



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Apr 24, 2017 – 12:15 PM EDT

PDB ID : 5X58
EMDB ID: : EMD-6703
Title : Prefusion structure of SARS-CoV spike glycoprotein, conformation 1
Authors : Yuan, Y.; Cao, D.; Zhang, Y.; Ma, J.; Qi, J.; Wang, Q.; Lu, G.; Wu, Y.; Yan, J.; Shi, Y.; Zhang, X.; Gao, G.F.
Deposited on : 2017-02-15
Resolution : 3.20 Å(reported)
Based on PDB ID : 5X4S, 2AJF

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029077

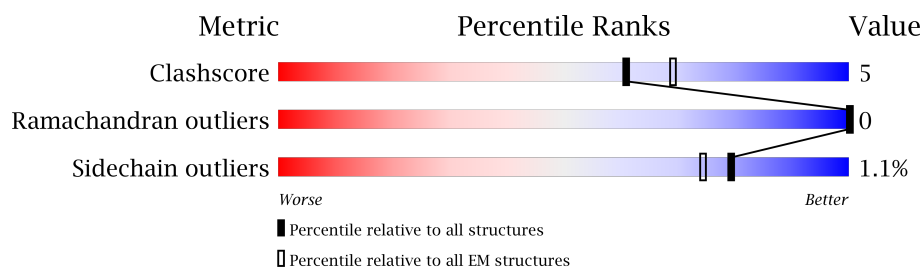
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	1228	72% 14% 14%
1	B	1228	72% 13% 14%
1	C	1228	71% 14% 14%

2 Entry composition [i](#)

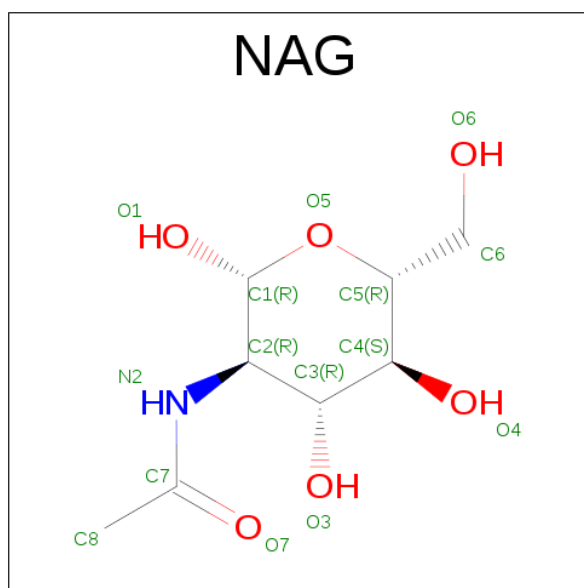
There are 2 unique types of molecules in this entry. The entry contains 25265 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1054	Total	C	N	O	S	0	0
			8234	5260	1363	1567	44		
1	B	1053	Total	C	N	O	S	0	0
			8226	5256	1362	1564	44		
1	C	1052	Total	C	N	O	S	0	0
			8217	5250	1360	1563	44		

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			196	112	14	70	
2	A	1	Total	C	N	O	0
			196	112	14	70	
2	A	1	Total	C	N	O	0
			196	112	14	70	
2	A	1	Total	C	N	O	0
			196	112	14	70	

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Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			196	112	14	70	
2	A	1	Total	C	N	O	0
			196	112	14	70	
2	A	1	Total	C	N	O	0
			196	112	14	70	
2	A	1	Total	C	N	O	0
			196	112	14	70	
2	A	1	Total	C	N	O	0
			196	112	14	70	
2	A	1	Total	C	N	O	0
			196	112	14	70	
2	A	1	Total	C	N	O	0
			196	112	14	70	
2	A	1	Total	C	N	O	0
			196	112	14	70	
2	B	1	Total	C	N	O	0
			196	112	14	70	
2	B	1	Total	C	N	O	0
			196	112	14	70	
2	B	1	Total	C	N	O	0
			196	112	14	70	
2	B	1	Total	C	N	O	0
			196	112	14	70	
2	B	1	Total	C	N	O	0
			196	112	14	70	
2	B	1	Total	C	N	O	0
			196	112	14	70	
2	B	1	Total	C	N	O	0
			196	112	14	70	
2	B	1	Total	C	N	O	0
			196	112	14	70	
2	B	1	Total	C	N	O	0
			196	112	14	70	

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Mol	Chain	Residues	Atoms				AltConf
2	B	1	Total	C	N	O	0
			196	112	14	70	
2	B	1	Total	C	N	O	0
			196	112	14	70	
2	B	1	Total	C	N	O	0
			196	112	14	70	
2	C	1	Total	C	N	O	0
			196	112	14	70	
2	C	1	Total	C	N	O	0
			196	112	14	70	
2	C	1	Total	C	N	O	0
			196	112	14	70	
2	C	1	Total	C	N	O	0
			196	112	14	70	
2	C	1	Total	C	N	O	0
			196	112	14	70	
2	C	1	Total	C	N	O	0
			196	112	14	70	
2	C	1	Total	C	N	O	0
			196	112	14	70	
2	C	1	Total	C	N	O	0
			196	112	14	70	
2	C	1	Total	C	N	O	0
			196	112	14	70	
2	C	1	Total	C	N	O	0
			196	112	14	70	
2	C	1	Total	C	N	O	0
			196	112	14	70	
2	C	1	Total	C	N	O	0
			196	112	14	70	

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	60000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	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: NAG

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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.38	0/8432	0.62	8/11475 (0.1%)
1	B	0.38	0/8424	0.62	8/11464 (0.1%)
1	C	0.38	0/8415	0.62	8/11453 (0.1%)
All	All	0.38	0/25271	0.62	24/34392 (0.1%)

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 outliers	#Planarity outliers
1	A	0	4
1	B	0	4
1	C	0	4
All	All	0	12

There are no bond length outliers.

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	515	LEU	CA-CB-CG	8.31	134.43	115.30
1	C	515	LEU	CA-CB-CG	8.31	134.42	115.30
1	B	515	LEU	CA-CB-CG	8.31	134.40	115.30
1	A	920	LEU	CA-CB-CG	7.47	132.49	115.30
1	B	920	LEU	CA-CB-CG	7.46	132.46	115.30

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	316	PHE	Peptide
1	A	512	GLY	Peptide
1	A	616	THR	Peptide
1	A	741	PHE	Peptide
1	B	316	PHE	Peptide

5.2 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 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	A	8234	0	8002	95	0
1	B	8226	0	7997	95	0
1	C	8217	0	7984	94	0
2	A	196	0	180	3	0
2	B	196	0	180	3	0
2	C	196	0	180	3	0
All	All	25265	0	24523	264	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 5.

The worst 5 of 264 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:953:GLY:HA3	1:A:977:ARG:HH11	1.61	0.66
1:C:953:GLY:HA3	1:C:977:ARG:HH11	1.61	0.66
1:B:891:ILE:HD12	1:B:1029:TYR:HB3	1.78	0.65
1:C:891:ILE:HD12	1:C:1029:TYR:HB3	1.78	0.65
1:A:891:ILE:HD12	1:A:1029:TYR:HB3	1.78	0.63

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 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 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	Percentiles	
1	A	1046/1228 (85%)	950 (91%)	96 (9%)	0	100	100
1	B	1045/1228 (85%)	950 (91%)	95 (9%)	0	100	100
1	C	1044/1228 (85%)	948 (91%)	96 (9%)	0	100	100
All	All	3135/3684 (85%)	2848 (91%)	287 (9%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 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 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	A	914/1073 (85%)	904 (99%)	10 (1%)	78	92
1	B	913/1073 (85%)	903 (99%)	10 (1%)	78	92
1	C	912/1073 (85%)	902 (99%)	10 (1%)	78	92
All	All	2739/3219 (85%)	2709 (99%)	30 (1%)	79	92

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	522	ASN
1	B	733	ASN
1	C	772	LYS
1	B	721	ASN
1	B	772	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	599	GLN
1	B	733	ASN
1	C	766	GLN
1	B	614	GLN
1	B	641	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

42 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	A	1301	-	14,14,15	0.54	0	15,19,21	1.01	1 (6%)
2	NAG	A	1302	1	14,14,15	0.76	0	15,19,21	1.09	2 (13%)
2	NAG	A	1303	1	14,14,15	0.35	0	15,19,21	1.01	1 (6%)
2	NAG	A	1304	1	14,14,15	1.49	2 (14%)	15,19,21	1.94	2 (13%)
2	NAG	A	1305	1	14,14,15	0.41	0	15,19,21	1.06	1 (6%)
2	NAG	A	1306	1	14,14,15	0.45	0	15,19,21	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	A	1307	1	14,14,15	0.44	0	15,19,21	0.68	0
2	NAG	A	1308	1	14,14,15	0.48	0	15,19,21	0.68	1 (6%)
2	NAG	A	1309	1	14,14,15	0.36	0	15,19,21	0.39	0
2	NAG	A	1310	1	14,14,15	0.32	0	15,19,21	0.57	0
2	NAG	A	1311	1	14,14,15	0.38	0	15,19,21	0.63	0
2	NAG	A	1312	1	14,14,15	0.66	1 (7%)	15,19,21	0.61	0
2	NAG	A	1313	1	14,14,15	0.41	0	15,19,21	0.58	0
2	NAG	A	1314	-	14,14,15	0.39	0	15,19,21	0.45	0
2	NAG	B	1301	1	14,14,15	0.86	1 (7%)	15,19,21	1.18	2 (13%)
2	NAG	B	1302	1	14,14,15	0.80	2 (14%)	15,19,21	1.09	2 (13%)
2	NAG	B	1303	1	14,14,15	0.35	0	15,19,21	1.00	1 (6%)
2	NAG	B	1304	1	14,14,15	1.49	2 (14%)	15,19,21	1.94	3 (20%)
2	NAG	B	1305	1	14,14,15	0.34	0	15,19,21	1.05	1 (6%)
2	NAG	B	1306	1	14,14,15	0.45	0	15,19,21	0.43	0
2	NAG	B	1307	1	14,14,15	0.44	0	15,19,21	0.67	0
2	NAG	B	1308	1	14,14,15	0.46	0	15,19,21	0.69	1 (6%)
2	NAG	B	1309	1	14,14,15	0.37	0	15,19,21	0.39	0
2	NAG	B	1310	1	14,14,15	0.32	0	15,19,21	0.56	0
2	NAG	B	1311	1	14,14,15	0.36	0	15,19,21	0.65	0
2	NAG	B	1312	1	14,14,15	0.65	0	15,19,21	0.61	0
2	NAG	B	1313	1	14,14,15	0.40	0	15,19,21	0.59	0
2	NAG	B	1314	-	14,14,15	0.38	0	15,19,21	0.47	0
2	NAG	C	1301	1	14,14,15	0.90	1 (7%)	15,19,21	1.25	2 (13%)
2	NAG	C	1302	1	14,14,15	0.75	0	15,19,21	1.09	2 (13%)
2	NAG	C	1303	1	14,14,15	0.33	0	15,19,21	1.00	1 (6%)
2	NAG	C	1304	1	14,14,15	1.49	2 (14%)	15,19,21	1.95	3 (20%)
2	NAG	C	1305	1	14,14,15	0.34	0	15,19,21	1.05	1 (6%)
2	NAG	C	1306	1	14,14,15	0.43	0	15,19,21	0.43	0
2	NAG	C	1307	1	14,14,15	0.43	0	15,19,21	0.67	0
2	NAG	C	1308	1	14,14,15	0.47	0	15,19,21	0.66	1 (6%)
2	NAG	C	1309	1	14,14,15	0.37	0	15,19,21	0.39	0
2	NAG	C	1310	1	14,14,15	0.32	0	15,19,21	0.56	0
2	NAG	C	1311	1	14,14,15	0.36	0	15,19,21	0.64	0
2	NAG	C	1312	1	14,14,15	0.66	0	15,19,21	0.62	0
2	NAG	C	1313	1	14,14,15	0.41	0	15,19,21	0.58	0
2	NAG	C	1314	-	14,14,15	0.38	0	15,19,21	0.44	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. '-' means

no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	1301	-	-	0/6/23/26	0/1/1/1
2	NAG	A	1302	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1303	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1304	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1305	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1306	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1307	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1308	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1309	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1310	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1311	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1312	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1313	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1314	-	-	0/6/23/26	0/1/1/1
2	NAG	B	1301	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1302	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1303	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1304	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1305	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1306	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1307	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1308	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1309	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1310	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1311	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1312	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1313	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1314	-	-	0/6/23/26	0/1/1/1
2	NAG	C	1301	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1302	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1303	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1304	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1305	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1306	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1307	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1308	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1309	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1310	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1311	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1312	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1313	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1314	-	-	0/6/23/26	0/1/1/1

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1302	NAG	O5-C1	2.04	1.47	1.43
2	B	1302	NAG	C1-C2	2.05	1.55	1.52
2	A	1312	NAG	C1-C2	2.07	1.55	1.52
2	B	1301	NAG	C1-C2	2.73	1.56	1.52
2	C	1301	NAG	C1-C2	2.90	1.56	1.52

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1304	NAG	C3-C4-C5	2.05	113.83	110.22
2	B	1302	NAG	C1-O5-C5	2.08	115.03	112.17
2	C	1304	NAG	C3-C4-C5	2.08	113.89	110.22
2	A	1302	NAG	C1-O5-C5	2.09	115.05	112.17
2	C	1302	NAG	C1-O5-C5	2.09	115.05	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1310	NAG	1	0
2	A	1312	NAG	1	0
2	A	1314	NAG	1	0
2	B	1310	NAG	1	0
2	B	1312	NAG	1	0
2	B	1314	NAG	1	0
2	C	1310	NAG	1	0
2	C	1312	NAG	1	0
2	C	1314	NAG	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.