



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 26, 2024 – 11:40 AM EDT

PDB ID : 6E4X  
Title : Human antibody S5V2-29 in complex with influenza hemagglutinin A/Texas/50/2012 (H3N2)  
Authors : McCarthy, K.R.; Harrison, S.C.  
Deposited on : 2018-07-18  
Resolution : 2.25 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.20.1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

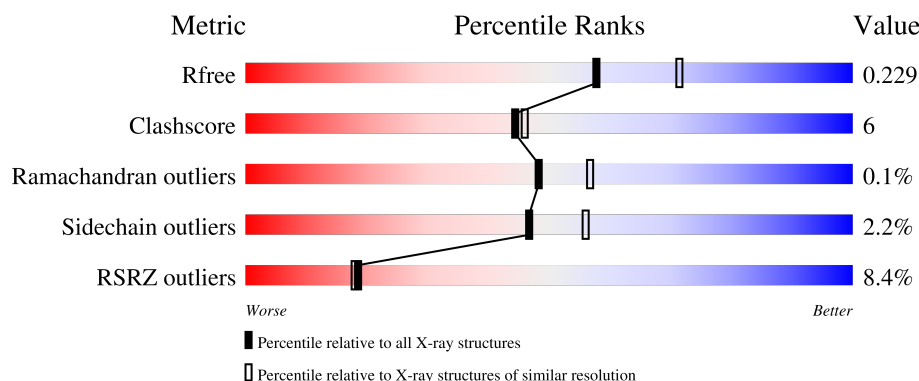
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


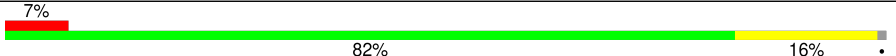
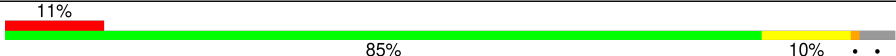


The reported resolution of this entry is 2.25 Å.

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))
$R_{free}$	164625	1763 (2.26-2.26)
Clashscore	180529	1919 (2.26-2.26)
Ramachandran outliers	177936	1884 (2.26-2.26)
Sidechain outliers	177891	1885 (2.26-2.26)
RSRZ outliers	164620	1763 (2.26-2.26)

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  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	291	
2	Y	210	
3	Z	241	
4	A	5	
5	C	3	

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Mol	Chain	Length	Quality of chain
6	D	4	 A horizontal bar chart showing the quality of chain D. The bar is divided into three segments: green (50%), yellow (25%), and orange (25%).

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 5835 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 Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	275	Total	C	N	O	S	0	0	0
			2180	1374	387	409	10			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	320	GLY	-	expression tag	UNP R4L1D1
B	321	ALA	-	expression tag	UNP R4L1D1
B	322	LEU	-	expression tag	UNP R4L1D1
B	323	GLU	-	expression tag	UNP R4L1D1
B	324	VAL	-	expression tag	UNP R4L1D1
B	325	LEU	-	expression tag	UNP R4L1D1
B	326	PHE	-	expression tag	UNP R4L1D1
B	327	GLN	-	expression tag	UNP R4L1D1

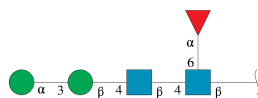
- Molecule 2 is a protein called S5V2-29 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	208	Total	C	N	O	S	0	0	0
			1586	988	268	325	5			

- Molecule 3 is a protein called S5V2-29 heavy chain.

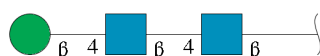
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Z	231	Total	C	N	O	S	0	0	0
			1739	1106	288	338	7			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



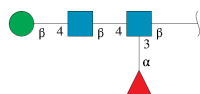
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	A	5	Total	C	N	O	0	0	0
			60	34	2	24			

- Molecule 5 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
5	C	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 6 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	D	4	Total	C	N	O	0	0	0
			49	28	2	19			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		

