Full wwPDB X-ray Structure Validation Report ⓘ

Oct 30, 2023 – 04:12 PM JST

PDB ID	:	8H5C
Title	:	Structure of SARS-CoV-2 Omicron BA.2.75 RBD in complex with human ACE2
Authors	:	Zhao, Z.N.; Bai, B.; Liu, K.F.; Qi, J.X.; Gao, G.F.
Deposited on	:	2022-10-12
Resolution	:	2.90 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp
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:

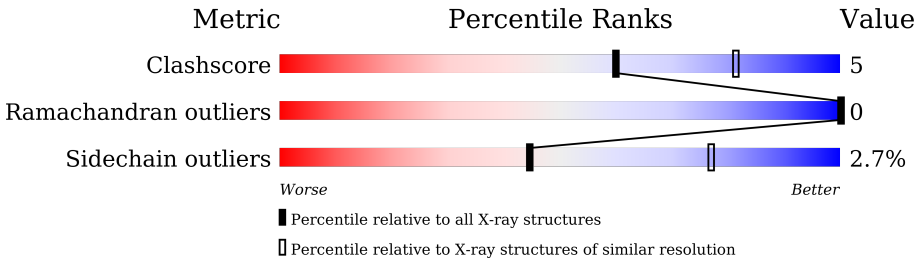
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	596	88% 12%
2	B	195	83% 17%
3	C	2	100%
4	D	3	100%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6546 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Processed angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	596	4877	3121	810	917	29	0	2	0

- Molecule 2 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	195	1560	1010	262	280	8	0	0	0

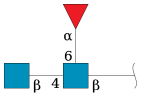
There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	339	HIS	GLY	conflict	UNP P0DTC2
B	371	PHE	SER	conflict	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	446	SER	GLY	variant	UNP P0DTC2
B	460	LYS	ASN	conflict	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	484	ALA	GLU	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 an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.

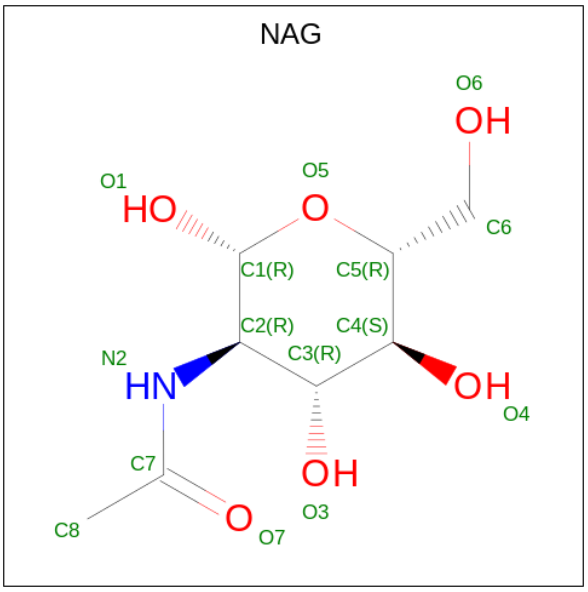


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Zn	0	0
			1	1		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



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

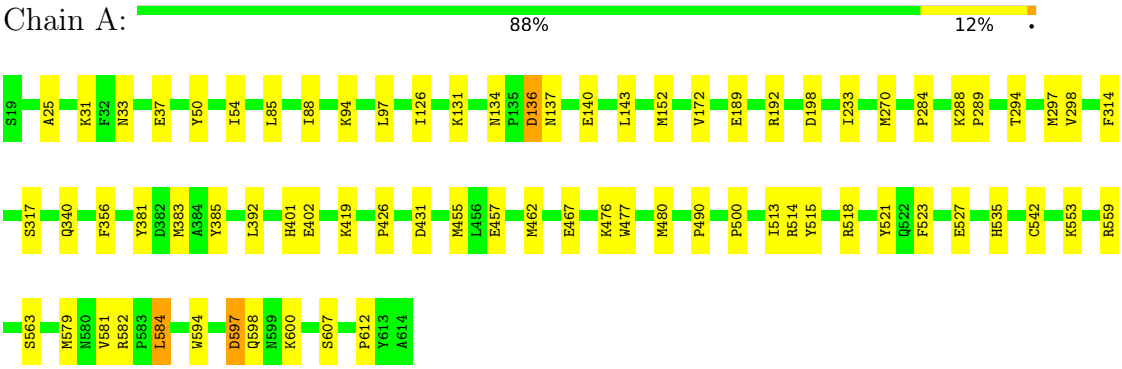
3 Residue-property plots (i)

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.

