Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	2HLW
Title	:	Solution Structure of the Human Ubiquitin-conjugating Enzyme Variant Uev1a
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Deposited on	:	2006-07-10

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 (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

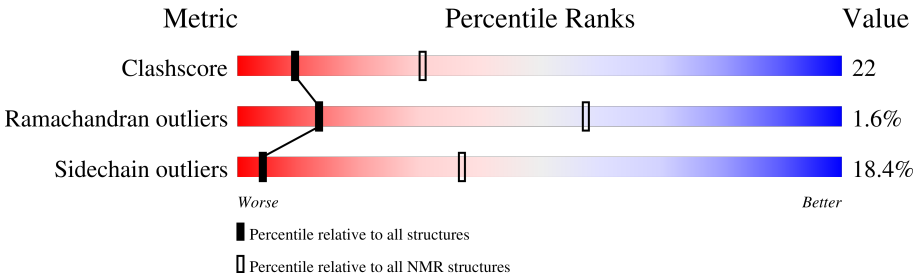
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

1 Overall quality at a glance (i)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	170	38% 32% • 27%

2 Ensemble composition and analysis

This entry contains 15 models. Model 9 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *minimized average structure*.

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:36-A:61, A:68-A:162, A:166-A:168 (124)	0.34	9

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 and 1 single-model cluster was found.

Cluster number	Models
1	1, 2, 4, 6, 7, 9, 10, 11, 12, 13
2	14, 15
3	3, 8
Single-model clusters	5

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2716 atoms, of which 1363 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Ubiquitin-conjugating enzyme E2 variant 1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	170	2716	852	1363	237	254	10	0

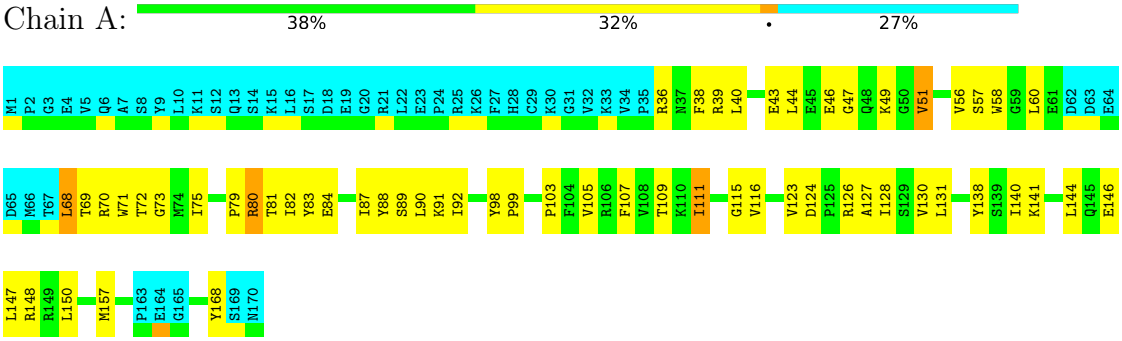
4 Residue-property plots

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-conjugating enzyme E2 variant 1

Chain A:



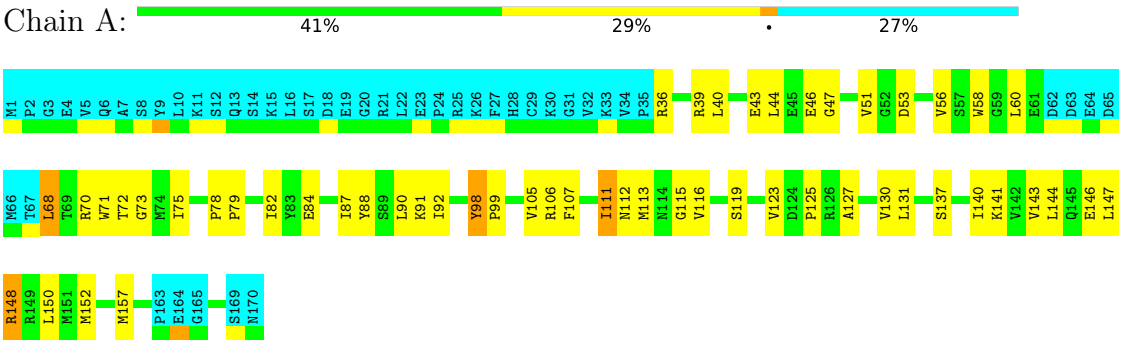
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Ubiquitin-conjugating enzyme E2 variant 1

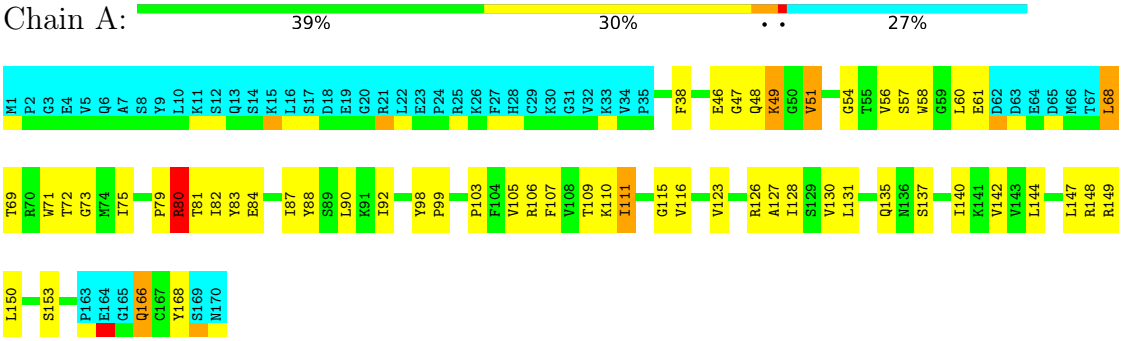
Chain A:



4.2.2 Score per residue for model 2

• Molecule 1: Ubiquitin-conjugating enzyme E2 variant 1

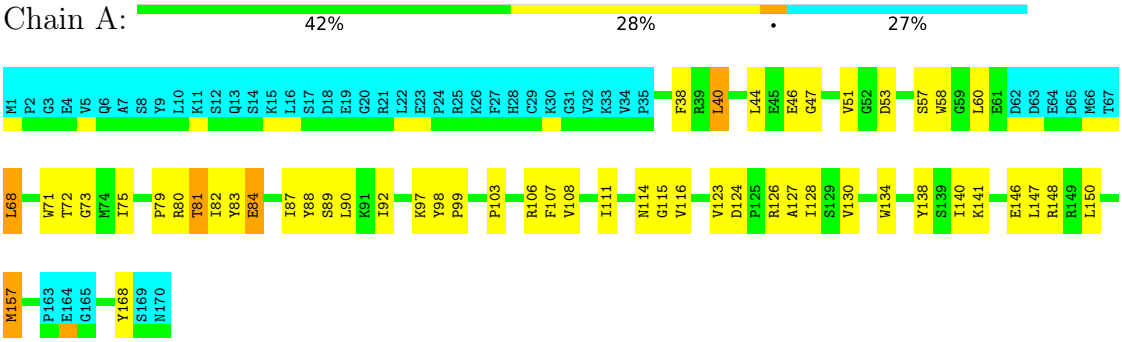
Chain A:



4.2.3 Score per residue for model 3

• Molecule 1: Ubiquitin-conjugating enzyme E2 variant 1

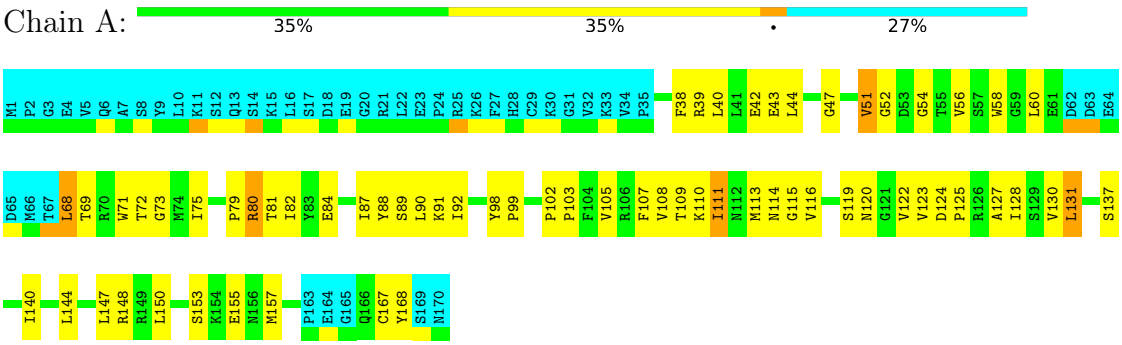
Chain A:



4.2.4 Score per residue for model 4

• Molecule 1: Ubiquitin-conjugating enzyme E2 variant 1

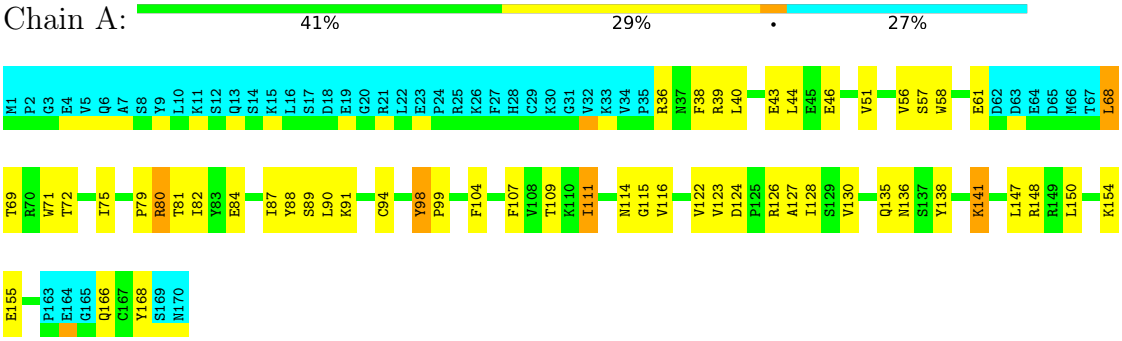
Chain A:



4.2.5 Score per residue for model 5

• Molecule 1: Ubiquitin-conjugating enzyme E2 variant 1

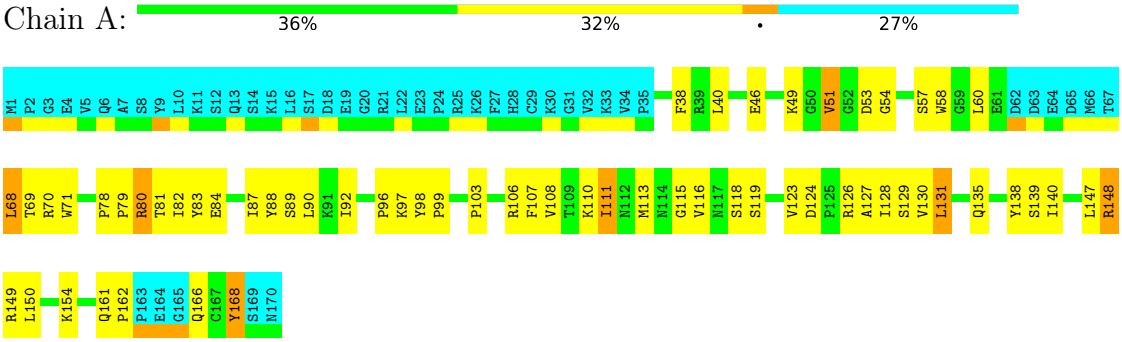
Chain A:



4.2.6 Score per residue for model 6

• Molecule 1: Ubiquitin-conjugating enzyme E2 variant 1

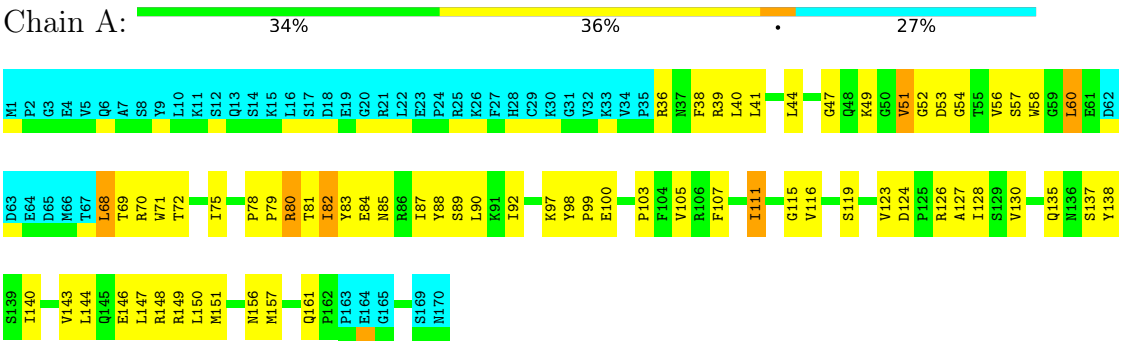
Chain A:



4.2.7 Score per residue for model 7

• Molecule 1: Ubiquitin-conjugating enzyme E2 variant 1

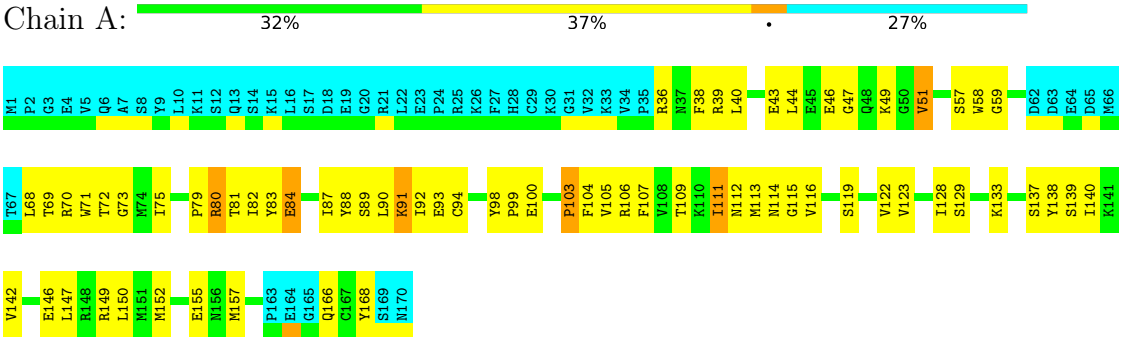
Chain A:



4.2.8 Score per residue for model 8

• Molecule 1: Ubiquitin-conjugating enzyme E2 variant 1

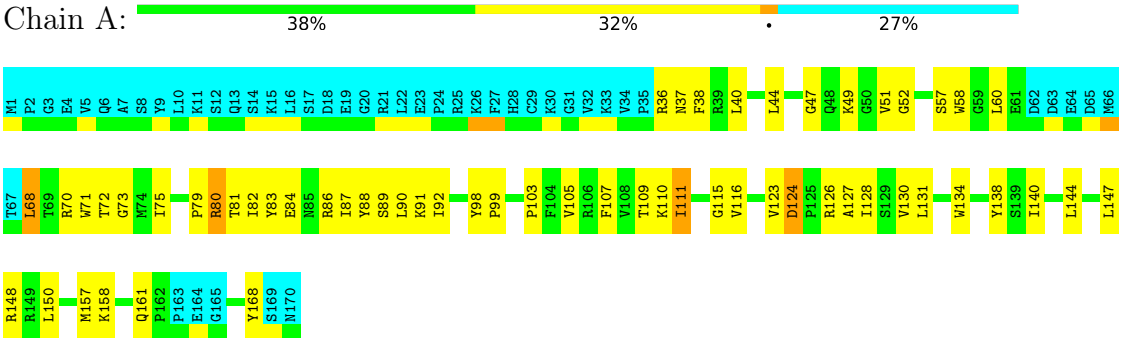
Chain A:



4.2.9 Score per residue for model 9 (medoid)

• Molecule 1: Ubiquitin-conjugating enzyme E2 variant 1

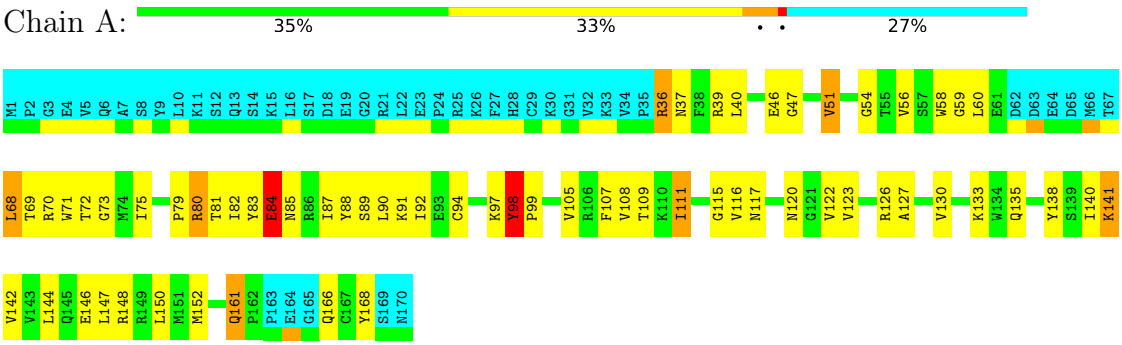
Chain A:



4.2.10 Score per residue for model 10

• Molecule 1: Ubiquitin-conjugating enzyme E2 variant 1

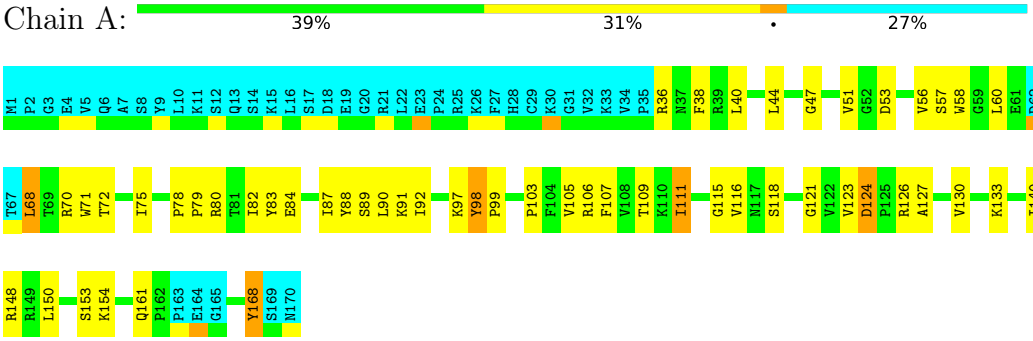
Chain A:



4.2.11 Score per residue for model 11

• Molecule 1: Ubiquitin-conjugating enzyme E2 variant 1

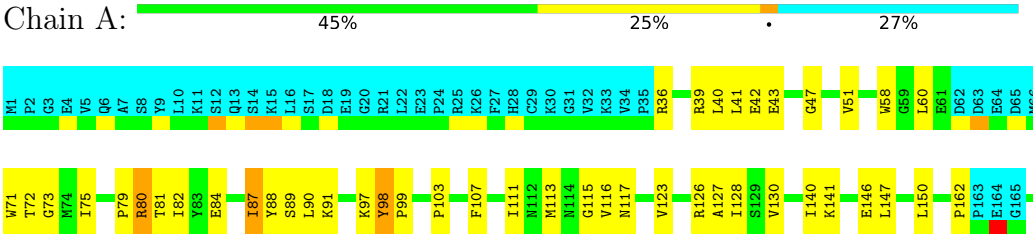
Chain A:



4.2.12 Score per residue for model 12

• Molecule 1: Ubiquitin-conjugating enzyme E2 variant 1

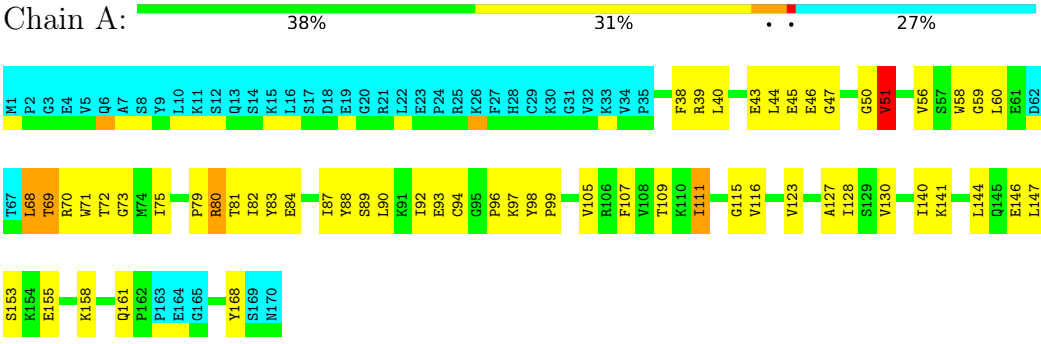
Chain A:



4.2.13 Score per residue for model 13

• Molecule 1: Ubiquitin-conjugating enzyme E2 variant 1

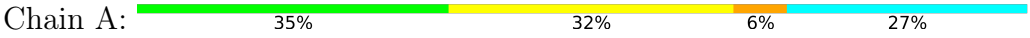
Chain A:

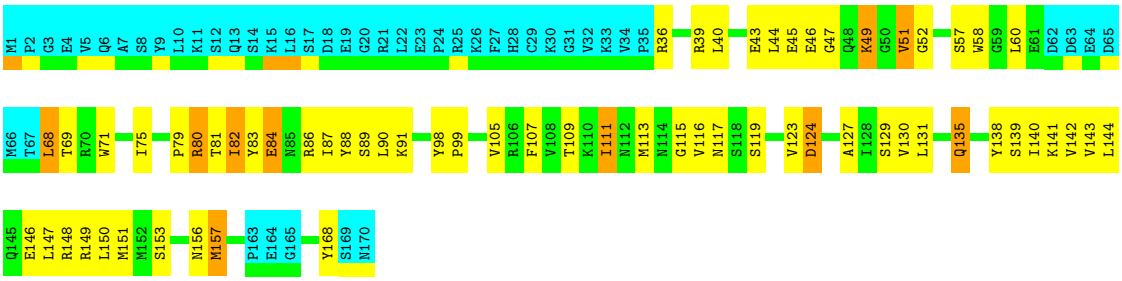


4.2.14 Score per residue for model 14

• Molecule 1: Ubiquitin-conjugating enzyme E2 variant 1

Chain A:

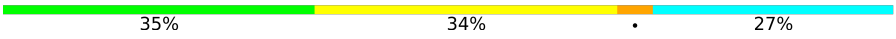


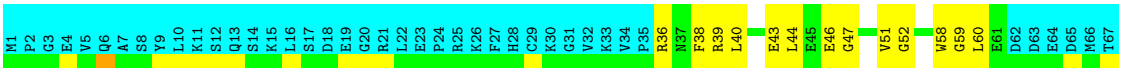


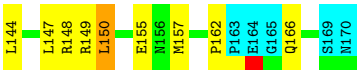
4.2.15 Score per residue for model 15

• Molecule 1: Ubiquitin-conjugating enzyme E2 variant 1

Chain A:







5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing torsion angle dynamics*.

Of the 200 calculated structures, 15 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
CNS	structure solution	1.1
Procheck	refinement	3.5.4

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	996	1016	1016	45±6
All	All	14940	15240	15240	676

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 22.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:60:LEU:HD11	1:A:68:LEU:HD23	1.08	1.25	15	10
1:A:107:PHE:CD2	1:A:111:ILE:HG21	1.01	1.90	12	15
1:A:116:VAL:HG22	1:A:123:VAL:HG13	0.90	1.38	6	15
1:A:107:PHE:CZ	1:A:147:LEU:HD13	0.86	2.06	3	4
1:A:90:LEU:HD21	1:A:107:PHE:CE2	0.84	2.07	4	13
1:A:75:ILE:CD1	1:A:147:LEU:HD11	0.83	2.03	7	9
1:A:107:PHE:CE1	1:A:147:LEU:HD13	0.80	2.11	8	6
1:A:88:TYR:CE2	1:A:111:ILE:HD12	0.80	2.12	3	1
1:A:138:TYR:CD1	1:A:142:VAL:HG11	0.79	2.13	8	3
1:A:92:ILE:HG23	1:A:105:VAL:HG22	0.78	1.52	8	8
1:A:75:ILE:HD13	1:A:147:LEU:HD11	0.78	1.55	7	9
1:A:107:PHE:CG	1:A:111:ILE:HG21	0.78	2.14	6	14
1:A:146:GLU:OE1	1:A:150:LEU:HD11	0.77	1.79	8	1
1:A:147:LEU:HA	1:A:150:LEU:HD12	0.77	1.55	6	15

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:147:LEU:HD12	1:A:148:ARG:N	0.77	1.93	2	9
1:A:69:THR:HG23	1:A:94:CYS:O	0.74	1.82	5	3
1:A:69:THR:HG22	1:A:94:CYS:O	0.73	1.83	15	1
1:A:116:VAL:CG2	1:A:123:VAL:HG13	0.72	2.14	1	8
1:A:40:LEU:HD21	1:A:98:TYR:CD2	0.71	2.20	8	3
1:A:40:LEU:HD22	1:A:71:TRP:CZ2	0.70	2.20	11	9
1:A:128:ILE:HG23	1:A:146:GLU:OE1	0.69	1.88	8	1
1:A:90:LEU:HD21	1:A:107:PHE:CZ	0.67	2.25	4	12
1:A:51:VAL:HG23	1:A:54:GLY:HA2	0.67	1.67	4	5
1:A:104:PHE:CZ	1:A:122:VAL:HG13	0.67	2.25	8	2
1:A:106:ARG:HA	1:A:123:VAL:HG23	0.65	1.66	8	2
1:A:60:LEU:CD1	1:A:68:LEU:HD23	0.65	2.22	2	3
1:A:56:VAL:HG12	1:A:75:ILE:HG12	0.64	1.69	11	8
1:A:115:GLY:HA3	1:A:127:ALA:HB3	0.64	1.70	6	14
1:A:60:LEU:HD11	1:A:68:LEU:CD2	0.63	2.23	2	4
1:A:60:LEU:HD21	1:A:68:LEU:HB3	0.62	1.72	15	7
1:A:71:TRP:CE3	1:A:140:ILE:HD13	0.59	2.33	15	6
1:A:115:GLY:CA	1:A:127:ALA:HB3	0.58	2.28	7	7
1:A:128:ILE:CG2	1:A:130:VAL:HG12	0.57	2.28	7	8
1:A:40:LEU:HD13	1:A:68:LEU:HB2	0.57	1.77	5	1
1:A:75:ILE:HD11	1:A:144:LEU:HD22	0.57	1.77	9	8
1:A:130:VAL:HG23	1:A:138:TYR:CD2	0.57	2.35	3	4
1:A:107:PHE:CE2	1:A:111:ILE:HD13	0.57	2.35	3	2
1:A:130:VAL:HG21	1:A:142:VAL:HG12	0.56	1.77	10	2
1:A:51:VAL:HG21	1:A:56:VAL:O	0.56	2.00	10	1
1:A:130:VAL:HG23	1:A:138:TYR:CE2	0.56	2.36	5	5
1:A:88:TYR:CD2	1:A:111:ILE:HD12	0.56	2.36	3	1
1:A:68:LEU:HD12	1:A:68:LEU:N	0.56	2.15	4	1
1:A:60:LEU:HD21	1:A:68:LEU:HA	0.56	1.78	7	2
1:A:80:ARG:O	1:A:81:THR:HG23	0.55	2.02	2	5
1:A:107:PHE:HE2	1:A:111:ILE:HD13	0.55	1.61	3	2
1:A:147:LEU:HD12	1:A:147:LEU:C	0.55	2.22	14	8
1:A:40:LEU:HD22	1:A:68:LEU:HB2	0.54	1.79	3	1
1:A:116:VAL:HG22	1:A:123:VAL:HA	0.54	1.77	1	1
1:A:87:ILE:HG22	1:A:88:TYR:N	0.54	2.18	9	15
1:A:130:VAL:CG2	1:A:142:VAL:HG12	0.54	2.32	2	2
1:A:51:VAL:HG11	1:A:58:TRP:CH2	0.54	2.38	14	3
1:A:107:PHE:CD1	1:A:116:VAL:HG11	0.54	2.38	10	3
1:A:36:ARG:HD3	1:A:40:LEU:HD11	0.53	1.80	9	2
1:A:60:LEU:HD11	1:A:68:LEU:HB3	0.53	1.79	2	1
1:A:92:ILE:HG13	1:A:105:VAL:HG13	0.52	1.81	8	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:98:TYR:HB3	1:A:99:PRO:HD3	0.52	1.81	8	12
1:A:105:VAL:HG21	1:A:143:VAL:HG11	0.52	1.82	14	3
1:A:125:PRO:HB3	1:A:131:LEU:HD23	0.52	1.81	1	1
1:A:71:TRP:CE2	1:A:140:ILE:HD11	0.52	2.40	3	2
1:A:71:TRP:O	1:A:91:LYS:HA	0.52	2.05	8	5
1:A:36:ARG:NH1	1:A:40:LEU:HD11	0.51	2.19	10	1
1:A:73:GLY:CA	1:A:144:LEU:HD11	0.51	2.35	1	1
1:A:79:PRO:O	1:A:80:ARG:HB2	0.51	2.05	12	2
1:A:87:ILE:O	1:A:88:TYR:CD1	0.51	2.63	1	13
1:A:71:TRP:CD2	1:A:140:ILE:CD1	0.51	2.93	9	8
1:A:130:VAL:HG13	1:A:146:GLU:HG2	0.51	1.83	1	4
1:A:89:SER:C	1:A:90:LEU:HD12	0.50	2.27	6	1
1:A:79:PRO:HA	1:A:84:GLU:HB2	0.50	1.83	2	12
1:A:58:TRP:CH2	1:A:141:LYS:CB	0.50	2.95	10	7
1:A:107:PHE:HZ	1:A:147:LEU:HD13	0.50	1.67	1	4
1:A:47:GLY:CA	1:A:58:TRP:CE2	0.50	2.95	15	12
1:A:89:SER:O	1:A:90:LEU:HG	0.50	2.07	5	12
1:A:41:LEU:HD23	1:A:68:LEU:HD21	0.49	1.84	7	2
1:A:73:GLY:O	1:A:90:LEU:HD12	0.49	2.07	4	10
1:A:36:ARG:HH11	1:A:40:LEU:HD11	0.49	1.67	10	1
1:A:94:CYS:CB	1:A:98:TYR:CD2	0.49	2.96	15	1
1:A:40:LEU:O	1:A:44:LEU:HB2	0.49	2.08	7	10
1:A:98:TYR:CD1	1:A:98:TYR:C	0.48	2.84	5	7
1:A:40:LEU:HD23	1:A:71:TRP:CZ2	0.48	2.43	3	1
1:A:130:VAL:HG13	1:A:131:LEU:HD12	0.48	1.85	6	1
1:A:79:PRO:HA	1:A:84:GLU:HG3	0.48	1.85	3	3
1:A:79:PRO:HA	1:A:84:GLU:CG	0.48	2.38	10	3
1:A:130:VAL:HG13	1:A:146:GLU:CG	0.48	2.39	1	3
1:A:98:TYR:HB3	1:A:99:PRO:CD	0.48	2.38	11	7
1:A:107:PHE:CE1	1:A:116:VAL:HG21	0.47	2.44	12	1
1:A:39:ARG:O	1:A:43:GLU:HG3	0.47	2.09	14	2
1:A:130:VAL:HG22	1:A:146:GLU:HG2	0.47	1.86	14	2
1:A:128:ILE:HG22	1:A:130:VAL:HG12	0.47	1.86	6	5
1:A:75:ILE:HD12	1:A:90:LEU:HD11	0.47	1.86	8	2
1:A:98:TYR:CE1	1:A:103:PRO:HB3	0.47	2.44	3	7
1:A:83:TYR:O	1:A:84:GLU:C	0.47	2.52	3	3
1:A:104:PHE:CE2	1:A:122:VAL:HG13	0.47	2.45	8	1
1:A:98:TYR:CB	1:A:99:PRO:CD	0.47	2.93	10	7
1:A:113:MET:HE1	1:A:147:LEU:HB2	0.47	1.86	1	1
1:A:71:TRP:CE3	1:A:140:ILE:CD1	0.47	2.98	2	4
1:A:40:LEU:HD21	1:A:98:TYR:CE2	0.47	2.44	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:92:ILE:HD12	1:A:92:ILE:N	0.47	2.25	2	8
1:A:113:MET:O	1:A:115:GLY:N	0.47	2.47	8	1
1:A:43:GLU:O	1:A:58:TRP:NE1	0.46	2.48	8	4
1:A:58:TRP:CZ3	1:A:141:LYS:CB	0.46	2.99	14	3
1:A:75:ILE:HG23	1:A:148:ARG:HG3	0.46	1.87	7	1
1:A:94:CYS:HB2	1:A:98:TYR:CG	0.46	2.46	8	1
1:A:111:ILE:HD13	1:A:112:ASN:N	0.46	2.26	1	3
