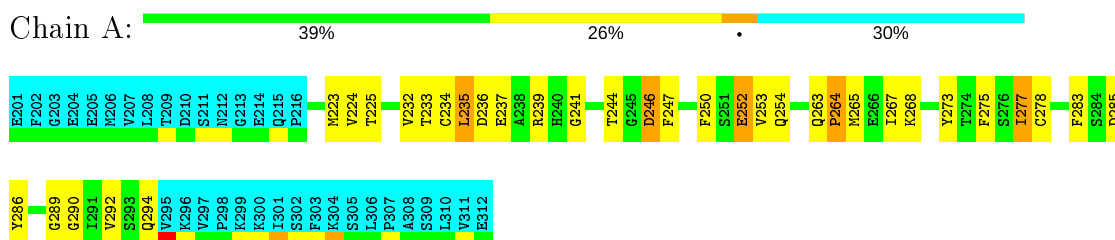
4.2.10 Score per residue for model 10

- Molecule 1: UBIQUITIN-ACTIVATING ENZYME E1 X



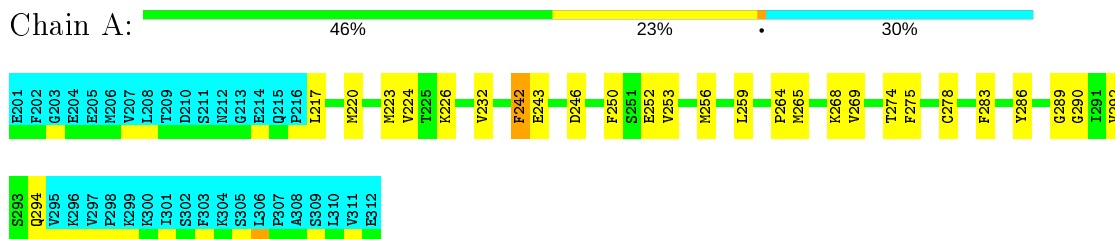
4.2.11 Score per residue for model 11

- Molecule 1: UBIQUITIN-ACTIVATING ENZYME E1 X



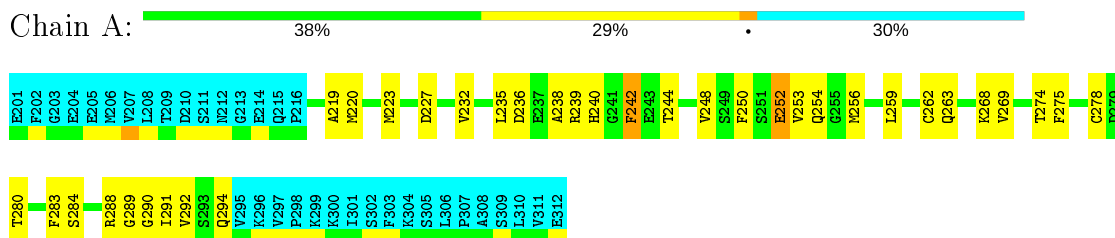
4.2.12 Score per residue for model 12

- Molecule 1: UBIQUITIN-ACTIVATING ENZYME E1 X



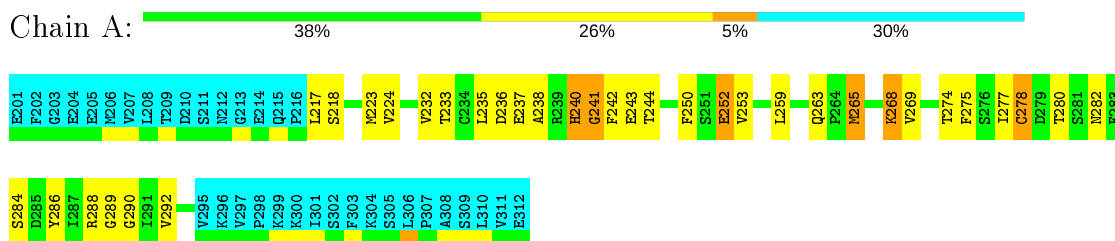
4.2.13 Score per residue for model 13

- Molecule 1: UBIQUITIN-ACTIVATING ENZYME E1 X



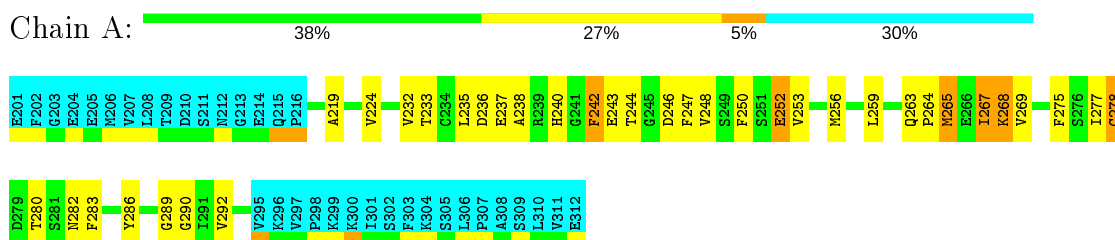
4.2.14 Score per residue for model 14

- Molecule 1: UBIQUITIN-ACTIVATING ENZYME E1 X



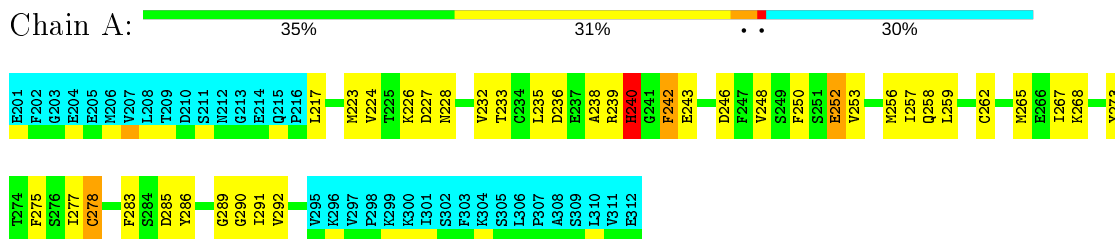
4.2.15 Score per residue for model 15 (medoid)

