Full wwPDB EM Validation Report ⓘ

Oct 7, 2024 – 02:23 PM JST

PDB ID	:	8XSJ
EMDB ID	:	EMD-38620
Title	:	SARS-CoV-2 Omicron BA.4 RBD + IMCAS-316 + ACE2
Authors	:	Tong, Z.; Cui, Y.; Xie, Y.; Tong, J.; Gao, G.F.; Qi, J.
Deposited on	:	2024-01-09
Resolution	:	2.61 Å(reported)

This is a Full wwPDB EM Validation 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:

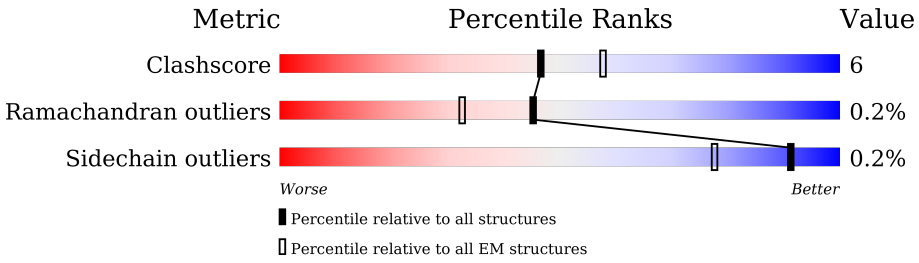
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.61 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	805	64% 10% 26%
2	B	223	76% 11% 13%
3	H	230	74% 17% 8%
4	L	215	80% 18% .
5	C	2	100%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9740 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 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	596	4869	3116	807	917	29	1	0

- Molecule 2 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	195	1554	1001	263	282	8	0	0

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	339	ASP	GLY	variant	UNP P0DTC2
B	371	PHE	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	376	ALA	THR	variant	UNP P0DTC2
B	405	ASN	ASP	variant	UNP P0DTC2
B	408	SER	ARG	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	452	ARG	LEU	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	484	ALA	GLU	variant	UNP P0DTC2
B	486	VAL	PHE	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2

- Molecule 3 is a protein called IMCAS-316 H chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	211	Total	C	N	O	S	0	0
			1583	1000	269	307	7		

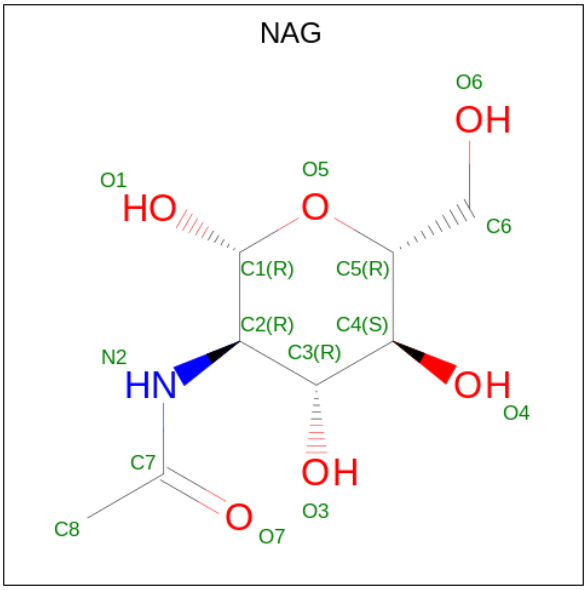
- Molecule 4 is a protein called IMCAS-316 L chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	213	Total	C	N	O	S	0	0
			1621	1011	269	336	5		

- Molecule 5 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
5	C	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

Continued on next page...

Continued from previous page...

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

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

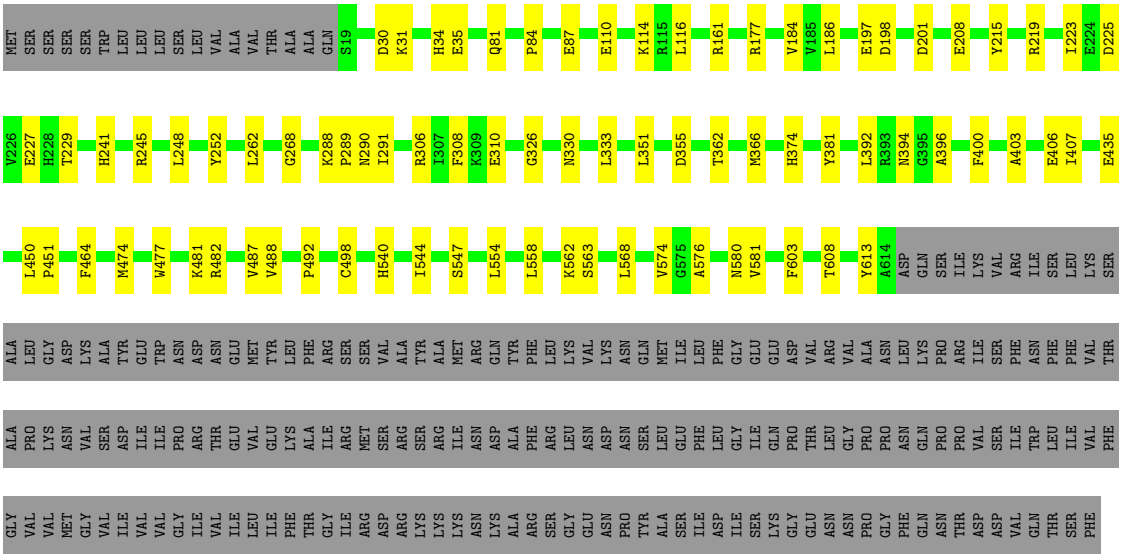
Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total	Zn	0
			1	1	

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.

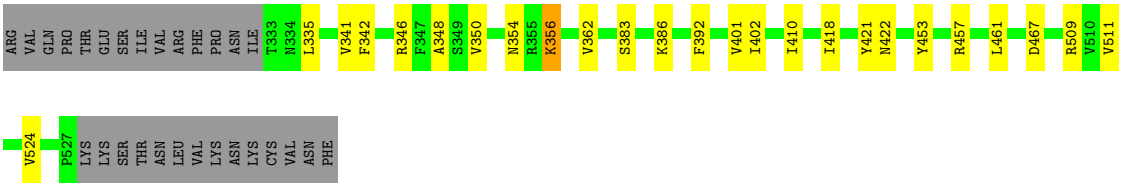
- Molecule 1: Angiotensin-converting enzyme 2

Chain A:



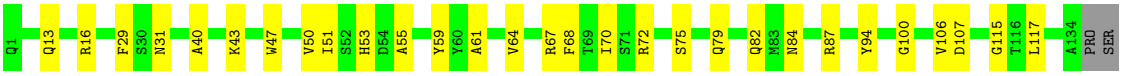
- Molecule 2: Spike protein S1

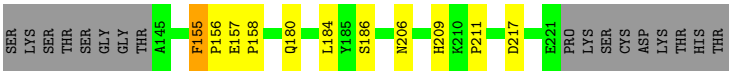
Chain B:



- Molecule 3: IMCAS-316 H chain

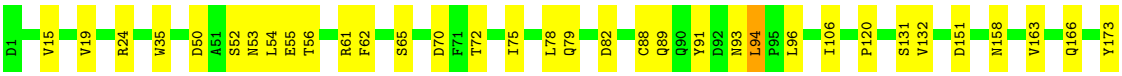
Chain H:





• Molecule 4: IMCAS-316 L chain

Chain L:



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

4 Experimental information (i)

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 ($e^-/Å^2$)	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	0.26	0/5010	0.46	0/6807
2	B	0.29	0/1601	0.51	0/2180
3	H	0.27	0/1621	0.53	0/2206
4	L	0.27	0/1655	0.49	0/2249
All	All	0.27	0/9887	0.48	0/13442

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
3	H	0	1
4	L	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	H	155	PHE	Peptide
4	L	94	LEU	Peptide

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	4869	0	4640	50	0
2	B	1554	0	1476	15	0
3	H	1583	0	1535	24	0
4	L	1621	0	1556	24	0
5	C	28	0	25	0	0
6	A	70	0	65	1	0
6	B	14	0	13	0	0
7	A	1	0	0	0	0
All	All	9740	0	9310	112	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 6.

All (112) 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:L:131:SER:HA	4:L:179:LEU:O	1.78	0.83
1:A:31:LYS:NZ	1:A:35:GLU:OE2	2.20	0.71
2:B:457:ARG:NH1	2:B:467:ASP:OD2	2.24	0.69
1:A:381:TYR:HD1	1:A:558:LEU:HD22	1.59	0.68
4:L:78:LEU:HD21	4:L:106:ILE:HD12	1.77	0.65
4:L:61:ARG:NH1	4:L:82:ASP:OD2	2.29	0.65
2:B:383:SER:H	2:B:386:LYS:HE2	1.62	0.63
1:A:482:ARG:HG2	1:A:488:VAL:HG12	1.81	0.62
1:A:574:VAL:HG23	1:A:576:ALA:H	1.64	0.62
3:H:206:ASN:ND2	3:H:217:ASP:OD1	2.31	0.61
1:A:116:LEU:HD13	1:A:186:LEU:HD23	1.84	0.59
1:A:208:GLU:OE1	1:A:219:ARG:NH1	2.36	0.59
1:A:81:GLN:HG2	6:A:903:NAG:H3	1.84	0.59
1:A:30:ASP:O	1:A:34[A]:HIS:ND1	2.35	0.59
3:H:13:GLN:OE1	3:H:16:ARG:NH2	2.36	0.59
4:L:50:ASP:OD1	4:L:91:TYR:OH	2.19	0.58
3:H:51:ILE:HD13	3:H:72:ARG:HG3	1.85	0.58
1:A:225:ASP:O	1:A:229:THR:HG23	2.05	0.57
1:A:435:GLU:OE2	1:A:540:HIS:NE2	2.36	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:29:PHE:O	3:H:72:ARG:NH2	2.38	0.57
3:H:82:GLN:NE2	3:H:84:ASN:OD1	2.37	0.57
2:B:422:ASN:ND2	2:B:453:TYR:HB2	2.21	0.56
2:B:418:ILE:HD13	2:B:422:ASN:HD22	1.70	0.56
2:B:392:PHE:O	2:B:524:VAL:N	2.39	0.56
1:A:396:ALA:HB3	1:A:400:PHE:CE2	2.42	0.55
1:A:306:ARG:NH1	1:A:310:GLU:OE2	2.18	0.55
3:H:106:VAL:O	4:L:91:TYR:HB2	2.06	0.55
1:A:381:TYR:CD1	1:A:558:LEU:HD22	2.40	0.54
3:H:157:GLU:HB2	3:H:211:PRO:HG2	1.90	0.54
1:A:326:GLY:O	1:A:330:ASN:ND2	2.40	0.54
4:L:55:GLU:HG2	4:L:56:THR:H	1.73	0.54
4:L:91:TYR:HA	4:L:96:LEU:HD22	1.88	0.53
2:B:421:TYR:HA	2:B:461:LEU:HD13	1.90	0.53
3:H:67:ARG:HG3	3:H:68:PHE:CD1	2.44	0.53
4:L:89:GLN:HE21	4:L:96:LEU:HB3	1.72	0.53
3:H:157:GLU:HB3	3:H:158:PRO:HD3	1.91	0.53
2:B:350:VAL:HG12	2:B:422:ASN:HB3	1.91	0.52
4:L:24:ARG:NH1	4:L:70:ASP:OD1	2.42	0.52
1:A:177:ARG:HH11	1:A:177:ARG:HG2	1.74	0.52
1:A:580:ASN:OD1	1:A:581:VAL:N	2.42	0.52
2:B:335:LEU:HD23	2:B:362:VAL:HG13	1.92	0.52
1:A:374:HIS:HE1	1:A:406:GLU:HG3	1.74	0.51
2:B:402:ILE:HD13	2:B:410:ILE:HD11	1.92	0.51
3:H:209:HIS:CD2	3:H:211:PRO:HD2	2.45	0.51
2:B:401:VAL:HG22	2:B:509:ARG:HG2	1.91	0.51
1:A:474:MET:HE3	1:A:498:CYS:HA	1.93	0.50
3:H:31:ASN:HA	3:H:53:HIS:HB2	1.94	0.50
3:H:40:ALA:HB3	3:H:43:LYS:HB2	1.93	0.50
3:H:157:GLU:HB3	3:H:158:PRO:CD	2.42	0.50
1:A:241:HIS:NE2	1:A:262:LEU:HD13	2.26	0.50
3:H:156:PRO:HG2	3:H:209:HIS:HE2	1.76	0.50
1:A:223:ILE:O	1:A:227:GLU:HG3	2.12	0.50
1:A:351:LEU:HB2	1:A:355:ASP:HB3	1.93	0.49
4:L:65:SER:OG	4:L:72:THR:OG1	2.27	0.49
3:H:70:ILE:HD11	3:H:79:GLN:HE21	1.78	0.49
1:A:184:VAL:HG13	1:A:464:PHE:HD1	1.78	0.49
1:A:248:LEU:HD22	1:A:252:TYR:HE2	1.77	0.49
1:A:245:ARG:HB2	1:A:262:LEU:HD11	1.95	0.48
4:L:52:SER:OG	4:L:52:SER:O	2.31	0.48
4:L:15:VAL:HA	4:L:78:LEU:HD22	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:61:ALA:HB3	3:H:64:VAL:HG22	1.96	0.48
1:A:374:HIS:CE1	1:A:406:GLU:HG3	2.48	0.47
1:A:492:PRO:HG3	1:A:613:TYR:CE2	2.49	0.47
3:H:67:ARG:HH22	3:H:87:ARG:NH2	2.11	0.47
3:H:94:TYR:O	3:H:115:GLY:HA2	2.14	0.47
1:A:290:ASN:OD1	1:A:291:ILE:N	2.41	0.47
4:L:35:TRP:CZ3	4:L:88:CYS:HB3	2.50	0.47
4:L:163:VAL:HG22	4:L:175:LEU:HD12	1.97	0.47
1:A:84:PRO:HB2	1:A:87:GLU:OE1	2.14	0.46
1:A:481:LYS:HD3	1:A:487:VAL:HG23	1.97	0.46
1:A:110:GLU:HG2	1:A:114:LYS:HE3	1.96	0.46
2:B:342:PHE:CZ	2:B:511:VAL:HG11	2.51	0.45
1:A:544:ILE:O	1:A:547:SER:OG	2.34	0.45
3:H:47:TRP:HZ2	3:H:50:VAL:HB	1.81	0.45
1:A:474:MET:HA	1:A:477:TRP:HB3	1.99	0.45
1:A:198:ASP:N	1:A:198:ASP:OD1	2.50	0.45
3:H:155:PHE:HB2	3:H:184:LEU:HD23	1.99	0.44
4:L:52:SER:O	4:L:53:ASN:ND2	2.47	0.44
4:L:54:LEU:HD21	4:L:62:PHE:O	2.16	0.44
4:L:151:ASP:N	4:L:191:VAL:O	2.44	0.44
1:A:197:GLU:HB2	1:A:201:ASP:OD2	2.17	0.44
1:A:608:THR:HG22	1:A:608:THR:O	2.17	0.44
4:L:93:ASN:CG	4:L:94:LEU:H	2.21	0.44
1:A:245:ARG:NH2	1:A:603:PHE:O	2.51	0.43
1:A:554:LEU:HG	1:A:558:LEU:HD21	2.00	0.43
2:B:422:ASN:HD21	2:B:453:TYR:HB2	1.82	0.43
1:A:333:LEU:O	1:A:362:THR:HG22	2.18	0.43
1:A:177:ARG:HG2	1:A:177:ARG:NH1	2.34	0.43
1:A:291:ILE:HG22	1:A:366:MET:HE1	2.00	0.43
1:A:161:ARG:NH2	1:A:268:GLY:H	2.16	0.43
3:H:117:LEU:HD21	3:H:157:GLU:OE1	2.19	0.42
1:A:394:ASN:HB2	1:A:562:LYS:HD2	2.01	0.42
4:L:19:VAL:HB	4:L:75:ILE:HD13	2.02	0.42
4:L:61:ARG:HH12	4:L:79:GLN:HB2	1.84	0.42
2:B:383:SER:N	2:B:386:LYS:HE2	2.33	0.42
3:H:100:GLY:N	3:H:107:ASP:HB3	2.35	0.42
4:L:120:PRO:HD3	4:L:132:VAL:HG22	2.01	0.42
4:L:166:GLN:HB2	4:L:173:TYR:CZ	2.55	0.42
1:A:184:VAL:HG13	1:A:464:PHE:CD1	2.54	0.42
1:A:403:ALA:O	1:A:407:ILE:HG23	2.21	0.41
3:H:50:VAL:HG12	3:H:59:TYR:HB2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:LYS:HA	1:A:289:PRO:HD3	1.94	0.41
2:B:348:ALA:HB2	2:B:354:ASN:HB2	2.01	0.41
1:A:308:PHE:CZ	1:A:333:LEU:HD22	2.56	0.41
4:L:195:GLU:HG2	4:L:206:THR:HG23	2.03	0.41
4:L:158:ASN:HD22	4:L:181:LEU:HD21	1.86	0.41
1:A:392:LEU:HD13	1:A:563:SER:HA	2.03	0.41
1:A:215:TYR:HE2	1:A:568:LEU:HD13	1.87	0.40
3:H:180:GLN:NE2	3:H:186:SER:HB2	2.36	0.40
1:A:396:ALA:HB3	1:A:400:PHE:HE2	1.87	0.40
1:A:450:LEU:HB2	1:A:451:PRO:HD3	2.04	0.40
2:B:341:VAL:CG2	2:B:356:LYS:HD3	2.52	0.40

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	595/805 (74%)	579 (97%)	16 (3%)	0	100 100
2	B	193/223 (86%)	185 (96%)	8 (4%)	0	100 100
3	H	207/230 (90%)	190 (92%)	15 (7%)	2 (1%)	13 26
4	L	211/215 (98%)	197 (93%)	14 (7%)	0	100 100
All	All	1206/1473 (82%)	1151 (95%)	53 (4%)	2 (0%)	45 65

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	55	ALA
3	H	75	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	527/711 (74%)	527 (100%)	0	100 100
2	B	167/195 (86%)	165 (99%)	2 (1%)	67 84
3	H	174/192 (91%)	174 (100%)	0	100 100
4	L	184/187 (98%)	184 (100%)	0	100 100
All	All	1052/1285 (82%)	1050 (100%)	2 (0%)	91 98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	346	ARG
2	B	356	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
3	H	79	GLN
4	L	89	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)

2 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	$\#\|Z\| > 2$
5	NAG	C	1	1,5	14,14,15	0.22	0	17,19,21	0.44	0
5	NAG	C	2	5	14,14,15	0.22	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. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	C	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	C	2	5	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

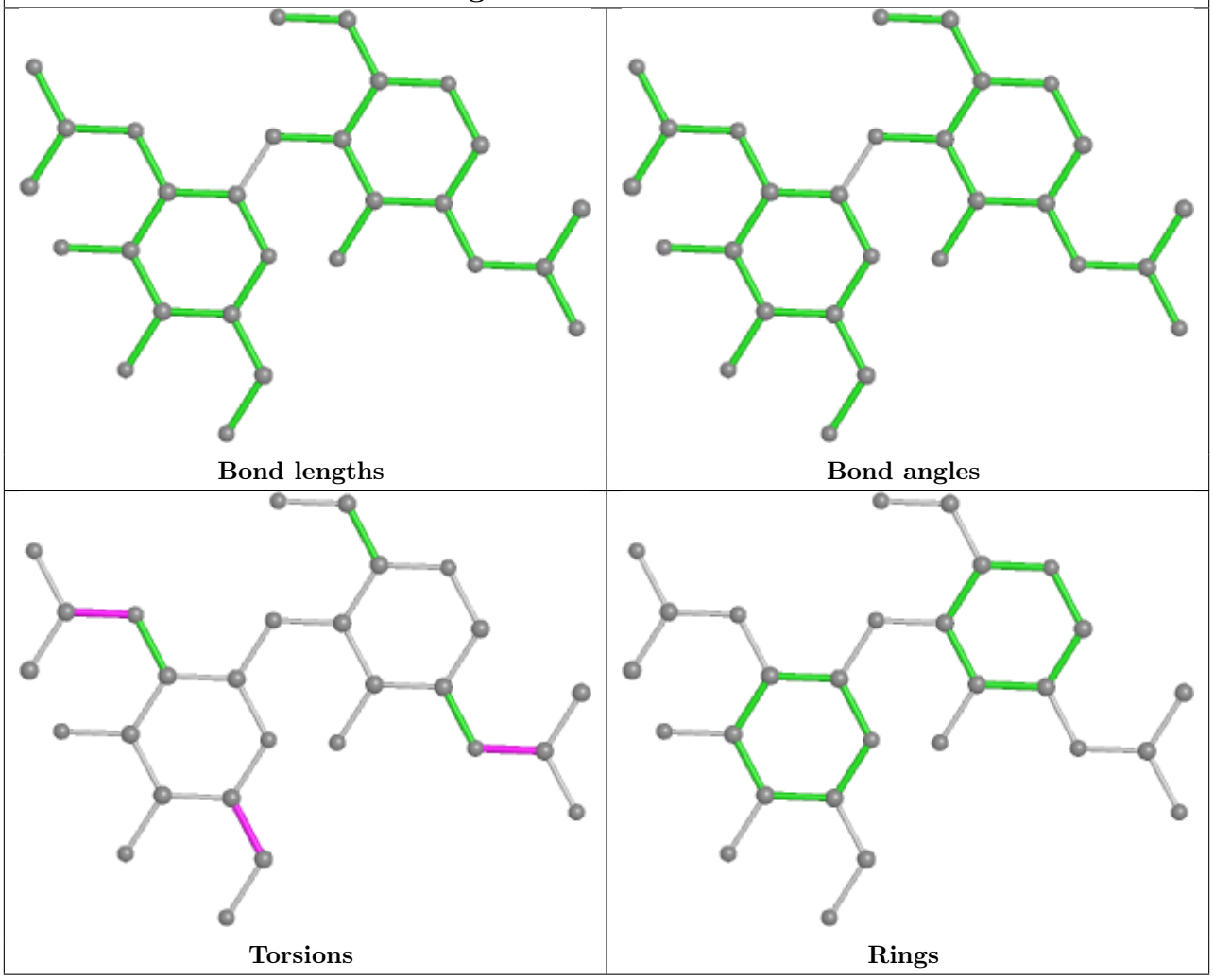
Mol	Chain	Res	Type	Atoms
5	C	1	NAG	C8-C7-N2-C2
5	C	1	NAG	O7-C7-N2-C2
5	C	2	NAG	C8-C7-N2-C2
5	C	2	NAG	O7-C7-N2-C2
5	C	2	NAG	O5-C5-C6-O6
5	C	2	NAG	C4-C5-C6-O6

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.

Oligosaccharide Chain C



5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 for Mogul analysis.

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	A	901	1	14,14,15	0.20	0	17,19,21	0.39	0
6	NAG	B	601	2	14,14,15	0.20	0	17,19,21	0.43	0
6	NAG	A	902	1	14,14,15	0.19	0	17,19,21	0.38	0
6	NAG	A	903	1	14,14,15	0.21	0	17,19,21	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	NAG	A	905	1	14,14,15	0.27	0	17,19,21	0.50	0
6	NAG	A	904	1	14,14,15	0.28	0	17,19,21	0.47	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	A	901	1	-	2/6/23/26	0/1/1/1
6	NAG	B	601	2	-	2/6/23/26	0/1/1/1
6	NAG	A	902	1	-	2/6/23/26	0/1/1/1
6	NAG	A	903	1	-	0/6/23/26	0/1/1/1
6	NAG	A	905	1	-	3/6/23/26	0/1/1/1
6	NAG	A	904	1	-	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 (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	904	NAG	O5-C5-C6-O6
6	A	901	NAG	C4-C5-C6-O6
6	A	905	NAG	C4-C5-C6-O6
6	A	904	NAG	C4-C5-C6-O6
6	A	901	NAG	O5-C5-C6-O6
6	A	902	NAG	O5-C5-C6-O6
6	A	905	NAG	O5-C5-C6-O6
6	B	601	NAG	C4-C5-C6-O6
6	B	601	NAG	O5-C5-C6-O6
6	A	905	NAG	C3-C2-N2-C7
6	A	902	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	903	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.