



Full wwPDB NMR Structure Validation Report ⓘ

Mar 26, 2026 – 03:40 AM UTC

PDB ID : 2KR0 / pdb_00002kr0
Title : Solution structure of the proteasome ubiquitin receptor Rpn13
Authors : Chen, X.; Lee, B.; Finley, D.; Walters, K.J.
Deposited on : 2009-11-25

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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

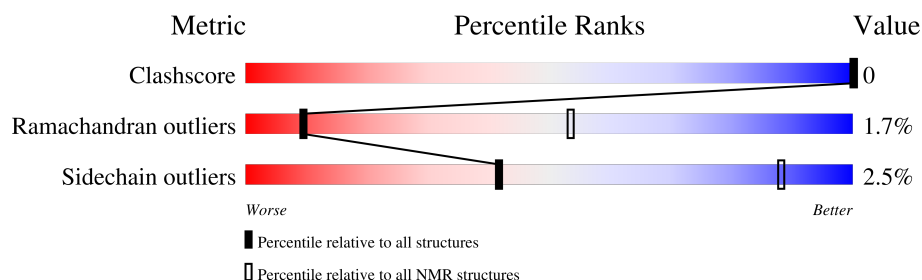
1 Overall quality at a glance

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	411	

2 Ensemble composition and analysis

This entry contains 31 models. Model 4 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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:22-A:131, A:286-A:385 (210)	0.87	4

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 1 single-model cluster was found.

Cluster number	Models
1	2, 6, 8, 11, 12, 13, 15, 17, 19, 22, 23, 27, 29
2	3, 4, 5, 9, 10, 18, 25, 26, 28
3	7, 16, 21, 24, 30, 31
4	1, 14
Single-model clusters	20

3 Entry composition [i](#)

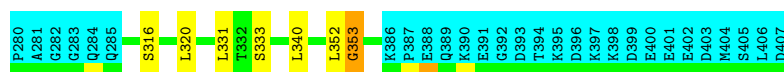
There is only 1 type of molecule in this entry. The entry contains 5853 atoms, of which 2901 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Proteasomal ubiquitin receptor ADRM1.

Mol	Chain	Residues	Atoms						Trace
1	A	407	Total	C	H	N	O	S	0
			5853	1825	2901	506	604	17	

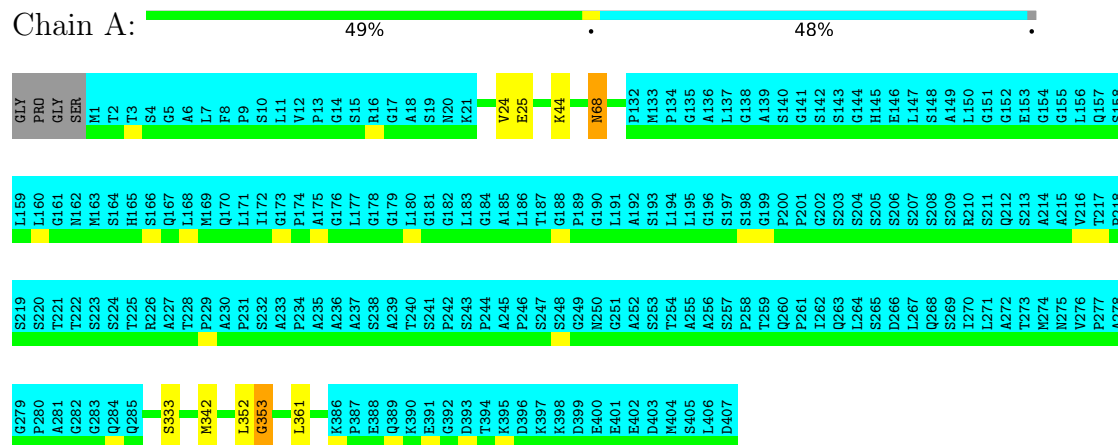
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP Q16186
A	-2	PRO	-	expression tag	UNP Q16186
A	-1	GLY	-	expression tag	UNP Q16186
A	0	SER	-	expression tag	UNP Q16186



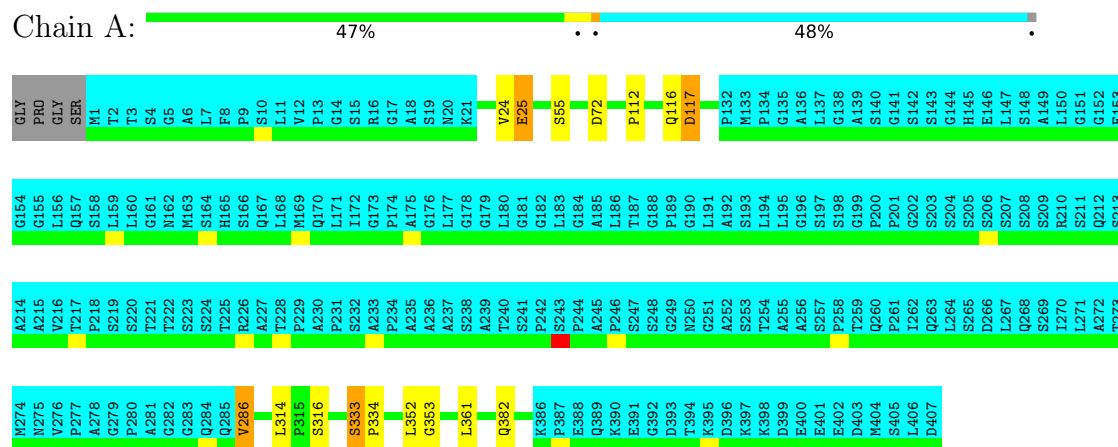
4.2.2 Score per residue for model 2

- Molecule 1: Proteasomal ubiquitin receptor ADRM1



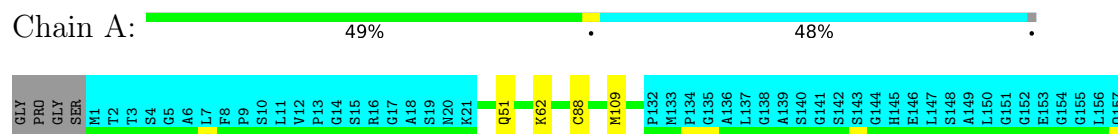
4.2.3 Score per residue for model 3

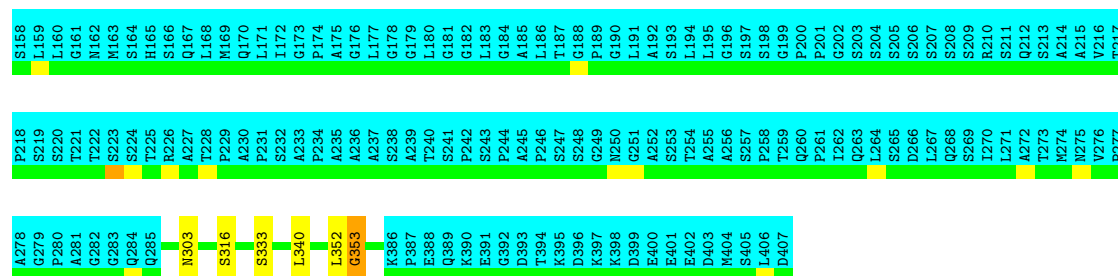
- Molecule 1: Proteasomal ubiquitin receptor ADRM1



4.2.4 Score per residue for model 4 (medoid)

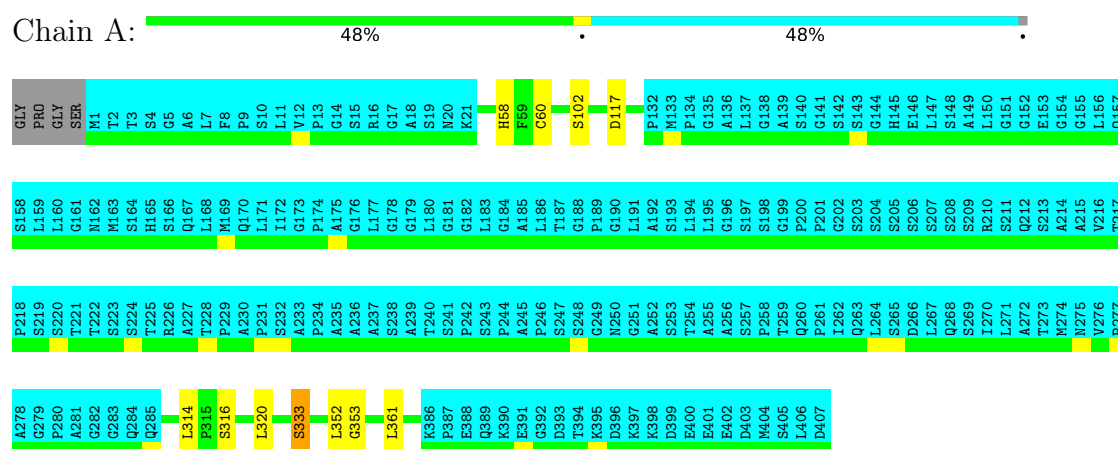
- Molecule 1: Proteasomal ubiquitin receptor ADRM1





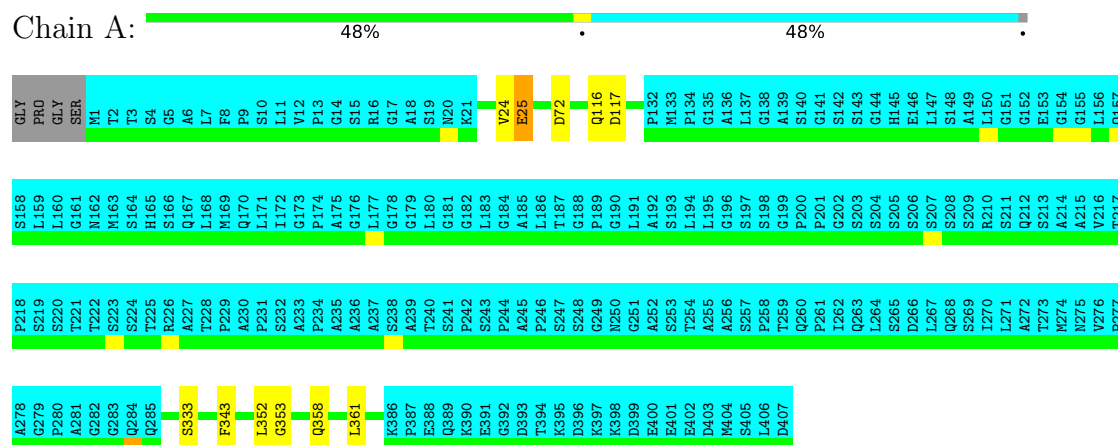
4.2.5 Score per residue for model 5

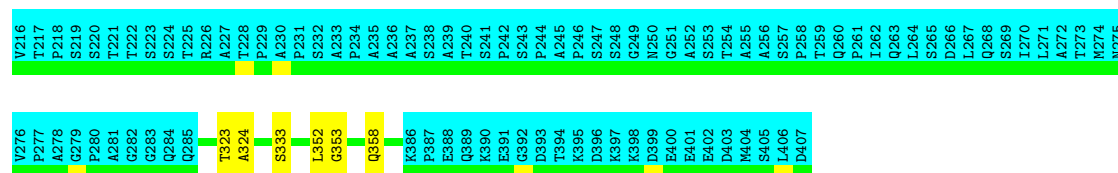
- Molecule 1: Proteasomal ubiquitin receptor ADRM1



4.2.6 Score per residue for model 6

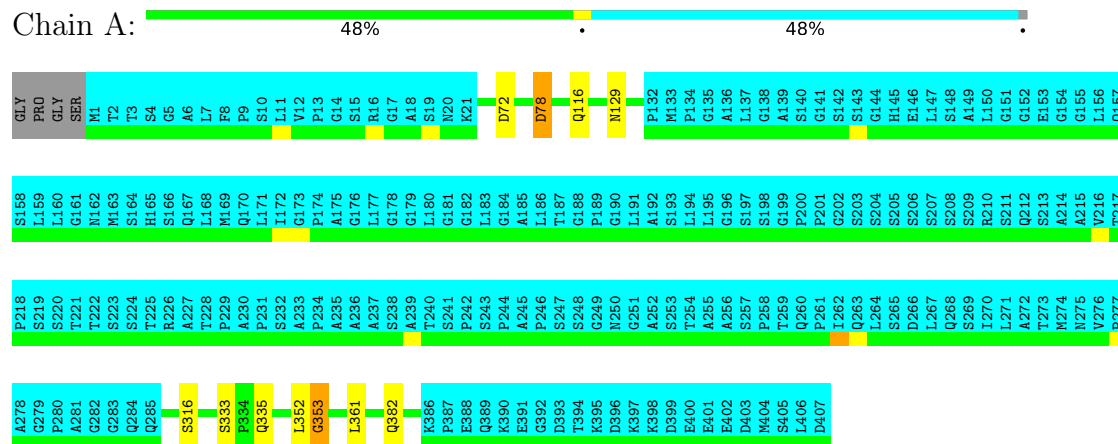
- Molecule 1: Proteasomal ubiquitin receptor ADRM1





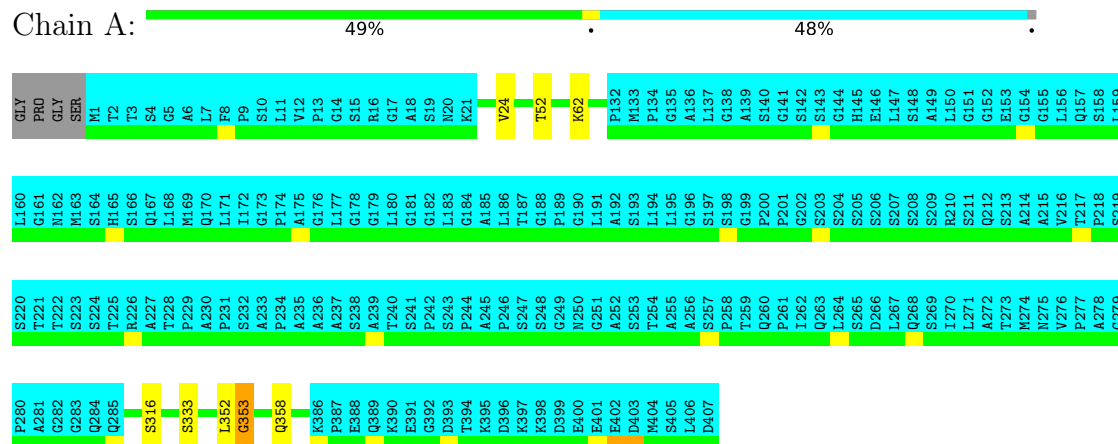
4.2.10 Score per residue for model 10

- Molecule 1: Proteasomal ubiquitin receptor ADRM1



4.2.11 Score per residue for model 11

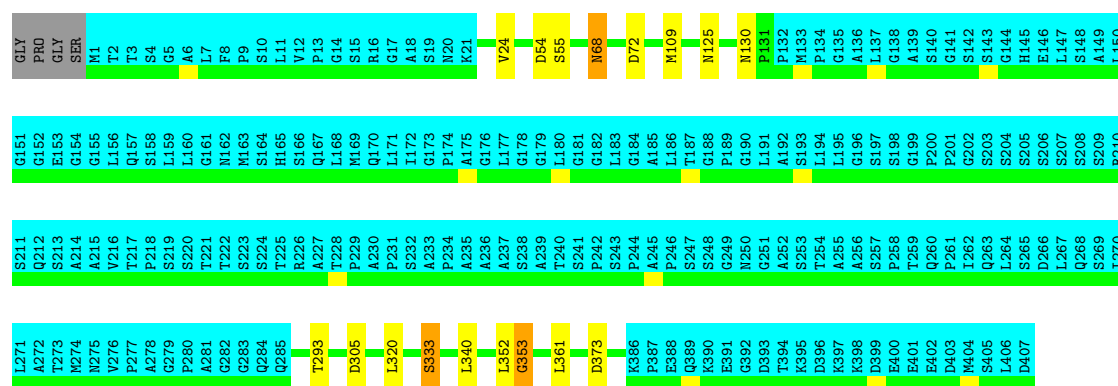
- Molecule 1: Proteasomal ubiquitin receptor ADRM1



4.2.12 Score per residue for model 12

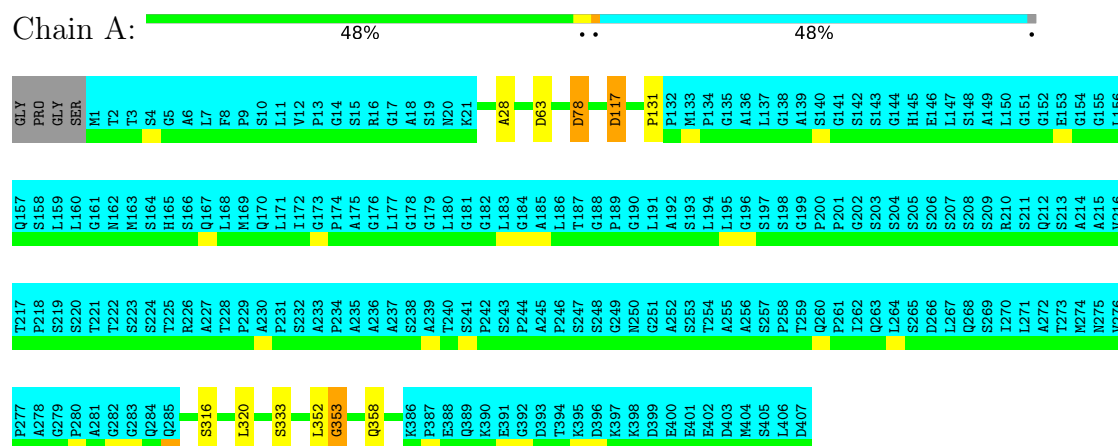
- Molecule 1: Proteasomal ubiquitin receptor ADRM1





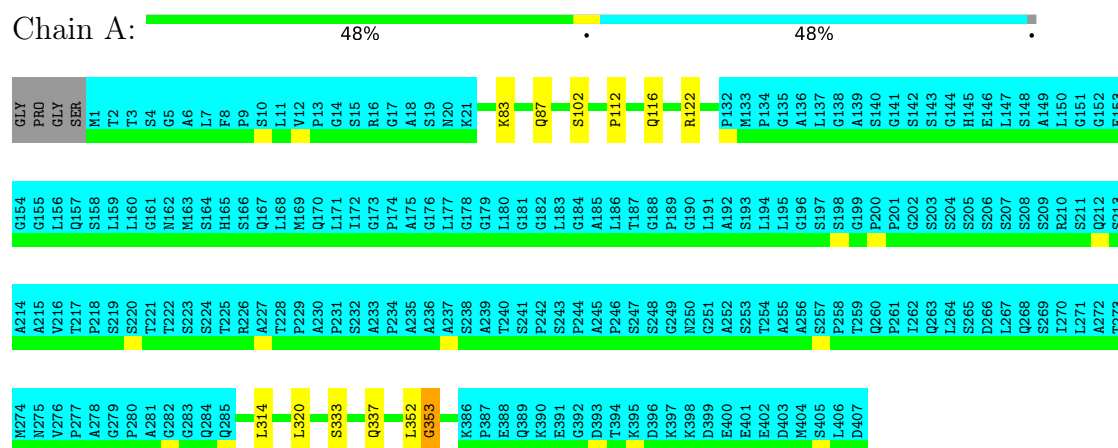
4.2.13 Score per residue for model 13

- Molecule 1: Proteasomal ubiquitin receptor ADRM1



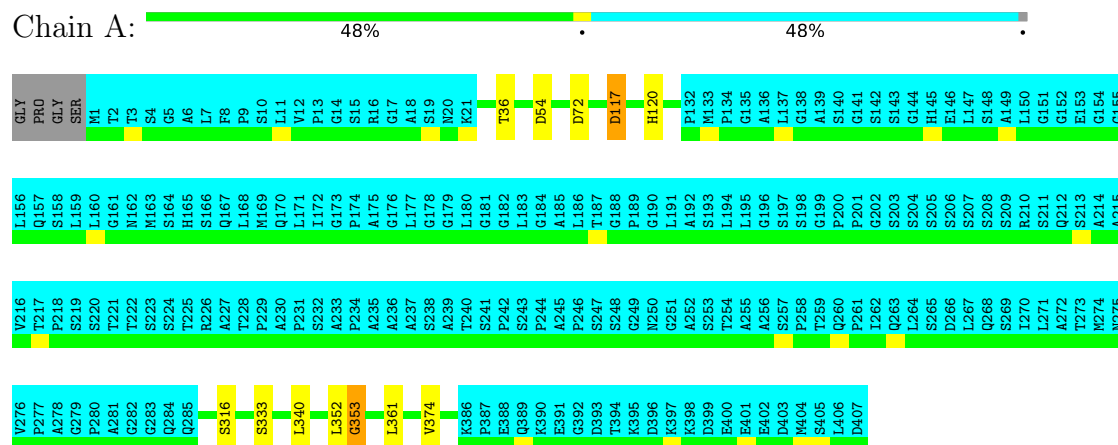
4.2.14 Score per residue for model 14

- Molecule 1: Proteasomal ubiquitin receptor ADRM1



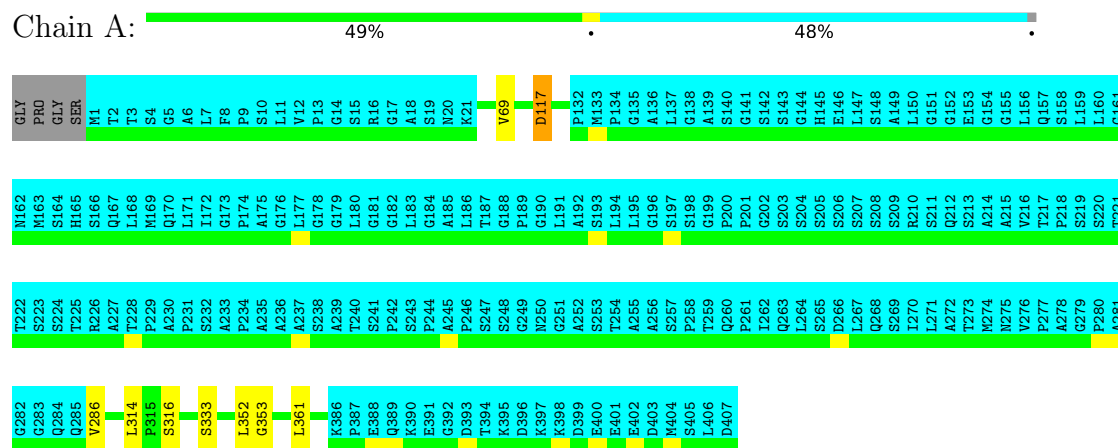
4.2.15 Score per residue for model 15

- Molecule 1: Proteasomal ubiquitin receptor ADRM1



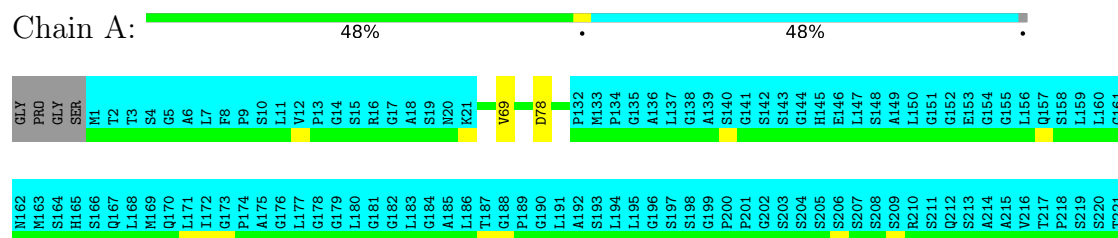
4.2.16 Score per residue for model 16

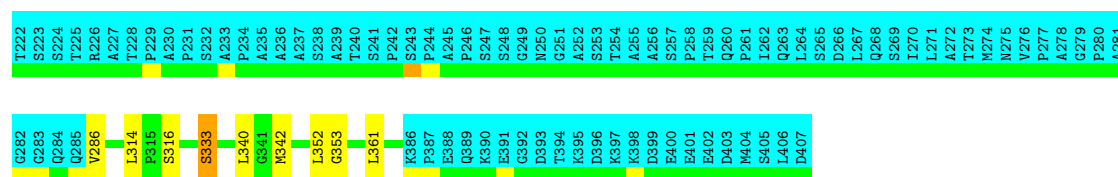
- Molecule 1: Proteasomal ubiquitin receptor ADRM1



4.2.17 Score per residue for model 17

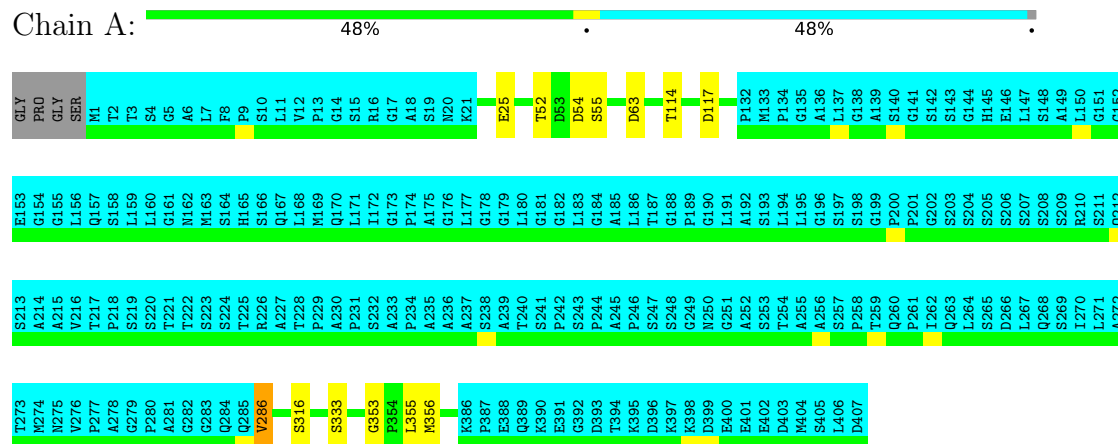
- Molecule 1: Proteasomal ubiquitin receptor ADRM1





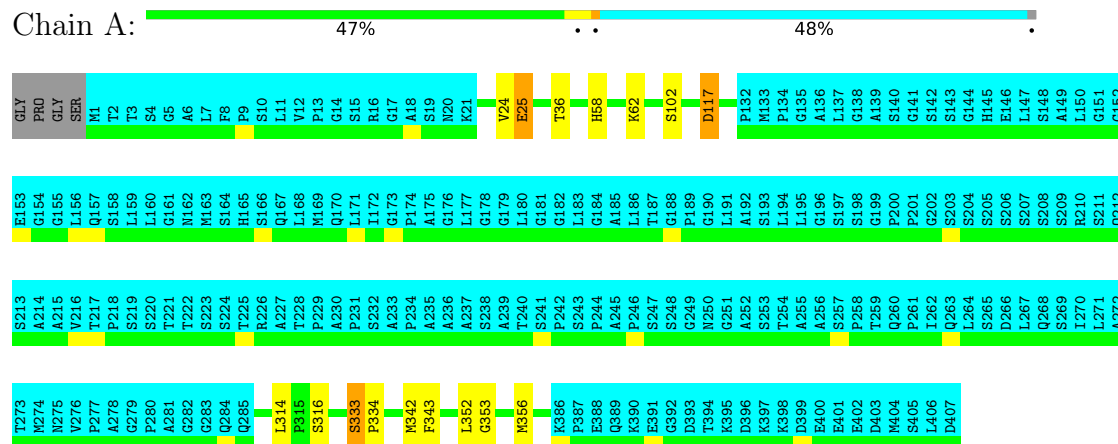
4.2.18 Score per residue for model 18

- Molecule 1: Proteasomal ubiquitin receptor ADRM1



4.2.19 Score per residue for model 19

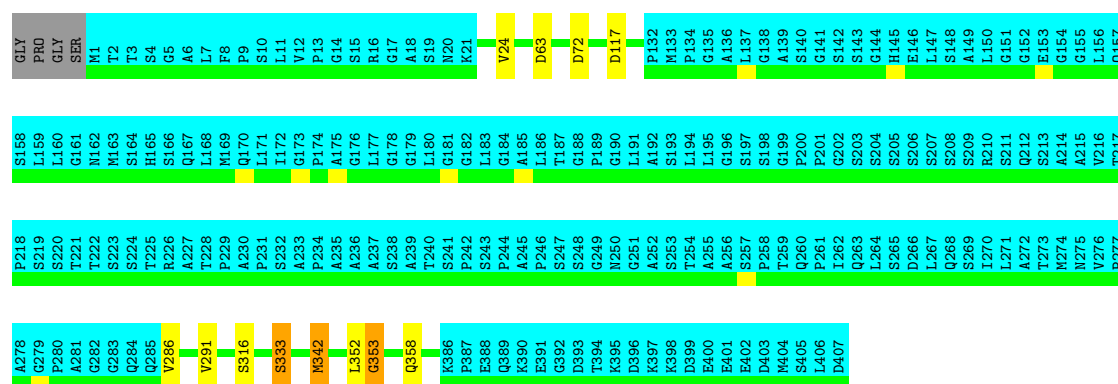
- Molecule 1: Proteasomal ubiquitin receptor ADRM1



4.2.20 Score per residue for model 20

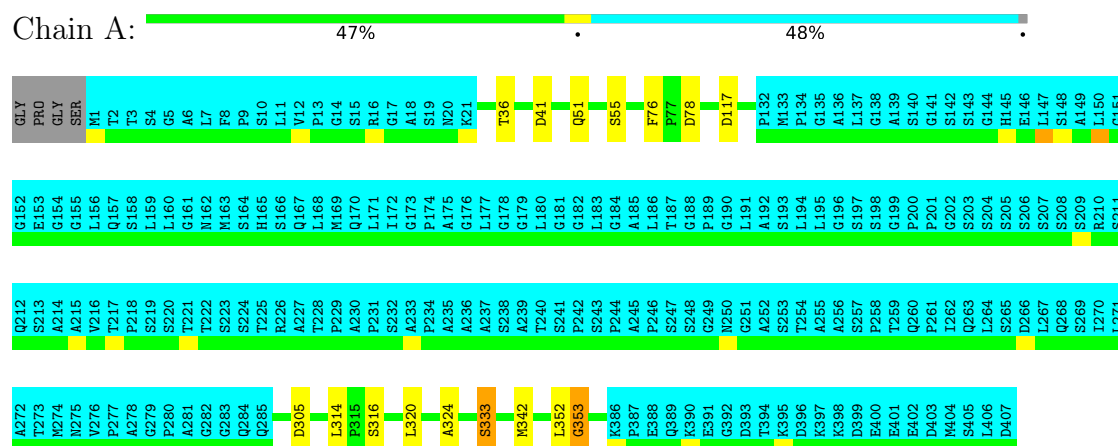
- Molecule 1: Proteasomal ubiquitin receptor ADRM1





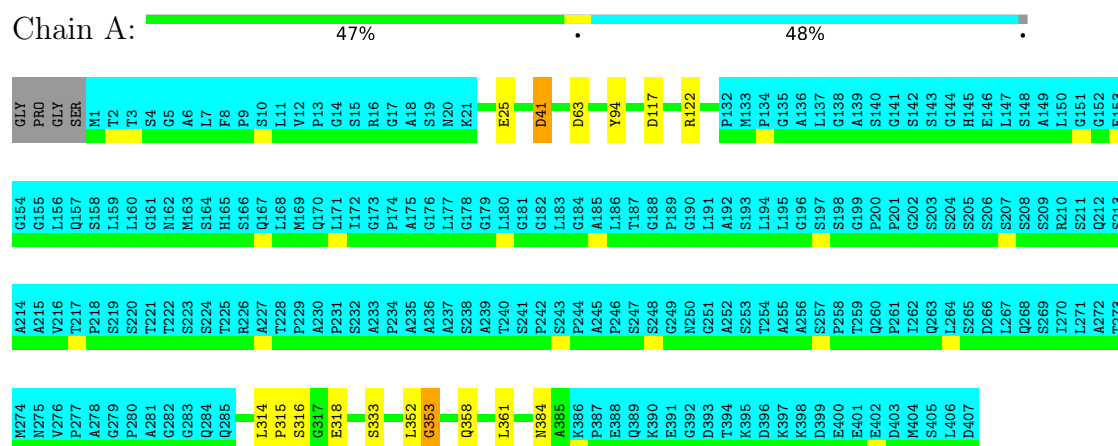
4.2.21 Score per residue for model 21

- Molecule 1: Proteasomal ubiquitin receptor ADRM1



4.2.22 Score per residue for model 22

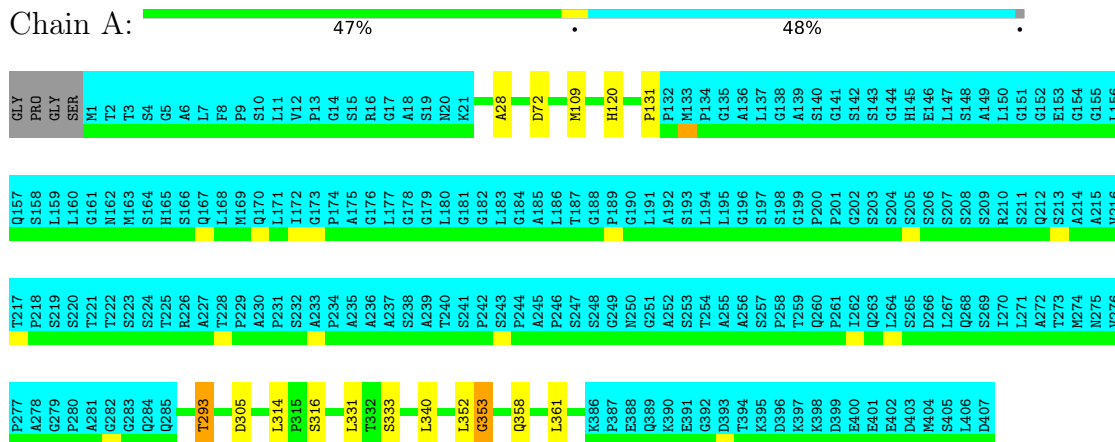
- Molecule 1: Proteasomal ubiquitin receptor ADRM1



4.2.23 Score per residue for model 23

- Molecule 1: Proteasomal ubiquitin receptor ADRM1

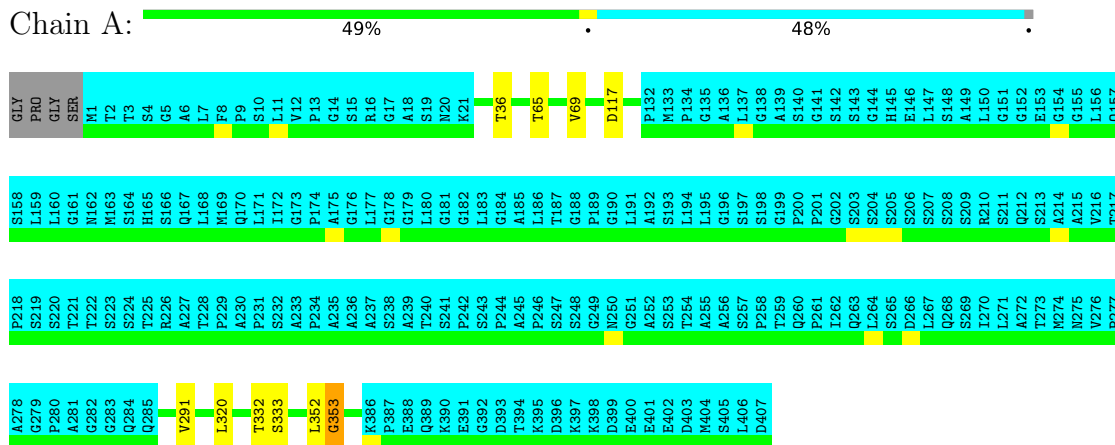
Chain A:



4.2.24 Score per residue for model 24

- Molecule 1: Proteasomal ubiquitin receptor ADRM1

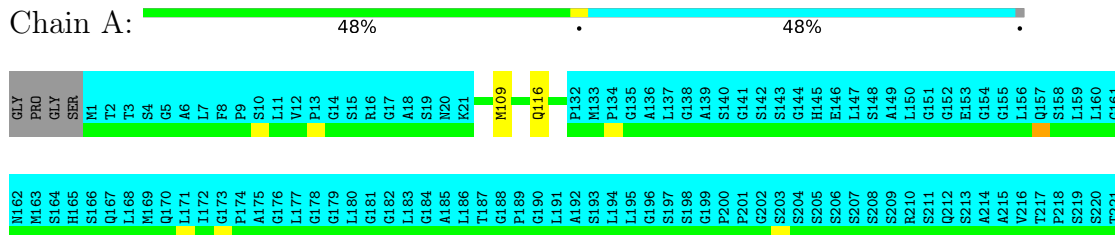
Chain A:

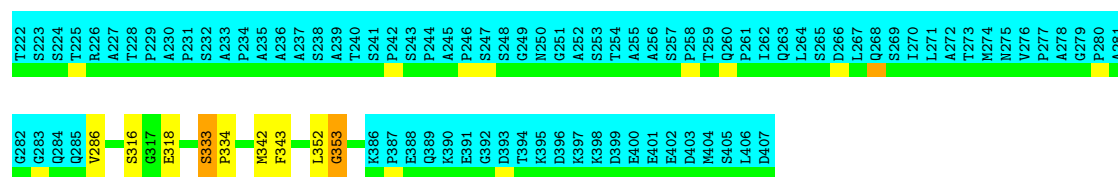


4.2.25 Score per residue for model 25

- Molecule 1: Proteasomal ubiquitin receptor ADRM1

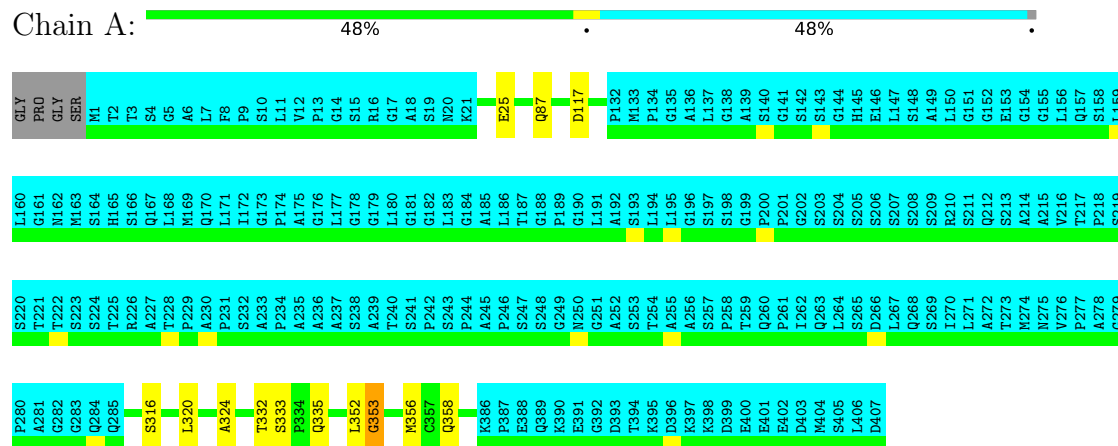
Chain A:





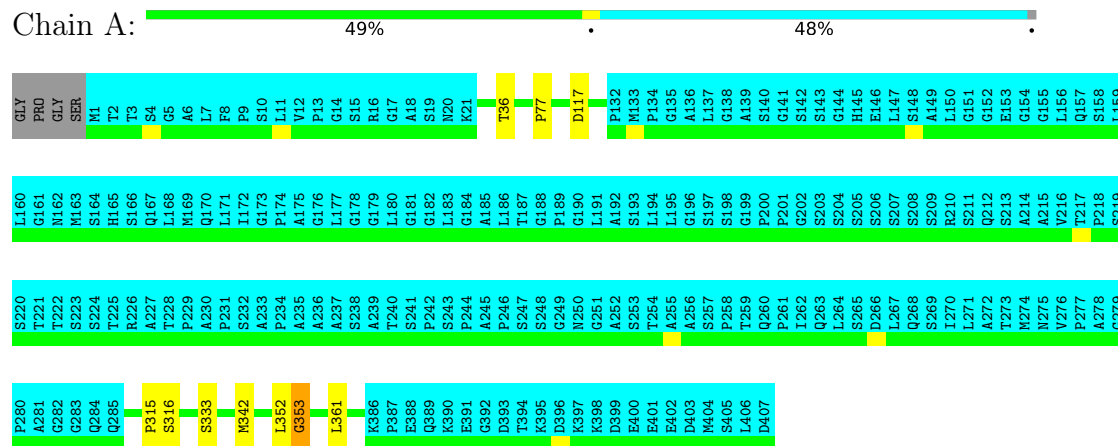
4.2.26 Score per residue for model 26

- Molecule 1: Proteasomal ubiquitin receptor ADRM1



4.2.27 Score per residue for model 27

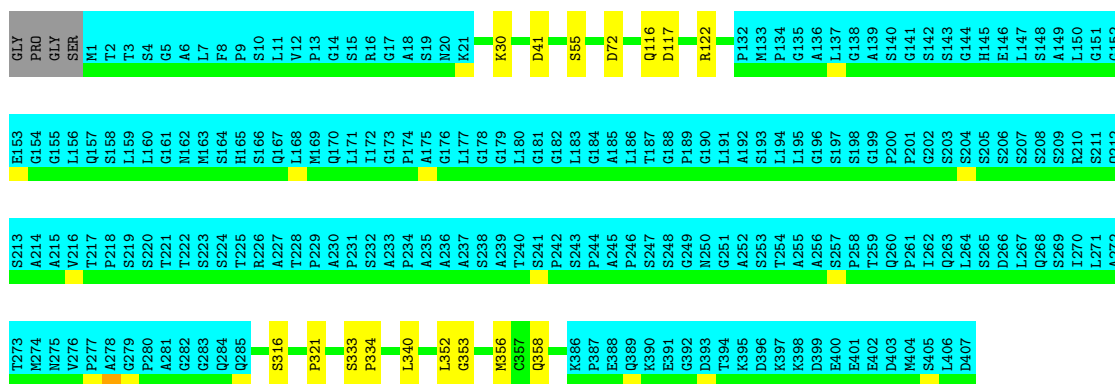
- Molecule 1: Proteasomal ubiquitin receptor ADRM1



4.2.28 Score per residue for model 28

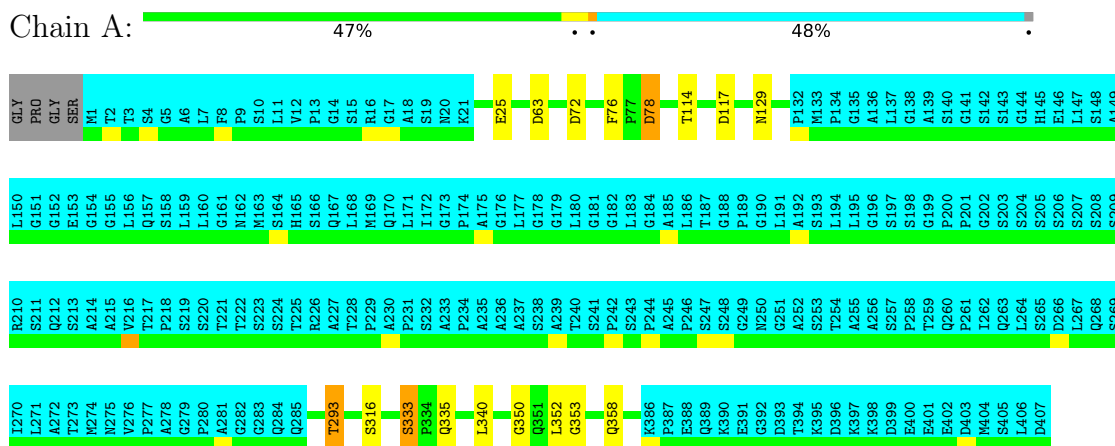
- Molecule 1: Proteasomal ubiquitin receptor ADRM1





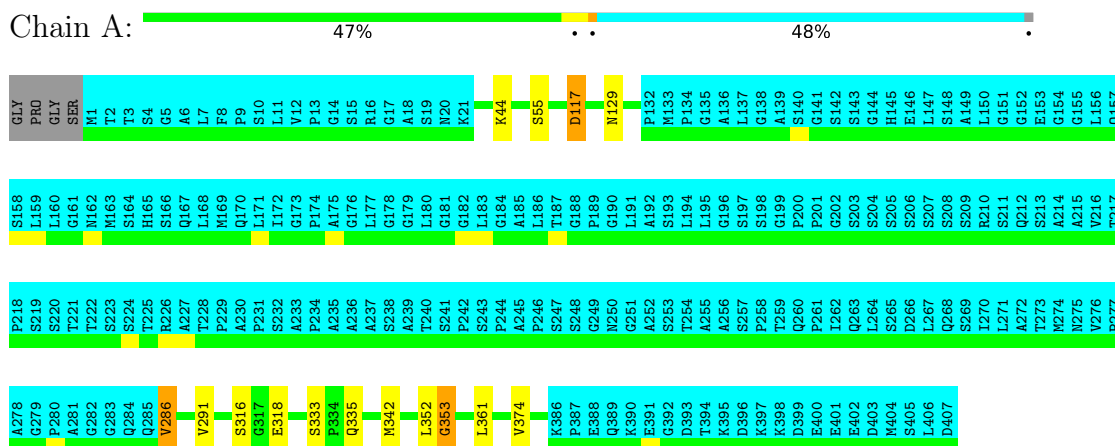
4.2.29 Score per residue for model 29

- Molecule 1: Proteasomal ubiquitin receptor ADRM1



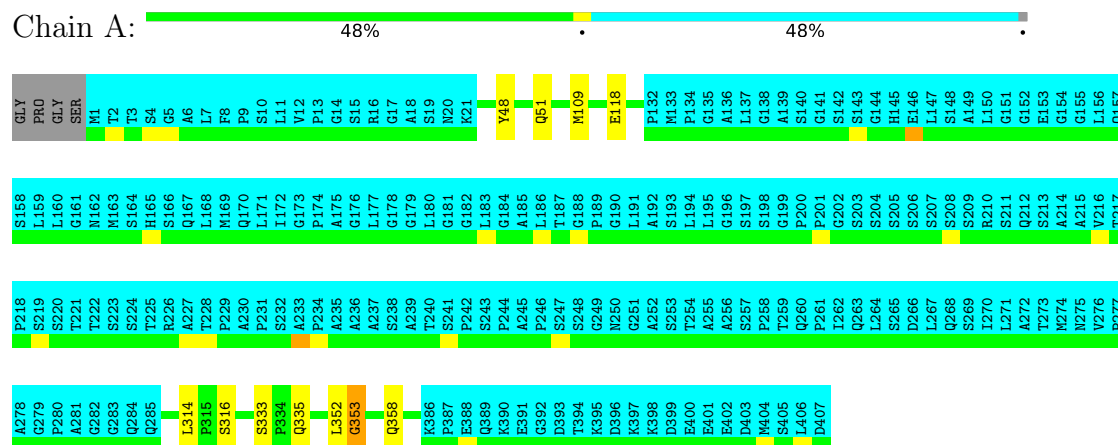
4.2.30 Score per residue for model 30

- Molecule 1: Proteasomal ubiquitin receptor ADRM1



4.2.31 Score per residue for model 31

● Molecule 1: Proteasomal ubiquitin receptor ADRM1



5 Refinement protocol and experimental data overview

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

Of the 50 calculated structures, 31 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
X-PLOR NIH	refinement	
X-PLOR NIH	structure solution	

No chemical shift data was provided.

6 Model quality

6.1 Standard geometry

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	0.86±0.01	0±0/1676 (0.0± 0.0%)	1.54±0.02	10±3/2274 (0.4± 0.1%)
All	All	0.86	0/51956 (0.0%)	1.54	316/70494 (0.4%)