- Molecule 1: UBIQUITIN-ACTIVATING ENZYME E1 X



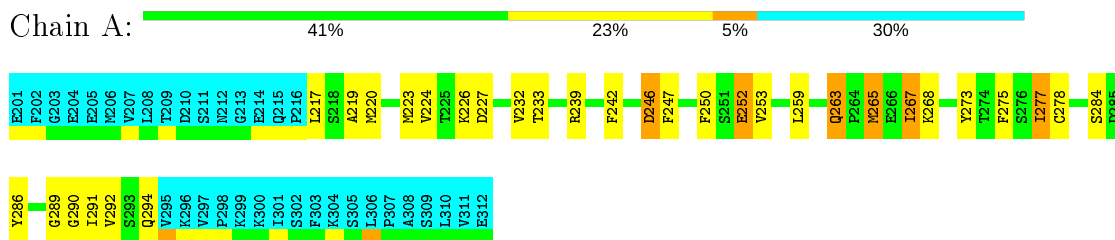
4.2.16 Score per residue for model 16

- Molecule 1: UBIQUITIN-ACTIVATING ENZYME E1 X



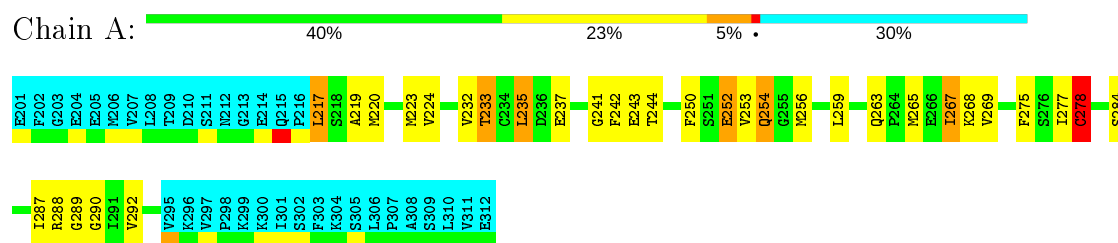
4.2.17 Score per residue for model 17

- Molecule 1: UBIQUITIN-ACTIVATING ENZYME E1 X



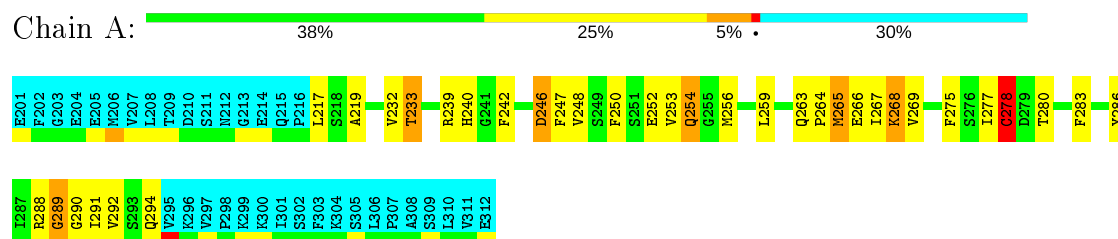
4.2.18 Score per residue for model 18

- Molecule 1: UBIQUITIN-ACTIVATING ENZYME E1 X



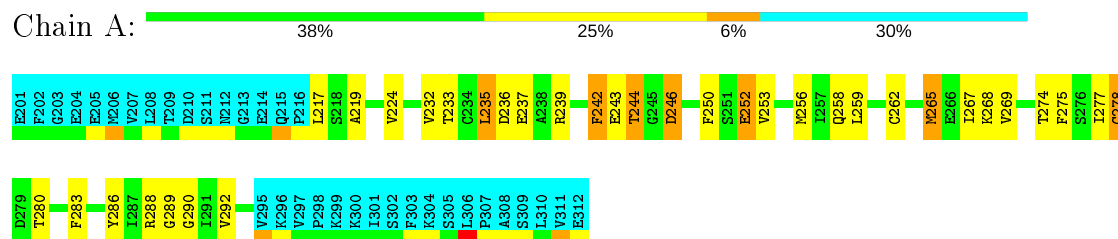
4.2.19 Score per residue for model 19

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

6 Model quality

6.1 Standard geometry

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	589	569	568	20±4
All	All	11780	11380	11360	406