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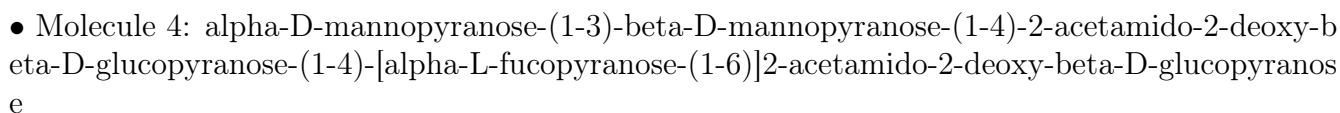
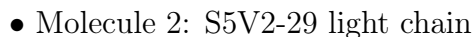
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	Y	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	71	Total	O	0	0
			71	71		
9	Y	45	Total	O	0	0
			45	45		
9	Z	28	Total	O	0	0
			28	28		



- Molecule 1: Hemagglutinin







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

Chain C:  100%



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  50% 25% 25%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	115.74Å 163.48Å 136.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.37 – 2.25 46.37 – 2.25	Depositor EDS
% Data completeness (in resolution range)	97.7 (46.37-2.25) 97.7 (46.37-2.25)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.87 (at 2.24Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, $R_{free}$	0.203 , 0.225 0.207 , 0.229	Depositor DCC
$R_{free}$ test set	2961 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	54.6	Xtriage
Anisotropy	0.401	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 48.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5835	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: NAG, MAN, GOL, FUC, BMA

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	B	0.27	0/2234	0.47	0/3036
2	Y	0.31	1/1618 (0.1%)	0.53	2/2195 (0.1%)
3	Z	0.31	0/1783	0.57	1/2431 (0.0%)
All	All	0.30	1/5635 (0.0%)	0.52	3/7662 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Y	190	CYS	CB-SG	5.33	1.91	1.82

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	190	CYS	CA-CB-SG	5.48	123.86	114.00
3	Z	75	MET	CG-SD-CE	-5.13	92.00	100.20
2	Y	130	CYS	CA-CB-SG	5.12	123.21	114.00

