



wwPDB EM Validation Summary Report ⓘ

Apr 30, 2024 – 04:09 PM JST

PDB ID : 8HPV
EMDB ID : EMD-34945
Title : Cryo-EM structure of SARS-CoV-2 Omicron Prototype S-trimer in complex with fab L4.65 and L5.34
Authors : Gao, G.F.; Liu, S.
Deposited on : 2022-12-13
Resolution : 2.65 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

EMDB validation analysis : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
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) : 2.36.2

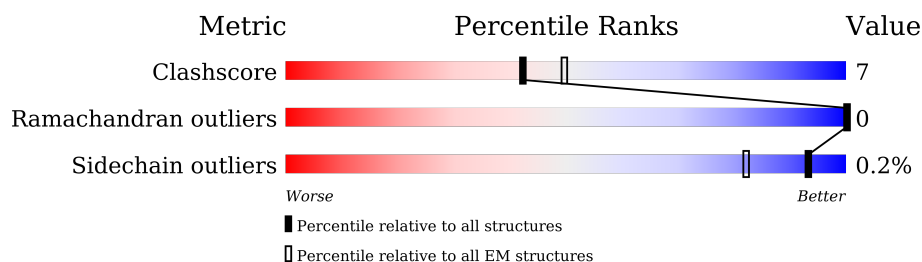
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.65 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.










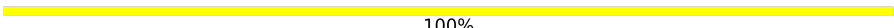
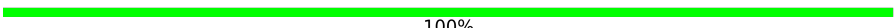
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	1134	81% 11% 8%
1	B	1134	81% 10% 8%
1	C	1134	82% 9% 8%
2	E	225	71% 29%
2	M	225	72% 28%
2	R	225	80% 20%
3	F	216	77% 23%
3	N	216	70% 30%
3	S	216	74% 26%

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Mol	Chain	Length	Quality of chain
4	H	231	 73%27%
4	I	231	 74%25%.
4	P	231	 79%21%
5	J	215	 75%25%
5	L	215	 71%29%
5	Q	215	 77%23%
6	D	2	 50%50%
6	G	2	 100%
6	K	2	 100%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 44640 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 protein S2'.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1040	Total	C	N	O	S	0	0
			8131	5194	1355	1545	37		
1	B	1040	Total	C	N	O	S	0	0
			8131	5194	1355	1545	37		
1	C	1040	Total	C	N	O	S	0	0
			8131	5194	1355	1545	37		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	817	PRO	PHE	conflict	UNP P0DTC2
A	892	PRO	ALA	conflict	UNP P0DTC2
A	899	PRO	ALA	conflict	UNP P0DTC2
A	942	PRO	ALA	conflict	UNP P0DTC2
A	986	PRO	LYS	conflict	UNP P0DTC2
A	987	PRO	VAL	conflict	UNP P0DTC2
B	817	PRO	PHE	conflict	UNP P0DTC2
B	892	PRO	ALA	conflict	UNP P0DTC2
B	899	PRO	ALA	conflict	UNP P0DTC2
B	942	PRO	ALA	conflict	UNP P0DTC2
B	986	PRO	LYS	conflict	UNP P0DTC2
B	987	PRO	VAL	conflict	UNP P0DTC2
C	817	PRO	PHE	conflict	UNP P0DTC2
C	892	PRO	ALA	conflict	UNP P0DTC2
C	899	PRO	ALA	conflict	UNP P0DTC2
C	942	PRO	ALA	conflict	UNP P0DTC2
C	986	PRO	LYS	conflict	UNP P0DTC2
C	987	PRO	VAL	conflict	UNP P0DTC2

- Molecule 2 is a protein called fab L5.34.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	225	Total	C	N	O	S	0	0
			1665	1045	280	332	8		
2	E	225	Total	C	N	O	S	0	0
			1665	1045	280	332	8		
2	R	225	Total	C	N	O	S	0	0
			1665	1045	280	332	8		

- Molecule 3 is a protein called fab L5.34.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	216	Total	C	N	O	S	0	0
			1642	1020	280	336	6		
3	F	216	Total	C	N	O	S	0	0
			1642	1020	280	336	6		
3	S	216	Total	C	N	O	S	0	0
			1642	1020	280	336	6		

- Molecule 4 is a protein called fab L4.65.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	231	Total	C	N	O	S	0	0
			1756	1115	287	347	7		
4	P	231	Total	C	N	O	S	0	0
			1756	1115	287	347	7		
4	I	231	Total	C	N	O	S	0	0
			1756	1115	287	347	7		

- Molecule 5 is a protein called fab L4.65.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	215	Total	C	N	O	S	0	0
			1658	1036	281	336	5		
5	Q	215	Total	C	N	O	S	0	0
			1658	1036	281	336	5		
5	J	215	Total	C	N	O	S	0	0
			1658	1036	281	336	5		

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

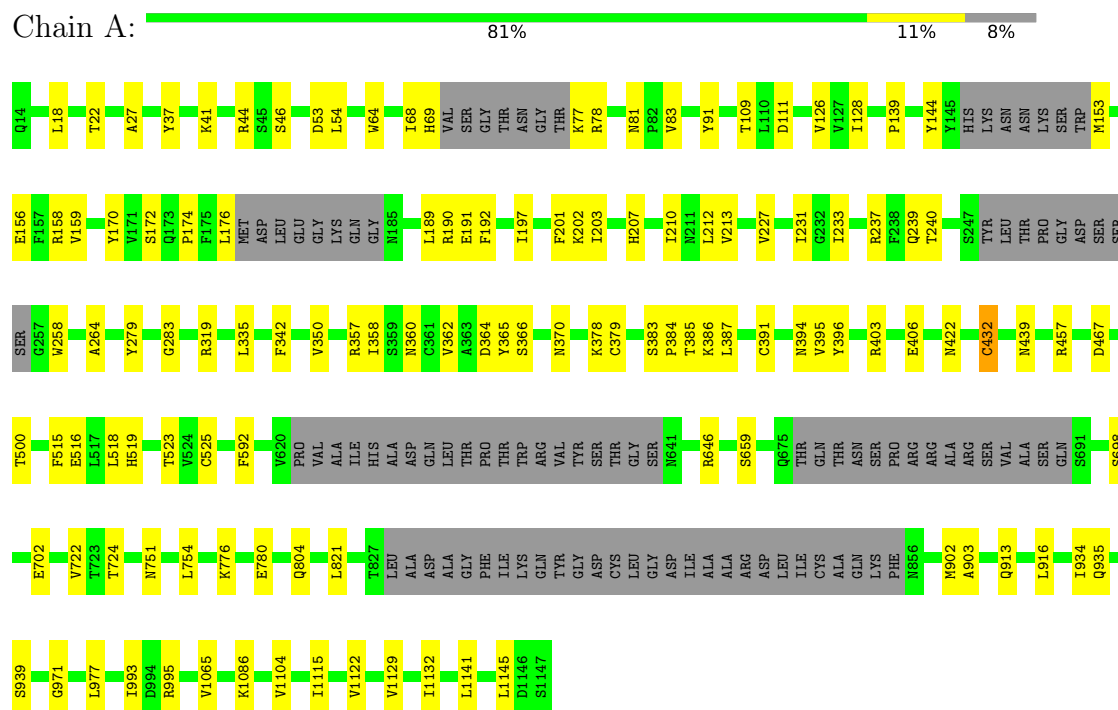


Mol	Chain	Residues	Atoms				AltConf	Trace
6	D	2	Total 28	C 16	N 2	O 10	0	0
6	G	2	Total 28	C 16	N 2	O 10	0	0
6	K	2	Total 28	C 16	N 2	O 10	0	0

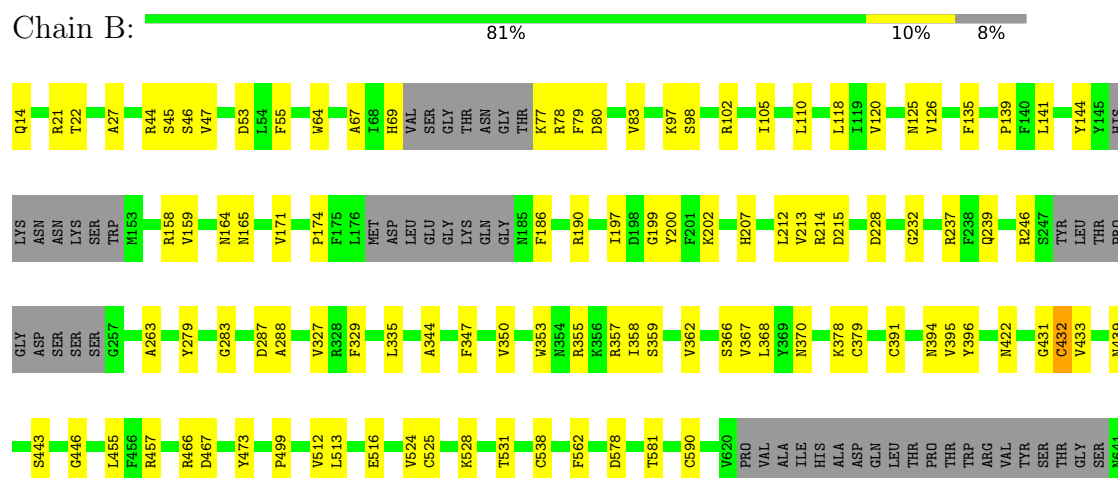
3 Residue-property plots


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.

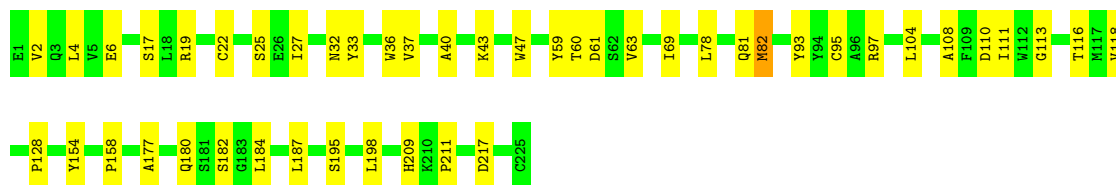
• Molecule 1: Spike protein S2'



• Molecule 1: Spike protein S2'

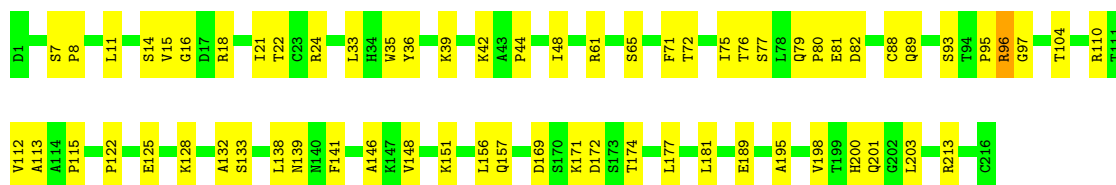


Chain R:  80% 20%




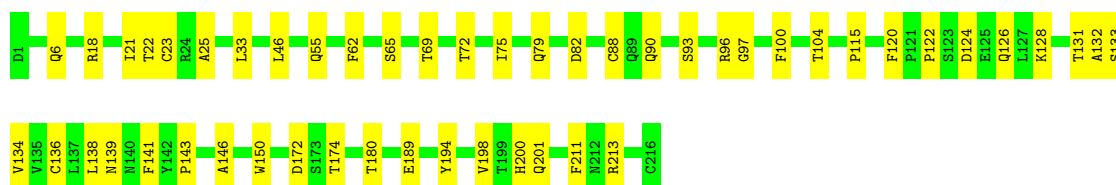
- Molecule 3: fab L5.34

Chain N:  70% 30%



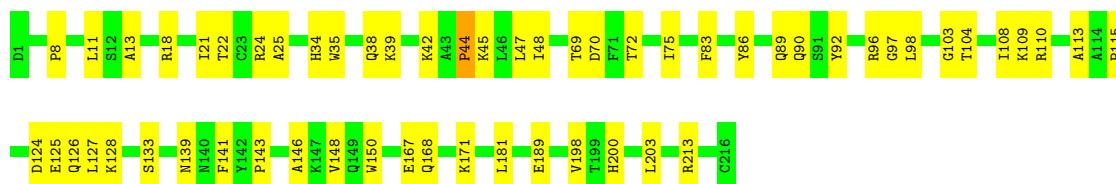
- Molecule 3: fab L5.34

Chain F:  77% 23%



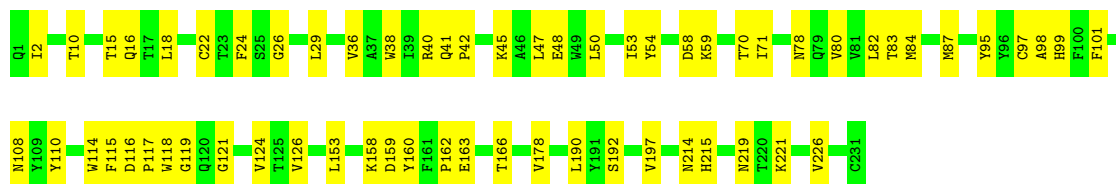
- Molecule 3: fab L5.34

Chain S:  74% 26%




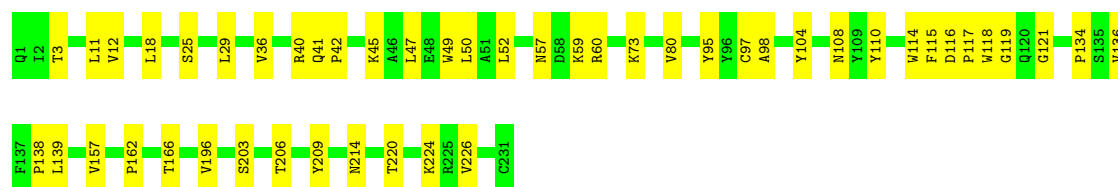
- Molecule 4: fab L4.65

Chain H:  73% 27%



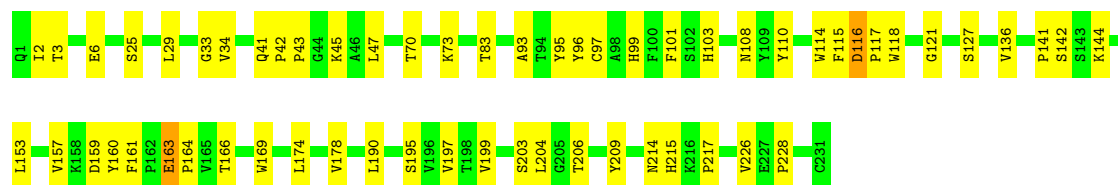
- Molecule 4: fab L4.65

Chain P:  79% 21%



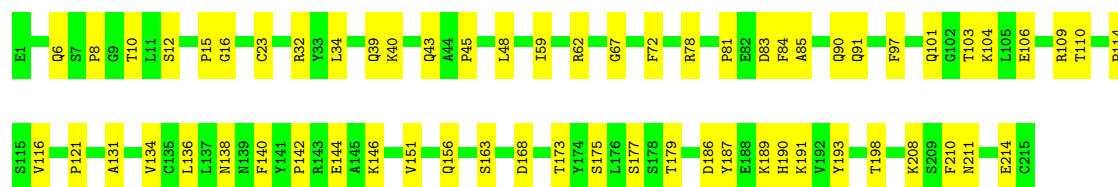
• Molecule 4: fab L4.65

Chain I:  74% 25%




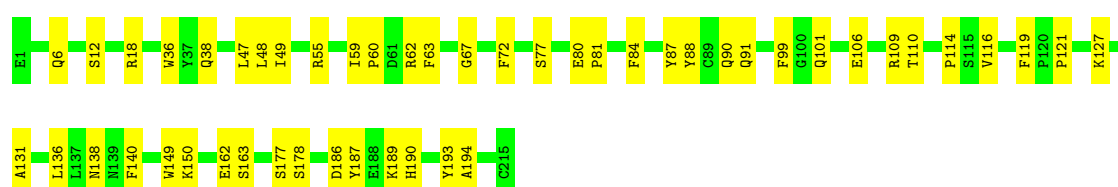
• Molecule 5: fab L4.65

Chain L:  71% 29%



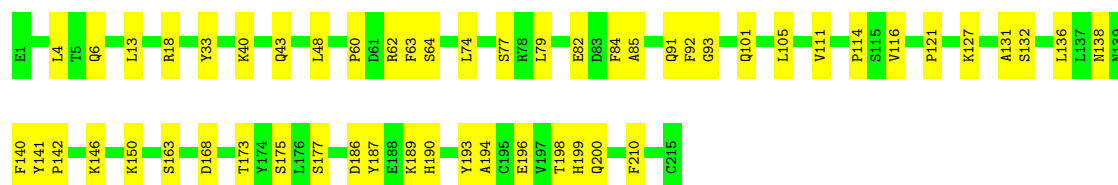
• Molecule 5: fab L4.65

Chain Q:  77% 23%



• Molecule 5: fab L4.65

Chain J:  75% 25%




- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  50% 50%

MAG1
MAG2

- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  100%

MAG1
MAG2

- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  100%

MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	615800	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.39	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k 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: 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	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.29	0/8319	0.51	1/11324 (0.0%)
1	B	0.29	0/8319	0.51	1/11324 (0.0%)
1	C	0.29	0/8319	0.51	1/11324 (0.0%)
2	E	0.25	0/1703	0.51	0/2320
2	M	0.26	0/1703	0.53	0/2320
2	R	0.27	0/1703	0.54	1/2320 (0.0%)
3	F	0.25	0/1676	0.49	0/2272
3	N	0.25	0/1676	0.50	0/2272
3	S	0.47	2/1676 (0.1%)	0.67	3/2272 (0.1%)
4	H	0.26	0/1805	0.51	0/2471
4	I	0.26	0/1805	0.58	2/2471 (0.1%)
4	P	0.26	0/1805	0.49	0/2471
5	J	0.26	0/1694	0.50	0/2294
5	L	0.26	0/1694	0.53	0/2294
5	Q	0.25	0/1694	0.50	0/2294
All	All	0.29	2/45591 (0.0%)	0.52	9/62043 (0.0%)

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
4	I	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	S	44	PRO	CG-CD	-14.39	1.03	1.50
3	S	44	PRO	N-CD	6.51	1.56	1.47

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	S	44	PRO	N-CD-CG	-15.09	80.56	103.20
3	S	44	PRO	CA-N-CD	-10.76	96.43	111.50
4	I	164	PRO	CA-N-CD	-8.68	99.34	111.50
3	S	44	PRO	CA-CB-CG	-8.40	88.03	104.00
2	R	158	PRO	CA-N-CD	-7.93	100.39	111.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	I	116	ASP	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	8131	0	7932	75	0
1	B	8131	0	7932	71	0
1	C	8131	0	7932	71	0
2	E	1665	0	1629	43	0
2	M	1665	0	1629	40	0
2	R	1665	0	1629	32	0
3	F	1642	0	1599	33	0
3	N	1642	0	1599	46	0
3	S	1642	0	1599	34	0
4	H	1756	0	1713	44	0
4	I	1756	0	1713	40	0
4	P	1756	0	1713	32	0
5	J	1658	0	1599	32	0
5	L	1658	0	1599	37	0
5	Q	1658	0	1599	35	0
6	D	28	0	25	1	0
6	G	28	0	25	1	0
6	K	28	0	25	0	0
All	All	44640	0	43491	637	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 7.

The worst 5 of 637 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)
4:H:95:TYR:O	4:H:121:GLY:HA2	1.68	0.93
4:P:95:TYR:O	4:P:121:GLY:HA2	1.73	0.89
2:M:33:TYR:HB2	2:M:98:GLU:HB2	1.55	0.86
1:C:81:ASN:HD21	1:C:242:LEU:HD13	1.41	0.86
3:S:39:LYS:HB2	3:S:42:LYS:HE3	1.61	0.83

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	Percentiles	
1	A	1022/1134 (90%)	987 (97%)	35 (3%)	0	100	100
1	B	1022/1134 (90%)	987 (97%)	35 (3%)	0	100	100
1	C	1022/1134 (90%)	996 (98%)	26 (2%)	0	100	100
2	E	223/225 (99%)	211 (95%)	12 (5%)	0	100	100
2	M	223/225 (99%)	214 (96%)	9 (4%)	0	100	100
2	R	223/225 (99%)	211 (95%)	12 (5%)	0	100	100
3	F	214/216 (99%)	204 (95%)	10 (5%)	0	100	100
3	N	214/216 (99%)	203 (95%)	11 (5%)	0	100	100
3	S	214/216 (99%)	204 (95%)	10 (5%)	0	100	100
4	H	229/231 (99%)	213 (93%)	16 (7%)	0	100	100
4	I	229/231 (99%)	219 (96%)	10 (4%)	0	100	100
4	P	229/231 (99%)	213 (93%)	16 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	J	213/215 (99%)	208 (98%)	5 (2%)	0	100	100
5	L	213/215 (99%)	206 (97%)	7 (3%)	0	100	100
5	Q	213/215 (99%)	207 (97%)	6 (3%)	0	100	100
All	All	5703/6063 (94%)	5483 (96%)	220 (4%)	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	910/988 (92%)	909 (100%)	1 (0%)	93	97
1	B	910/988 (92%)	910 (100%)	0	100	100
1	C	910/988 (92%)	910 (100%)	0	100	100
2	E	188/188 (100%)	188 (100%)	0	100	100
2	M	188/188 (100%)	186 (99%)	2 (1%)	73	85
2	R	188/188 (100%)	187 (100%)	1 (0%)	88	94
3	F	189/189 (100%)	189 (100%)	0	100	100
3	N	189/189 (100%)	188 (100%)	1 (0%)	88	94
3	S	189/189 (100%)	188 (100%)	1 (0%)	88	94
4	H	204/204 (100%)	204 (100%)	0	100	100
4	I	204/204 (100%)	203 (100%)	1 (0%)	88	94
4	P	204/204 (100%)	204 (100%)	0	100	100
5	J	186/186 (100%)	185 (100%)	1 (0%)	88	94
5	L	186/186 (100%)	185 (100%)	1 (0%)	88	94
5	Q	186/186 (100%)	185 (100%)	1 (0%)	88	94
All	All	5031/5265 (96%)	5021 (100%)	10 (0%)	93	97

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	J	127	LYS
2	R	82	MET
3	S	171	LYS
3	N	96	ARG
5	L	43	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	717	ASN
1	C	901	GLN
2	R	81	GLN
1	C	1011	GLN
1	C	81	ASN

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](#)

6 monosaccharides 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	$\# Z > 2$
6	NAG	D	1	1,6	14,14,15	0.18	0	17,19,21	0.44	0
6	NAG	D	2	6	14,14,15	0.23	0	17,19,21	0.38	0
6	NAG	G	1	1,6	14,14,15	0.22	0	17,19,21	0.43	0
6	NAG	G	2	6	14,14,15	0.22	0	17,19,21	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	K	1	1,6	14,14,15	0.17	0	17,19,21	0.48	0
6	NAG	K	2	6	14,14,15	0.23	0	17,19,21	0.43	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. 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
6	NAG	D	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	D	2	6	-	2/6/23/26	0/1/1/1
6	NAG	G	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	G	2	6	-	0/6/23/26	0/1/1/1
6	NAG	K	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	K	2	6	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

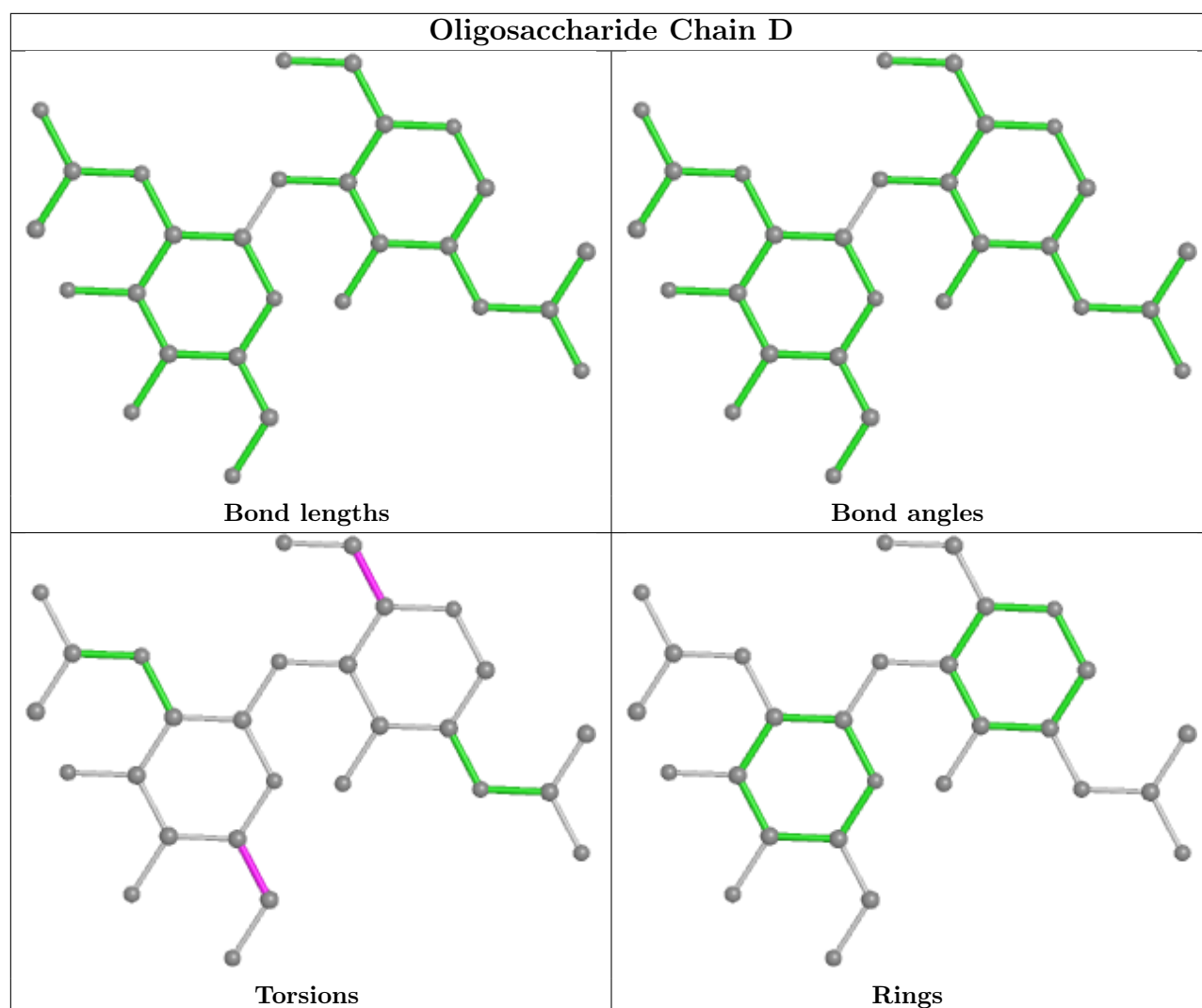
Mol	Chain	Res	Type	Atoms
6	D	2	NAG	O5-C5-C6-O6
6	K	2	NAG	O5-C5-C6-O6
6	K	2	NAG	C4-C5-C6-O6
6	D	2	NAG	C4-C5-C6-O6
6	D	1	NAG	C4-C5-C6-O6

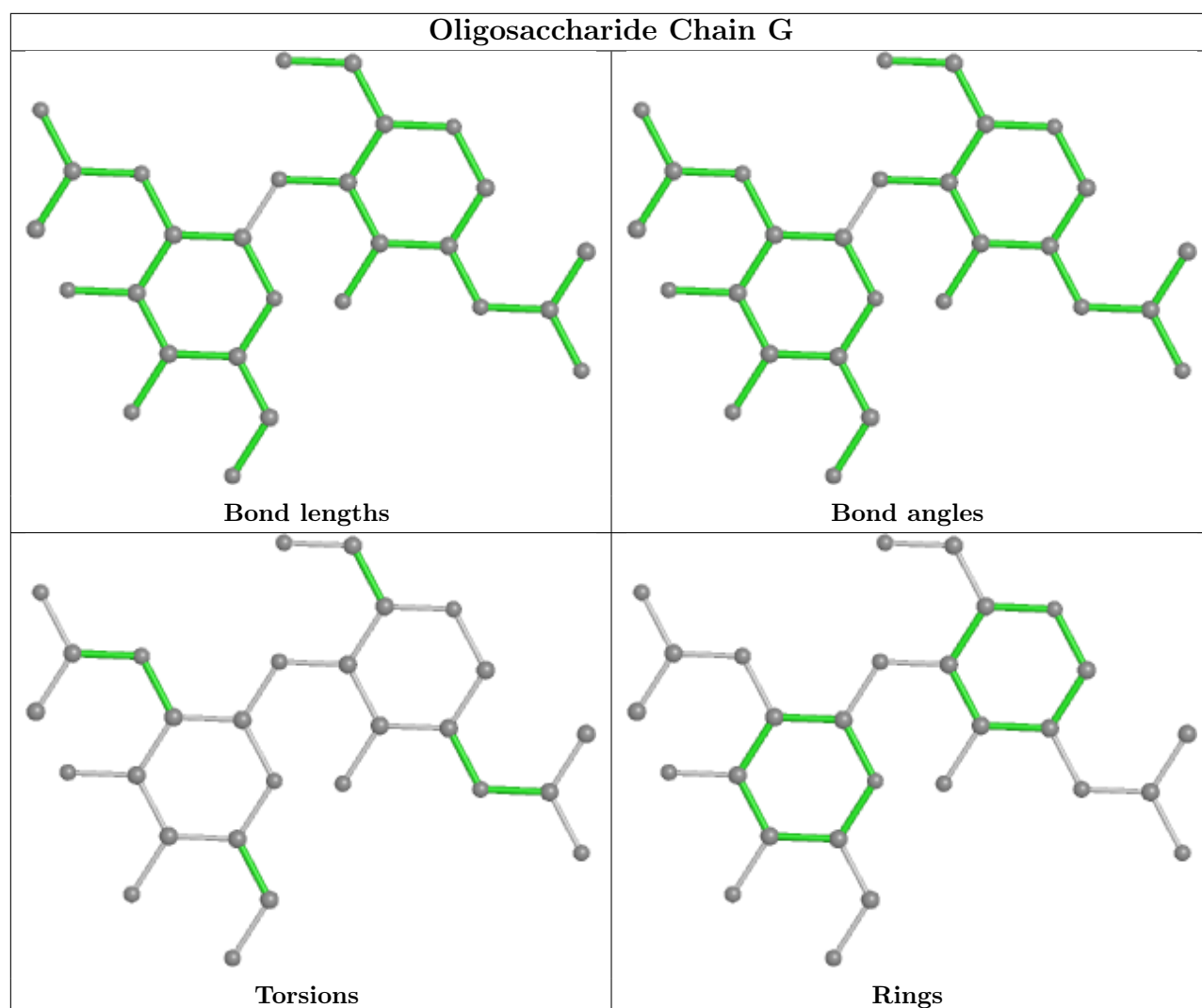
There are no ring outliers.

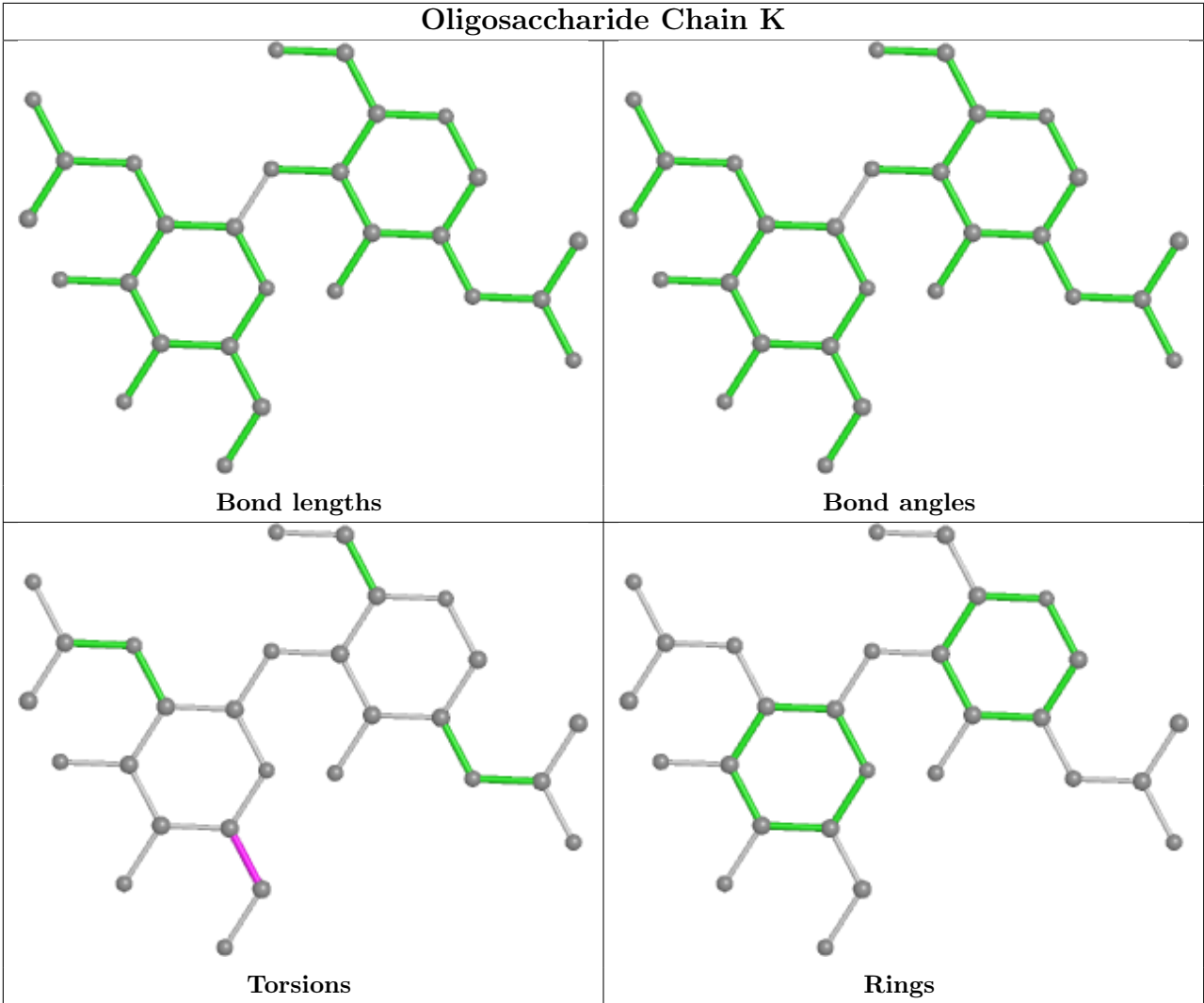
3 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	1	NAG	1	0
6	G	1	NAG	1	0
6	G	2	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.







5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
1	C	1

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Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	700:GLY	C	701:ALA	N	3.05
1	C	700:GLY	C	701:ALA	N	3.04
1	B	700:GLY	C	701:ALA	N	3.02