1:A:83:TYR:CE1	1:A:151:MET:CE	0.45	2.99	14	1
1:A:107:PHE:HE1	1:A:147:LEU:HD13	0.45	1.65	11	2
1:A:103:PRO:CD	1:A:134:TRP:CZ3	0.45	3.00	9	1
1:A:138:TYR:HD1	1:A:142:VAL:HG11	0.45	1.64	8	1
1:A:75:ILE:HB	1:A:88:TYR:HB2	0.45	1.88	11	1
1:A:81:THR:HG22	1:A:157:MET:CB	0.45	2.42	3	1
1:A:71:TRP:CD2	1:A:140:ILE:HD11	0.45	2.47	4	2
1:A:135:GLN:NE2	1:A:138:TYR:CZ	0.45	2.85	14	1
1:A:116:VAL:HG22	1:A:123:VAL:CG1	0.45	2.37	1	3
1:A:110:LYS:CG	1:A:166:GLN:O	0.45	2.65	2	1
1:A:58:TRP:CH2	1:A:141:LYS:HB2	0.44	2.48	13	3
1:A:80:ARG:N	1:A:84:GLU:HG3	0.44	2.27	3	3
1:A:90:LEU:CD2	1:A:147:LEU:HD12	0.44	2.42	11	1
1:A:113:MET:HE1	1:A:147:LEU:O	0.44	2.13	14	2
1:A:59:GLY:O	1:A:71:TRP:CE3	0.44	2.71	10	4
1:A:88:TYR:CD2	1:A:109:THR:HG21	0.44	2.48	2	1
1:A:105:VAL:HG21	1:A:143:VAL:CG1	0.44	2.42	14	1
1:A:58:TRP:CZ2	1:A:141:LYS:HB3	0.44	2.48	11	1
1:A:102:PRO:HB3	1:A:131:LEU:HD23	0.44	1.90	4	1
1:A:107:PHE:CD2	1:A:111:ILE:CG2	0.44	2.95	11	2
1:A:58:TRP:O	1:A:58:TRP:CD1	0.44	2.70	2	6
1:A:98:TYR:OH	1:A:140:ILE:CG1	0.44	2.66	15	2
1:A:80:ARG:O	1:A:81:THR:CG2	0.44	2.66	12	8
1:A:110:LYS:CG	1:A:166:GLN:CG	0.44	2.96	6	1
1:A:50:GLY:O	1:A:51:VAL:O	0.43	2.36	13	1
1:A:108:VAL:HG12	1:A:167:CYS:HB2	0.43	1.89	4	1
1:A:91:LYS:HE3	1:A:108:VAL:HG21	0.43	1.89	10	1
1:A:87:ILE:CG2	1:A:88:TYR:N	0.43	2.81	15	11
1:A:82:ILE:HG22	1:A:83:TYR:CD1	0.43	2.48	7	1
1:A:39:ARG:O	1:A:43:GLU:HG2	0.43	2.14	1	2
1:A:125:PRO:HB3	1:A:131:LEU:HD22	0.43	1.91	4	1
1:A:40:LEU:HB3	1:A:68:LEU:HD13	0.43	1.88	11	1
1:A:44:LEU:HD13	1:A:71:TRP:CZ3	0.43	2.48	5	3
1:A:73:GLY:O	1:A:90:LEU:CD1	0.43	2.67	13	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:120:ASN:CG	1:A:122:VAL:HG23	0.43	2.34	4	1
1:A:123:VAL:HG12	1:A:128:ILE:HG13	0.43	1.91	6	1
1:A:98:TYR:OH	1:A:140:ILE:HG12	0.43	2.14	8	1
1:A:82:ILE:HB	1:A:157:MET:O	0.43	2.14	14	1
1:A:40:LEU:CD2	1:A:68:LEU:HB2	0.43	2.42	3	1
1:A:75:ILE:HD12	1:A:90:LEU:CD1	0.43	2.43	8	1
1:A:130:VAL:HG23	1:A:131:LEU:CD2	0.43	2.44	14	1
1:A:58:TRP:CZ3	1:A:141:LYS:HB2	0.42	2.48	1	2
1:A:75:ILE:O	1:A:88:TYR:N	0.42	2.52	3	5
1:A:47:GLY:HA3	1:A:58:TRP:NE1	0.42	2.28	7	1
1:A:116:VAL:HG13	1:A:121:GLY:O	0.42	2.14	11	1
1:A:78:PRO:O	1:A:84:GLU:CB	0.42	2.67	7	5
1:A:107:PHE:CG	1:A:111:ILE:CG2	0.42	2.98	6	2
1:A:83:TYR:CD1	1:A:161:GLN:OE1	0.42	2.73	9	2
1:A:71:TRP:CD2	1:A:140:ILE:HD13	0.42	2.48	14	2
1:A:109:THR:O	1:A:168:TYR:CE2	0.42	2.72	11	9
1:A:148:ARG:HG3	1:A:149:ARG:N	0.42	2.30	6	1
1:A:44:LEU:HD13	1:A:60:LEU:HG	0.42	1.89	7	1
1:A:118:SER:O	1:A:168:TYR:CZ	0.42	2.73	11	1
1:A:73:GLY:HA3	1:A:144:LEU:HD11	0.42	1.90	1	1
1:A:40:LEU:HD22	1:A:71:TRP:HE1	0.42	1.74	8	1
1:A:110:LYS:HG2	1:A:166:GLN:O	0.42	2.15	2	1
1:A:39:ARG:O	1:A:43:GLU:CG	0.42	2.68	4	3
1:A:56:VAL:HG23	1:A:58:TRP:CZ3	0.42	2.50	5	1
1:A:146:GLU:CD	1:A:150:LEU:HD11	0.42	2.33	8	1
1:A:79:PRO:O	1:A:80:ARG:CB	0.42	2.67	15	1
1:A:83:TYR:CE2	1:A:161:GLN:OE1	0.42	2.72	13	1
1:A:115:GLY:O	1:A:124:ASP:N	0.41	2.52	4	5
1:A:130:VAL:HG13	1:A:146:GLU:CD	0.41	2.35	1	1
1:A:109:THR:OG1	1:A:110:LYS:N	0.41	2.53	4	2
1:A:148:ARG:CZ	1:A:152:MET:CE	0.41	2.99	1	1
1:A:58:TRP:CH2	1:A:141:LYS:HB3	0.41	2.50	3	2
1:A:103:PRO:CD	1:A:134:TRP:CE3	0.41	3.03	3	1
1:A:108:VAL:O	1:A:168:TYR:CD2	0.41	2.73	3	2
1:A:98:TYR:OH	1:A:140:ILE:N	0.41	2.54	11	1
1:A:71:TRP:HB2	1:A:92:ILE:O	0.41	2.15	3	1
1:A:83:TYR:CE1	1:A:161:GLN:OE1	0.41	2.74	6	2
1:A:90:LEU:CD2	1:A:107:PHE:CE2	0.41	2.97	9	1
1:A:36:ARG:HG3	1:A:37:ASN:N	0.41	2.30	10	1
1:A:81:THR:O	1:A:84:GLU:HB3	0.41	2.16	2	1
1:A:83:TYR:CE2	1:A:88:TYR:CZ	0.41	3.09	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:71:TRP:CE2	1:A:140:ILE:CD1	0.41	3.03	3	1
1:A:47:GLY:CA	1:A:58:TRP:NE1	0.41	2.84	7	1
1:A:83:TYR:CZ	1:A:161:GLN:OE1	0.41	2.74	10	1
1:A:40:LEU:HD22	1:A:71:TRP:HZ2	0.41	1.68	11	1
1:A:128:ILE:CG2	1:A:130:VAL:CG2	0.41	2.99	13	1
1:A:92:ILE:N	1:A:92:ILE:HD12	0.41	2.31	6	1
1:A:83:TYR:CE1	1:A:151:MET:O	0.41	2.75	7	1
1:A:120:ASN:HB3	1:A:122:VAL:HG23	0.41	1.92	10	1
1:A:115:GLY:CA	1:A:127:ALA:CB	0.41	2.99	12	1
1:A:58:TRP:CD1	1:A:58:TRP:O	0.40	2.74	8	1
1:A:82:ILE:HG23	1:A:161:GLN:HG3	0.40	1.94	7	1
1:A:98:TYR:CE1	1:A:103:PRO:HG3	0.40	2.52	8	1
1:A:109:THR:O	1:A:168:TYR:CD2	0.40	2.74	13	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	124/170 (73%)	105±4 (85±3%)	17±3 (13±3%)	2±1 (2±1%)	13	57
All	All	1860/2550 (73%)	1580 (85%)	250 (13%)	30 (2%)	13	57

All 12 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	52	GLY	5
1	A	98	TYR	4
1	A	49	LYS	3
1	A	80	ARG	3
1	A	84	GLU	3
1	A	103	PRO	3
1	A	96	PRO	3
1	A	119	SER	2
1	A	114	ASN	1

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Mol	Chain	Res	Type	Models (Total)
1	A	87	ILE	1
1	A	51	VAL	1
1	A	79	PRO	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	111/152 (73%)	91±4 (82±3%)	20±4 (18±3%)	4 37
All	All	1665/2280 (73%)	1358 (82%)	307 (18%)	4 37

All 64 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	51	VAL	15
1	A	68	LEU	15
1	A	82	ILE	15
1	A	111	ILE	13
1	A	72	THR	12
1	A	38	PHE	11
1	A	80	ARG	11
1	A	46	GLU	10
1	A	126	ARG	10
1	A	70	ARG	9
1	A	57	SER	9
1	A	36	ARG	8
1	A	157	MET	8
1	A	69	THR	8
1	A	97	LYS	7
1	A	124	ASP	7
1	A	91	LYS	6
1	A	148	ARG	6
1	A	135	GLN	6
1	A	53	ASP	5
1	A	106	ARG	5
1	A	119	SER	5

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Mol	Chain	Res	Type	Models (Total)
1	A	137	SER	5
1	A	49	LYS	5
1	A	149	ARG	5
1	A	153	SER	5
1	A	166	GLN	5
1	A	155	GLU	5
1	A	131	LEU	4
1	A	146	GLU	4
1	A	139	SER	4
1	A	114	ASN	3
1	A	154	LYS	3
1	A	129	SER	3
1	A	39	ARG	3
1	A	100	GLU	3
1	A	93	GLU	3
1	A	133	LYS	3
1	A	117	ASN	3
1	A	61	GLU	2
1	A	42	GLU	2
1	A	113	MET	2
1	A	98	TYR	2
1	A	136	ASN	2
1	A	141	LYS	2
1	A	168	TYR	2
1	A	85	ASN	2
1	A	156	ASN	2
1	A	152	MET	2
1	A	86	ARG	2
1	A	158	LYS	2
1	A	84	GLU	2
1	A	45	GLU	2
1	A	150	LEU	2
1	A	48	GLN	1
1	A	40	LEU	1
1	A	81	THR	1
1	A	118	SER	1
1	A	60	LEU	1
1	A	89	SER	1
1	A	37	ASN	1
1	A	110	LYS	1
1	A	161	GLN	1
1	A	120	ASN	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 monosaccharides 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 (i)

No chemical shift data were provided