



wwPDB EM Validation Summary Report ⓘ

Oct 7, 2024 – 02:30 PM JST

PDB ID : 8XSL
EMDB ID : EMD-38621
Title : SARS-CoV-2 spike + IMCAS-123
Authors : Tong, Z.; Cui, Y.; Xie, Y.; Tong, J.; Gao, G.F.; Qi, J.
Deposited on : 2024-01-09
Resolution : 3.20 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 : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

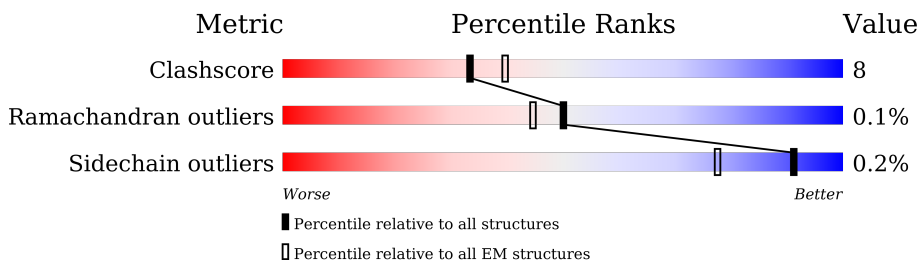
1 Overall quality at a glance

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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1273	
1	B	1273	
1	C	1273	
2	H	226	
2	M	226	
3	L	215	
3	N	215	
4	D	2	
4	E	2	

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 30267 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
			Total	C	N	O	S		
1	A	1001	7817	4991	1300	1491	35	1	0
1	B	1001	7817	4991	1300	1491	35	1	0
1	C	1002	7829	5000	1301	1493	35	1	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	986	PRO	LYS	variant	UNP P0DTC2
A	987	PRO	VAL	variant	UNP P0DTC2
B	986	PRO	LYS	variant	UNP P0DTC2
B	987	PRO	VAL	variant	UNP P0DTC2
C	986	PRO	LYS	variant	UNP P0DTC2
C	987	PRO	VAL	variant	UNP P0DTC2

- Molecule 2 is a protein called IMCAS-123 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	H	223	1658	1044	281	326	7	0	0
2	M	223	1658	1044	281	326	7	0	0

- Molecule 3 is a protein called IMCAS-123 light chain.

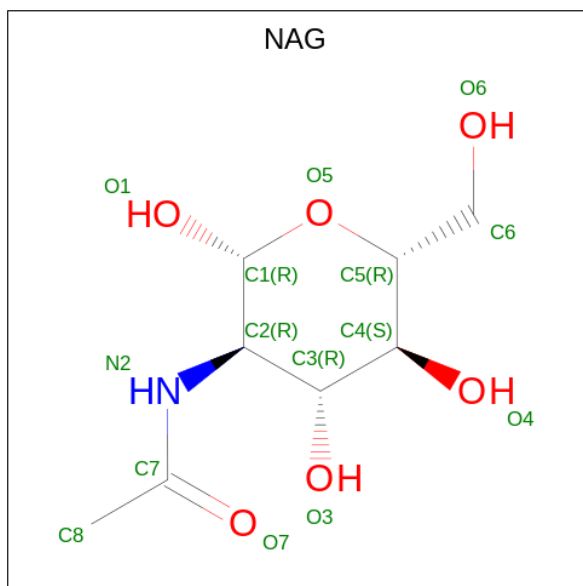
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	L	212	1611	1008	272	326	5	0	0
3	N	212	1611	1008	272	326	5	0	0

- Molecule 4 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
			Total	C	N	O		
4	D	2	28	16	2	10	0	0
4	E	2	28	16	2	10	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
5	A	1	14	8	1	5	0
5	A	1	14	8	1	5	0
5	A	1	14	8	1	5	0
5	A	1	14	8	1	5	0
5	A	1	14	8	1	5	0
5	B	1	14	8	1	5	0

Continued on next page...