Note EDS was not executed.

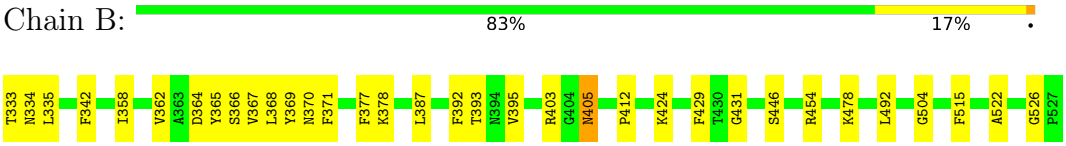
• Molecule 1: Processed angiotensin-converting enzyme 2

Chain A:



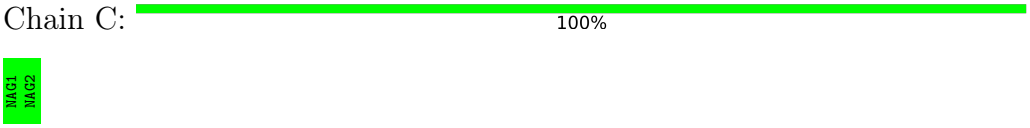
• Molecule 2: Spike protein S1

Chain B:



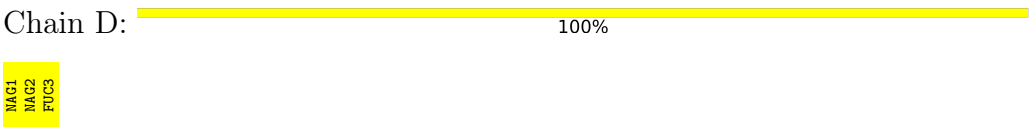
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:



• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	105.77Å 105.77Å 228.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.04 – 2.90	Depositor
% Data completeness (in resolution range)	91.6 (39.04-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.197 , 0.242	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6546	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, FUC, 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	0/5021	0.45	1/6821 (0.0%)
2	B	0.30	0/1609	0.56	0/2190
All	All	0.27	0/6630	0.48	1/9011 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	289	PRO	N-CD-CG	-5.21	95.38	103.20

There are no chirality outliers.

There are no planarity outliers.

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	4877	0	4654	39	1
2	B	1560	0	1487	19	0
3	C	28	0	25	0	0
4	D	38	0	34	1	0
5	A	1	0	0	0	0
6	A	42	0	39	1	0
All	All	6546	0	6239	59	1

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.

All (59) 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:B:366:SER:O	2:B:369:TYR:HD1	1.60	0.84
2:B:366:SER:HA	2:B:369:TYR:HE1	1.48	0.78
1:A:419:LYS:HE2	1:A:426:PRO:HA	1.71	0.72
2:B:366:SER:HA	2:B:369:TYR:CE1	2.24	0.71
2:B:403:ARG:NH1	2:B:405:ASN:OD1	2.22	0.68
1:A:33:ASN:O	1:A:37:GLU:HG3	1.94	0.66
1:A:131:LYS:HB3	1:A:143:LEU:HD23	1.78	0.65
1:A:527:GLU:OE2	1:A:582:ARG:NH2	2.25	0.64
1:A:597:ASP:O	1:A:600:LYS:HD3	1.98	0.63
1:A:294:THR:O	1:A:298:VAL:HG23	2.03	0.59
1:A:490:PRO:HA	1:A:612:PRO:HG2	1.85	0.58
2:B:362:VAL:HG23	2:B:526:GLY:HA3	1.86	0.58
2:B:358:ILE:HB	2:B:395:VAL:HB	1.85	0.57
2:B:368:LEU:O	2:B:370:ASN:N	2.38	0.56
2:B:335:LEU:HD13	2:B:362:VAL:HG13	1.88	0.55
1:A:535:HIS:CD2	1:A:542:CYS:HB2	2.41	0.55
1:A:140:GLU:O	1:A:140:GLU:HG3	2.07	0.55
2:B:365:TYR:CD2	2:B:387:LEU:HD23	2.43	0.54
1:A:189:GLU:HG2	1:A:192[B]:ARG:HH22	1.74	0.53
1:A:288:LYS:HE3	1:A:431:ASP:OD2	2.08	0.52
2:B:393:THR:HA	2:B:522:ALA:HA	1.92	0.51
1:A:136:ASP:N	1:A:136:ASP:OD1	2.41	0.51
1:A:402:GLU:HB3	1:A:518:ARG:HD2	1.92	0.50
2:B:366:SER:O	2:B:369:TYR:CD1	2.52	0.48
1:A:50:TYR:CE1	1:A:54:ILE:HG23	2.49	0.48
1:A:85:LEU:O	1:A:94:LYS:HE2	2.14	0.47
2:B:334:ASN:OD1	2:B:334:ASN:N	2.45	0.47
1:A:137:ASN:HB3	1:A:140:GLU:HG2	1.97	0.47
1:A:462:MET:HG2	1:A:467:GLU:OE1	2.15	0.47
1:A:521:TYR:HE1	1:A:579:MET:HB2	1.79	0.47
2:B:431:GLY:HA2	2:B:515:PHE:CD2	2.49	0.46
1:A:126:ILE:HG22	1:A:172:VAL:HG13	1.97	0.46
1:A:50:TYR:HE1	1:A:54:ILE:HG23	1.80	0.45
2:B:364:ASP:O	2:B:367:VAL:N	2.45	0.45
1:A:356:PHE:CE2	1:A:383:MET:HG2	2.52	0.45
1:A:476:LYS:HG3	1:A:480:MET:HE2	1.97	0.45
1:A:284:PRO:HB3	1:A:594:TRP:CH2	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:342:PHE:HB3	2:B:371:PHE:CZ	2.53	0.44
1:A:523:PHE:CD2	1:A:584:LEU:HD12	2.53	0.43
1:A:152:MET:HG3	1:A:270:MET:HA	1.99	0.43
1:A:340:GLN:OE1	6:A:702:NAG:H82	2.18	0.43
1:A:514:ARG:HG2	1:A:515:TYR:N	2.34	0.43
1:A:457:GLU:HG2	1:A:513:ILE:HB	1.99	0.43
2:B:454:ARG:HA	2:B:492:LEU:HD23	2.01	0.43
1:A:233:ILE:HG13	1:A:581:VAL:HG21	2.01	0.43
1:A:314:PHE:O	1:A:317:SER:OG	2.30	0.43
1:A:392:LEU:HD13	1:A:563:SER:HA	2.00	0.43
2:B:392:PHE:CE1	2:B:515:PHE:HB3	2.54	0.42
1:A:189:GLU:HG2	1:A:192[B]:ARG:NH2	2.34	0.42
1:A:25:ALA:HB1	1:A:97:LEU:HD11	2.00	0.42
2:B:405:ASN:HD21	2:B:504:GLY:HA3	1.83	0.42
2:B:412:PRO:HG3	2:B:429:PHE:HB3	2.02	0.42
1:A:477:TRP:CE2	1:A:500:PRO:HD3	2.55	0.41
1:A:88:ILE:CD1	1:A:97:LEU:HD12	2.51	0.41
1:A:294:THR:HA	1:A:297:MET:HE2	2.01	0.41
1:A:137:ASN:OD1	1:A:140:GLU:N	2.54	0.40
4:D:1:NAG:H61	4:D:2:NAG:HN2	1.86	0.40
1:A:476:LYS:HG3	1:A:480:MET:CE	2.51	0.40
1:A:594:TRP:CH2	1:A:598:GLN:HG3	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:607:SER:OG	1:A:607:SER:OG[8_554]	2.02	0.18

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 X-ray entries followed by that with respect to entries of similar resolution.

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	596/596 (100%)	584 (98%)	12 (2%)	0	100	100
2	B	193/195 (99%)	177 (92%)	16 (8%)	0	100	100
All	All	789/791 (100%)	761 (96%)	28 (4%)	0	100	100

There are no Ramachandran outliers to report.

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 X-ray entries followed by that with respect to entries of similar resolution.