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	B	2180	0	2126	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Y	1586	0	1538	26	0
3	Z	1739	0	1722	21	0
4	A	60	0	52	0	0
5	C	39	0	34	0	0
6	D	49	0	43	1	0
7	B	14	0	13	0	0
8	B	18	0	24	3	0
8	Y	6	0	8	0	0
9	B	71	0	0	2	0
9	Y	45	0	0	1	0
9	Z	28	0	0	1	0
All	All	5835	0	5560	66	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 (66) 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:Y:51:ALA:O	9:Y:401:HOH:O	1.89	0.90
2:Y:2:ILE:HD11	2:Y:27:GLN:H	1.43	0.83
2:Y:2:ILE:HG21	2:Y:90:GLN:HE21	1.46	0.80
3:Z:212:ILE:CD1	3:Z:227:ARG:HB2	2.17	0.75
1:B:158:ASN:O	9:B:501:HOH:O	2.05	0.75
1:B:95:SER:H	3:Z:107:LEU:HD21	1.52	0.74
1:B:264:LYS:O	1:B:264:LYS:HD3	1.87	0.73
3:Z:29:VAL:HG12	3:Z:55:HIS:NE2	2.04	0.72
1:B:264:LYS:O	1:B:264:LYS:CD	2.39	0.71
2:Y:2:ILE:HG21	2:Y:90:GLN:NE2	2.07	0.68
3:Z:106:MET:O	9:Z:301:HOH:O	2.15	0.65
1:B:307:ARG:NH2	9:B:505:HOH:O	2.30	0.64
1:B:264:LYS:NZ	1:B:302:TYR:CZ	2.63	0.64
2:Y:2:ILE:CG2	2:Y:90:GLN:HE21	2.11	0.64
2:Y:104:ARG:NH2	2:Y:105:THR:OG1	2.31	0.63
3:Z:212:ILE:HD13	3:Z:227:ARG:HA	1.81	0.61
6:D:2:NAG:H83	6:D:2:NAG:H3	1.81	0.61
2:Y:78:LEU:HD11	2:Y:100:LEU:HD21	1.84	0.60
3:Z:212:ILE:HD11	3:Z:227:ARG:HB2	1.82	0.60
1:B:262:SER:H	8:B:416:GOL:H32	1.68	0.58
2:Y:115:PRO:HG2	3:Z:231:LYS:HE3	1.87	0.57
3:Z:188:GLN:HG2	3:Z:192:LEU:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:LYS:HD3	1:B:257:TYR:CG	2.40	0.56
3:Z:212:ILE:HD13	3:Z:227:ARG:HB2	1.86	0.56
3:Z:30:SER:HB3	3:Z:75:MET:CE	2.36	0.54
3:Z:212:ILE:HD13	3:Z:227:ARG:CA	2.37	0.54
2:Y:83:PHE:HB2	2:Y:102:ILE:HD13	1.89	0.53
3:Z:45:LYS:O	3:Z:45:LYS:HD3	2.08	0.53
3:Z:65:LEU:O	3:Z:67:SER:N	2.40	0.53
2:Y:24:ARG:NH1	2:Y:70:ASP:OD2	2.36	0.52
2:Y:2:ILE:HD11	2:Y:27:GLN:N	2.19	0.52
1:B:295:GLN:HB2	1:B:306:PRO:HB2	1.93	0.50
2:Y:80:PRO:HA	2:Y:102:ILE:HG12	1.94	0.50
2:Y:141:LYS:HB3	2:Y:193:THR:OG1	2.11	0.50
3:Z:212:ILE:HD13	3:Z:227:ARG:CB	2.42	0.50
3:Z:62:ASN:HB3	3:Z:65:LEU:HD12	1.96	0.48
2:Y:4:MET:O	2:Y:96:GLN:NE2	2.40	0.47
8:B:416:GOL:O3	8:B:416:GOL:O1	2.21	0.47
1:B:288:ILE:HG22	1:B:289:PRO:O	2.15	0.47
2:Y:2:ILE:HD12	2:Y:2:ILE:HA	1.75	0.47
2:Y:104:ARG:HG2	2:Y:105:THR:N	2.30	0.47
1:B:262:SER:O	1:B:262:SER:OG	2.32	0.46
3:Z:30:SER:HB3	3:Z:75:MET:HE2	1.97	0.46
2:Y:193:THR:HG22	2:Y:200:PRO:HG3	1.97	0.46
1:B:115:SER:OG	1:B:260:ILE:HD12	2.16	0.45
2:Y:159:VAL:HG22	2:Y:171:LEU:HD12	1.99	0.45
3:Z:66:LYS:H	3:Z:66:LYS:HG2	1.48	0.45
2:Y:2:ILE:HD13	2:Y:27:GLN:HB3	1.99	0.44
2:Y:121:LEU:O	2:Y:179:LYS:HD2	2.17	0.44
1:B:167:THR:HA	1:B:243:LEU:O	2.19	0.43
1:B:241:ASP:OD1	1:B:242:ILE:N	2.51	0.43
1:B:176:LYS:HD3	1:B:257:TYR:CD1	2.54	0.42
1:B:75:GLN:NE2	1:B:94:TYR:O	2.52	0.42
3:Z:107:LEU:HD23	3:Z:107:LEU:HA	1.55	0.42
2:Y:101:GLU:HG2	2:Y:102:ILE:N	2.34	0.42
2:Y:136:TYR:CG	2:Y:137:PRO:HA	2.54	0.42
1:B:182:VAL:HG21	1:B:213:VAL:HG11	2.01	0.41
2:Y:40:PRO:HG3	2:Y:83:PHE:HE2	1.85	0.41
2:Y:96:GLN:H	2:Y:96:GLN:CD	2.23	0.41
3:Z:41:GLN:HB2	3:Z:47:LEU:HD23	2.02	0.41
1:B:90:ARG:O	3:Z:109:ALA:HB2	2.21	0.41
2:Y:2:ILE:HD12	2:Y:26:SER:OG	2.20	0.41
1:B:135:THR:O	8:B:414:GOL:H12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:8:GLY:HA3	3:Z:20:LEU:HD23	2.02	0.40
2:Y:36:TYR:HE1	2:Y:89:GLN:HB3	1.86	0.40
1:B:186:VAL:HG23	1:B:219:PHE:HA	2.03	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 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	B	273/291 (94%)	266 (97%)	7 (3%)	0	100	100
2	Y	206/210 (98%)	199 (97%)	7 (3%)	0	100	100
3	Z	229/241 (95%)	219 (96%)	9 (4%)	1 (0%)	30	32
All	All	708/742 (95%)	684 (97%)	23 (3%)	1 (0%)	48	57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	Z	66	LYS