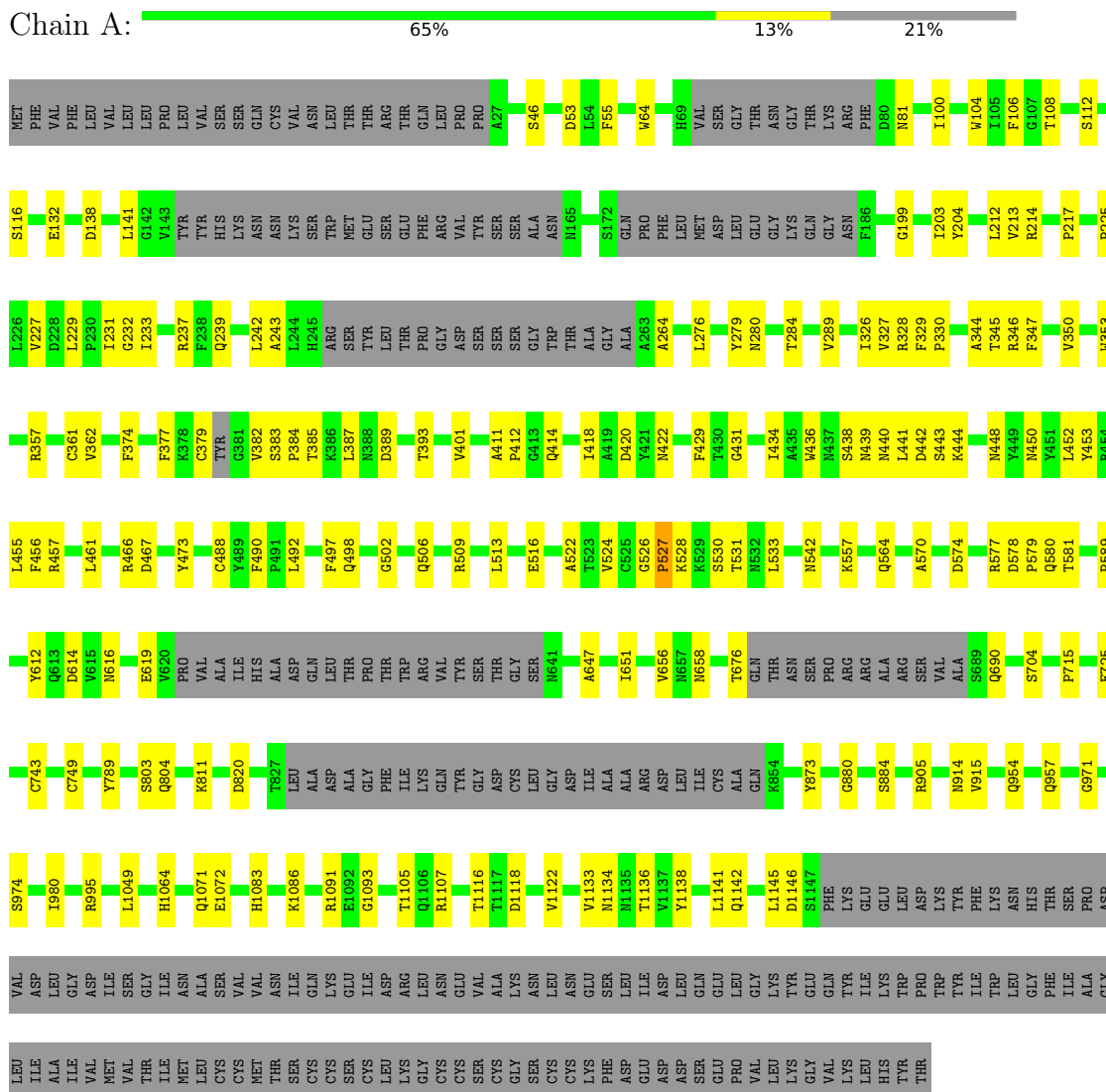
Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	