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	528/526 (100%)	516 (98%)	12 (2%)	50	80
2	B	168/168 (100%)	161 (96%)	7 (4%)	30	63
All	All	696/694 (100%)	677 (97%)	19 (3%)	44	77

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LYS
1	A	134	ASN
1	A	136	ASP
1	A	198	ASP
1	A	381	TYR
1	A	385	TYR
1	A	401	HIS
1	A	455	MET
1	A	553	LYS
1	A	559	ARG
1	A	584	LEU
1	A	597	ASP
2	B	333	THR
2	B	377	PHE
2	B	378	LYS
2	B	405	ASN
2	B	424	LYS
2	B	446	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	478	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	ASN
1	A	325	GLN
1	A	552	GLN
2	B	360	ASN
2	B	487	ASN

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

5 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	$\#\|Z\| > 2$
3	NAG	C	1	3,1	14,14,15	0.40	0	17,19,21	0.62	0
3	NAG	C	2	3	14,14,15	0.23	0	17,19,21	0.63	0
4	NAG	D	1	4,1	14,14,15	0.41	0	17,19,21	0.53	0
4	NAG	D	2	4	14,14,15	0.27	0	17,19,21	0.42	0
4	FUC	D	3	4	10,10,11	0.88	1 (10%)	14,14,16	0.93	1 (7%)

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	C	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	4/6/23/26	0/1/1/1
4	NAG	D	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	FUC	D	3	4	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	3	FUC	C1-C2	2.31	1.57	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	3	FUC	C1-C2-C3	2.07	112.21	109.67

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	2	NAG	O5-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
3	C	2	NAG	C3-C2-N2-C7
3	C	2	NAG	C1-C2-N2-C7
4	D	1	NAG	O5-C5-C6-O6

There are no ring outliers.

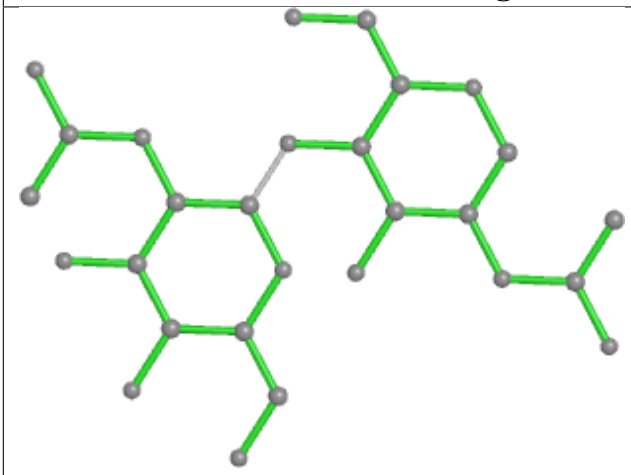
2 monomers are involved in 1 short contact:

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

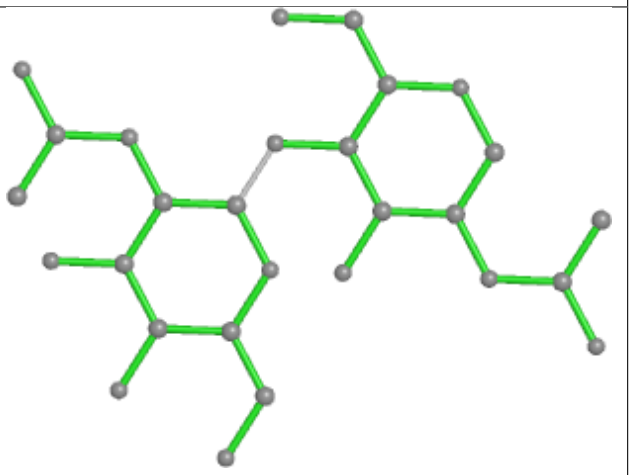
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for oligosaccharide.

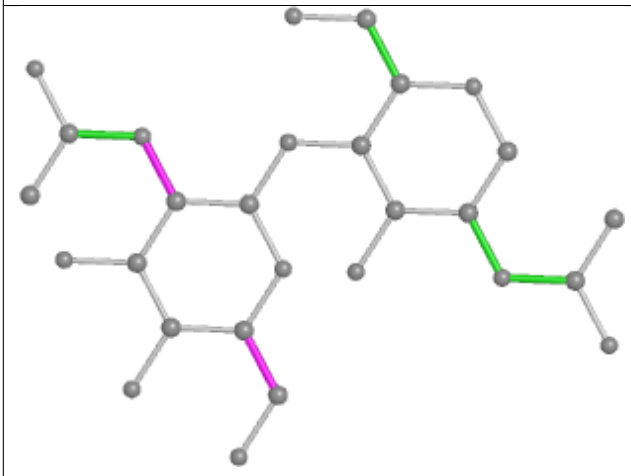
Oligosaccharide Chain C



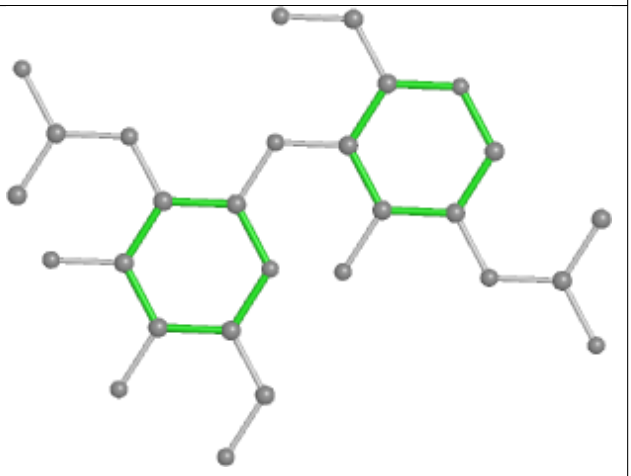
Bond lengths



Bond angles

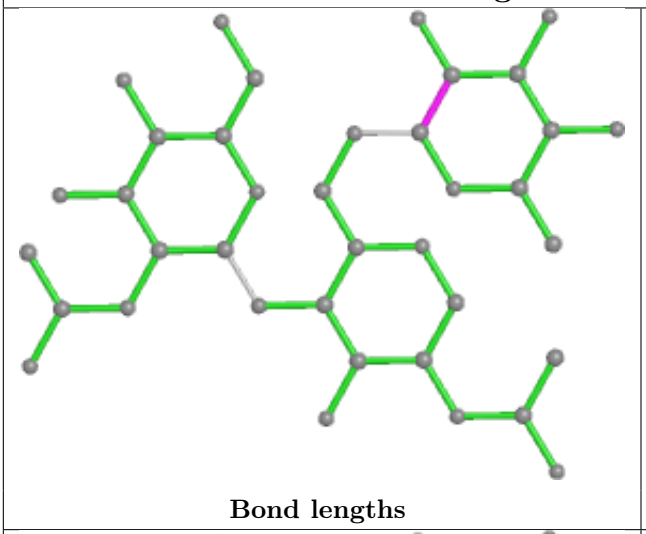


Torsions

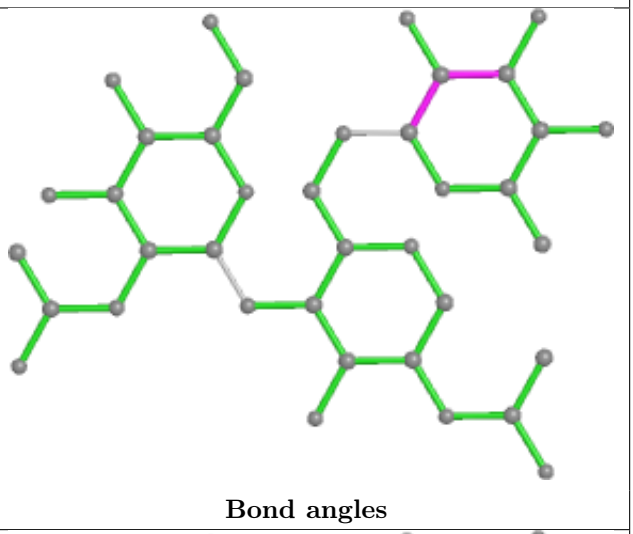


Rings

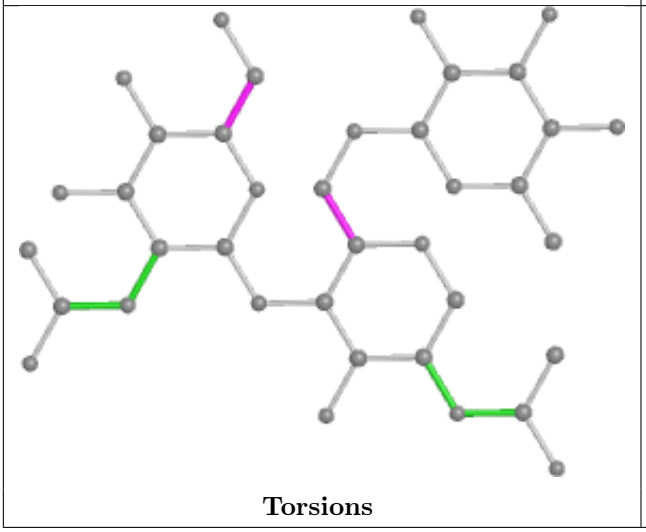
Oligosaccharide Chain D



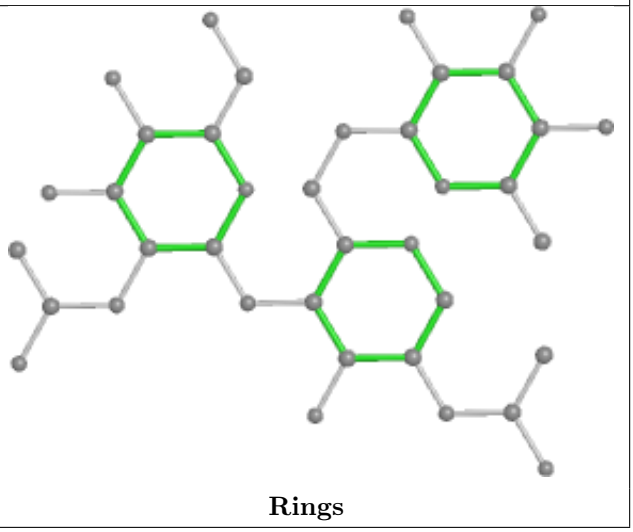
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	703	1	14,14,15	0.46	0	17,19,21	0.52	0
6	NAG	A	704	1	14,14,15	0.27	0	17,19,21	0.53	0
