

wwPDB EM Validation Summary Report (i)

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PDB ID	:	8XZB
EMDB ID	:	EMD-38792
Title	:	The structure of fox ACE2 and SARS-CoV RBD complex
Authors	:	sun, J.Q.
Deposited on		
Resolution	:	3.12 Å(reported)

This is a wwPDB EM 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/EMValidationReportHelp with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

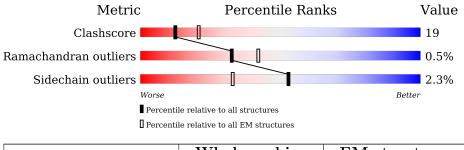
EMDB validation analysis	:	FAILED
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $ELECTRON\ MICROSCOPY$

The reported resolution of this entry is 3.12 Å.

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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f EM} {f structures} \ (\#{f Entries})$	
Clashscore	158937	4297	
Ramachandran outliers	154571	4023	
Sidechain outliers	154315	3826	

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	А	613	76%		21%	·	
2	С	228	53%	30%	• 16%		



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6412 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

• Molecule 1 is a protein called Angiotensin-converting enzyme.

Mol	Chain	Residues	Atoms				AltConf	Trace	
1	А	596	Total 4885	C 3123	N 810	0 923	S 29	0	0

• Molecule 2 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms			AltConf	Trace		
2	С	191	Total	С	Ν	0	S	0	0
	U	191	1526	987	248	282	9	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
С	528	HIS	-	expression tag	UNP P59594
С	529	HIS	-	expression tag	UNP P59594
С	530	HIS	-	expression tag	UNP P59594
С	531	HIS	-	expression tag	UNP P59594
С	532	HIS	-	expression tag	UNP P59594
С	533	HIS	-	expression tag	UNP P59594

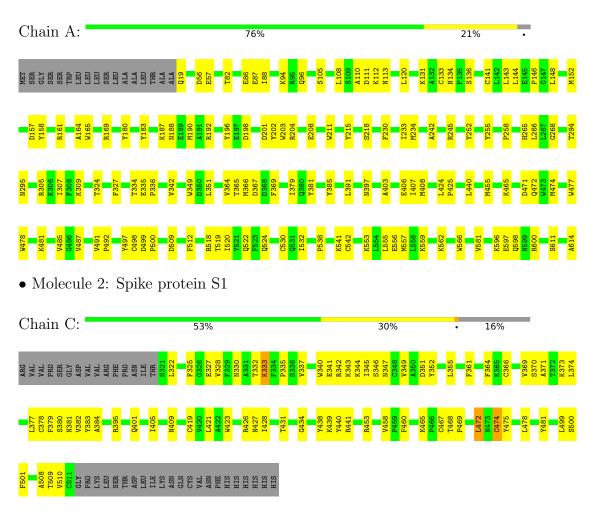
• Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
3	А	1	Total Zn 1 1	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-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 outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.



• Molecule 1: Angiotensin-converting enzyme



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	345875	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor



5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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 root-mean-square of all Z scores of the bond lengths (or angles).

Mal	Mol Chain		lengths	Bond angles		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.32	0/5027	0.69	0/6830	
2	С	0.35	0/1574	0.83	0/2149	
All	All	0.33	0/6601	0.73	0/8979	

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 the 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 within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	4885	0	4654	138	0
2	С	1526	0	1457	98	0
3	А	1	0	0	0	0
All	All	6412	0	6111	236	0

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 19.

The worst 5 of 236 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:LYS:HG2	1:A:141:CYS:SG	1.45	1.57
2:C:361:PHE:CZ	2:C:421:LEU:HD13	1.54	1.39
2:C:361:PHE:CE1	2:C:421:LEU:HB3	1.67	1.29
2:C:440:TYR:HB3	2:C:481:TYR:CZ	1.67	1.29
2:C:440:TYR:HB3	2:C:481:TYR:OH	1.33	1.25

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 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 EM 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	Perce	entiles
1	А	594/613~(97%)	586~(99%)	6 (1%)	2~(0%)	41	73
2	С	189/228~(83%)	180 (95%)	7 (4%)	2(1%)	14	45
All	All	783/841~(93%)	766~(98%)	13 (2%)	4 (0%)	32	63

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	146	PRO
2	С	469	PRO
1	А	258	PRO
2	С	460	PHE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM 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	А	530/542~(98%)	521 (98%)	9~(2%)	60 83
2	С	167/202~(83%)	160 (96%)	7 (4%)	30 62
All	All	697/744~(94%)	681 (98%)	16 (2%)	53 76

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	С	474	CYS
2	С	472	LEU
1	А	557	MET
2	С	468	THR
1	А	532	ILE

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such side chains are listed below:

Mol	Chain	Res	Type
2	С	330	ASN
2	С	401	GLN
1	А	345	HIS
1	А	397	ASN
1	А	522	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis. There are no bond length outliers.



There are no bond angle outliers. There are no chirality outliers. There are no torsion outliers. There are no ring outliers. No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

