



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 14, 2020 – 02:51 PM BST

PDB ID : 6XC7
Title : Crystal structure of SARS-CoV-2 receptor binding domain in complex with antibodies CC12.3 and CR3022
Authors : Yuan, M.; Liu, H.; Wu, N.C.; Zhu, X.; Wilson, I.A.
Deposited on : 2020-06-08
Resolution : 2.88 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 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) : 1.13
EDS : **FAILED**
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) : 2.14.4.dev1

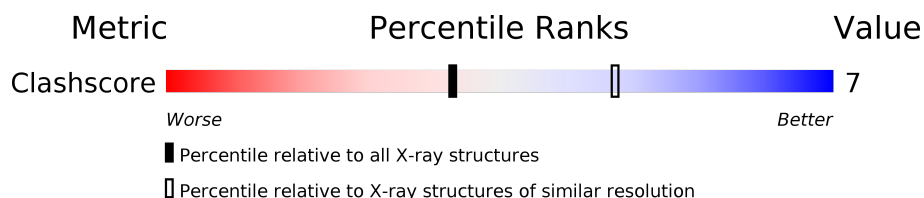
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.88 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	2947 (2.90-2.86)

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 on 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 $\leq 5\%$.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	231	71% 13% 16%
2	H	222	91% 7% .
3	L	221	86% 14%
4	C	220	82% 17% .
5	D	215	73% 26% .
6	B	3	100%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8191 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 Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	193	Total	C	N	O	S	0	0	0
			1537	987	256	286	8			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	542	SER	-	expression tag	UNP P0DTC2
A	543	GLY	-	expression tag	UNP P0DTC2
A	544	HIS	-	expression tag	UNP P0DTC2
A	545	HIS	-	expression tag	UNP P0DTC2
A	546	HIS	-	expression tag	UNP P0DTC2
A	547	HIS	-	expression tag	UNP P0DTC2
A	548	HIS	-	expression tag	UNP P0DTC2
A	549	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called CR3022 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	218	Total	C	N	O	S	0	0	0
			1619	1027	263	320	9			

- Molecule 3 is a protein called CR3022 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	221	Total	C	N	O	S	0	0	0
			1716	1076	284	351	5			

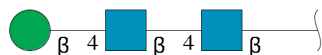
- Molecule 4 is a protein called CC12.3 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	C	220	Total	C	N	O	S	0	0	0
			1645	1040	272	326	7			

- Molecule 5 is a protein called CC12.3 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	213	Total	C	N	O	S	0	0	0
			1635	1021	279	331	4			

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



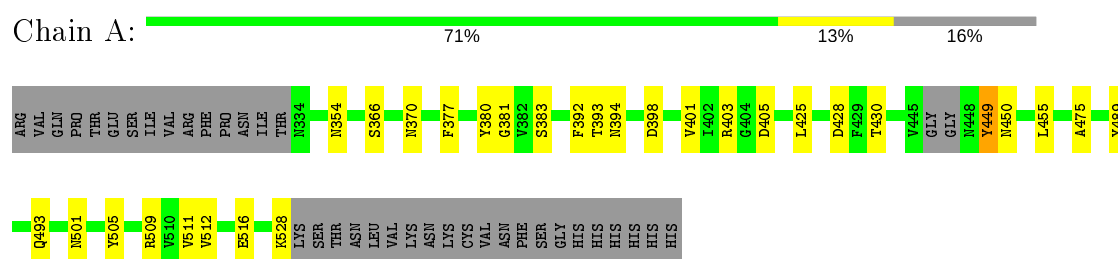
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	B	3	Total	C	N	O	0	0	0
			39	22	2	15			

3 Residue-property plots

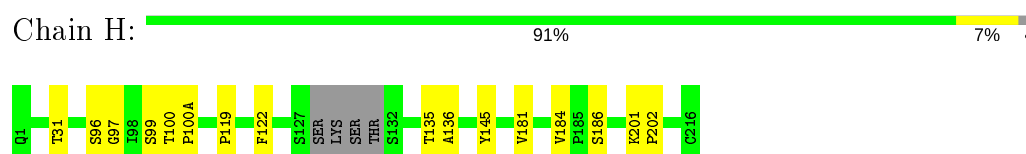
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS failed to run properly.

