



## wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Dec 10, 2019 – 02:43 PM EST

PDB ID : 6CS2  
EMDB ID: : EMD-7582  
Title : SARS Spike Glycoprotein - human ACE2 complex, Stabilized variant, all ACE2-bound particles  
Authors : Kirchdoerfer, R.N.; Wang, N.; Pallesen, J.; Turner, H.L.; Cottrell, C.A.; McLellan, J.S.; Ward, A.B.  
Deposited on : 2018-03-19  
Resolution : 4.40 Å (reported)  
Based on PDB ID : 5I08, 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](mailto: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 ⓘ symbol.

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MolProbity : 4.02b-467  
Mogul : 1.8.0 (224370), CSD as540be (2019)  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.4

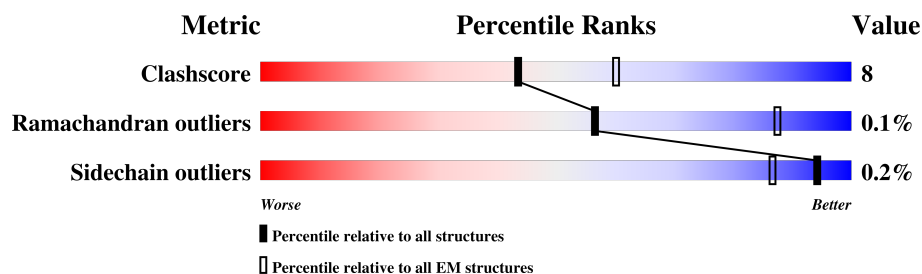
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.40 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	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

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  $\geq 3$ , 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	1215	61% 12% 27%
1	B	1215	69% 19% 11%
1	C	1215	58% 15% 27%
2	D	605	73% 17% 10%

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 27858 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,Fibritin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	891	Total	C	N	O	S	0	0
			6914	4403	1146	1328	37		
1	B	1076	Total	C	N	O	S	0	0
			8405	5371	1389	1599	46		
1	C	893	Total	C	N	O	S	0	0
			6927	4409	1149	1332	37		

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	577	ALA	SER	conflict	UNP P59594
A	968	PRO	LYS	engineered mutation	UNP P59594
A	969	PRO	VAL	engineered mutation	UNP P59594
A	1191	GLY	-	linker	UNP P59594
A	1192	SER	ALA	linker	UNP D9IEJ2
A	1220	GLY	-	expression tag	UNP D9IEJ2
A	1221	ARG	-	expression tag	UNP D9IEJ2
A	1222	SER	-	expression tag	UNP D9IEJ2
A	1223	LEU	-	expression tag	UNP D9IEJ2
A	1224	GLU	-	expression tag	UNP D9IEJ2
A	1225	VAL	-	expression tag	UNP D9IEJ2
A	1226	LEU	-	expression tag	UNP D9IEJ2
A	1227	PHE	-	expression tag	UNP D9IEJ2
A	1228	GLN	-	expression tag	UNP D9IEJ2
B	577	ALA	SER	conflict	UNP P59594
B	968	PRO	LYS	engineered mutation	UNP P59594
B	969	PRO	VAL	engineered mutation	UNP P59594
B	1191	GLY	-	linker	UNP P59594
B	1192	SER	ALA	linker	UNP D9IEJ2
B	1220	GLY	-	expression tag	UNP D9IEJ2
B	1221	ARG	-	expression tag	UNP D9IEJ2
B	1222	SER	-	expression tag	UNP D9IEJ2
B	1223	LEU	-	expression tag	UNP D9IEJ2
B	1224	GLU	-	expression tag	UNP D9IEJ2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1225	VAL	-	expression tag	UNP D9IEJ2
B	1226	LEU	-	expression tag	UNP D9IEJ2
B	1227	PHE	-	expression tag	UNP D9IEJ2
B	1228	GLN	-	expression tag	UNP D9IEJ2
C	577	ALA	SER	conflict	UNP P59594
C	968	PRO	LYS	engineered mutation	UNP P59594
C	969	PRO	VAL	engineered mutation	UNP P59594
C	1191	GLY	-	linker	UNP P59594
C	1192	SER	ALA	linker	UNP D9IEJ2
C	1220	GLY	-	expression tag	UNP D9IEJ2
C	1221	ARG	-	expression tag	UNP D9IEJ2
C	1222	SER	-	expression tag	UNP D9IEJ2
C	1223	LEU	-	expression tag	UNP D9IEJ2
C	1224	GLU	-	expression tag	UNP D9IEJ2
C	1225	VAL	-	expression tag	UNP D9IEJ2
C	1226	LEU	-	expression tag	UNP D9IEJ2
C	1227	PHE	-	expression tag	UNP D9IEJ2
C	1228	GLN	-	expression tag	UNP D9IEJ2

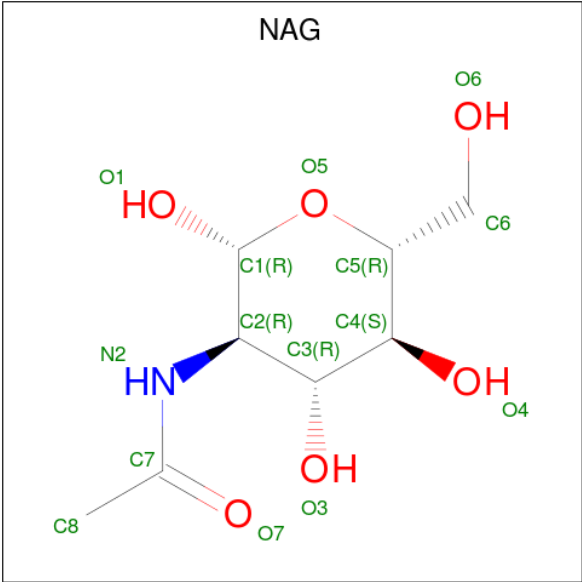
- Molecule 2 is a protein called Angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	544	Total	C	N	O	S	0	0
			4431	2828	736	839	28		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	616	GLY	-	expression tag	UNP Q9BYF1
D	617	SER	-	expression tag	UNP Q9BYF1
D	618	LEU	-	expression tag	UNP Q9BYF1
D	619	GLU	-	expression tag	UNP Q9BYF1
D	620	VAL	-	expression tag	UNP Q9BYF1
D	621	LEU	-	expression tag	UNP Q9BYF1
D	622	PHE	-	expression tag	UNP Q9BYF1
D	623	GLN	-	expression tag	UNP Q9BYF1

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			280	160	20	100	
3	A	1	Total	C	N	O	0
			280	160	20	100	
3	A	1	Total	C	N	O	0
			280	160	20	100	
3	A	1	Total	C	N	O	0
			280	160	20	100	
3	A	1	Total	C	N	O	0
			280	160	20	100	
3	A	1	Total	C	N	O	0
			280	160	20	100	
3	A	1	Total	C	N	O	0
			280	160	20	100	
3	A	1	Total	C	N	O	0
			280	160	20	100	
3	A	1	Total	C	N	O	0
			280	160	20	100	
3	A	1	Total	C	N	O	0
			280	160	20	100	
3	A	1	Total	C	N	O	0
			280	160	20	100	
3	A	1	Total	C	N	O	0
			280	160	20	100	

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Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			280	160	20	100	
3	A	1	Total	C	N	O	0
			280	160	20	100	
3	A	1	Total	C	N	O	0
			280	160	20	100	
3	A	1	Total	C	N	O	0
			280	160	20	100	
3	A	1	Total	C	N	O	0
			280	160	20	100	
3	B	1	Total	C	N	O	0
			280	160	20	100	
3	B	1	Total	C	N	O	0
			280	160	20	100	
3	B	1	Total	C	N	O	0
			280	160	20	100	
3	B	1	Total	C	N	O	0
			280	160	20	100	
3	B	1	Total	C	N	O	0
			280	160	20	100	
3	B	1	Total	C	N	O	0
			280	160	20	100	
3	B	1	Total	C	N	O	0
			280	160	20	100	
3	B	1	Total	C	N	O	0
			280	160	20	100	
3	B	1	Total	C	N	O	0
			280	160	20	100	
3	B	1	Total	C	N	O	0
			280	160	20	100	
3	B	1	Total	C	N	O	0
			280	160	20	100	
3	B	1	Total	C	N	O	0
			280	160	20	100	
3	B	1	Total	C	N	O	0
			280	160	20	100	

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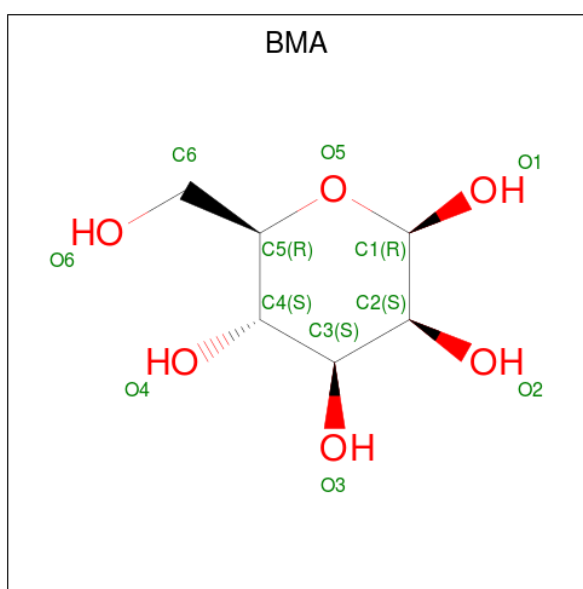
Mol	Chain	Residues	Atoms				AltConf
3	B	1	Total	C	N	O	0
			280	160	20	100	
3	B	1	Total	C	N	O	0
			280	160	20	100	
3	B	1	Total	C	N	O	0
			280	160	20	100	
3	B	1	Total	C	N	O	0
			280	160	20	100	
3	B	1	Total	C	N	O	0
			280	160	20	100	
3	C	1	Total	C	N	O	0
			280	160	20	100	
3	C	1	Total	C	N	O	0
			280	160	20	100	
3	C	1	Total	C	N	O	0
			280	160	20	100	
3	C	1	Total	C	N	O	0
			280	160	20	100	
3	C	1	Total	C	N	O	0
			280	160	20	100	
3	C	1	Total	C	N	O	0
			280	160	20	100	
3	C	1	Total	C	N	O	0
			280	160	20	100	
3	C	1	Total	C	N	O	0
			280	160	20	100	
3	C	1	Total	C	N	O	0
			280	160	20	100	
3	C	1	Total	C	N	O	0
			280	160	20	100	
3	C	1	Total	C	N	O	0
			280	160	20	100	
3	C	1	Total	C	N	O	0
			280	160	20	100	
3	C	1	Total	C	N	O	0
			280	160	20	100	
3	C	1	Total	C	N	O	0
			280	160	20	100	
3	C	1	Total	C	N	O	0
			280	160	20	100	

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Mol	Chain	Residues	Atoms				AltConf
3	C	1	Total	C	N	O	0
			280	160	20	100	
3	C	1	Total	C	N	O	0
			280	160	20	100	
3	C	1	Total	C	N	O	0
			280	160	20	100	
3	C	1	Total	C	N	O	0
			280	160	20	100	

- Molecule 4 is BETA-D-MANNOSE (three-letter code: BMA) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	C	O	0
			77	42	35	
4	A	1	Total	C	O	0
			77	42	35	
4	A	1	Total	C	O	0
			77	42	35	
4	A	1	Total	C	O	0
			77	42	35	
4	A	1	Total	C	O	0
			77	42	35	
4	A	1	Total	C	O	0
			77	42	35	
4	A	1	Total	C	O	0
			77	42	35	

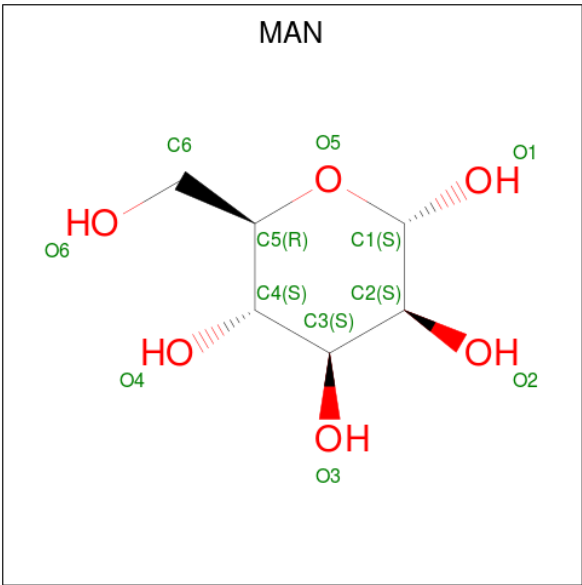
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Mol	Chain	Residues	Atoms			AltConf
4	B	1	Total	C	O	0
			77	42	35	
4	B	1	Total	C	O	0
			77	42	35	
4	B	1	Total	C	O	0
			77	42	35	
4	B	1	Total	C	O	0
			77	42	35	
4	B	1	Total	C	O	0
			77	42	35	
4	B	1	Total	C	O	0
			77	42	35	
4	C	1	Total	C	O	0
			66	36	30	
4	C	1	Total	C	O	0
			66	36	30	
4	C	1	Total	C	O	0
			66	36	30	
4	C	1	Total	C	O	0
			66	36	30	
4	C	1	Total	C	O	0
			66	36	30	
4	C	1	Total	C	O	0
			66	36	30	

- Molecule 5 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).

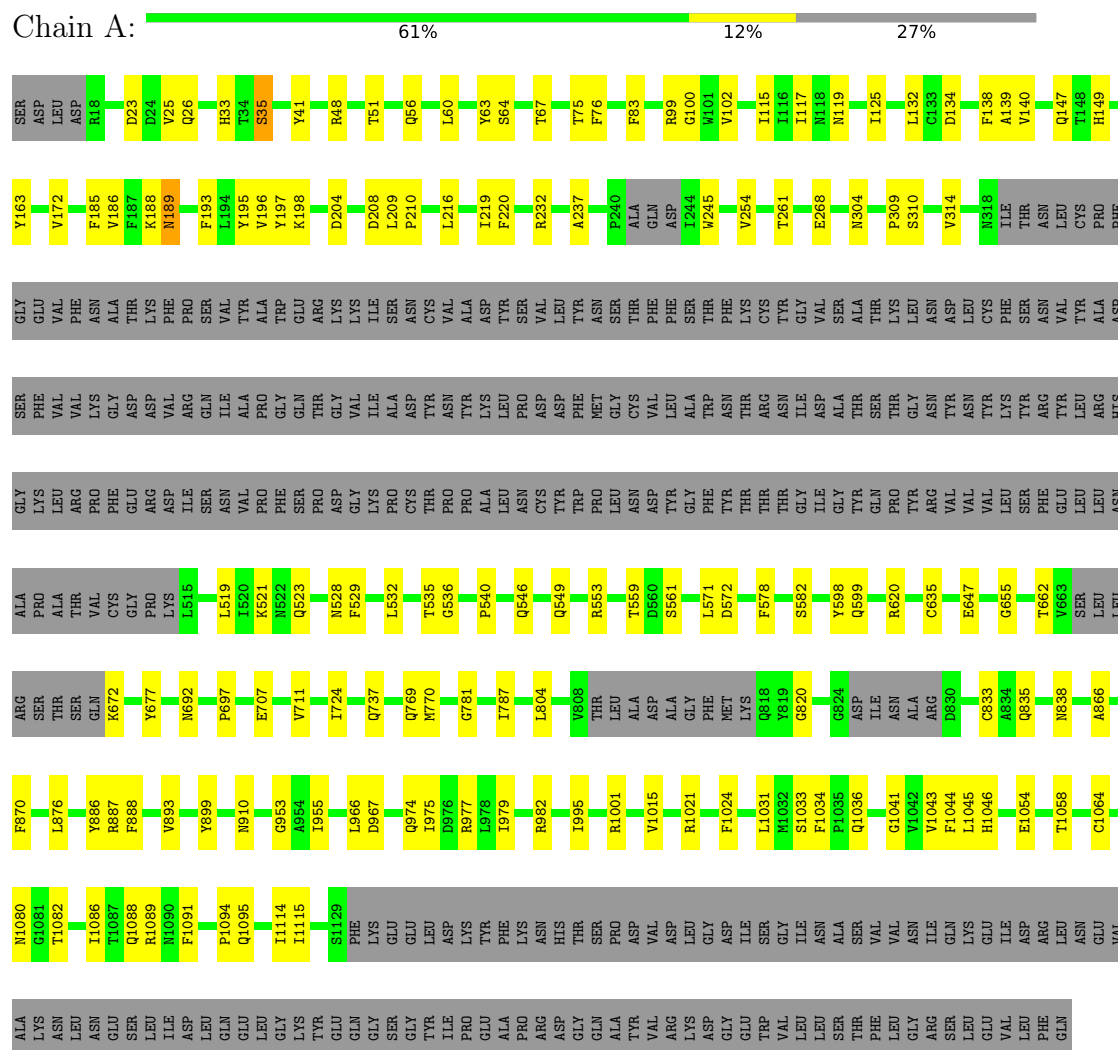


Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	C	O	0
			44	24	20	
5	A	1	Total	C	O	0
			44	24	20	
5	A	1	Total	C	O	0
			44	24	20	
5	A	1	Total	C	O	0
			44	24	20	
5	B	1	Total	C	O	0
			33	18	15	
5	B	1	Total	C	O	0
			33	18	15	
5	B	1	Total	C	O	0
			33	18	15	
5	C	1	Total	C	O	0
			44	24	20	
5	C	1	Total	C	O	0
			44	24	20	
5	C	1	Total	C	O	0
			44	24	20	
5	C	1	Total	C	O	0
			44	24	20	

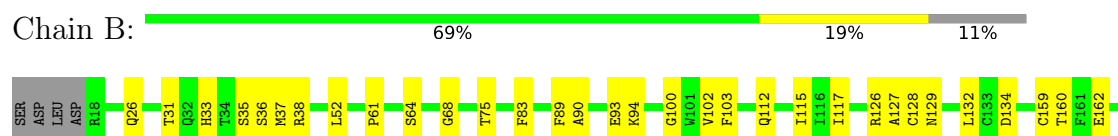
### 3 Residue-property plots

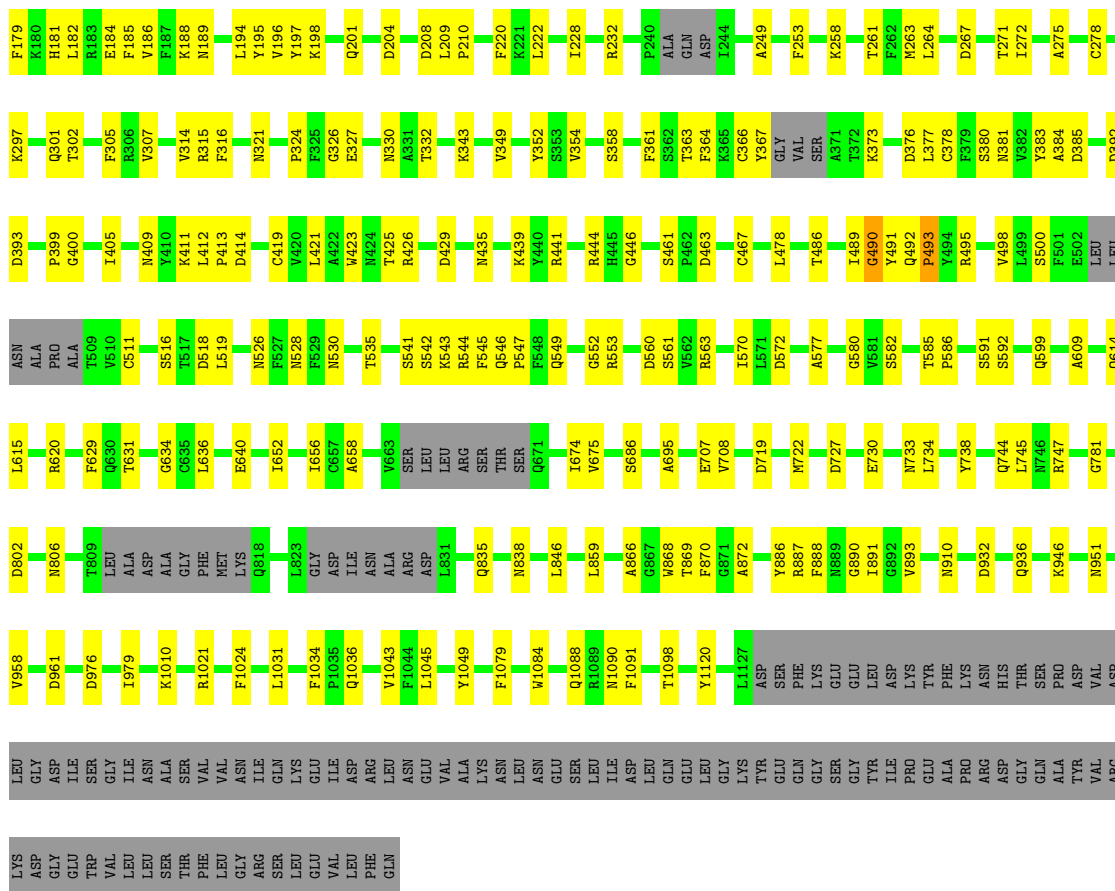
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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: Spike glycoprotein,Fibrin

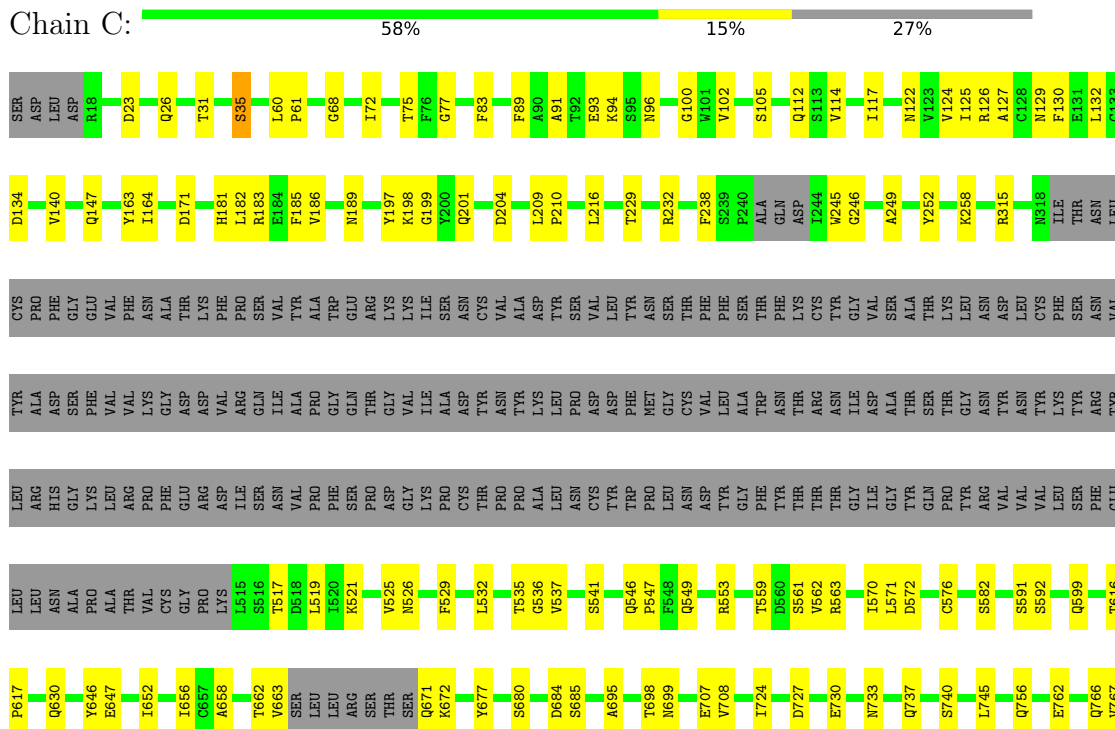


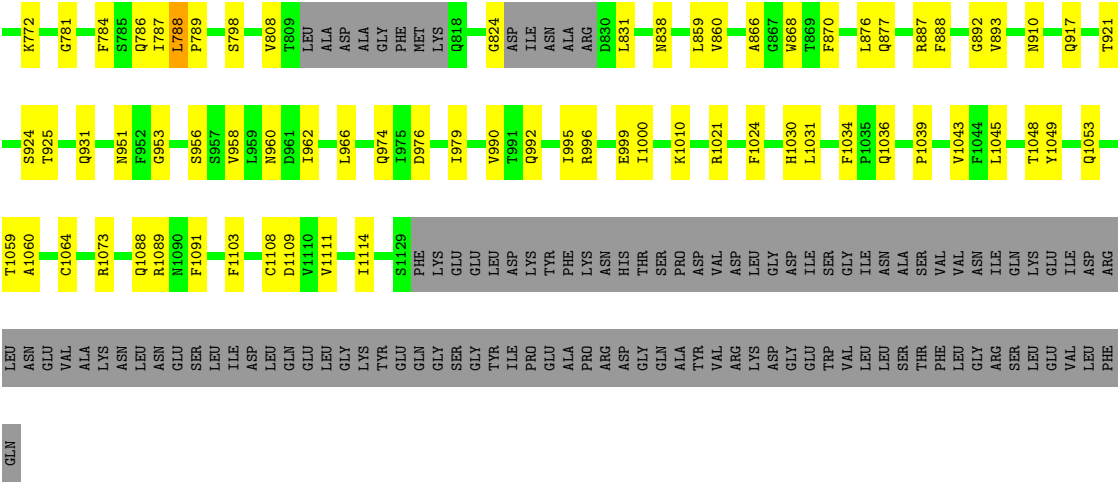
- Molecule 1: Spike glycoprotein,Fibrin



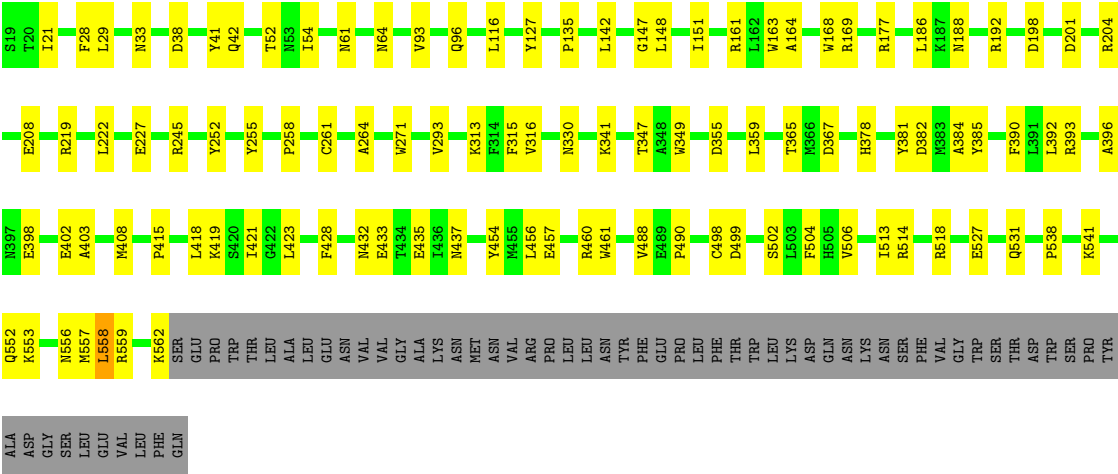


- Molecule 1: Spike glycoprotein, Fibrin





● Molecule 2: Angiotensin-converting enzyme 2



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	66771	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	65	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	29000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, MAN

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	0.39	0/7067	0.57	0/9612
1	B	0.37	0/8606	0.56	0/11712
1	C	0.38	0/7080	0.56	0/9630
2	D	0.28	0/4551	0.51	0/6176
All	All	0.36	0/27304	0.55	0/37130

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	2
1	B	0	2
1	C	0	2
All	All	0	6

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	35	SER	Peptide
1	A	83	PHE	Peptide
1	B	35	SER	Peptide
1	B	83	PHE	Peptide
1	C	35	SER	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	6914	0	6723	90	0
1	B	8405	0	8145	145	0
1	C	6927	0	6729	124	0
2	D	4431	0	4231	73	0
3	A	280	0	244	2	0
3	B	280	0	244	0	0
3	C	280	0	245	2	0
4	A	77	0	66	0	0
4	B	77	0	67	0	0
4	C	66	0	56	1	0
5	A	44	0	40	0	0
5	B	33	0	30	0	0
5	C	44	0	40	0	0
All	All	27858	0	26860	413	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 8.

The worst 5 of 413 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:B:425:THR:OG1	1:B:493:PRO:O	1.97	0.81
2:D:381:TYR:HD1	2:D:558:LEU:CD1	1.94	0.81
1:A:966:LEU:O	1:A:967:ASP:OD1	2.02	0.77
1:A:955:ILE:H	1:A:974:GLN:HE22	1.33	0.76
1:C:727:ASP:O	1:C:727:ASP:OD1	2.03	0.76

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	879/1215 (72%)	821 (93%)	58 (7%)	0	100	100
1	B	1062/1215 (87%)	973 (92%)	87 (8%)	2 (0%)	49	84
1	C	881/1215 (72%)	811 (92%)	70 (8%)	0	100	100
2	D	542/605 (90%)	521 (96%)	21 (4%)	0	100	100
All	All	3364/4250 (79%)	3126 (93%)	236 (7%)	2 (0%)	56	87

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	490	GLY
1	B	493	PRO

### 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	771/1053 (73%)	769 (100%)	2 (0%)	93	95
1	B	934/1053 (89%)	933 (100%)	1 (0%)	94	96
1	C	772/1053 (73%)	770 (100%)	2 (0%)	93	95
2	D	479/534 (90%)	477 (100%)	2 (0%)	92	95
All	All	2956/3693 (80%)	2949 (100%)	7 (0%)	94	96

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	189	ASN
2	D	558	LEU
1	C	788	LEU
1	A	1114	ILE
2	D	456	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	806	ASN
1	B	1088	GLN
2	D	64	ASN
1	B	935	ASN
1	A	974	GLN

### 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 ⓘ

91 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	$\# Z  > 2$
3	NAG	A	1301	1	14,14,15	0.36	0	17,19,21	0.53	0
3	NAG	A	1302	1,3	14,14,15	0.34	0	17,19,21	0.79	1 (5%)
3	NAG	A	1303	3,4	14,14,15	0.28	0	17,19,21	0.45	0
4	BMA	A	1304	3	11,11,12	0.80	0	15,15,17	0.98	1 (6%)
3	NAG	A	1305	1,3	14,14,15	0.34	0	17,19,21	0.43	0
3	NAG	A	1306	3,4	14,14,15	0.19	0	17,19,21	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	BMA	A	1307	3	11,11,12	0.83	0	15,15,17	1.36	3 (20%)
3	NAG	A	1308	1	14,14,15	0.44	0	17,19,21	0.42	0
3	NAG	A	1309	1,3	14,14,15	0.41	0	17,19,21	0.58	0
3	NAG	A	1310	3	14,14,15	0.23	0	17,19,21	0.55	0
3	NAG	A	1311	1,3	14,14,15	0.37	0	17,19,21	0.42	0
3	NAG	A	1312	3,4	14,14,15	0.40	0	17,19,21	0.40	0
4	BMA	A	1313	3,5	11,11,12	0.81	0	15,15,17	0.83	0
5	MAN	A	1314	4	11,11,12	0.79	0	15,15,17	1.06	2 (13%)
3	NAG	A	1315	1,3	14,14,15	0.62	1 (7%)	17,19,21	0.76	0
3	NAG	A	1316	3,4	14,14,15	0.21	0	17,19,21	0.51	0
4	BMA	A	1317	3,5	11,11,12	0.46	0	15,15,17	1.15	1 (6%)
5	MAN	A	1318	4	11,11,12	0.89	1 (9%)	15,15,17	1.48	2 (13%)
3	NAG	A	1319	1,3	14,14,15	0.30	0	17,19,21	0.61	0
3	NAG	A	1320	3	14,14,15	0.33	0	17,19,21	0.62	1 (5%)
3	NAG	A	1321	1,3	14,14,15	0.67	1 (7%)	17,19,21	0.86	1 (5%)
3	NAG	A	1322	3,4	14,14,15	0.21	0	17,19,21	0.47	0
4	BMA	A	1323	3,5	11,11,12	0.73	0	15,15,17	0.92	1 (6%)
5	MAN	A	1324	4	11,11,12	0.85	0	15,15,17	1.09	2 (13%)
3	NAG	A	1325	1,3	14,14,15	0.75	1 (7%)	17,19,21	0.70	0
3	NAG	A	1326	3,4	14,14,15	0.17	0	17,19,21	0.52	0
4	BMA	A	1327	3,5	11,11,12	0.77	0	15,15,17	0.95	1 (6%)
5	MAN	A	1328	4	11,11,12	0.92	0	15,15,17	1.08	2 (13%)
3	NAG	A	1329	1,3	14,14,15	0.56	0	17,19,21	0.67	0
3	NAG	A	1330	3,4	14,14,15	0.24	0	17,19,21	0.56	0
4	BMA	A	1331	3	11,11,12	0.74	0	15,15,17	0.93	1 (6%)
3	NAG	B	1301	1,3	14,14,15	0.46	0	17,19,21	0.58	0
3	NAG	B	1302	3	14,14,15	0.39	0	17,19,21	0.56	0
3	NAG	B	1303	1,3	14,14,15	0.30	0	17,19,21	0.49	0
3	NAG	B	1304	3,4	14,14,15	0.25	0	17,19,21	0.41	0
4	BMA	B	1305	3	11,11,12	0.71	0	15,15,17	0.91	1 (6%)
3	NAG	B	1306	1,3	14,14,15	0.55	0	17,19,21	0.67	0
3	NAG	B	1307	3,4	14,14,15	0.42	0	17,19,21	0.90	1 (5%)
4	BMA	B	1308	3,5	11,11,12	0.59	0	15,15,17	1.16	2 (13%)
5	MAN	B	1309	4	11,11,12	0.69	0	15,15,17	1.03	2 (13%)
3	NAG	B	1310	1	14,14,15	0.24	0	17,19,21	0.57	0
3	NAG	B	1311	1,3	14,14,15	0.73	1 (7%)	17,19,21	0.76	0
3	NAG	B	1312	3,4	14,14,15	0.18	0	17,19,21	0.60	0
4	BMA	B	1313	3	11,11,12	0.79	0	15,15,17	1.33	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	B	1314	1,3	14,14,15	0.32	0	17,19,21	0.48	0
3	NAG	B	1315	3	14,14,15	0.25	0	17,19,21	0.59	1 (5%)
3	NAG	B	1316	1,3	14,14,15	0.95	1 (7%)	17,19,21	0.77	0
3	NAG	B	1317	3,4	14,14,15	0.28	0	17,19,21	0.48	0
4	BMA	B	1318	3,5	11,11,12	0.56	0	15,15,17	1.07	2 (13%)
5	MAN	B	1319	4	11,11,12	0.86	0	15,15,17	1.05	2 (13%)
3	NAG	B	1320	1	14,14,15	0.47	0	17,19,21	0.62	0
3	NAG	B	1321	1,3	14,14,15	0.69	1 (7%)	17,19,21	0.63	0
3	NAG	B	1322	3,4	14,14,15	0.23	0	17,19,21	0.44	0
4	BMA	B	1323	3	11,11,12	0.59	0	15,15,17	0.89	1 (6%)
3	NAG	B	1324	1,3	14,14,15	0.31	0	17,19,21	0.54	0
3	NAG	B	1325	3,4	14,14,15	0.25	0	17,19,21	0.66	0
4	BMA	B	1326	3,5	11,11,12	0.87	0	15,15,17	1.33	2 (13%)
5	MAN	B	1327	4	11,11,12	1.09	1 (9%)	15,15,17	1.48	3 (20%)
3	NAG	B	1328	1,3	14,14,15	0.35	0	17,19,21	0.56	0
3	NAG	B	1329	3,4	14,14,15	0.23	0	17,19,21	0.52	0
4	BMA	B	1330	3	11,11,12	0.60	0	15,15,17	1.14	2 (13%)
3	NAG	C	1301	1,3	14,14,15	0.21	0	17,19,21	0.60	0
3	NAG	C	1302	3,4	14,14,15	0.29	0	17,19,21	0.59	0
4	BMA	C	1303	3	11,11,12	0.62	0	15,15,17	0.80	0
3	NAG	C	1304	1,3	14,14,15	0.24	0	17,19,21	0.59	0
3	NAG	C	1305	3,4	14,14,15	0.26	0	17,19,21	0.54	0
4	BMA	C	1306	3	11,11,12	0.85	0	15,15,17	0.80	0
3	NAG	C	1307	1,3	14,14,15	0.29	0	17,19,21	0.61	0
3	NAG	C	1308	3	14,14,15	0.23	0	17,19,21	0.53	0
3	NAG	C	1309	1	14,14,15	0.26	0	17,19,21	0.44	0
3	NAG	C	1310	1,3	14,14,15	0.52	0	17,19,21	0.55	0
3	NAG	C	1311	3	14,14,15	0.36	0	17,19,21	0.63	1 (5%)
3	NAG	C	1312	1,3	14,14,15	0.40	0	17,19,21	0.46	0
3	NAG	C	1313	3,4	14,14,15	0.25	0	17,19,21	0.55	0
4	BMA	C	1314	3,5	11,11,12	0.78	0	15,15,17	1.30	2 (13%)
5	MAN	C	1315	4	11,11,12	0.91	0	15,15,17	0.93	1 (6%)
3	NAG	C	1316	1,3	14,14,15	0.43	0	17,19,21	0.47	0
3	NAG	C	1317	3,4	14,14,15	0.23	0	17,19,21	0.45	0
4	BMA	C	1318	3,5	11,11,12	0.86	1 (9%)	15,15,17	1.22	1 (6%)
5	MAN	C	1319	4	11,11,12	0.82	0	15,15,17	0.98	2 (13%)
3	NAG	C	1320	1	14,14,15	0.33	0	17,19,21	0.44	0
3	NAG	C	1321	1,3	14,14,15	0.47	0	17,19,21	0.72	0
3	NAG	C	1322	3	14,14,15	0.47	0	17,19,21	0.41	0
3	NAG	C	1323	1,3	14,14,15	0.26	0	17,19,21	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	C	1324	3,4	14,14,15	0.20	0	17,19,21	0.66	1 (5%)
4	BMA	C	1325	3,5	11,11,12	0.53	0	15,15,17	0.94	2 (13%)
5	MAN	C	1326	4	11,11,12	0.71	0	15,15,17	1.27	2 (13%)
3	NAG	C	1327	1,3	14,14,15	0.47	0	17,19,21	0.54	0
3	NAG	C	1328	3,4	14,14,15	0.20	0	17,19,21	0.44	0
4	BMA	C	1329	3,5	11,11,12	0.69	0	15,15,17	0.85	1 (6%)
5	MAN	C	1330	4	11,11,12	0.85	1 (9%)	15,15,17	1.21	2 (13%)

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. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1301	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1302	1,3	-	2/6/23/26	0/1/1/1
3	NAG	A	1303	3,4	-	2/6/23/26	0/1/1/1
4	BMA	A	1304	3	-	0/2/19/22	0/1/1/1
3	NAG	A	1305	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1306	3,4	-	2/6/23/26	0/1/1/1
4	BMA	A	1307	3	-	2/2/19/22	0/1/1/1
3	NAG	A	1308	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1309	1,3	-	2/6/23/26	0/1/1/1
3	NAG	A	1310	3	-	0/6/23/26	0/1/1/1
3	NAG	A	1311	1,3	-	2/6/23/26	0/1/1/1
3	NAG	A	1312	3,4	-	2/6/23/26	0/1/1/1
4	BMA	A	1313	3,5	-	0/2/19/22	0/1/1/1
5	MAN	A	1314	4	-	0/2/19/22	0/1/1/1
3	NAG	A	1315	1,3	-	2/6/23/26	0/1/1/1
3	NAG	A	1316	3,4	-	1/6/23/26	0/1/1/1
4	BMA	A	1317	3,5	-	0/2/19/22	0/1/1/1
5	MAN	A	1318	4	-	2/2/19/22	0/1/1/1
3	NAG	A	1319	1,3	-	2/6/23/26	0/1/1/1
3	NAG	A	1320	3	-	2/6/23/26	0/1/1/1
3	NAG	A	1321	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1322	3,4	-	0/6/23/26	0/1/1/1
4	BMA	A	1323	3,5	-	2/2/19/22	0/1/1/1
5	MAN	A	1324	4	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1325	1,3	-	1/6/23/26	0/1/1/1
3	NAG	A	1326	3,4	-	2/6/23/26	0/1/1/1
4	BMA	A	1327	3,5	-	2/2/19/22	0/1/1/1
5	MAN	A	1328	4	-	0/2/19/22	0/1/1/1
3	NAG	A	1329	1,3	-	2/6/23/26	0/1/1/1
3	NAG	A	1330	3,4	-	2/6/23/26	0/1/1/1
4	BMA	A	1331	3	-	2/2/19/22	0/1/1/1
3	NAG	B	1301	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	1302	3	-	0/6/23/26	0/1/1/1
3	NAG	B	1303	1,3	-	2/6/23/26	0/1/1/1
3	NAG	B	1304	3,4	-	2/6/23/26	0/1/1/1
4	BMA	B	1305	3	-	0/2/19/22	0/1/1/1
3	NAG	B	1306	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	1307	3,4	-	2/6/23/26	0/1/1/1
4	BMA	B	1308	3,5	-	2/2/19/22	0/1/1/1
5	MAN	B	1309	4	-	0/2/19/22	0/1/1/1
3	NAG	B	1310	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1311	1,3	-	1/6/23/26	0/1/1/1
3	NAG	B	1312	3,4	-	2/6/23/26	0/1/1/1
4	BMA	B	1313	3	-	2/2/19/22	0/1/1/1
3	NAG	B	1314	1,3	-	2/6/23/26	0/1/1/1
3	NAG	B	1315	3	-	2/6/23/26	0/1/1/1
3	NAG	B	1316	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	1317	3,4	-	2/6/23/26	0/1/1/1
4	BMA	B	1318	3,5	-	2/2/19/22	0/1/1/1
5	MAN	B	1319	4	-	0/2/19/22	0/1/1/1
3	NAG	B	1320	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1321	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	1322	3,4	-	2/6/23/26	0/1/1/1
4	BMA	B	1323	3	-	0/2/19/22	0/1/1/1
3	NAG	B	1324	1,3	-	1/6/23/26	0/1/1/1
3	NAG	B	1325	3,4	-	2/6/23/26	0/1/1/1
4	BMA	B	1326	3,5	-	0/2/19/22	0/1/1/1
5	MAN	B	1327	4	-	0/2/19/22	0/1/1/1
3	NAG	B	1328	1,3	-	2/6/23/26	0/1/1/1
3	NAG	B	1329	3,4	-	2/6/23/26	0/1/1/1
4	BMA	B	1330	3	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	1301	1,3	-	2/6/23/26	0/1/1/1
3	NAG	C	1302	3,4	-	2/6/23/26	0/1/1/1
4	BMA	C	1303	3	-	0/2/19/22	0/1/1/1
3	NAG	C	1304	1,3	-	2/6/23/26	0/1/1/1
3	NAG	C	1305	3,4	-	0/6/23/26	0/1/1/1
4	BMA	C	1306	3	-	0/2/19/22	0/1/1/1
3	NAG	C	1307	1,3	-	2/6/23/26	0/1/1/1
3	NAG	C	1308	3	-	2/6/23/26	0/1/1/1
3	NAG	C	1309	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1310	1,3	-	2/6/23/26	0/1/1/1
3	NAG	C	1311	3	-	2/6/23/26	0/1/1/1
3	NAG	C	1312	1,3	-	2/6/23/26	0/1/1/1
3	NAG	C	1313	3,4	-	1/6/23/26	0/1/1/1
4	BMA	C	1314	3,5	-	2/2/19/22	0/1/1/1
5	MAN	C	1315	4	-	0/2/19/22	0/1/1/1
3	NAG	C	1316	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	1317	3,4	-	2/6/23/26	0/1/1/1
4	BMA	C	1318	3,5	-	2/2/19/22	0/1/1/1
5	MAN	C	1319	4	-	0/2/19/22	0/1/1/1
3	NAG	C	1320	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1321	1,3	-	2/6/23/26	0/1/1/1
3	NAG	C	1322	3	-	1/6/23/26	0/1/1/1
3	NAG	C	1323	1,3	-	2/6/23/26	0/1/1/1
3	NAG	C	1324	3,4	-	2/6/23/26	0/1/1/1
4	BMA	C	1325	3,5	-	0/2/19/22	0/1/1/1
5	MAN	C	1326	4	-	2/2/19/22	0/1/1/1
3	NAG	C	1327	1,3	-	2/6/23/26	0/1/1/1
3	NAG	C	1328	3,4	-	1/6/23/26	0/1/1/1
4	BMA	C	1329	3,5	-	2/2/19/22	0/1/1/1
5	MAN	C	1330	4	-	2/2/19/22	0/1/1/1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1316	NAG	O5-C1	-3.45	1.38	1.43
5	B	1327	MAN	C1-C2	3.05	1.59	1.52
5	A	1318	MAN	O5-C5	2.57	1.48	1.43
3	B	1311	NAG	O5-C1	-2.57	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1325	NAG	O5-C1	-2.56	1.39	1.43

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1318	MAN	C1-O5-C5	4.61	118.47	112.20
5	C	1326	MAN	C1-O5-C5	3.76	117.31	112.20
5	C	1330	MAN	C1-O5-C5	3.66	117.18	112.20
4	B	1313	BMA	C1-O5-C5	3.40	116.82	112.20
4	A	1307	BMA	C1-O5-C5	3.18	116.52	112.20

There are no chirality outliers.

5 of 113 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1308	NAG	O5-C5-C6-O6
3	C	1321	NAG	O5-C5-C6-O6
5	C	1330	MAN	C4-C5-C6-O6
3	A	1326	NAG	O5-C5-C6-O6
3	B	1315	NAG	O5-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1302	NAG	1	0
3	A	1321	NAG	1	0
4	C	1314	BMA	1	0
3	C	1323	NAG	2	0

## 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.