3 Residue-property plots [i](#)

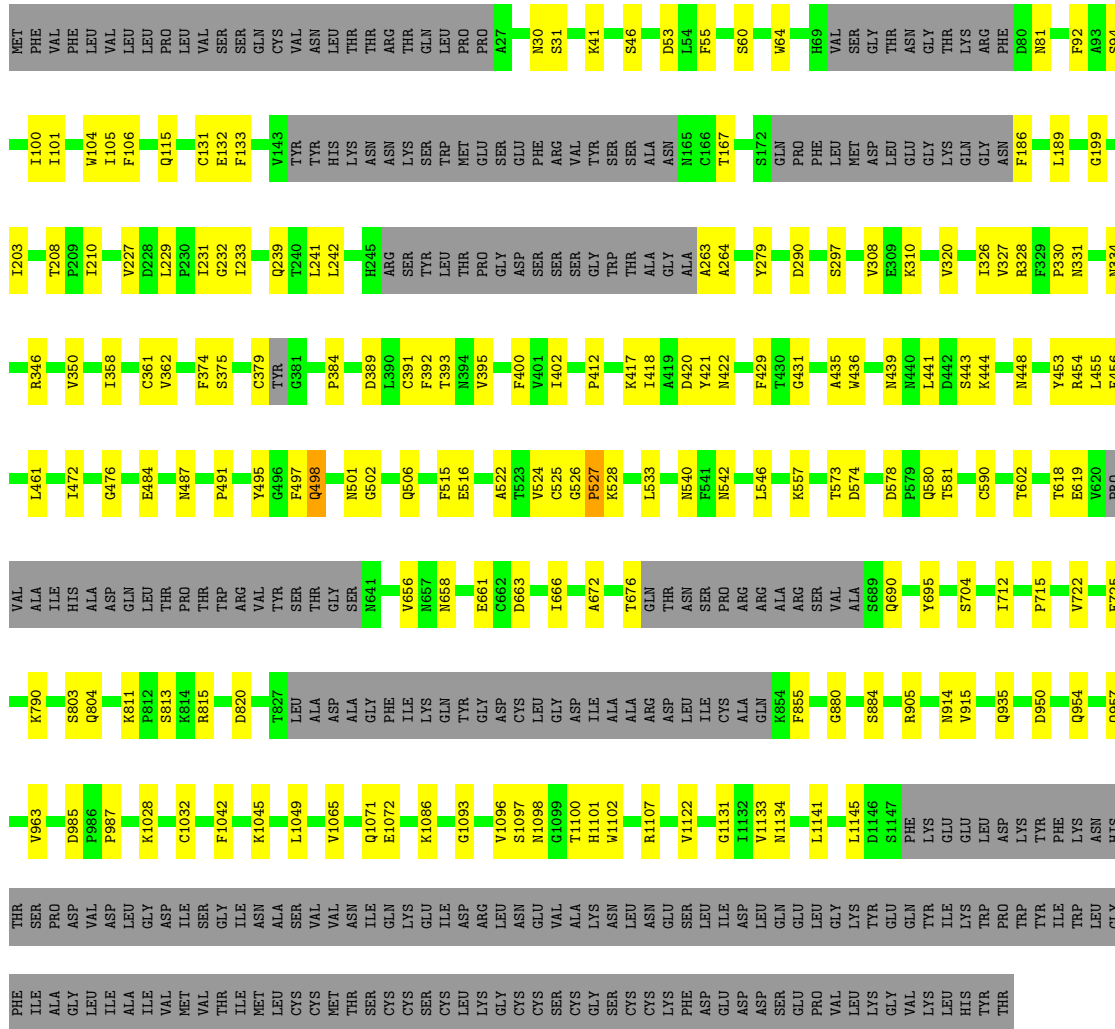
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