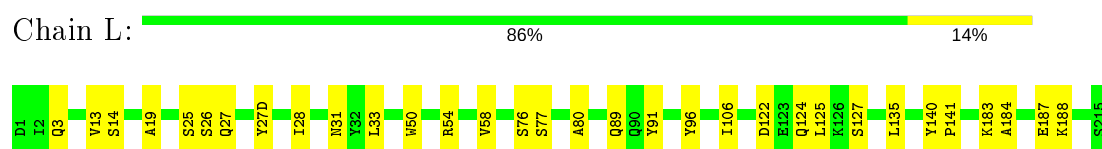
- Molecule 1: Spike protein S1



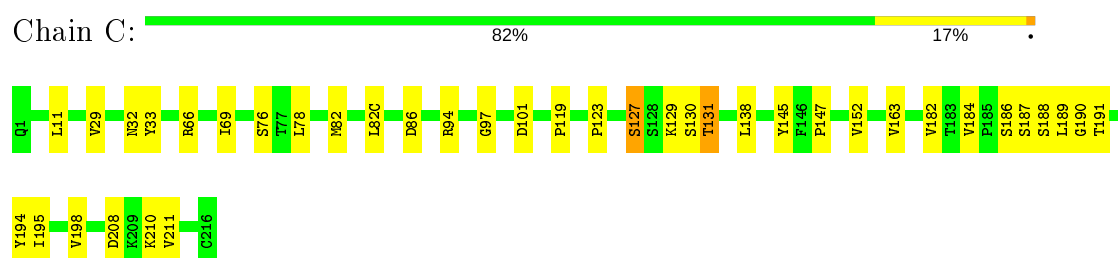
- Molecule 2: CR3022 heavy chain



- Molecule 3: CR3022 light chain

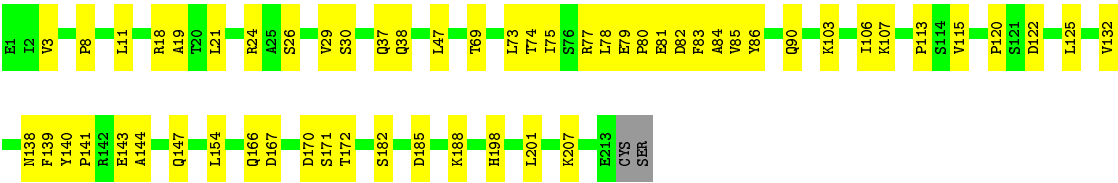


- Molecule 4: CC12.3 heavy chain



- Molecule 5: CC12.3 light chain





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

Chain B:

100%



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	110.87Å 110.87Å 228.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.25 – 2.88	Depositor
% Data completeness (in resolution range)	99.7 (42.25-2.88)	Depositor
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.219 , 0.259	Depositor
Wilson B-factor (Å ²)	79.5	Xtriage
Anisotropy	0.084	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8191	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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

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	0.27	0/1580	0.47	0/2149
2	H	0.26	0/1660	0.49	0/2259
3	L	0.27	0/1754	0.50	0/2383
4	C	0.30	0/1685	0.56	1/2292 (0.0%)
5	D	0.29	0/1670	0.56	0/2266
All	All	0.28	0/8349	0.52	1/11349 (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
1	A	0	1
2	H	0	1
4	C	0	2
5	D	0	1
All	All	0	5

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	131	THR	N-CA-C	-6.09	94.56	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	449	TYR	Peptide
4	C	127	SER	Peptide
4	C	129	LYS	Peptide
5	D	30	SER	Peptide
2	H	135	THR	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	1537	0	1458	19	0
2	H	1619	0	1591	11	0
3	L	1716	0	1658	20	0
4	C	1645	0	1604	30	0
5	D	1635	0	1592	38	0
6	B	39	0	34	0	0
All	All	8191	0	7937	109	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.

All (109) 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)
5:D:77:ARG:O	5:D:79:GLU:OE1	1.86	0.94
1:A:383:SER:HB2	2:H:96:SER:HB3	1.58	0.85
4:C:188:SER:HG	4:C:194:TYR:HH	1.22	0.84
3:L:3:GLN:H	3:L:26:SER:HB3	1.50	0.76
5:D:80:PRO:HA	5:D:83:PHE:HE2	1.51	0.75
5:D:78:LEU:C	5:D:79:GLU:OE2	2.28	0.73
5:D:143:GLU:OE2	5:D:143:GLU:C	2.28	0.71
4:C:66:ARG:NH2	4:C:86:ASP:OD2	2.24	0.70
4:C:187:SER:HA	4:C:189:LEU:HD22	1.72	0.69
4:C:186:SER:O	4:C:189:LEU:HB3	1.92	0.69
5:D:77:ARG:O	5:D:79:GLU:CD	2.30	0.69
2:H:201:LYS:HG2	2:H:202:PRO:HD3	1.78	0.66
1:A:455:LEU:HD12	1:A:493:GLN:HG3	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:122:ASP:HA	5:D:125:LEU:HB2	1.79	0.65
1:A:381:GLY:HA3	1:A:430:THR:HG22	1.80	0.63
5:D:113:PRO:HD2	5:D:201:LEU:HD11	1.80	0.63
5:D:78:LEU:O	5:D:79:GLU:OE2	2.17	0.63
3:L:54:ARG:HG2	3:L:58:VAL:HB	1.82	0.62
4:C:11:LEU:HB2	4:C:147:PRO:HG3	1.81	0.62
5:D:185:ASP:HA	5:D:188:LYS:HD2	1.82	0.62
4:C:152:VAL:HG22	4:C:198:VAL:HG13	1.82	0.61
4:C:29:VAL:HG21	4:C:76:SER:HA	1.83	0.60
4:C:119:PRO:HB3	4:C:145:TYR:HB3	1.83	0.60
5:D:182:SER:HG	5:D:185:ASP:H	1.51	0.59
4:C:163:VAL:HG22	4:C:182:VAL:HG12	1.85	0.59
4:C:184:VAL:HG11	4:C:194:TYR:OH	2.03	0.58
4:C:189:LEU:HD23	4:C:190:GLY:H	1.69	0.58
5:D:106:ILE:H	5:D:166:GLN:HE22	1.52	0.58
1:A:393:THR:O	1:A:394:ASN:ND2	2.38	0.57
5:D:8:PRO:HD2	5:D:11:LEU:HD11	1.87	0.57
3:L:80:ALA:HA	3:L:106:ILE:HD11	1.87	0.56
4:C:82:MET:HB3	4:C:82(C):LEU:HD21	1.88	0.56
5:D:3:VAL:H	5:D:26:SER:HB3	1.71	0.55
5:D:77:ARG:O	5:D:79:GLU:OE2	2.25	0.54
3:L:25:SER:OG	3:L:27:GLN:O	2.26	0.54
1:A:489:TYR:OH	4:C:94:ARG:NH2	2.32	0.54
4:C:195:ILE:HG22	4:C:210:LYS:HA	1.92	0.52
5:D:38:GLN:O	5:D:84:ALA:HB1	2.10	0.52
5:D:198:HIS:HB3	5:D:201:LEU:CD1	2.40	0.52
3:L:13:VAL:HG21	3:L:19:ALA:HB2	1.90	0.52
4:C:123:PRO:HB3	4:C:211:VAL:HG12	1.92	0.51
1:A:501:ASN:HB3	1:A:505:TYR:HB2	1.93	0.50
3:L:76:SER:OG	3:L:77:SER:N	2.44	0.50
5:D:29:VAL:HG11	5:D:90:GLN:HB2	1.93	0.50
5:D:85:VAL:HG22	5:D:103:LYS:HG3	1.94	0.50
1:A:403:ARG:NH2	1:A:405:ASP:OD2	2.45	0.49
5:D:21:LEU:HD13	5:D:73:LEU:HD23	1.95	0.49
4:C:188:SER:HA	4:C:191:THR:OG1	2.13	0.48
4:C:195:ILE:HD12	4:C:208:ASP:HB3	1.95	0.48
4:C:187:SER:C	4:C:189:LEU:H	2.16	0.48
2:H:97:GLY:O	2:H:100:THR:OG1	2.32	0.48
1:A:354:ASN:O	1:A:398:ASP:HA	2.14	0.48
3:L:27(D):TYR:HB3	3:L:28:ILE:HG22	1.94	0.48
4:C:189:LEU:HD23	4:C:190:GLY:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:198:HIS:HB3	5:D:201:LEU:HD12	1.95	0.47
1:A:425:LEU:HD21	1:A:512:VAL:HG11	1.96	0.47
5:D:113:PRO:HB3	5:D:139:PHE:CD1	2.50	0.47
3:L:13:VAL:HG12	3:L:14:SER:O	2.15	0.47
1:A:449:TYR:HD2	1:A:450:ASN:HA	1.80	0.47
5:D:80:PRO:HA	5:D:83:PHE:CE2	2.40	0.47
2:H:136:ALA:HB2	2:H:186:SER:HB3	1.97	0.47
5:D:147:GLN:HG2	5:D:154:LEU:HD13	1.96	0.46
3:L:31:ASN:O	3:L:50:TRP:HA	2.15	0.46
3:L:183:LYS:O	3:L:187:GLU:HG3	2.16	0.46
