

wwPDB NMR Structure Validation Summary Report (i)

Oct 2, 2021 – 08:15 PM EDT

PDB ID : 2KU2

Title: Dynamic Regulation of Archaeal Proteasome Gate Opening as Studied by

TROSY-NMR

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Deposited on : 2010-02-11

This is a wwPDB NMR Structure Validation Summary 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 : 2.23.2

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

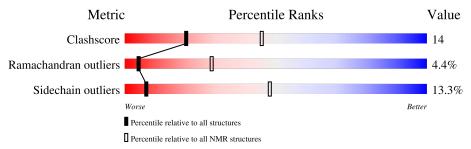
Validation Pipeline (wwPDB-VP) : 2.23.2

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 $(\# \mathrm{Entries})$	$ m 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	237	55%	32%	5% • 6%			
1	В	237	59%	27%	7% 6%			
1	С	237	61%	27%	6% 6%			
1	D	237	60%	26%	7% 6%			
1	Е	237	55%	32%	7% 6%			
1	F	237	59%	30%	5% • 6%			
1	G	237	58%	32%	• 6%			



2 Ensemble composition and analysis (i)

This entry contains 50 models. Model 10 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:12-A:233, B:12-B:233,	0.04	10					
	C:12-C:233, D:12-D:233,							
	E:12-E:233, F:12-F:233,							
	G:12-G:233 (1554)							

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 9 clusters and 1 single-model cluster was found.

Cluster number	Models
1	5, 6, 9, 10, 15, 16, 17, 19, 21, 26, 37, 39, 45, 47
2	2, 13, 29, 41, 42, 44, 48, 49, 50
3	14, 18, 32, 36, 38
4	7, 8, 25, 34, 43
5	11, 22, 23, 24, 40
6	27, 28, 31, 33
7	1, 3, 4
8	12, 20
9	35, 46
Single-model clusters	30



3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 25802 atoms, of which 13027 are hydrogens and 0 are deuteriums.

• Molecule 1 is a protein called Proteasome subunit alpha.

Mol	Chain	Residues		\mathbf{Atoms}					Trace
1	Λ	237	Total	С	Н	N	О	S	0
1	A	231	3686	1153	1861	312	354	6	0
1	В	237	Total	С	Н	N	О	S	0
1	Б	231	3686	1153	1861	312	354	6	0
1	С	237	Total	С	Н	N	О	S	0
1		231	3686	1153	1861	312	354	6	0
1	D	237	Total	С	Н	N	О	S	0
1	ט		3686	1153	1861	312	354	6	0
1	Е	237	Total	С	Н	N	О	S	0
1	<u> 1</u> 2	231	3686	1153	1861	312	354	6	0
1	F	227	Total	С	Н	N	О	S	0
	237	3686	1153	1861	312	354	6	0	
1	1 0	237	Total	С	Н	N	О	S	0
1	G	231	3686	1153	1861	312	354	6	

There are 42 discrepancies between the modelled and reference sequences:

Cl :-	D ! .l	N / L . 1 . 11 1	A -41	C	D . C
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP P25156
A	-2	ALA	-	expression tag	UNP P25156
A	-1	MET	-	expression tag	UNP P25156
A	0	GLY	-	expression tag	UNP P25156
A	8	GLY	TYR	engineered mutation	UNP P25156
A	9	GLY	ASP	engineered mutation	UNP P25156
В	-3	GLY	_	expression tag	UNP P25156
В	-2	ALA	-	expression tag	UNP P25156
В	-1	MET	_	expression tag	UNP P25156
В	0	GLY	_	expression tag	UNP P25156
В	8	GLY	TYR	engineered mutation	UNP P25156
В	9	GLY	ASP	engineered mutation	UNP P25156
С	-3	GLY	-	expression tag	UNP P25156
С	-2	ALA	-	expression tag	UNP P25156
С	-1	MET	-	expression tag	UNP P25156
С	0	GLY	-	expression tag	UNP P25156
С	8	GLY	TYR	engineered mutation	UNP P25156
С	9	GLY	ASP	engineered mutation	UNP P25156
D	-3	GLY	-	expression tag	UNP P25156

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	ALA	-	expression tag	UNP P25156
D	-1	MET	-	expression tag	UNP P25156
D	0	GLY	-	expression tag	UNP P25156
D	8	GLY	TYR	engineered mutation	UNP P25156
D	9	GLY	ASP	engineered mutation	UNP P25156
Е	-3	GLY	-	expression tag	UNP P25156
Е	-2	ALA	-	expression tag	UNP P25156
Е	-1	MET	-	expression tag	UNP P25156
Е	0	GLY	-	expression tag	UNP P25156
Е	8	GLY	TYR	engineered mutation	UNP P25156
Е	9	GLY	ASP	engineered mutation	UNP P25156
F	-3	GLY	-	expression tag	UNP P25156
F	-2	ALA	-	expression tag	UNP P25156
F	-1	MET	-	expression tag	UNP P25156
F	0	GLY	-	expression tag	UNP P25156
F	8	GLY	TYR	engineered mutation	UNP P25156
F	9	GLY	ASP	engineered mutation	UNP P25156
G	-3	GLY	-	expression tag	UNP P25156
G	-2	ALA	-	expression tag	UNP P25156
G	-1	MET	-	expression tag	UNP P25156
G	0	GLY	-	expression tag	UNP P25156
G	8	GLY	TYR	engineered mutation	UNP P25156
G	9	GLY	ASP	engineered mutation	UNP P25156

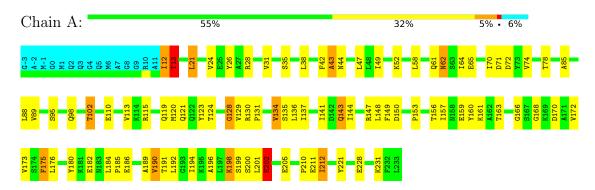


4 Residue-property plots (i)

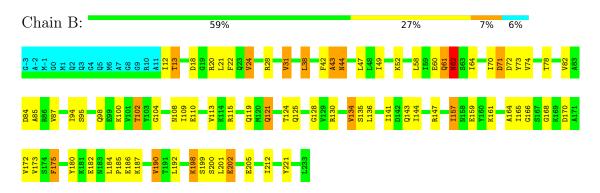
4.1 Average score per residue in the NMR ensemble

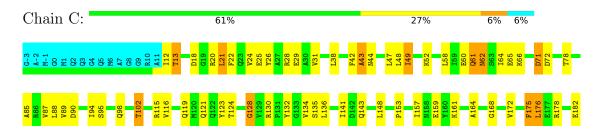
These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for 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: Proteasome subunit alpha



• Molecule 1: Proteasome subunit alpha

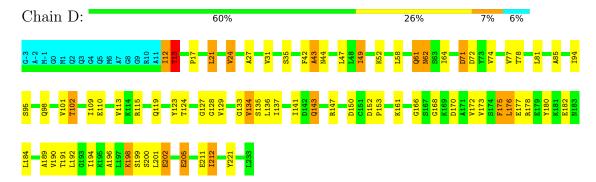




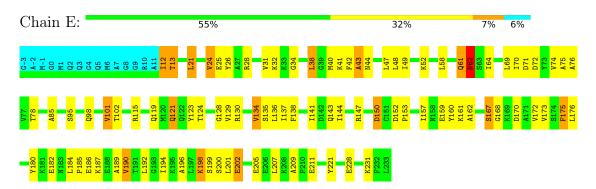




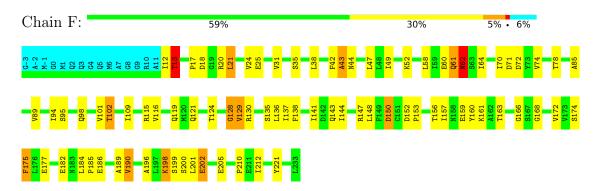
• Molecule 1: Proteasome subunit alpha

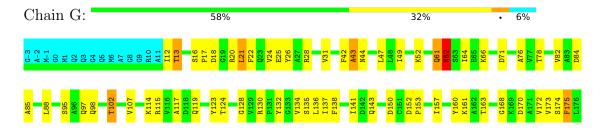


• Molecule 1: Proteasome subunit alpha



• Molecule 1: Proteasome subunit alpha





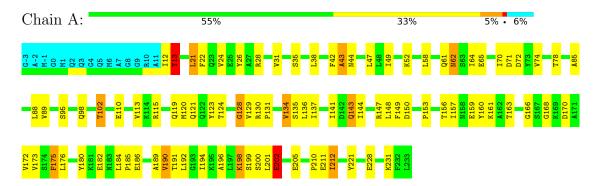


E177 Y180 K181 R183 L184 P185 P186 P186 P186 P186 P187 P187

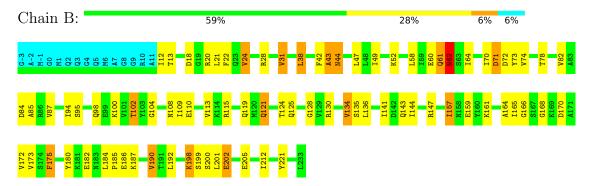
4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 10. Colouring as in section 4.1 above.

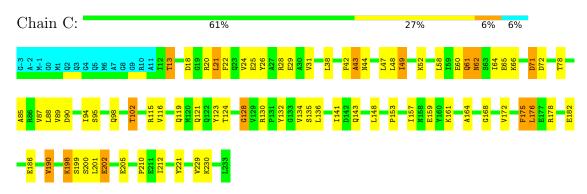
• Molecule 1: Proteasome subunit alpha



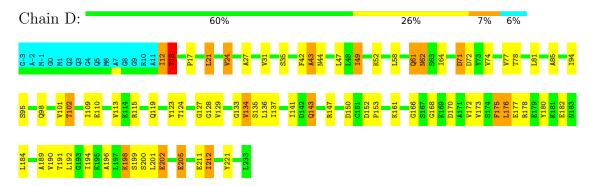
• Molecule 1: Proteasome subunit alpha



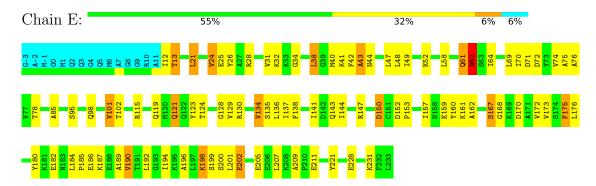
• Molecule 1: Proteasome subunit alpha



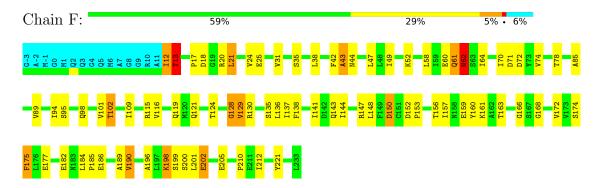


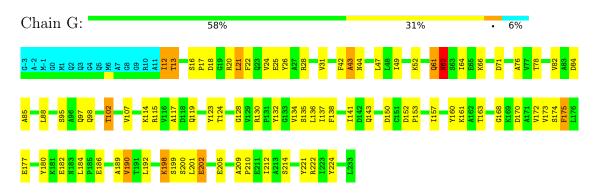


• Molecule 1: Proteasome subunit alpha



• Molecule 1: Proteasome subunit alpha







Refinement protocol and experimental data overview (i) 5



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

Of the 166 calculated structures, 50 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	structure solution	2.23
X-PLOR NIH	refinement	2.23

No chemical shift data was provided.



6 Model quality (i)

6.1 Standard geometry (i)

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		I	Bond lengths	Bond angles		
WIOI	Chain	RMSZ	#Z>5	RMSZ	#Z>5	
1	A	0.53 ± 0.00	$0\pm0/1751~(~0.0\pm~0.0\%)$	0.72 ± 0.00	$1\pm0/2359$ ($0.0\pm$ 0.0%)	
1	В	0.51 ± 0.00	$0\pm0/1751~(~0.0\pm~0.0\%)$	0.71 ± 0.00	$0\pm0/2359$ ($0.0\pm$ 0.0%)	
1	С	0.53 ± 0.00	$0\pm0/1751~(~0.0\pm~0.0\%)$	0.70 ± 0.00	$1\pm0/2359$ ($0.0\pm~0.0\%$)	
1	D	0.55 ± 0.00	$0\pm0/1751~(~0.0\pm~0.0\%)$	0.72 ± 0.00	$0\pm0/2359$ ($0.0\pm$ 0.0%)	
1	Е	0.53 ± 0.00	$0\pm0/1751~(~0.0\pm~0.0\%)$	0.71 ± 0.00	$0\pm0/2359$ ($0.0\pm$ 0.0%)	
1	F	0.54 ± 0.00	$0\pm0/1751~(~0.0\pm~0.0\%)$	0.69 ± 0.00	$0\pm0/2359~(~0.0\pm~0.0\%)$	
1	G	0.53 ± 0.00	$0\pm0/1751~(~0.0\pm~0.0\%)$	0.71 ± 0.00	$0\pm0/2359$ ($0.0\pm$ 0.0%)	
All	All	0.53	0/612850 ($0.0%$)	0.71	100/825650 (0.0%)	

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	Dog	Tuno	Atoma	7	$Observed(^{o}) \mid Ideal(^{o}) \mid Models$		dels	
MIOI	Chain	nes	Туре	Atoms Z		Z Observed(*)		Worst	Total
1	С	128	GLY	N-CA-C	5.36	126.49	113.10	1	50
1	A	128	GLY	N-CA-C	5.07	125.78	113.10	1	50

There are no chirality outliers.

There are no planarity outliers.

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	1728	1765	1765	59±1
1	В	1728	1765	1765	50±2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	С	1728	1765	1765	42±1
1	D	1728	1765	1765	46±1
1	Е	1728	1765	1765	56±1
1	F	1728	1765	1765	55±1
1	G	1728	1765	1765	49±1
All	All	604800	617750	617750	16650

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 14.

5 of 466 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total
1:A:12:ILE:HD12	1:A:12:ILE:N	0.77	1.94	4	2
1:F:12:ILE:HD13	1:F:12:ILE:H	0.76	1.39	21	1
1:A:52:LYS:NZ	1:A:62:ASN:HA	0.76	1.96	1	50
1:C:12:ILE:HD13	1:C:12:ILE:H	0.74	1.41	50	2
1:A:12:ILE:HD12	1:A:12:ILE:O	0.73	1.83	6	10

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	221/237~(93%)	186±1 (84±0%)	25±1 (11±0%)	10±1 (5±0%)	4 27
1	В	221/237 (93%)	187±1 (84±0%)	25±1 (11±0%)	10±1 (4±0%)	5 29
1	C	221/237~(93%)	185±1 (84±0%)	28±1 (13±0%)	8±1 (3±0%)	6 36
1	D	221/237 (93%)	189±1 (85±0%)	22±1 (10±0%)	10±1 (4±0%)	4 28
1	E	221/237~(93%)	184±1 (83±0%)	26±1 (12±0%)	12±1 (5±0%)	4 24
1	F	221/237 (93%)	187±1 (85±0%)	23±0 (10±0%)	11±1 (5±0%)	4 26
1	G	221/237~(93%)	188±1 (85±0%)	24±1 (11±0%)	9±0 (4±0%)	5 32
All	All	77350/82950 (93%)	65258 (84%)	8702 (11%)	3390 (4%)	4 29

5 of 77 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	43	ALA	50
1	A	72	ASP	50
1	A	128	GLY	50
1	A	129	VAL	50
1	A	182	GLU	50

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	185/192~(96%)	163±0 (88±0%)	22±0 (12±0%)	8	51
1	В	185/192~(96%)	160±0 (86±0%)	25±0 (14±0%)	7	47
1	С	185/192 (96%)	159±0 (86±0%)	26±0 (14±0%)	6	46
1	D	185/192~(96%)	158±1 (86±0%)	27±1 (14±0%)	6	45
1	E	185/192~(96%)	158±0 (85±0%)	27±0 (15±0%)	6	44
1	F	185/192~(96%)	162±0 (87±0%)	23±0 (13±0%)	8	49
1	G	185/192 (96%)	163±0 (88±0%)	22±0 (12±0%)	9	52
All	All	64750/67200 (96%)	56115 (87%)	8635 (13%)	7	48

5 of 178 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	13	THR	50
1	A	21	LEU	50
1	A	38	LEU	50
1	A	44	ASN	50
1	A	47	LEU	50

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 monosaccharides 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 (i)

No chemical shift data were provided