### 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	B	246/258 (95%)	240 (98%)	6 (2%)	44	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Y	180/182 (99%)	176 (98%)	4 (2%)	47	56
3	Z	198/208 (95%)	194 (98%)	4 (2%)	50	59
All	All	624/648 (96%)	610 (98%)	14 (2%)	47	56

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	54	SER
1	B	165	ASN
1	B	247	SER
1	B	264	LYS
1	B	295	GLN
1	B	307	ARG
2	Y	33	LEU
2	Y	90	GLN
2	Y	138	ARG
2	Y	199	SER
3	Z	35	TYR
3	Z	53	PHE
3	Z	112	GLN
3	Z	134	LYS

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

Mol	Chain	Res	Type
2	Y	27	GLN
2	Y	185	HIS

### 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 ⓘ

12 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	A	1	1,4	14,14,15	0.41	0	17,19,21	0.53	0
4	NAG	A	2	4	14,14,15	0.18	0	17,19,21	0.50	0
4	BMA	A	3	4	11,11,12	0.54	0	15,15,17	0.68	0
4	MAN	A	4	4	11,11,12	0.94	1 (9%)	15,15,17	1.13	2 (13%)
4	FUC	A	5	4	10,10,11	0.83	0	14,14,16	0.84	0
5	NAG	C	1	1,5	14,14,15	0.22	0	17,19,21	0.55	0
5	NAG	C	2	5	14,14,15	0.21	0	17,19,21	0.56	0
5	BMA	C	3	5	11,11,12	0.66	0	15,15,17	0.83	0
6	NAG	D	1	1,6	14,14,15	0.36	0	17,19,21	0.44	0
6	NAG	D	2	6	14,14,15	0.53	0	17,19,21	1.41	2 (11%)
6	BMA	D	3	6	11,11,12	0.68	0	15,15,17	0.83	0
6	FUC	D	4	6	10,10,11	0.93	1 (10%)	14,14,16	0.91	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
4	NAG	A	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	2	4	-	2/6/23/26	0/1/1/1
4	BMA	A	3	4	-	0/2/19/22	0/1/1/1
4	MAN	A	4	4	-	0/2/19/22	0/1/1/1
4	FUC	A	5	4	-	-	0/1/1/1
5	NAG	C	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	C	2	5	-	2/6/23/26	0/1/1/1
5	BMA	C	3	5	-	2/2/19/22	0/1/1/1
6	NAG	D	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	D	2	6	-	6/6/23/26	0/1/1/1
6	BMA	D	3	6	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	FUC	D	4	6	-	-	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	4	MAN	C1-C2	2.39	1.57	1.52
6	D	4	FUC	C1-C2	2.35	1.57	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	2	NAG	C2-N2-C7	4.71	129.21	122.90
4	A	4	MAN	C1-O5-C5	2.79	115.93	112.19
6	D	2	NAG	C1-C2-N2	2.14	113.80	110.43
4	A	4	MAN	O2-C2-C3	-2.11	105.79	110.15

There are no chirality outliers.

All (15) torsion outliers are listed below:

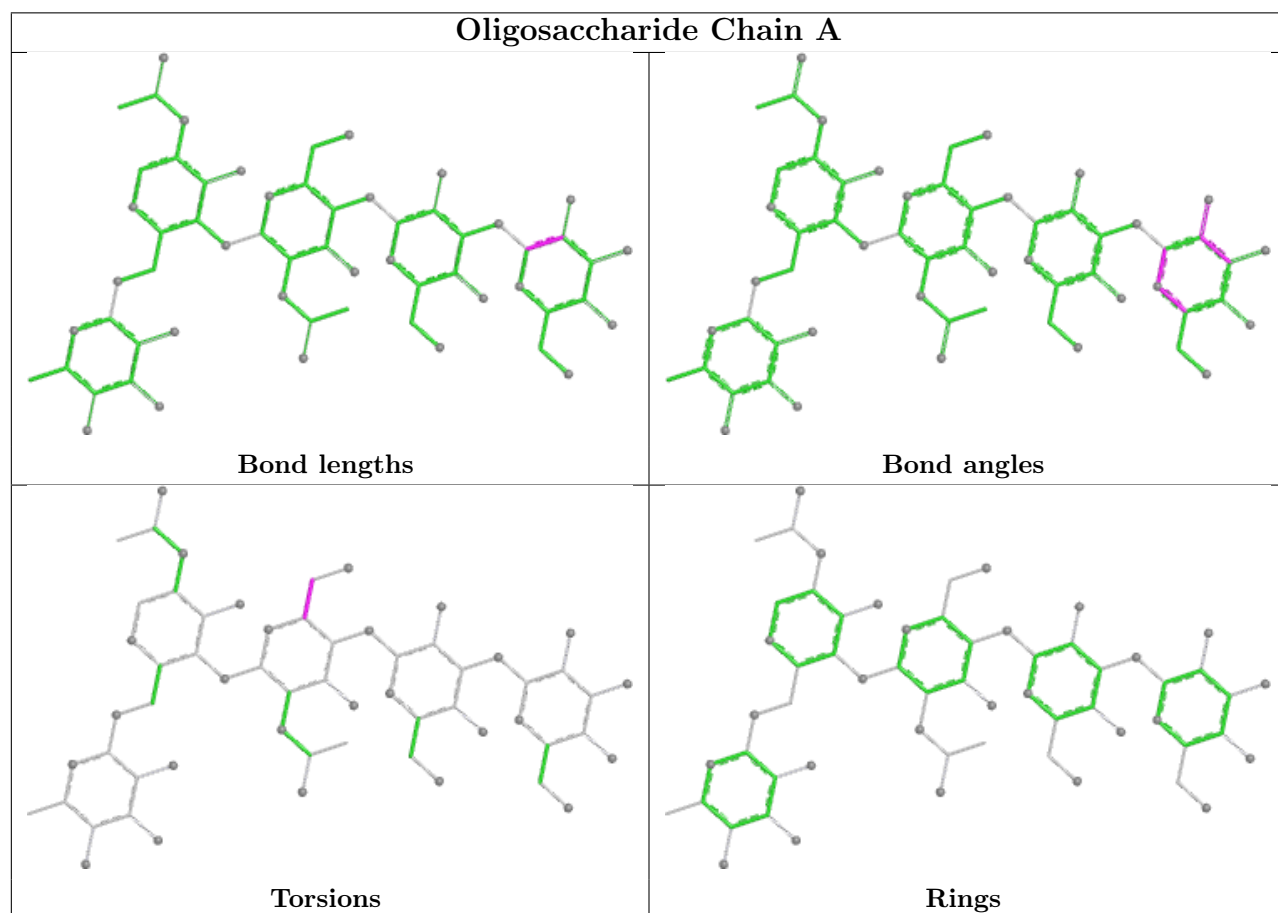
Mol	Chain	Res	Type	Atoms
5	C	1	NAG	O5-C5-C6-O6
6	D	2	NAG	O5-C5-C6-O6
5	C	2	NAG	C4-C5-C6-O6
5	C	2	NAG	O5-C5-C6-O6
5	C	1	NAG	C4-C5-C6-O6
4	A	2	NAG	O5-C5-C6-O6
5	C	3	BMA	O5-C5-C6-O6
6	D	2	NAG	C8-C7-N2-C2
6	D	2	NAG	O7-C7-N2-C2
5	C	3	BMA	C4-C5-C6-O6
4	A	2	NAG	C4-C5-C6-O6
6	D	2	NAG	C4-C5-C6-O6
6	D	2	NAG	C3-C2-N2-C7
6	D	2	NAG	C1-C2-N2-C7
6	D	3	BMA	O5-C5-C6-O6