6	NAG	A	702	1	14,14,15	0.19	0	17,19,21	0.69	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	703	1	-	3/6/23/26	0/1/1/1
6	NAG	A	704	1	-	1/6/23/26	0/1/1/1
6	NAG	A	702	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	703	NAG	O5-C5-C6-O6
6	A	704	NAG	O5-C5-C6-O6
6	A	703	NAG	C3-C2-N2-C7
6	A	703	NAG	C1-C2-N2-C7

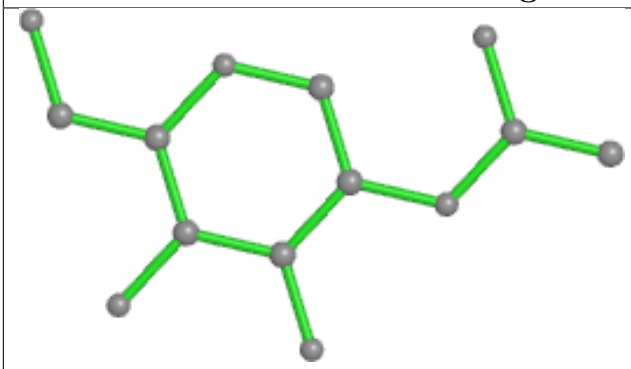
There are no ring outliers.

1 monomer is involved in 1 short contact:

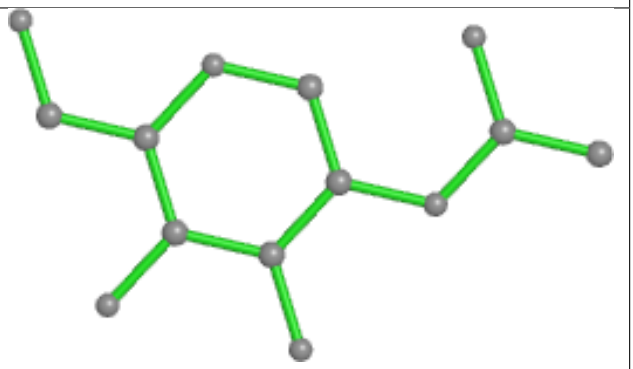
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	702	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