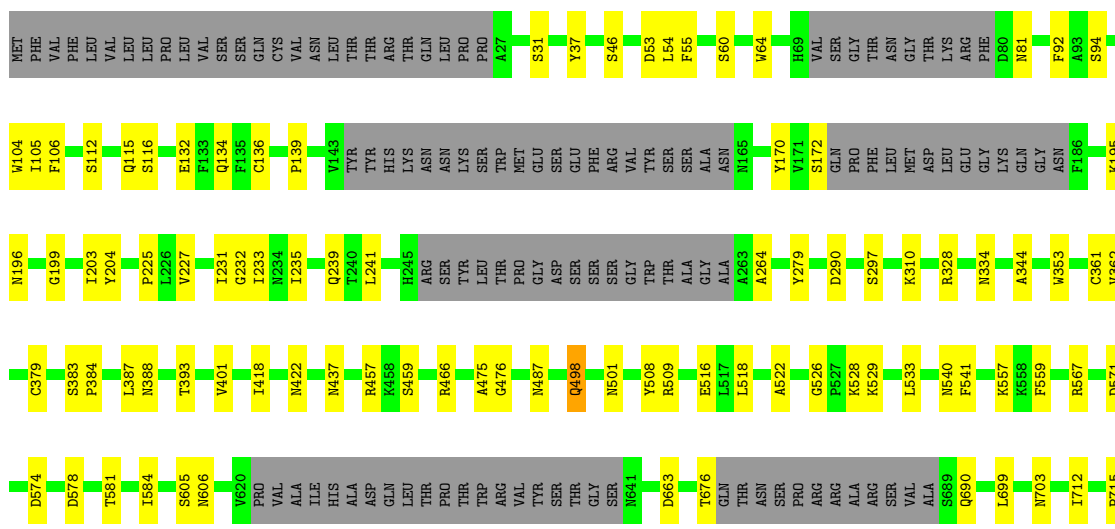


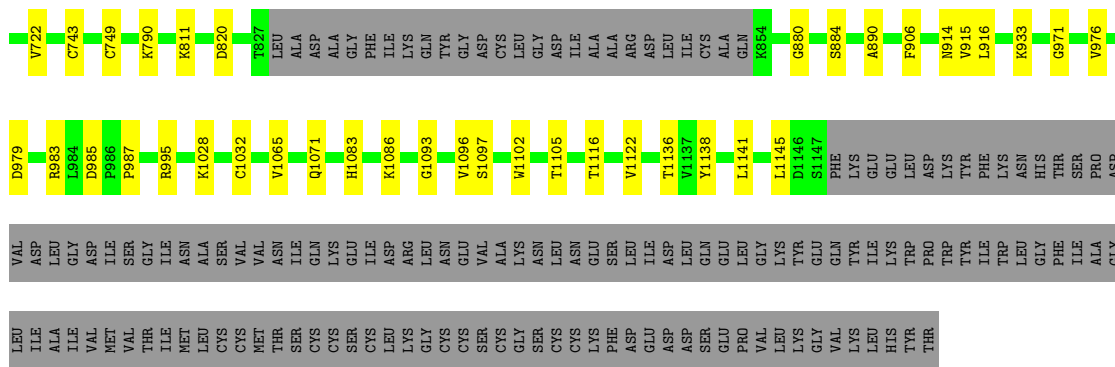
- Molecule 1: Spike glycoprotein



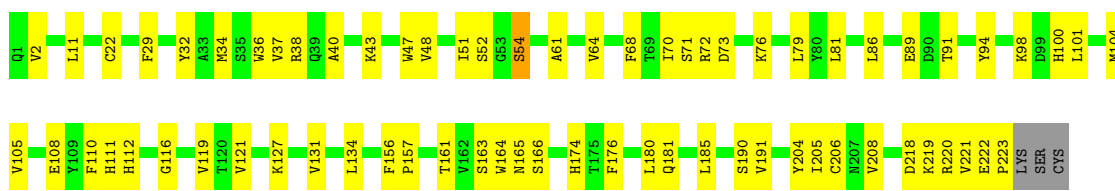


● Molecule 1: Spike glycoprotein





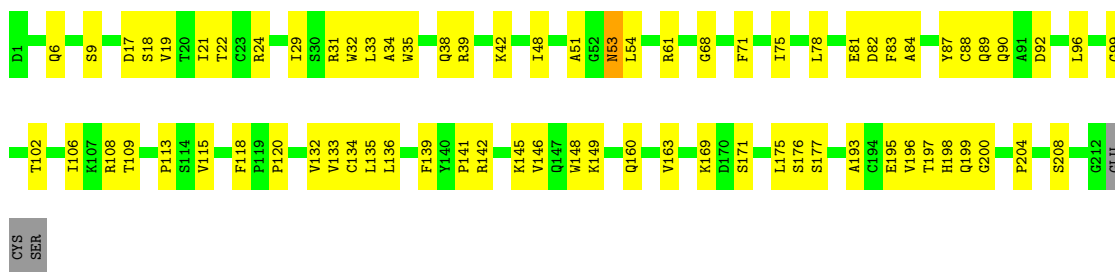
● Molecule 2: IMCAS-123 heavy chain



● Molecule 2: IMCAS-123 heavy chain

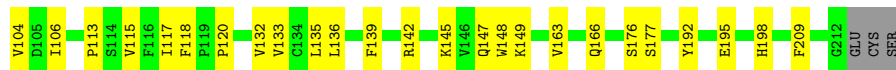
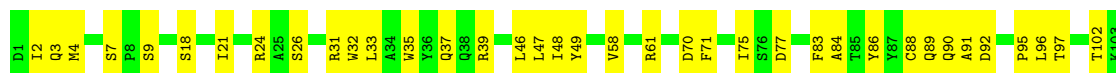


● Molecule 3: IMCAS-123 light chain



● Molecule 3: IMCAS-123 light chain

Chain N:  70% 29%



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

Chain D:  100%



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

Chain E:  100%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	583004	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 ($e^-/\text{\AA}^2$)	40	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: 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	0.33	0/7994	0.49	0/10877
1	B	0.33	0/7994	0.49	0/10877
1	C	0.34	0/8008	0.48	0/10898
2	H	0.26	0/1699	0.49	0/2314
2	M	0.26	0/1699	0.49	0/2314
3	L	0.28	0/1645	0.49	0/2234