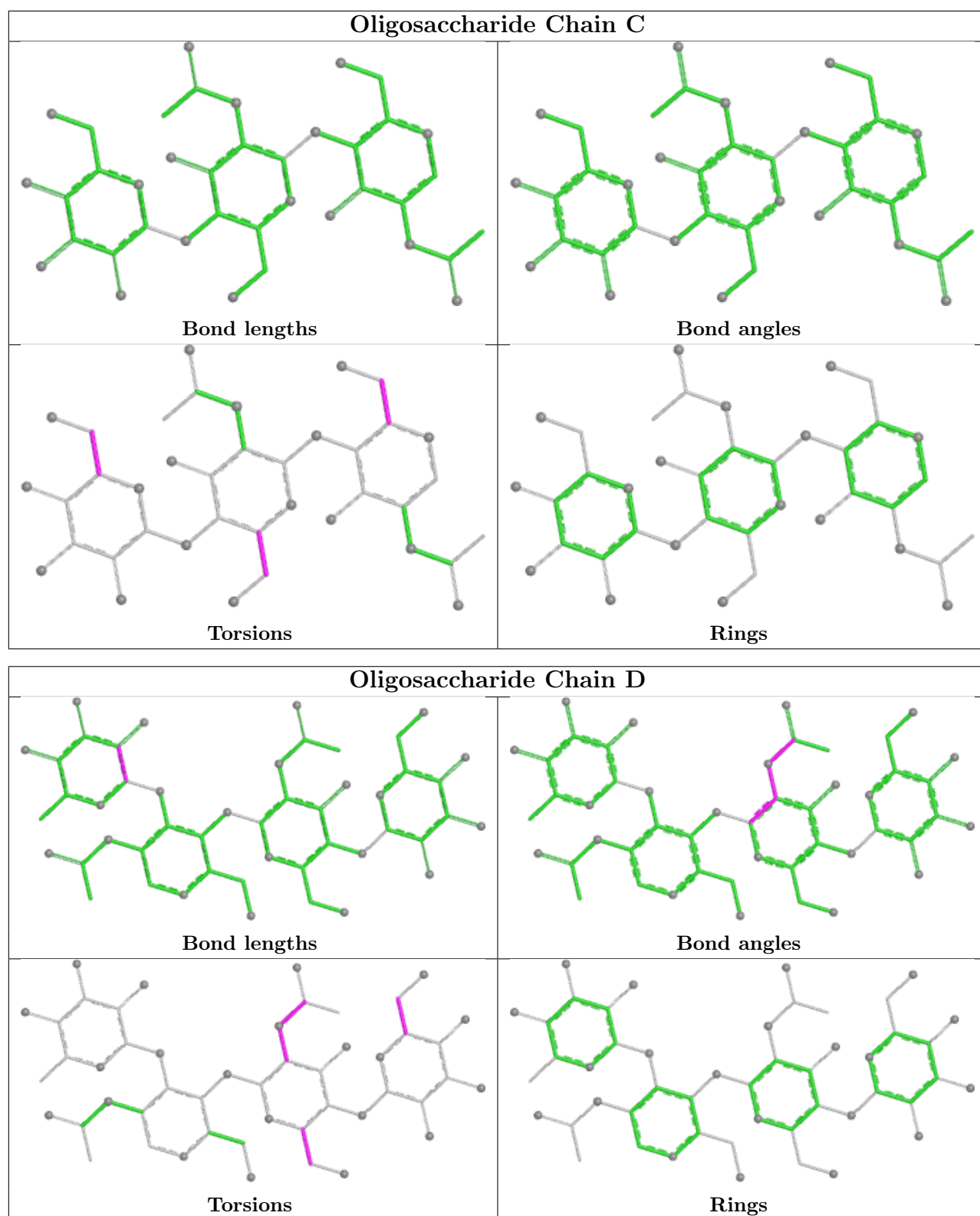
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	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 [i](#)