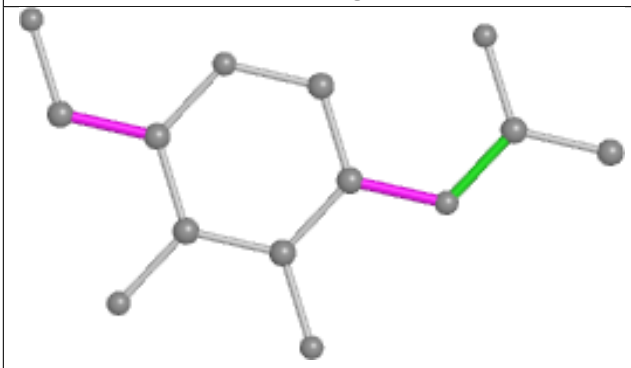
Ligand NAG A 703



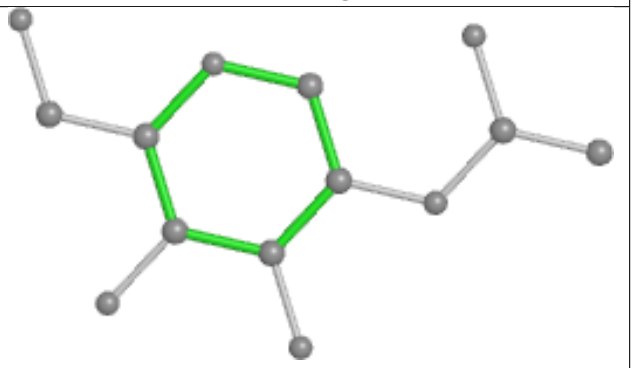
Bond lengths



Bond angles

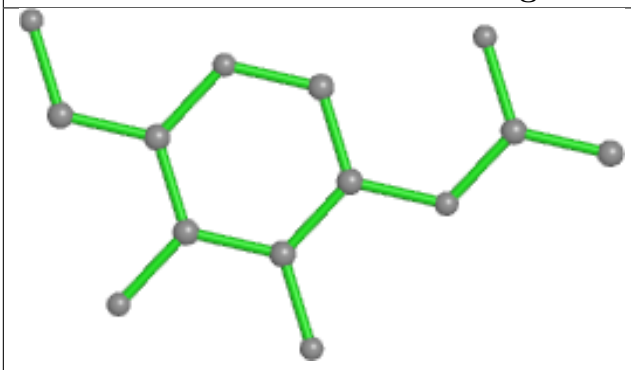


Torsions

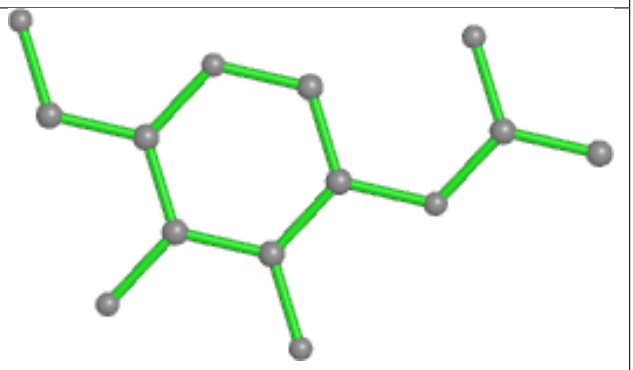


Rings

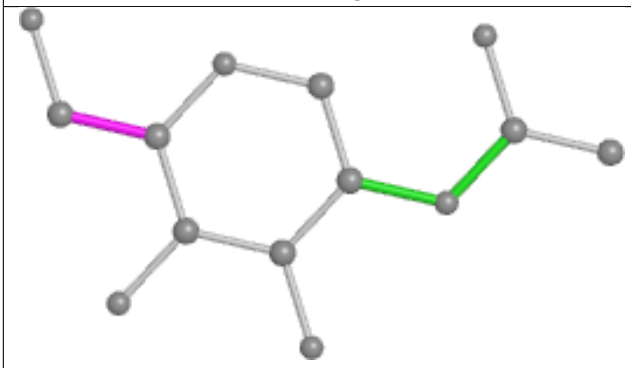
Ligand NAG A 704



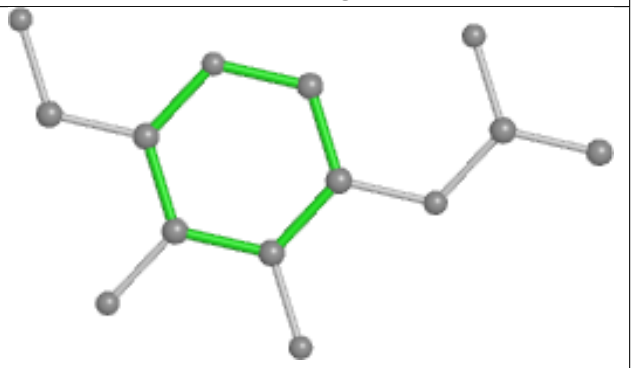
Bond lengths