1:A:428:ASP:O	3:L:27(D):TYR:OH	2.29	0.46
4:C:211:VAL:HG23	4:C:211:VAL:O	2.16	0.46
4:C:138:LEU:HD13	4:C:211:VAL:HG21	1.97	0.46
2:H:100(A):PRO:HD3	3:L:91:TYR:CZ	2.51	0.45
5:D:167:ASP:O	5:D:171:SER:HA	2.16	0.45
1:A:377:PHE:CG	2:H:31:THR:HG22	2.52	0.45
5:D:120:PRO:HD3	5:D:132:VAL:HG22	1.99	0.45
3:L:184:ALA:O	3:L:188:LYS:HG3	2.16	0.45
5:D:37:GLN:HB2	5:D:47:LEU:HD11	1.99	0.45
2:H:136:ALA:HB3	2:H:184:VAL:O	2.16	0.45
4:C:69:ILE:HD11	4:C:78:LEU:HD11	1.98	0.44
4:C:130:SER:O	4:C:131:THR:HG23	2.18	0.44
5:D:115:VAL:HG12	5:D:207:LYS:HG3	2.01	0.43
5:D:167:ASP:CG	5:D:170:ASP:OD2	2.57	0.43
4:C:101:ASP:OD1	4:C:101:ASP:N	2.47	0.43
4:C:33:TYR:CE1	4:C:97:GLY:HA2	2.55	0.42
1:A:401:VAL:HG22	1:A:509:ARG:HG2	2.02	0.42
5:D:106:ILE:HG22	5:D:107:LYS:N	2.34	0.42
5:D:138:ASN:HA	5:D:172:THR:HB	2.01	0.42
2:H:122:PHE:CE2	3:L:124:GLN:HG3	2.54	0.42
4:C:127:SER:HG	4:C:130:SER:HA	1.85	0.41
2:H:181:VAL:HG11	3:L:135:LEU:HD13	2.01	0.41
4:C:163:VAL:HG22	4:C:182:VAL:CG1	2.50	0.41
4:C:127:SER:OG	4:C:130:SER:HA	2.21	0.41
1:A:475:ALA:HB1	4:C:32:ASN:HD21	1.86	0.41
5:D:140:TYR:CG	5:D:141:PRO:HA	2.56	0.41
3:L:122:ASP:HA	3:L:125:LEU:HB2	2.03	0.41
5:D:143:GLU:OE2	5:D:144:ALA:N	2.54	0.41
5:D:81:GLU:C	5:D:83:PHE:H	2.22	0.41
1:A:366:SER:O	1:A:370:ASN:HB2	2.21	0.41
1:A:398:ASP:O	1:A:511:VAL:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:LYS:HB3	1:A:528:LYS:HE2	1.87	0.41
5:D:19:ALA:O	5:D:74:THR:HA	2.21	0.41
3:L:124:GLN:O	3:L:127:SER:OG	2.32	0.41
2:H:99:SER:N	3:L:96:TYR:OH	2.45	0.41
2:H:119:PRO:HB3	2:H:145:TYR:HB3	2.02	0.41
4:C:195:ILE:HG13	4:C:195:ILE:O	2.19	0.40
3:L:33:LEU:HD22	3:L:89:GLN:O	2.21	0.40
1:A:380:TYR:O	1:A:430:THR:HA	2.21	0.40
5:D:107:LYS:HA	5:D:140:TYR:OH	2.21	0.40
3:L:140:TYR:CG	3:L:141:PRO:HA	2.57	0.40
5:D:24:ARG:HA	5:D:69:THR:O	2.21	0.40
1:A:392:PHE:HB3	1:A:516:GLU:O	2.22	0.40
5:D:18:ARG:HB2	5:D:75:ILE:O	2.22	0.40
5:D:82:ASP:O	5:D:86:TYR:OH	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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](#)

3 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	B	1	1,6	14,14,15	0.37	0	17,19,21	0.43	0
6	NAG	B	2	6	14,14,15	0.20	0	17,19,21	0.46	0
6	BMA	B	3	6	11,11,12	0.64	0	15,15,17	0.76	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	B	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	B	2	6	-	2/6/23/26	0/1/1/1
6	BMA	B	3	6	-	0/2/19/22	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	B	2	NAG	O5-C5-C6-O6
6	B	2	NAG	C4-C5-C6-O6
6	B	1	NAG	C4-C5-C6-O6
6	B	1	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS failed to run properly - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS failed to run properly - this section is therefore empty.

6.4 Ligands [i](#)

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers [i](#)

EDS failed to run properly - this section is therefore empty.