5 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$
8	GOL	B	415	-	5,5,5	0.95	0	5,5,5	1.06	0
7	NAG	B	409	1	14,14,15	0.44	0	17,19,21	0.47	0
8	GOL	B	416	-	5,5,5	0.89	0	5,5,5	1.25	1 (20%)
8	GOL	B	414	-	5,5,5	1.02	0	5,5,5	1.02	0
8	GOL	Y	301	-	5,5,5	0.93	0	5,5,5	1.11	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
8	GOL	B	415	-	-	2/4/4/4	-
7	NAG	B	409	1	-	1/6/23/26	0/1/1/1
8	GOL	B	416	-	-	0/4/4/4	-
8	GOL	B	414	-	-	0/4/4/4	-
8	GOL	Y	301	-	-	2/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	416	GOL	C3-C2-C1	-2.18	103.82	111.80

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	409	NAG	O5-C5-C6-O6
8	B	415	GOL	C1-C2-C3-O3
8	Y	301	GOL	C1-C2-C3-O3
8	Y	301	GOL	O2-C2-C3-O3
8	B	415	GOL	O2-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	416	GOL	2	0
8	B	414	GOL	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.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	B	275/291 (94%)	0.30	19 (6%)	24 24	37, 56, 85, 136	0
2	Y	208/210 (99%)	0.42	14 (6%)	25 24	43, 59, 84, 120	0
3	Z	231/241 (95%)	0.69	27 (11%)	10 10	43, 62, 101, 119	0
All	All	714/742 (96%)	0.46	60 (8%)	18 18	37, 59, 92, 136	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Z	107	LEU	5.4
1	B	264	LYS	4.8
3	Z	231	LYS	4.6
3	Z	55	HIS	4.6
3	Z	43	PRO	4.6
3	Z	108	VAL	4.4
3	Z	29	VAL	4.2
3	Z	32	ASN	4.2
3	Z	150	GLY	3.9
3	Z	106	MET	3.8
2	Y	207	ARG	3.7
1	B	310	LYS	3.7
1	B	311	GLN	3.6
3	Z	218	LYS	3.6
3	Z	27	GLY	3.5
3	Z	75	MET	3.5
2	Y	208	GLY	3.4
1	B	208	ARG	3.3
3	Z	44	GLY	3.3
1	B	193	PHE	3.3
3	Z	149	SER	3.2
2	Y	206	ASN	3.1
1	B	37	THR	3.1

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Mol	Chain	Res	Type	RSRZ
3	Z	45	LYS	3.1
3	Z	104	ASN	3.0
3	Z	1	GLN	3.0
2	Y	2	ILE	2.7
2	Y	176	THR	2.7
3	Z	122	ARG	2.7
3	Z	46	GLY	2.7
3	Z	105	LEU	2.6
2	Y	12	SER	2.6
2	Y	4	MET	2.6
2	Y	99	LYS	2.6
1	B	225	ASN	2.5
3	Z	64	SER	2.5
1	B	104	ASP	2.5
2	Y	165	LYS	2.5
3	Z	31	SER	2.4
1	B	169	PRO	2.4
3	Z	109	ALA	2.4
1	B	288	ILE	2.4
1	B	39	ALA	2.4
1	B	105	TYR	2.3
2	Y	27	GLN	2.3
1	B	83	LYS	2.2
1	B	219	PHE	2.2
2	Y	24	ARG	2.2
1	B	91	SER	2.2
2	Y	103	LYS	2.1
3	Z	148	THR	2.1
3	Z	30	SER	2.1
3	Z	207	GLY	2.1
1	B	276	LYS	2.1
1	B	45	ASN	2.1
3	Z	76	SER	2.1
1	B	139	CYS	2.1
2	Y	184	LYS	2.0
1	B	38	ASN	2.0
2	Y	23	CYS	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

SUGAR-RSR INFOmissingINFO

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	NAG	B	409	14/15	0.71	0.21	94,107,111,111	0
8	GOL	B	414	6/6	0.85	0.19	66,74,85,88	0
8	GOL	B	416	6/6	0.85	0.18	70,73,78,82	0
8	GOL	B	415	6/6	0.89	0.20	79,82,96,102	0
8	GOL	Y	301	6/6	0.91	0.15	63,71,77,84	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.