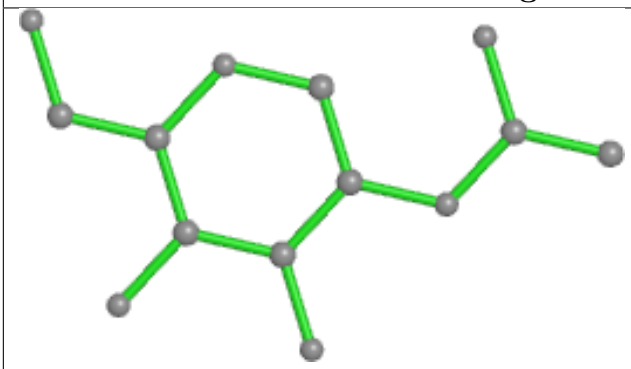
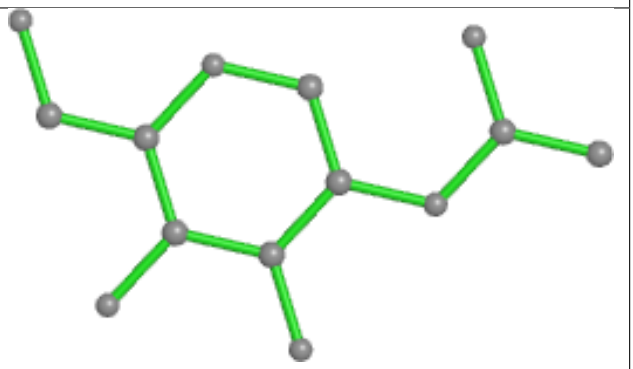
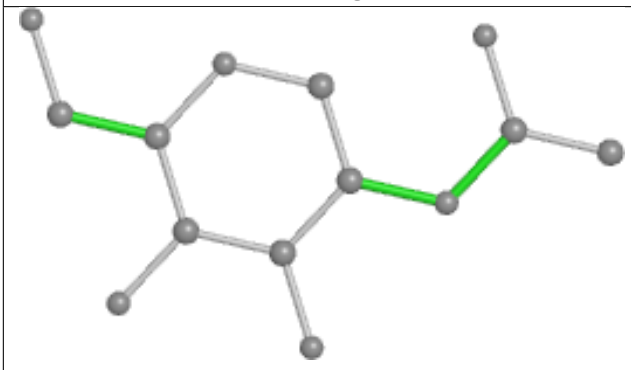
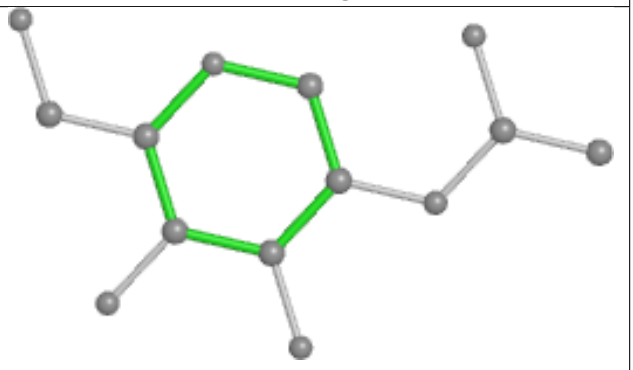
Bond angles



Torsions



Rings

Ligand NAG A 702	
	
Bond lengths	Bond angles
	
Torsions	Rings

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.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.