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: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
1:A:219:ALA:HB3	1:A:292:VAL:CG1	0.63	2.22	5	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:242:PHE:O	1:A:269:VAL:HG11	0.63	1.94	5	9
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	3
1:A:217:LEU:HD22	1:A:241:GLY:HA3	0.60	1.73	2	2
1:A:252:GLU:O	1:A:252:GLU:CG	0.60	2.49	6	2
1:A:217:LEU:HD21	1:A:241:GLY:C	0.59	2.17	14	1
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	10
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:292:VAL:O	1:A:292:VAL:HG13	0.55	2.02	18	8
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: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	7
1:A:253:VAL:O	1:A:257:ILE:HG22	0.51	2.05	16	1
1:A:269:VAL:O	1:A:269:VAL:HG23	0.50	2.06	10	7
1:A:269:VAL:HG23	1:A:269:VAL:O	0.50	2.06	5	3
1:A:259:LEU:N	1:A:259:LEU:HD22	0.50	2.21	20	8
1:A:277:ILE:HD11	1:A:280:THR:HG21	0.50	1.83	9	1
1:A:224:VAL:O	1:A:224:VAL:HG13	0.50	2.06	5	2
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
1:A:248:VAL:HB	1:A:292:VAL:HG23	0.48	1.84	13	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:217:LEU:HD22	1:A:241:GLY:CA	0.47	2.38	2	1
1:A:224:VAL:HG13	1:A:224:VAL:O	0.47	2.09	9	2
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:277:ILE:C	1:A:277:ILE:HD12	0.46	2.32	8	1
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:235:LEU:HD23	1:A:237:GLU:CG	0.45	2.41	4	1
1:A:224:VAL:HG12	1:A:286:TYR:CD1	0.45	2.46	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:N	1:A:242:PHE:CD1	0.45	2.82	15	2
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:242:PHE:CD1	1:A:242:PHE:N	0.44	2.83	13	1
1:A:257:ILE:HD13	1:A:257:ILE:H	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: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:CD2	1:A:259:LEU:N	0.41	2.83	9	2
1:A:242:PHE:HB2	1:A:267:ILE:HD13	0.41	1.91	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:254:GLN:N	1:A:288:ARG:O	0.41	2.51	18	2
1:A:232:VAL:CG2	1:A:233:THR:N	0.41	2.84	7	5
1:A:279:ASP:O	1:A:283:PHE:CE2	0.41	2.74	2	1
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:248:VAL:HG22	1:A:267:ILE:HG23	0.40	1.93	7	1
1:A:240:HIS:NE2	1:A:242:PHE:CD2	0.40	2.90	15	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	78/112 (70%)	62±3 (80±4%)	13±3 (16±4%)	3±2 (4±2%)	5	31
All	All	1560/2240 (70%)	1242 (80%)	256 (16%)	62 (4%)	5	31

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
1	A	264	PRO	2
1	A	240	HIS	2
1	A	283	PHE	2
1	A	229	PRO	1

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Mol	Chain	Res	Type	Models (Total)
1	A	294	GLN	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	68/99 (69%)	54±3 (80±4%)	14±3 (20±4%)	3 33
All	All	1360/1980 (69%)	1082 (80%)	278 (20%)	3 33

All 46 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	223	MET	14
1	A	278	CYS	13
1	A	242	PHE	13
1	A	284	SER	11
1	A	217	LEU	10
1	A	243	GLU	10
1	A	263	GLN	9
1	A	274	THR	9
1	A	236	ASP	9
1	A	265	MET	9
1	A	220	MET	9
1	A	288	ARG	9
1	A	226	LYS	8
1	A	268	LYS	8
1	A	246	ASP	8
1	A	227	ASP	7
1	A	244	THR	7
1	A	239	ARG	7
1	A	235	LEU	7
1	A	258	GLN	6
1	A	254	GLN	6
1	A	233	THR	6
1	A	240	HIS	5

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Mol	Chain	Res	Type	Models (Total)
1	A	267	ILE	5
1	A	262	CYS	5
1	A	294	GLN	5
1	A	280	THR	5
1	A	277	ILE	4
1	A	279	ASP	4
1	A	285	ASP	4
1	A	257	ILE	3
1	A	237	GLU	3
1	A	260	ASN	3
1	A	282	ASN	3
1	A	293	SER	2
1	A	225	THR	2
1	A	249	SER	2
1	A	266	GLU	2
1	A	234	CYS	2
1	A	228	ASN	2
1	A	283	PHE	1
1	A	251	SER	1
1	A	256	MET	1
1	A	218	SER	1
1	A	276	SER	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided