



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 2K7X
Title : solution structure of C-terminal domain of SARS-CoV main protease
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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

<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

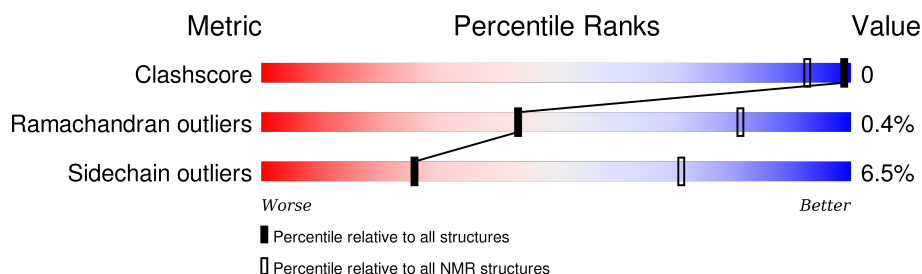
1 Overall quality at a glance

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	120	<div> <div style="width: 76%; background-color: green;"></div> <div style="width: 21%; background-color: cyan;"></div> <div style="width: 3%; background-color: yellow;"></div> <div style="width: 0%; background-color: orange;"></div> <div style="width: 0%; background-color: red;"></div> </div> <div>76% • 21%</div>

2 Ensemble composition and analysis

This entry contains 21 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:198-A:273, A:281-A:299 (95)	0.15	1

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. No single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 6, 8, 9, 10, 11, 12, 13, 14, 16, 18, 19, 20, 21
2	4, 5, 7, 15, 17

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1851 atoms, of which 918 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called SARS-CoV main protease.

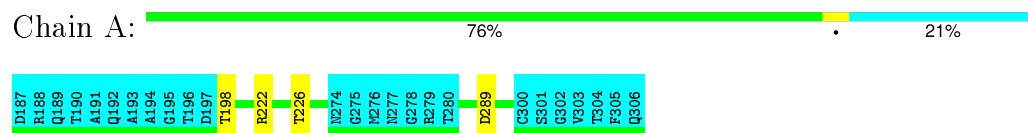
Mol	Chain	Residues	Atoms						Trace
1	A	120	Total	C	H	N	O	S	0
			1851	590	918	156	182	5	

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.

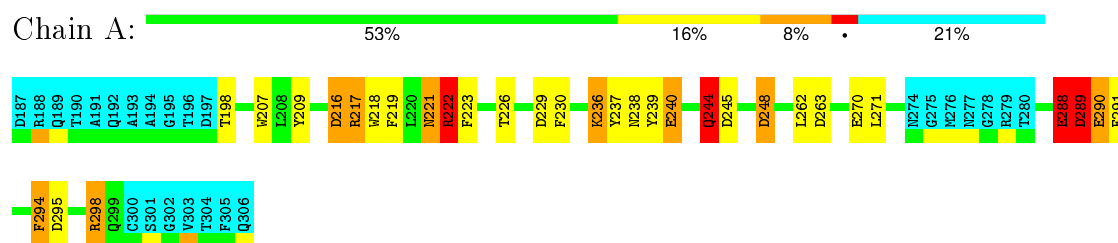
- Molecule 1: SARS-CoV main protease



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

The representative model is number 1. Colouring as in section 4.1 above.

- Molecule 1: SARS-CoV main protease



5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *molecular dynamics*.

Of the 100 calculated structures, 21 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
AMBER	refinement	
CYANA	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	0.68±0.28	2±8/770 (0.2±1.1%)	1.02±0.76	6±25/1055 (0.5±2.3%)
All	All	0.73	38/16170 (0.2%)	1.27	116/22155 (0.5%)

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	0.3±1.5
All	All	0	7

5 of 38 unique bond 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(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	298	ARG	CD-NE	-12.58	1.25	1.46	1	1
1	A	294	PHE	CB-CG	-12.12	1.30	1.51	1	1
1	A	217	ARG	CD-NE	-10.82	1.28	1.46	1	1
1	A	270	GLU	CG-CD	-9.73	1.37	1.51	1	1
1	A	217	ARG	NE-CZ	-9.67	1.20	1.33	1	1

5 of 116 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	240	GLU	OE1-CD-OE2	-38.02	77.67	123.30	1	1
1	A	290	GLU	OE1-CD-OE2	-30.37	86.86	123.30	1	1
1	A	298	ARG	NE-CZ-NH2	-27.99	106.30	120.30	1	1
1	A	288	GLU	OE1-CD-OE2	-27.28	90.56	123.30	1	1
1	A	217	ARG	NE-CZ-NH2	-23.98	108.31	120.30	1	1

There are no chirality outliers.

5 of 7 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	294	PHE	Sidechain	1
1	A	290	GLU	Sidechain	1
1	A	248	ASP	Sidechain	1
1	A	289	ASP	Sidechain	1
1	A	216	ASP	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	754	754	754	0±1
All	All	15834	15834	15834	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:222:ARG:O	1:A:222:ARG:HD3	0.60	1.96	1	1
1:A:217:ARG:HG3	1:A:217:ARG:O	0.52	2.04	1	1
1:A:244:GLN:HE21	1:A:244:GLN:HA	0.50	1.66	1	1
1:A:220:LEU:HD22	1:A:220:LEU:N	0.41	2.30	9	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	95/120 (79%)	90±1 (94±1%)	5±1 (5±1%)	0±1 (0±1%)	43	81
All	All	1995/2520 (79%)	1880 (94%)	108 (5%)	7 (0%)	43	81

All 2 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	251	GLY	4
1	A	217	ARG	3

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	83/101 (82%)	78±1 (94±2%)	5±1 (6±2%)	26	71
All	All	1743/2121 (82%)	1630 (94%)	113 (6%)	26	71

5 of 16 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	226	THR	21
1	A	222	ARG	20
1	A	198	THR	20
1	A	289	ASP	18
1	A	224	THR	9

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 [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