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	0.1±0.2
All	All	0	2

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	41	ASP	CA-CB-CG	8.53	121.13	112.60	21	2
1	A	78	ASP	CB-CA-C	8.42	118.17	109.83	13	3
1	A	129	ASN	CA-CB-CG	7.51	120.11	112.60	10	4
1	A	63	ASP	CA-CB-CG	7.45	120.05	112.60	20	1
1	A	117	ASP	CA-CB-CG	7.41	120.01	112.60	20	18
1	A	125	ASN	CA-CB-CG	6.54	119.14	112.60	12	1
1	A	352	LEU	CA-C-N	6.42	131.96	121.87	29	29
1	A	352	LEU	C-N-CA	6.42	131.96	121.87	29	29
1	A	28	ALA	CA-C-N	6.36	126.57	122.18	23	2
1	A	28	ALA	C-N-CA	6.36	126.57	122.18	23	2
1	A	324	ALA	CA-C-N	6.19	128.57	120.28	26	3
1	A	324	ALA	C-N-CA	6.19	128.57	120.28	26	3
1	A	343	PHE	CA-CB-CG	5.96	119.76	113.80	19	4
1	A	131	PRO	CA-C-N	5.96	125.44	119.24	23	3
1	A	131	PRO	C-N-CA	5.96	125.44	119.24	23	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	68	ASN	CA-CB-CG	5.95	118.55	112.60	2	2
1	A	52	THR	CA-C-N	5.88	128.97	120.38	11	3
1	A	52	THR	C-N-CA	5.88	128.97	120.38	11	3
1	A	54	ASP	CA-CB-CG	5.77	118.37	112.60	12	1
1	A	25	GLU	CB-CA-C	5.71	119.50	109.80	3	6
1	A	314	LEU	CA-C-N	5.70	125.81	119.32	21	9
1	A	314	LEU	C-N-CA	5.70	125.81	119.32	21	9
1	A	78	ASP	CA-C-N	5.66	128.19	120.54	21	2
1	A	78	ASP	C-N-CA	5.66	128.19	120.54	21	2
1	A	333	SER	CA-C-N	5.61	125.08	119.24	20	6
1	A	333	SER	C-N-CA	5.61	125.08	119.24	20	6
1	A	373	ASP	CA-CB-CG	5.57	118.17	112.60	12	1
1	A	361	LEU	CA-C-N	5.56	125.56	119.89	3	14
1	A	361	LEU	C-N-CA	5.56	125.56	119.89	3	14
1	A	353	GLY	CA-C-N	5.50	125.59	119.32	26	21
1	A	353	GLY	C-N-CA	5.50	125.59	119.32	26	21
1	A	72	ASP	CA-CB-CG	5.49	118.09	112.60	3	2
1	A	44	LYS	CA-C-N	5.46	125.94	122.18	30	1
1	A	44	LYS	C-N-CA	5.46	125.94	122.18	30	1
1	A	116	GLN	CA-C-N	5.46	127.85	120.38	14	5
1	A	116	GLN	C-N-CA	5.46	127.85	120.38	14	5
1	A	34	LYS	CA-C-N	5.41	128.20	122.63	1	1
1	A	34	LYS	C-N-CA	5.41	128.20	122.63	1	1
1	A	374	VAL	CA-C-N	5.39	127.45	120.44	15	2
1	A	374	VAL	C-N-CA	5.39	127.45	120.44	15	2
1	A	315	PRO	CA-C-N	5.36	131.78	121.54	22	2
1	A	315	PRO	C-N-CA	5.36	131.78	121.54	22	2
1	A	55	SER	CB-CA-C	5.36	118.13	110.04	3	2
1	A	342	MET	CA-C-N	5.34	127.44	120.28	19	7
1	A	342	MET	C-N-CA	5.34	127.44	120.28	19	7
1	A	76	PHE	CA-C-N	5.34	125.64	119.93	29	2
1	A	76	PHE	C-N-CA	5.34	125.64	119.93	29	2
1	A	323	THR	CA-C-N	5.31	127.65	120.38	9	1
1	A	323	THR	C-N-CA	5.31	127.65	120.38	9	1
1	A	291	VAL	N-CA-C	-5.30	106.63	111.67	20	3
1	A	120	HIS	CA-CB-CG	5.30	119.10	113.80	23	2
1	A	337	GLN	CA-C-N	5.29	127.31	120.44	14	1
1	A	337	GLN	C-N-CA	5.29	127.31	120.44	14	1
1	A	334	PRO	CA-C-N	5.28	127.61	120.38	28	1
1	A	334	PRO	C-N-CA	5.28	127.61	120.38	28	1
1	A	102	SER	CA-C-N	5.28	128.21	120.71	5	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	102	SER	C-N-CA	5.28	128.21	120.71	5	1
1	A	54	ASP	CA-C-N	5.21	131.49	121.54	18	1
1	A	54	ASP	C-N-CA	5.21	131.49	121.54	18	1
1	A	320	LEU	CA-C-N	5.19	126.33	119.84	5	2
1	A	320	LEU	C-N-CA	5.19	126.33	119.84	5	2
1	A	88	CYS	CA-C-N	5.13	125.16	119.32	4	1
1	A	88	CYS	C-N-CA	5.13	125.16	119.32	4	1
1	A	130	ASN	CA-C-N	5.12	125.66	120.38	12	1
1	A	130	ASN	C-N-CA	5.12	125.66	120.38	12	1
1	A	286	VAL	CA-C-N	5.11	131.29	121.54	18	2
1	A	286	VAL	C-N-CA	5.11	131.29	121.54	18	2
1	A	114	THR	CA-C-N	5.09	127.61	120.28	29	2
1	A	114	THR	C-N-CA	5.09	127.61	120.28	29	2
1	A	303	ASN	CA-C-N	5.08	127.09	120.28	4	1
1	A	303	ASN	C-N-CA	5.08	127.09	120.28	4	1
1	A	286	VAL	CB-CA-C	5.06	119.59	111.29	30	1
1	A	293	THR	CA-C-N	5.05	125.08	119.32	23	2
1	A	293	THR	C-N-CA	5.05	125.08	119.32	23	2
1	A	350	GLY	CA-C-N	5.04	127.54	120.28	29	1
1	A	350	GLY	C-N-CA	5.04	127.54	120.28	29	1
1	A	78	ASP	CA-CB-CG	5.03	117.63	112.60	10	1
1	A	118	GLU	CA-C-N	5.03	127.27	120.38	31	1
1	A	118	GLU	C-N-CA	5.03	127.27	120.38	31	1
1	A	355	LEU	CA-C-N	5.01	127.25	120.38	18	1
1	A	355	LEU	C-N-CA	5.01	127.25	120.38	18	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	94	TYR	Sidechain	1
1	A	48	TYR	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	1640	1615	1615	0±0
All	All	50840	50065	50065	4

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:333:SER:H	1:A:334:PRO:CD	0.47	2.22	19	3
1:A:333:SER:H	1:A:334:PRO:HD2	0.45	1.72	19	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	210/411 (51%)	199±2 (95±1%)	8±2 (4±1%)	4±1 (2±0%)	9	53
All	All	6510/12741 (51%)	6157 (95%)	243 (4%)	110 (2%)	9	53

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	333	SER	31
1	A	353	GLY	31
1	A	316	SER	24
1	A	286	VAL	8
1	A	55	SER	6
1	A	112	PRO	2
1	A	77	PRO	2
1	A	102	SER	2
1	A	332	THR	2
1	A	287	ASP	1
1	A	321	PRO	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	179/324 (55%)	174±2 (97±1%)	5±2 (3±1%)	42	88
All	All	5549/10044 (55%)	5409 (97%)	140 (3%)	42	88

All 40 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	358	GLN	11
1	A	25	GLU	10
1	A	320	LEU	8
1	A	340	LEU	8
1	A	24	VAL	8
1	A	72	ASP	8
1	A	117	ASP	7
1	A	63	ASP	6
1	A	109	MET	6
1	A	335	GLN	5
1	A	36	THR	5
1	A	69	VAL	4
1	A	356	MET	4
1	A	51	GLN	3
1	A	62	LYS	3
1	A	78	ASP	3
1	A	293	THR	3
1	A	305	ASP	3
1	A	122	ARG	3
1	A	318	GLU	3
1	A	331	LEU	2
1	A	44	LYS	2
1	A	68	ASN	2
1	A	382	GLN	2
1	A	58	HIS	2
1	A	116	GLN	2
1	A	87	GLN	2
1	A	342	MET	2
1	A	41	ASP	2

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Mol	Chain	Res	Type	Models (Total)
1	A	286	VAL	1
1	A	60	CYS	1
1	A	97	LYS	1
1	A	83	LYS	1
1	A	314	LEU	1
1	A	54	ASP	1
1	A	333	SER	1
1	A	384	ASN	1
1	A	65	THR	1
1	A	30	LYS	1
1	A	352	LEU	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 oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided