



Full wwPDB NMR Structure Validation Report ⓘ

Apr 27, 2016 – 12:30 AM BST

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

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
<http://wwpdb.org/validation/2016/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
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

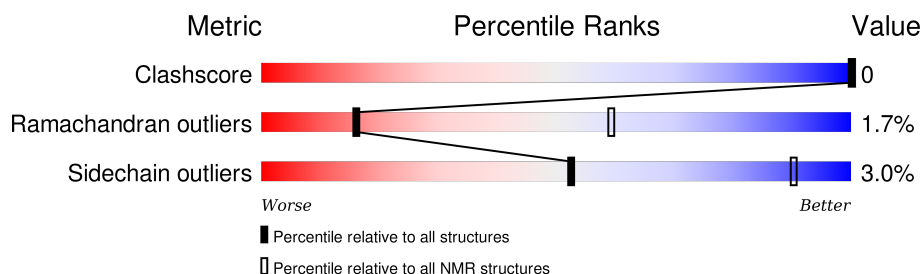
1 Overall quality at a glance

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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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	<div> <div>50%</div> <div>48%</div> </div>

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)	0.51	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](#)

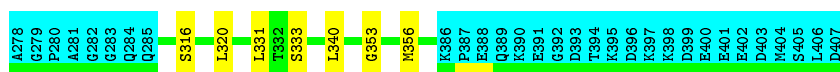
There is only 1 type of molecule in this entry. The entry contains 5853 atoms, of which 2901 are hydrogens and 0 are deuteriums.

- 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	

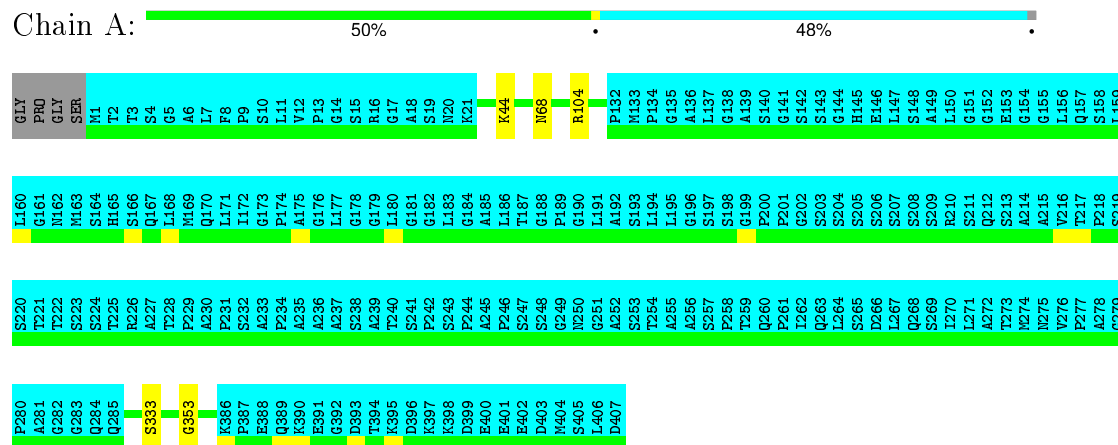
There are 4 discrepancies between the modelled and reference sequences:

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



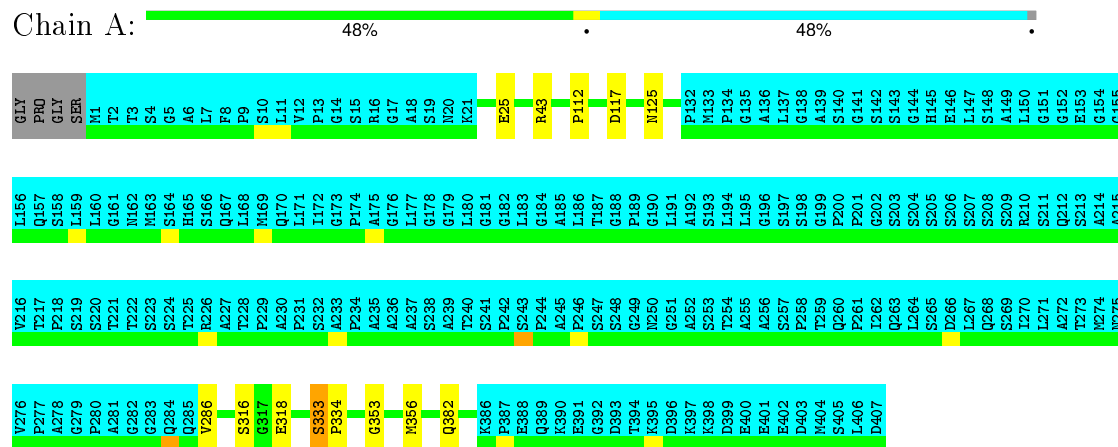
4.2.2 Score per residue for model 2

- Molecule 1: Proteasomal ubiquitin receptor ADRM1



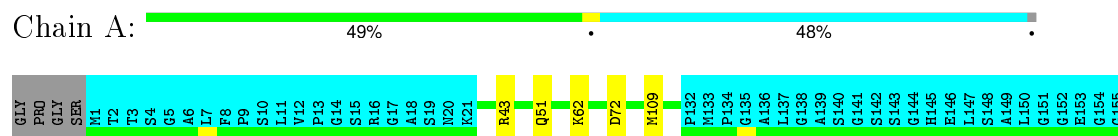
4.2.3 Score per residue for model 3

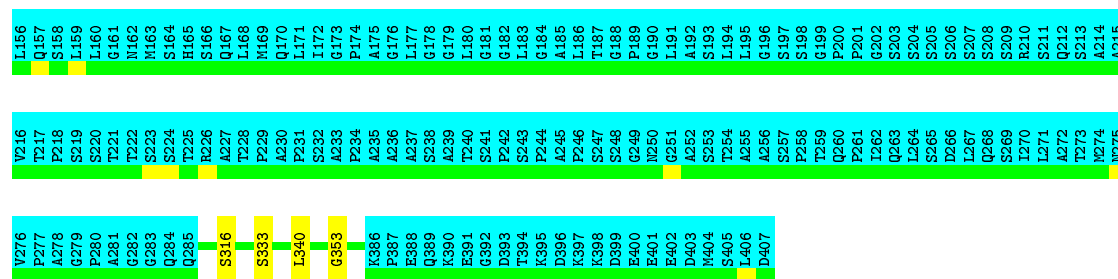
- Molecule 1: Proteasomal ubiquitin receptor ADRM1



4.2.4 Score per residue for model 4 (medoid)

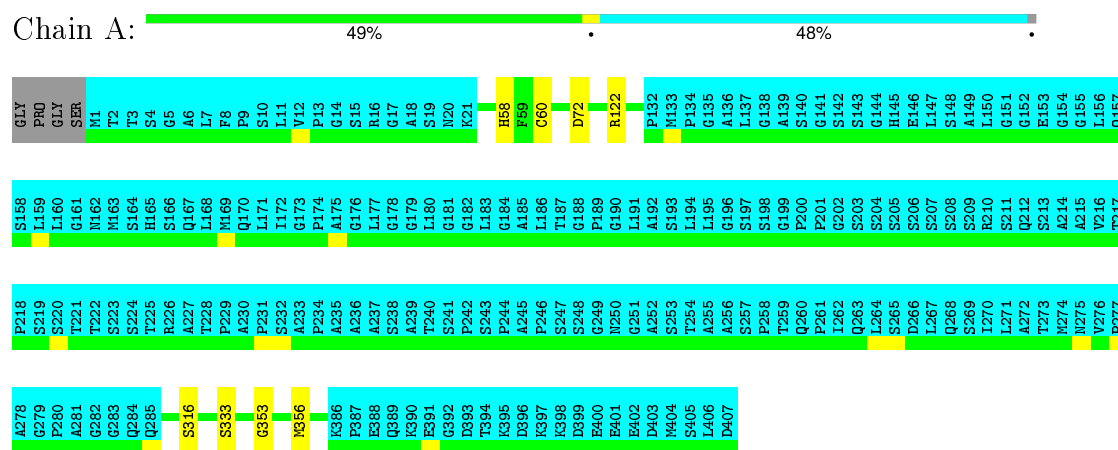
- Molecule 1: Proteasomal ubiquitin receptor ADRM1





4.2.5 Score per residue for model 5

- Molecule 1: Proteasomal ubiquitin receptor ADRM1



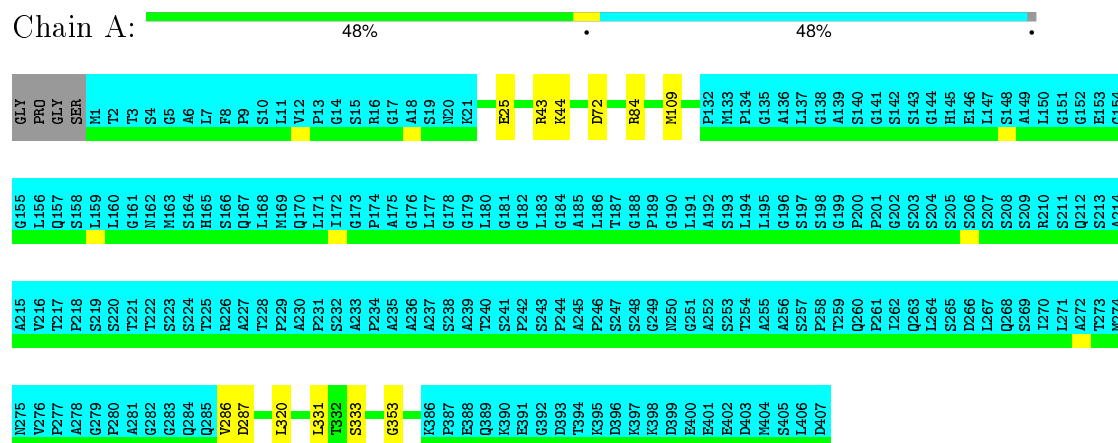
4.2.6 Score per residue for model 6

- Molecule 1: Proteasomal ubiquitin receptor ADRM1



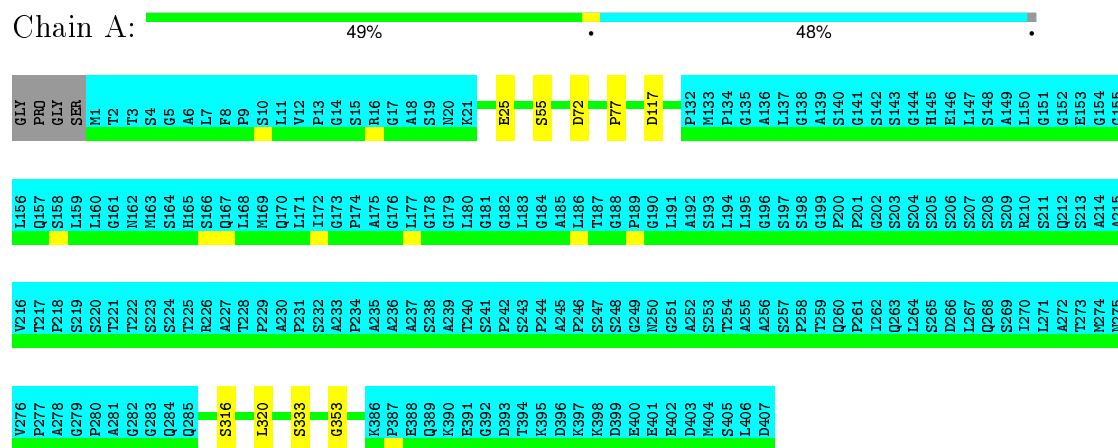
4.2.7 Score per residue for model 7

- Molecule 1: Proteasomal ubiquitin receptor ADRM1



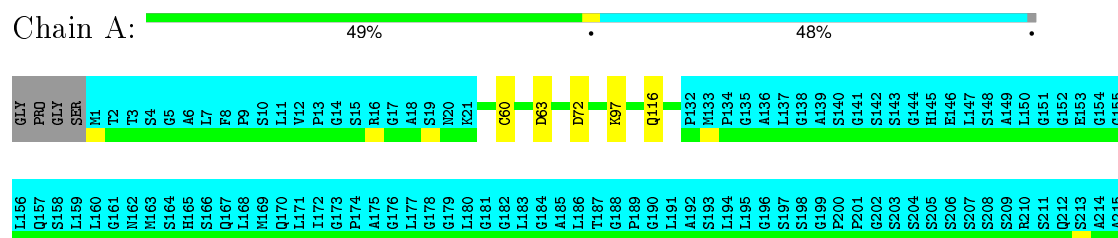
4.2.8 Score per residue for model 8

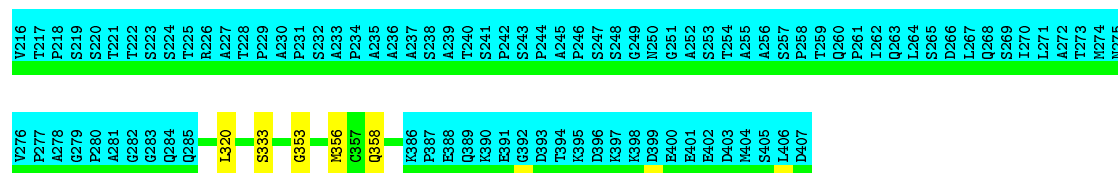
- Molecule 1: Proteasomal ubiquitin receptor ADRM1



4.2.9 Score per residue for model 9

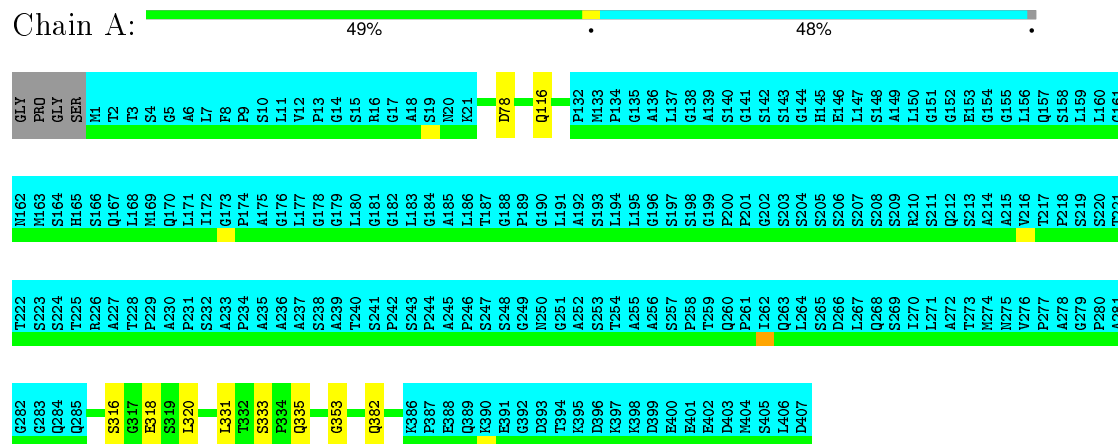
- Molecule 1: Proteasomal ubiquitin receptor ADRM1





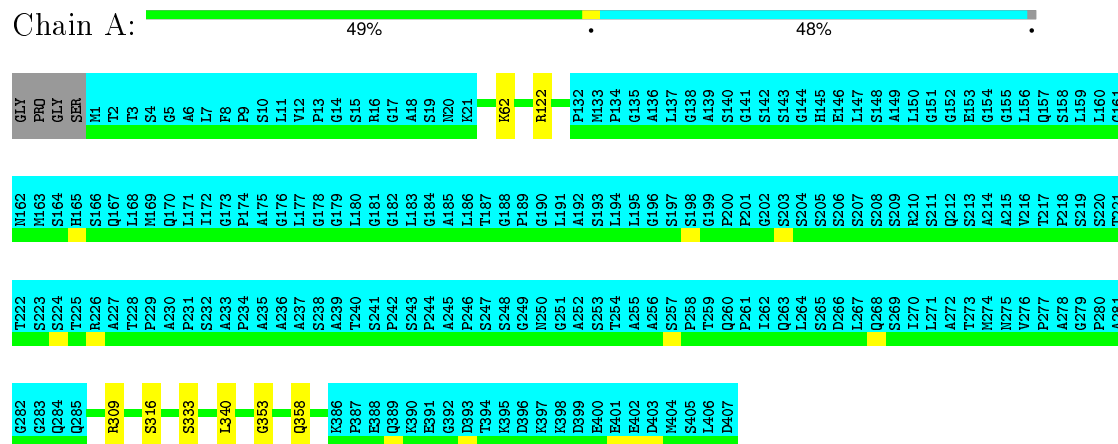
4.2.10 Score per residue for model 10

- Molecule 1: Proteasomal ubiquitin receptor ADRM1



4.2.11 Score per residue for model 11

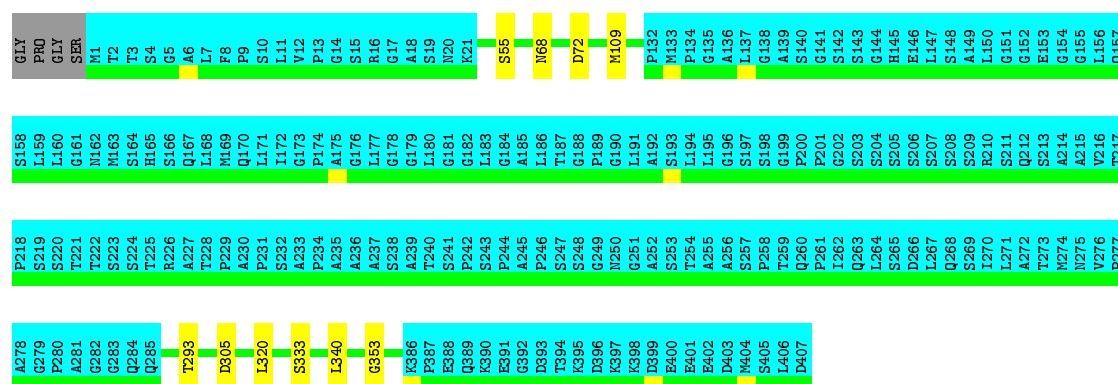
- Molecule 1: Proteasomal ubiquitin receptor ADRM1



4.2.12 Score per residue for model 12

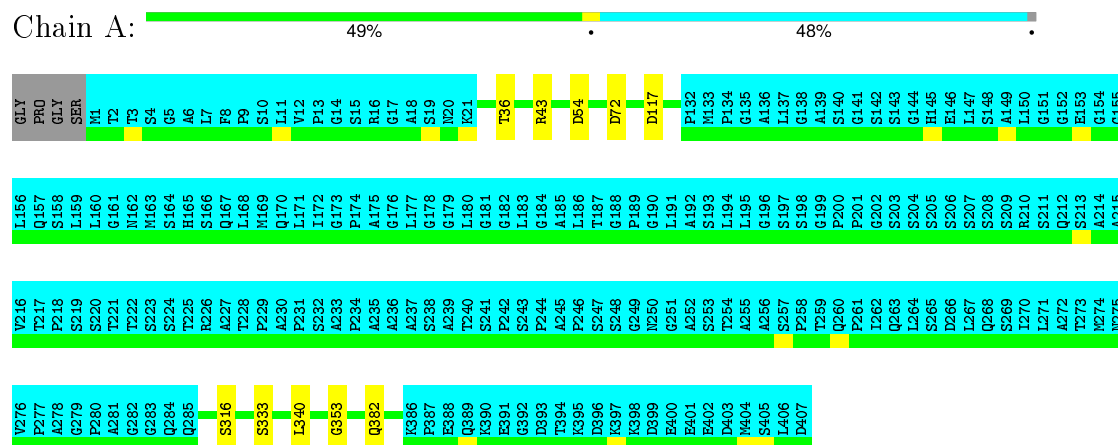
- Molecule 1: Proteasomal ubiquitin receptor ADRM1

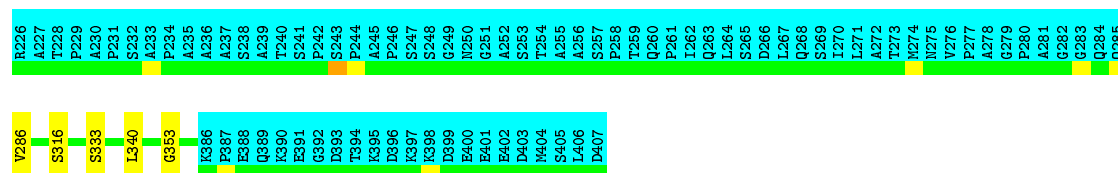




4.2.15 Score per residue for model 15

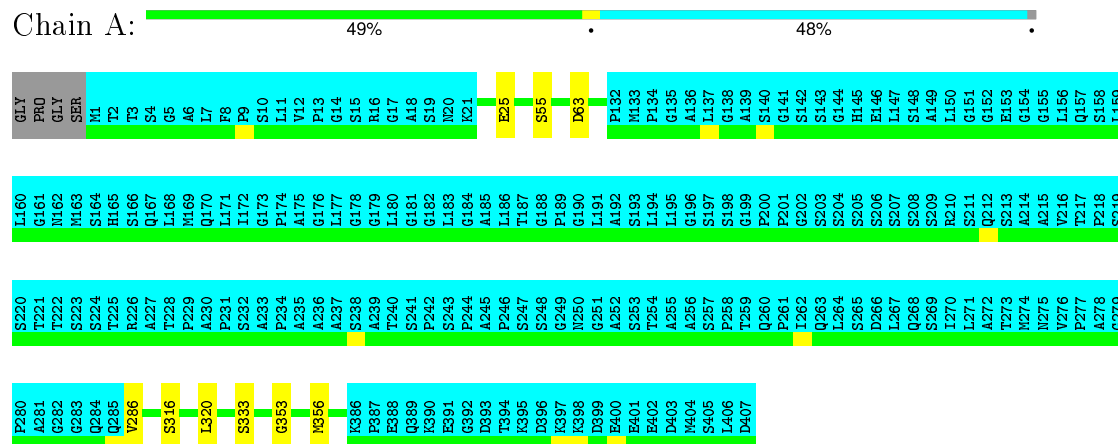
- Molecule 1: Proteasomal ubiquitin receptor ADRM1





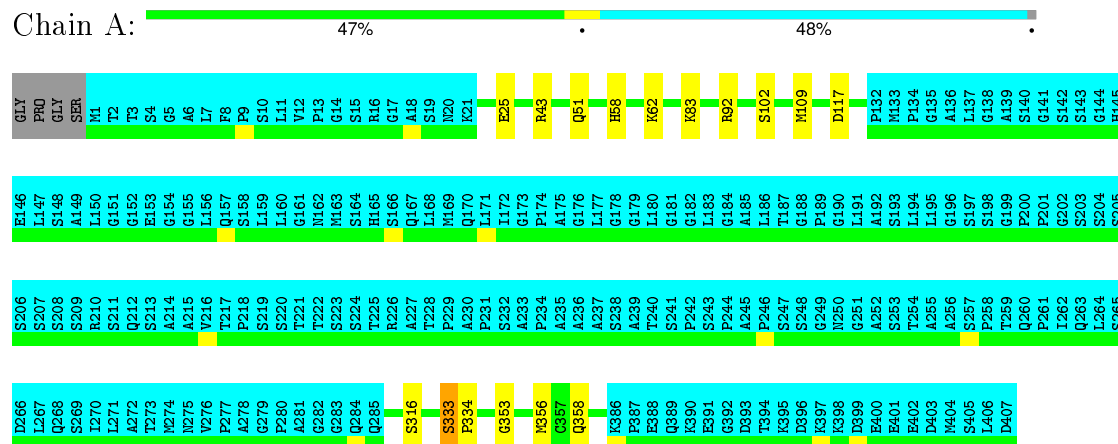
4.2.18 Score per residue for model 18

- 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

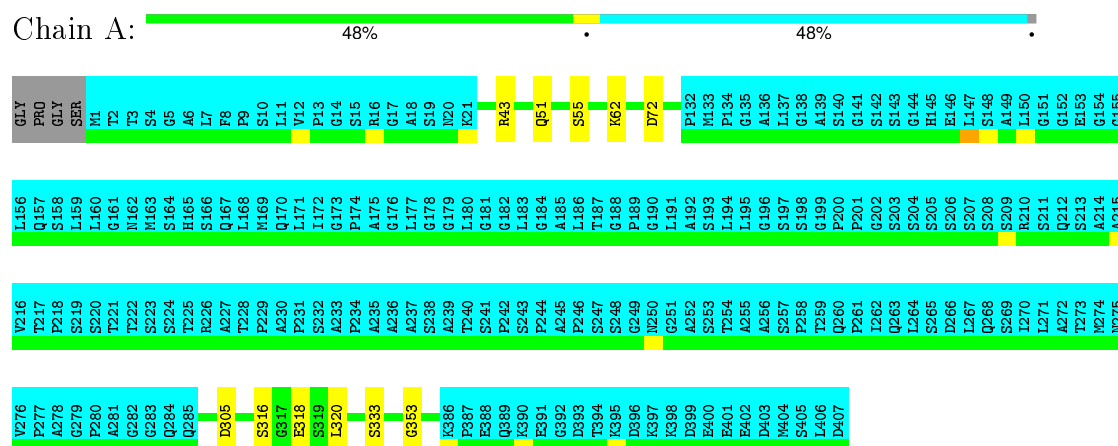
- Molecule 1: Proteasomal ubiquitin receptor ADRM1



Q284	Q285	V286	S316	S333	G353	Q358	K386	P387	E388	Q389	K390	E391	G392	D393	T394	K395	D396	K397	K398	D399	E400	E401	E402	D403	M404	S405	L406	D407	S164	H165	S166	Q167	M168	M169	Q170	L171	L172	G173	P174	A175	G176	L177	G178	G179	L180	G181	G182	L183	G184	A185	L186	T187	G188	P189	G190	L191	A192	S193	L194	L195	G196	S197	G198	G199	P200	P201	G202	S203	S204	S205	S206	S207	S208	S209	R210	L211	G212	S213	A214	G215	V216	T217	S218	S219	S220	T221	G222	M162	M163
																													M1	T2	T3	S4	G5	A6	L7	F8	P9	S10	L11	V12	P13	G14	S15	A16	G17	A18	S19	N20	K21	D72	P132	M133	P134	G135	A136	L137	G138	A139	S140	G141	G142	S143	G144	H145	E146	L147	S148	A149	L150	G151	G152	E153	G154	G155	L156	L157	S158	L159	L160	G161	N162								
S224	T225	R226	A227	T228	P229	A230	P231	S232	A233	P234	A235	A236	A237	S238	A239	T240	G241	P242	S243	P244	A245	P246	S247	S248	G249	N250	G251	A252	S253	T254	A255	A256	S257	P258	T259	Q260	P261	T262	Q263	L264	S265	D266	L267	Q268	S269	T270	L271	A272	T273	N274	N275	P276	P277	A278	G279	P280	A281	G282	G283																														
Q284	Q285	V286	S316	S333	G353	Q358	K386	P387	E388	Q389	K390	E391	G392	D393	T394	K395	D396	K397	K398	D399	E400	E401	E402	D403	M404	S405	L406	D407	P132	M133	P134	G135	A136	L137	G138	A139	S140	G141	G142	S143	G144	H145	E146	L147	S148	A149	L150	G151	G152	E153	G154	G155	L156	L157	S158	L159	L160	G161	N162																														

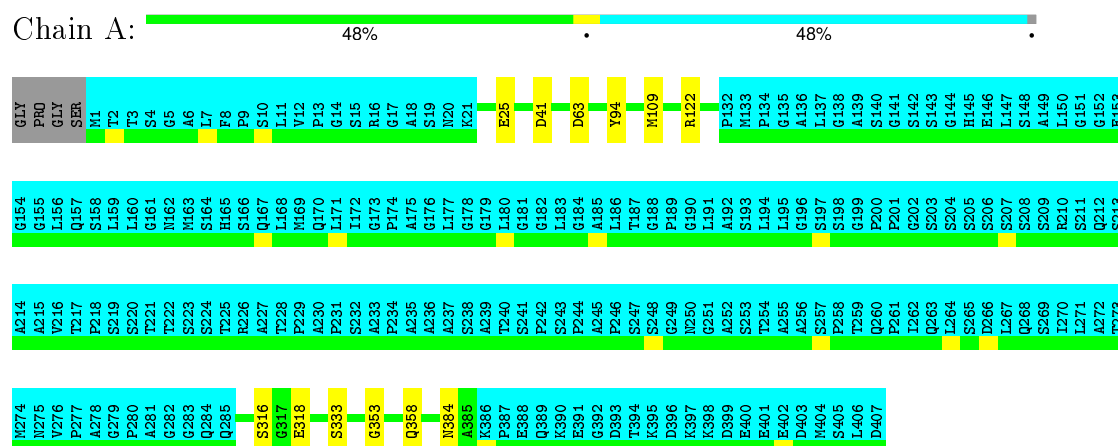
4.2.21 Score per residue for model 21

- Molecule 1: Proteasomal ubiquitin receptor ADRM1



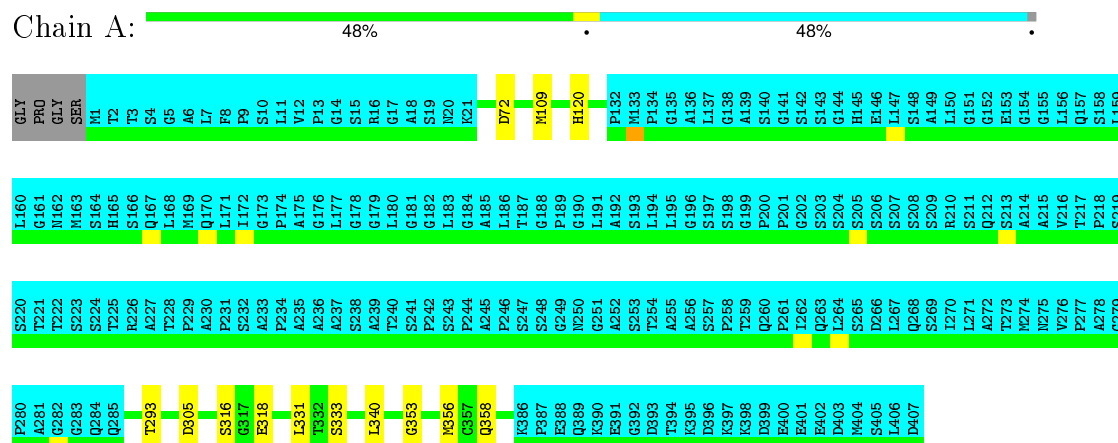
4.2.22 Score per residue for model 22

- Molecule 1: Proteasomal ubiquitin receptor ADRM1



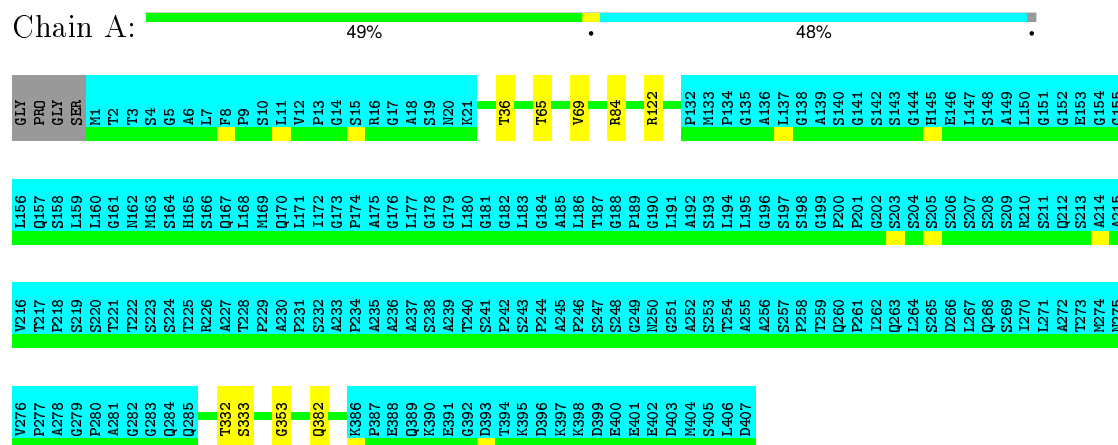
4.2.23 Score per residue for model 23

- Molecule 1: Proteasomal ubiquitin receptor ADRM1



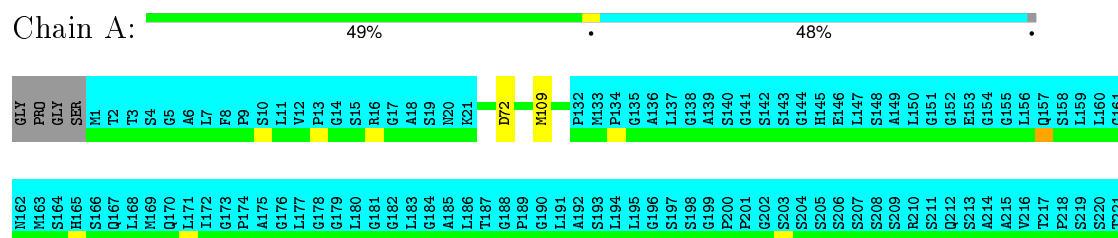
4.2.24 Score per residue for model 24

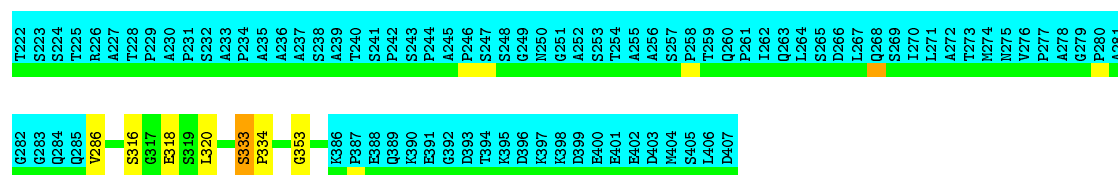
- Molecule 1: Proteasomal ubiquitin receptor ADRM1



4.2.25 Score per residue for model 25

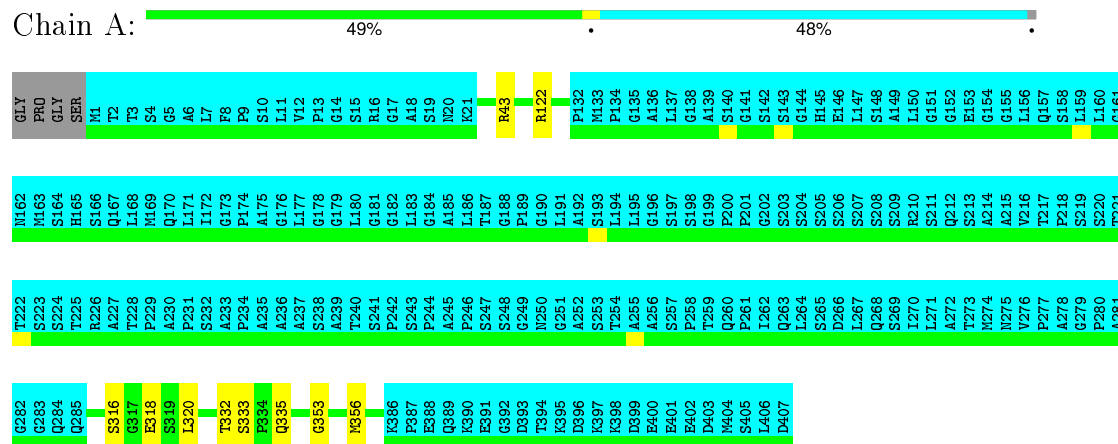
- Molecule 1: Proteasomal ubiquitin receptor ADRM1





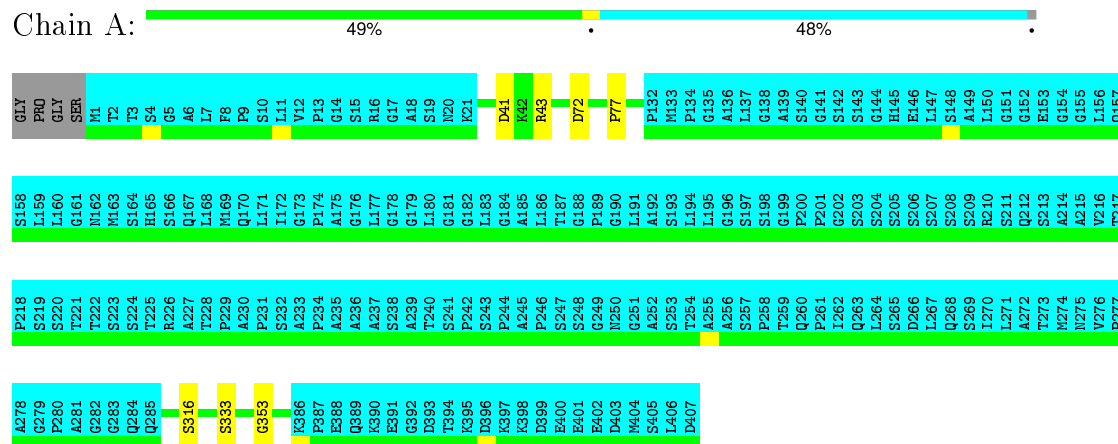
4.2.26 Score per residue for model 26

- Molecule 1: Proteasomal ubiquitin receptor ADRM1



4.2.27 Score per residue for model 27

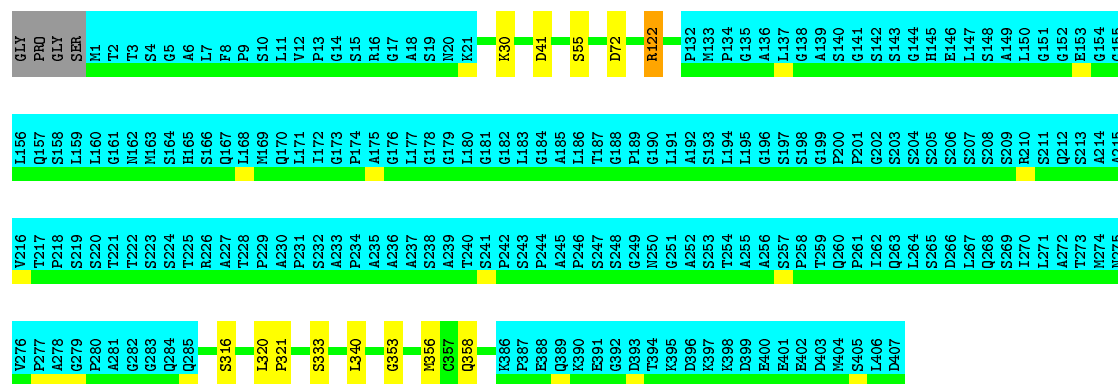
- Molecule 1: Proteasomal ubiquitin receptor ADRM1



4.2.28 Score per residue for model 28

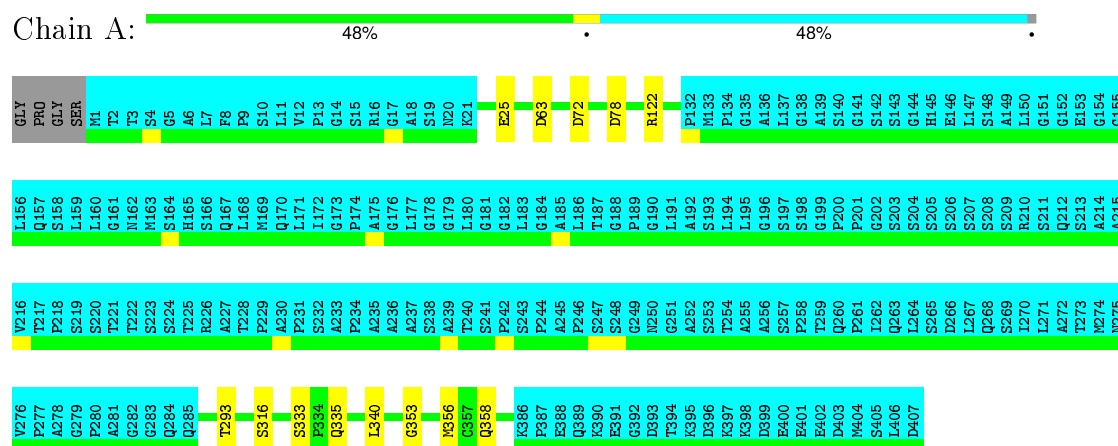
- Molecule 1: Proteasomal ubiquitin receptor ADRM1





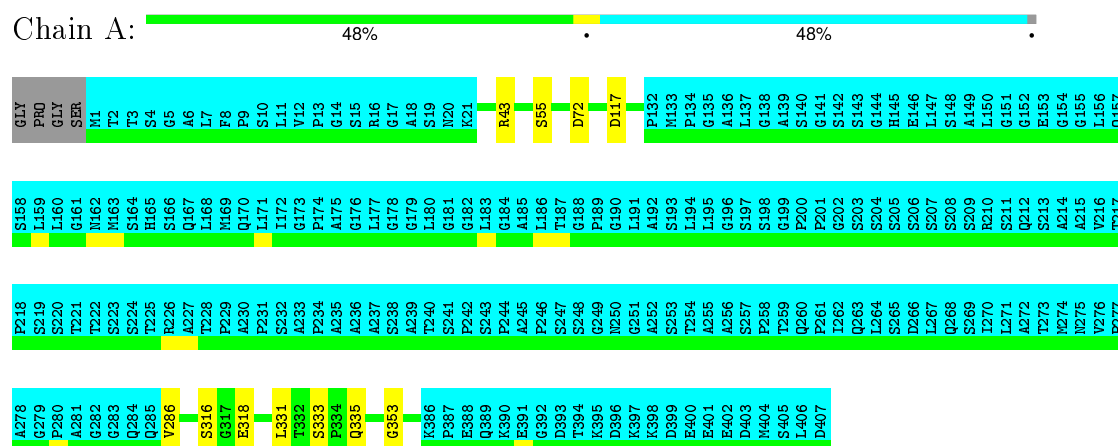
4.2.29 Score per residue for model 29

- Molecule 1: Proteasomal ubiquitin receptor ADRM1



4.2.30 Score per residue for model 30

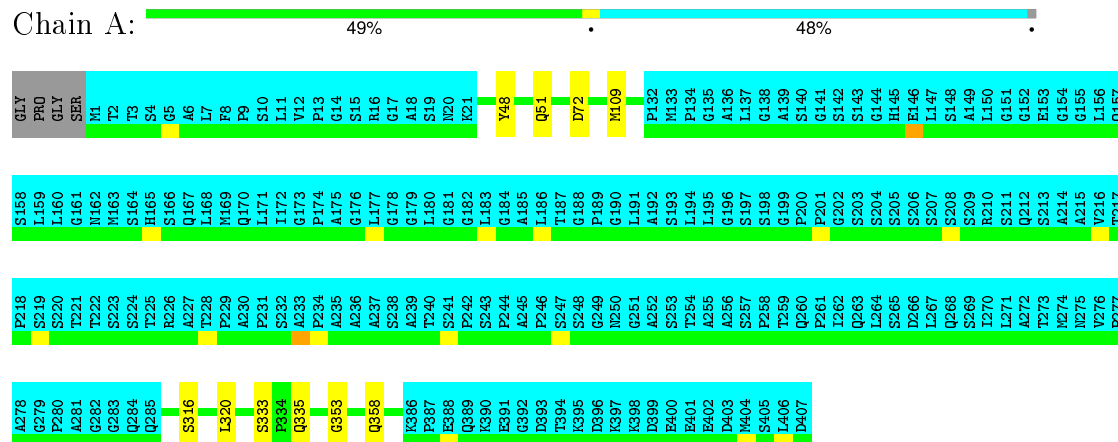
- Molecule 1: Proteasomal ubiquitin receptor ADRM1



4.2.31 Score per residue for model 31

• Molecule 1: Proteasomal ubiquitin receptor ADRM1

Chain A:



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

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	0.71±0.00	0±0/1676 (0.0±0.0%)	0.97±0.01	1±1/2274 (0.0±0.0%)
All	All	0.71	0/51956 (0.0%)	0.97	21/70494 (0.0%)

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	43	ARG	NE-CZ-NH2	-8.45	116.07	120.30	19	8
1	A	122	ARG	NE-CZ-NH2	-7.79	116.40	120.30	24	2
1	A	43	ARG	NE-CZ-NH1	6.72	123.66	120.30	15	2
1	A	309	ARG	NE-CZ-NH2	-6.53	117.03	120.30	11	1
1	A	92	ARG	NE-CZ-NH2	-6.26	117.17	120.30	6	1
1	A	84	ARG	NE-CZ-NH1	5.72	123.16	120.30	7	3
1	A	122	ARG	NE-CZ-NH1	5.23	122.92	120.30	29	2
1	A	104	ARG	CD-NE-CZ	5.12	130.76	123.60	2	1
1	A	316	SER	CB-CA-C	5.07	119.73	110.10	6	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	48	TYR	Sidechain	1
1	A	94	TYR	Sidechain	1

6.2 Too-close contacts [i](#)

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 [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	210/411 (51%)	199±2 (95±1%)	8±2 (4±1%)	4±1 (2±0%)	16	59
All	All	6510/12741 (51%)	6157 (95%)	243 (4%)	110 (2%)	16	59

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	353	GLY	31

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Mol	Chain	Res	Type	Models (Total)
1	A	333	SER	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%)	52	90
All	All	5549/10044 (55%)	5381 (97%)	168 (3%)	52	90

All 38 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	72	ASP	19
1	A	320	LEU	15
1	A	356	MET	11
1	A	358	GLN	11
1	A	340	LEU	9
1	A	25	GLU	8
1	A	109	MET	8
1	A	318	GLU	8
1	A	117	ASP	7
1	A	63	ASP	6
1	A	331	LEU	6
1	A	122	ARG	5
1	A	335	GLN	5
1	A	382	GLN	4
1	A	41	ASP	4

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Mol	Chain	Res	Type	Models (Total)
1	A	62	LYS	4
1	A	51	GLN	4
1	A	293	THR	3
1	A	305	ASP	3
1	A	78	ASP	3
1	A	58	HIS	2
1	A	116	GLN	2
1	A	68	ASN	2
1	A	30	LYS	2
1	A	36	THR	2
1	A	44	LYS	2
1	A	60	CYS	2
1	A	54	ASP	1
1	A	125	ASN	1
1	A	120	HIS	1
1	A	87	GLN	1
1	A	83	LYS	1
1	A	97	LYS	1
1	A	69	VAL	1
1	A	384	ASN	1
1	A	92	ARG	1
1	A	65	THR	1
1	A	314	LEU	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 carbohydrates in this entry.

6.6 Ligand geometry ⓘ

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