3	N	0.27	0/1645	0.50	0/2234
All	All	0.32	0/30684	0.49	0/41748

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	A	7817	0	7631	114	0
1	B	7817	0	7632	117	0
1	C	7829	0	7644	79	0
2	H	1658	0	1617	49	0
2	M	1658	0	1617	58	0
3	L	1611	0	1563	57	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	N	1611	0	1563	43	0
4	D	28	0	25	0	0
4	E	28	0	25	0	0
5	A	70	0	65	0	0
5	B	84	0	78	2	0
5	C	56	0	52	0	0
All	All	30267	0	29512	486	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 486 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)
2:H:91:THR:HA	2:H:119:VAL:O	1.69	0.93
1:B:362:VAL:HG13	1:B:526:GLY:HA2	1.58	0.86
2:H:94:TYR:O	2:H:116:GLY:HA2	1.79	0.82
1:B:326:ILE:HD11	1:B:533:LEU:HA	1.62	0.82
3:L:39:ARG:H	3:L:42:LYS:HE2	1.42	0.82

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	984/1273 (77%)	943 (96%)	40 (4%)	1 (0%)	48 80
1	B	984/1273 (77%)	935 (95%)	48 (5%)	1 (0%)	48 80
1	C	987/1273 (78%)	943 (96%)	44 (4%)	0	100 100
2	H	221/226 (98%)	202 (91%)	18 (8%)	1 (0%)	25 60
2	M	221/226 (98%)	208 (94%)	12 (5%)	1 (0%)	25 60

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	L	210/215 (98%)	205 (98%)	5 (2%)	0	100	100
3	N	210/215 (98%)	201 (96%)	9 (4%)	0	100	100
All	All	3817/4701 (81%)	3637 (95%)	176 (5%)	4 (0%)	50	80

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	527	PRO
1	B	527	PRO
2	H	54	SER
2	M	54	SER

5.3.2 Protein sidechains [i](#)

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	876/1112 (79%)	874 (100%)	2 (0%)	92	97
1	B	876/1112 (79%)	874 (100%)	2 (0%)	92	97
1	C	877/1112 (79%)	875 (100%)	2 (0%)	92	97
2	H	186/189 (98%)	186 (100%)	0	100	100
2	M	186/189 (98%)	185 (100%)	1 (0%)	86	93
3	L	180/184 (98%)	178 (99%)	2 (1%)	70	86
3	N	180/184 (98%)	179 (99%)	1 (1%)	84	92
All	All	3361/4082 (82%)	3351 (100%)	10 (0%)	91	96

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

Mol	Chain	Res	Type
3	L	169	LYS
2	M	219	LYS
3	N	7	SER
1	B	498[B]	GLN
1	C	498[A]	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
3	L	89	GLN
3	N	89	GLN
3	N	166	GLN
3	N	147	GLN
2	H	112	HIS

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](#)

4 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	$\# Z > 2$
4	NAG	D	1	1,4	14,14,15	0.36	0	17,19,21	0.53	0
4	NAG	D	2	4	14,14,15	0.23	0	17,19,21	0.48	0
4	NAG	E	1	1,4	14,14,15	0.22	0	17,19,21	0.46	0
4	NAG	E	2	4	14,14,15	0.20	0	17,19,21	0.41	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	NAG	E	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

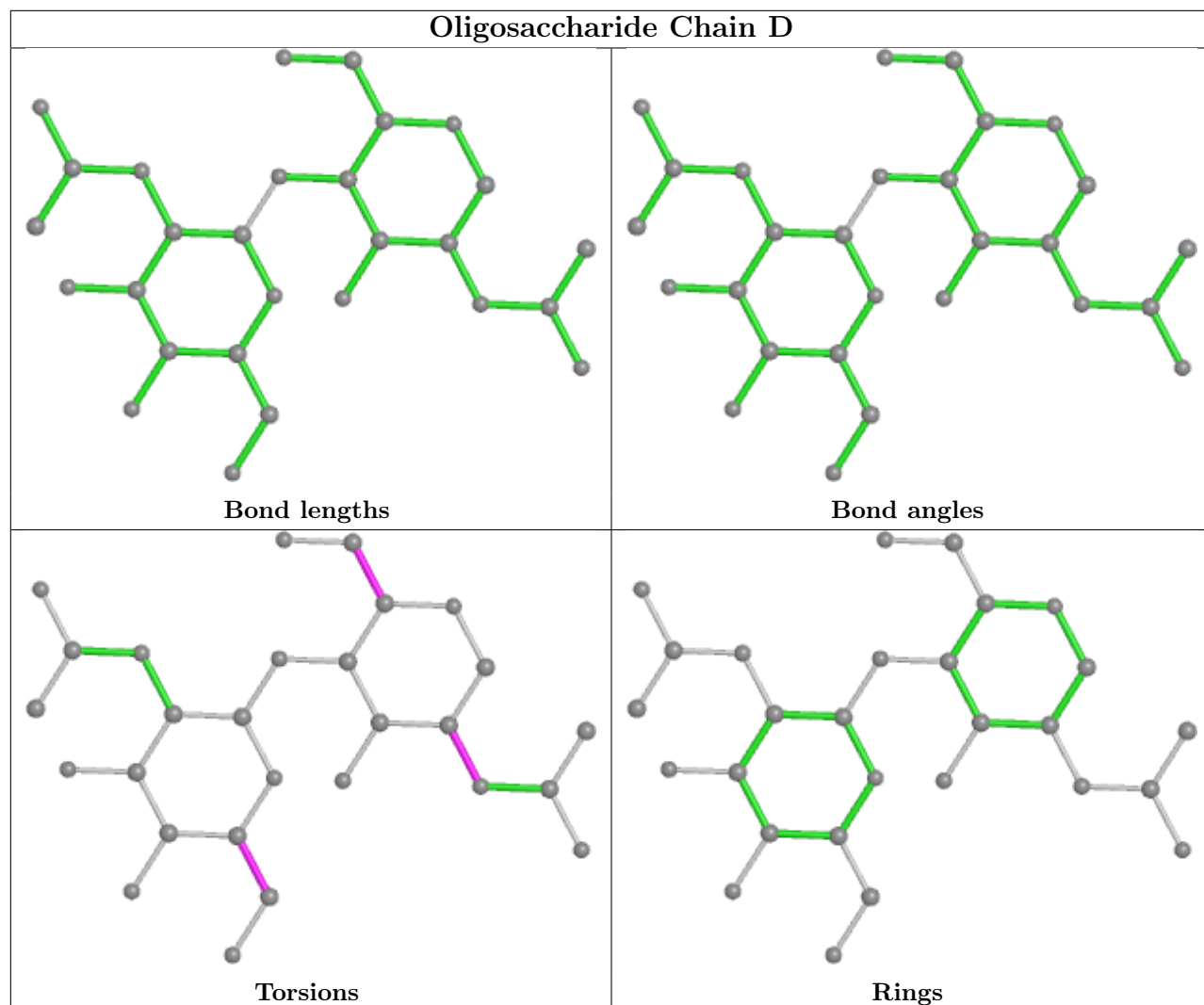
5 of 10 torsion outliers are listed below:

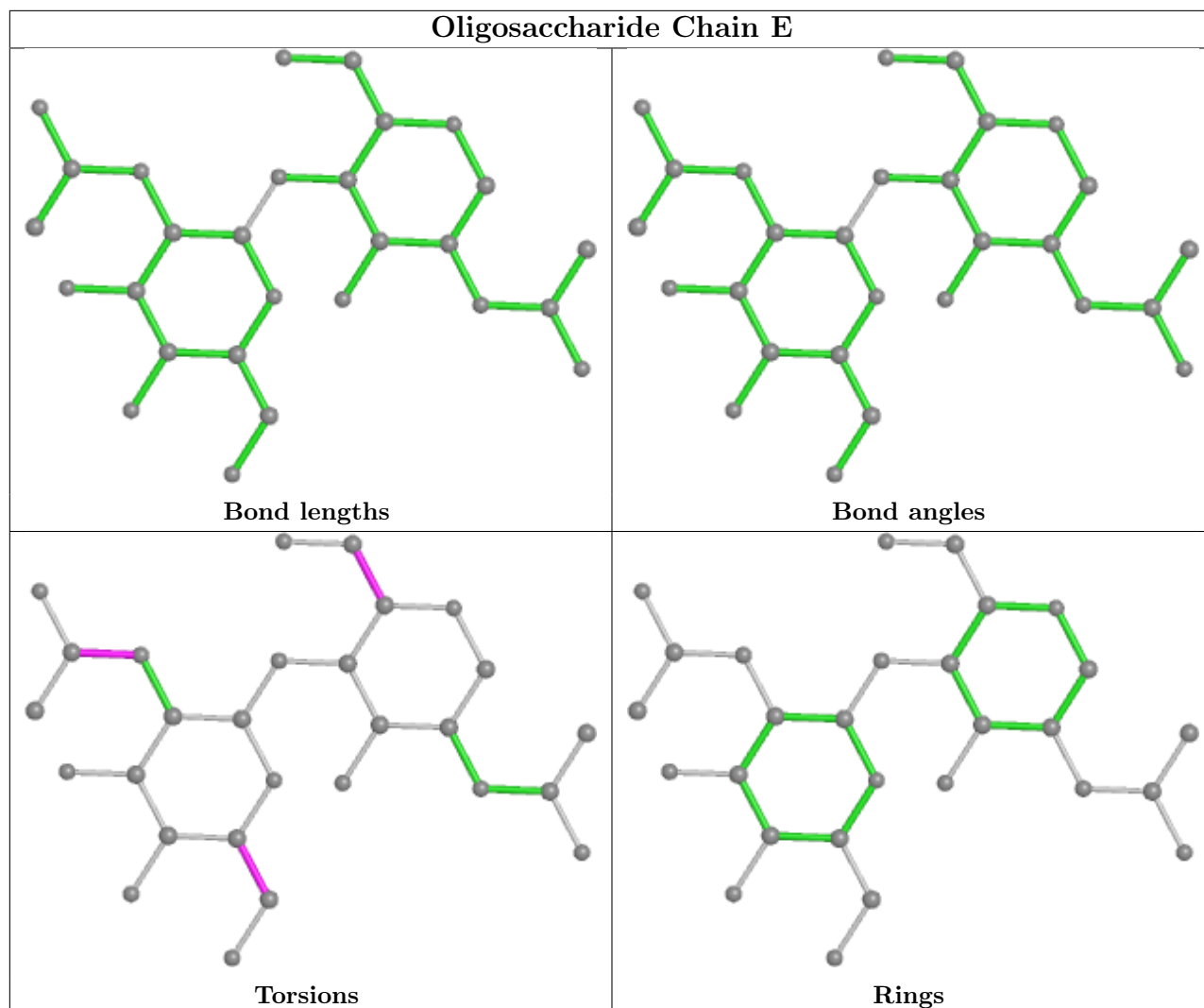
Mol	Chain	Res	Type	Atoms
4	D	2	NAG	O5-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
4	E	1	NAG	O5-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

15 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	$\# Z > 2$
5	NAG	A	1301	1	14,14,15	0.18	0	17,19,21	0.49	0
5	NAG	C	1303	1	14,14,15	0.19	0	17,19,21	0.55	0
5	NAG	A	1303	1	14,14,15	0.22	0	17,19,21	0.43	0
5	NAG	C	1301	1	14,14,15	0.20	0	17,19,21	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	B	1301	1	14,14,15	0.19	0	17,19,21	0.45	0
5	NAG	B	1303	1	14,14,15	0.21	0	17,19,21	0.51	0
5	NAG	C	1304	1	14,14,15	0.21	0	17,19,21	0.43	0
5	NAG	A	1304	1	14,14,15	0.23	0	17,19,21	0.40	0
5	NAG	B	1306	1	14,14,15	0.30	0	17,19,21	0.34	0
5	NAG	A	1302	1	14,14,15	0.21	0	17,19,21	0.44	0
5	NAG	B	1302	1	14,14,15	0.24	0	17,19,21	0.40	0
5	NAG	B	1304	1	14,14,15	0.19	0	17,19,21	0.42	0
5	NAG	B	1305	1	14,14,15	0.23	0	17,19,21	0.41	0
5	NAG	A	1305	1	14,14,15	0.22	0	17,19,21	0.45	0
5	NAG	C	1302	1	14,14,15	0.24	0	17,19,21	0.36	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
5	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1303	1	-	3/6/23/26	0/1/1/1
5	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1301	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1301	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1303	1	-	1/6/23/26	0/1/1/1
5	NAG	C	1304	1	-	1/6/23/26	0/1/1/1
5	NAG	A	1304	1	-	1/6/23/26	0/1/1/1
5	NAG	B	1306	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1302	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1305	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1305	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1302	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1305	NAG	C4-C5-C6-O6
5	A	1302	NAG	O5-C5-C6-O6
5	A	1303	NAG	O5-C5-C6-O6
5	A	1305	NAG	O5-C5-C6-O6
5	B	1304	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1306	NAG	1	0
5	B	1302	NAG	1	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.