



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 03:17 PM UTC

PDB ID : 9PHD / pdb\_00009phd  
Title : Crystal structure of the A/Puerto Rico/8/1934 (H1N1) influenza virus hemagglutinin in complex with fusion inhibitor cyclic peptide CP141076 (CP8)  
Authors : Kadam, R.U.; Wilson, I.A.  
Deposited on : 2025-07-09  
Resolution : 1.59 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 : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

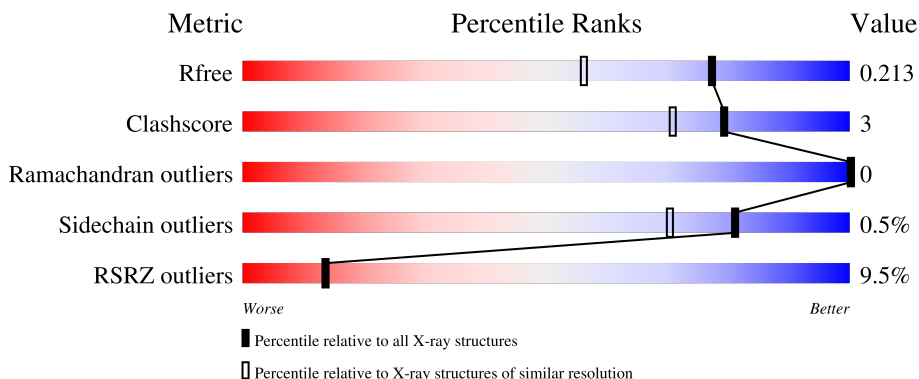
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.59 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))
$R_{free}$	180053	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	C	326	<div> <div>12%</div> <div> <div></div> <div>94%</div> <div>5%</div> </div> </div>
2	D	176	<div> <div>3%</div> <div> <div></div> <div>86%</div> <div>5%</div> <div>9%</div> </div> </div>
3	G	15	<div> <div>13%</div> <div> <div></div> <div>73%</div> <div>20%</div> <div>7%</div> </div> </div>
4	L	6	<div> <div></div> <div> <div></div> <div>50%</div> <div>50%</div> </div> </div>

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 4775 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	C	322	Total	C	N	O	S	0	13	0
			2605	1653	447	491	14			

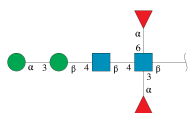
- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	160	Total	C	N	O	S	0	6	0
			1328	834	224	264	6			

- Molecule 3 is a protein called cyclic peptide CP141076.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	15	Total	C	N	O	S	0	3	0
			129	78	23	23	5			

- 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-(1-3)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



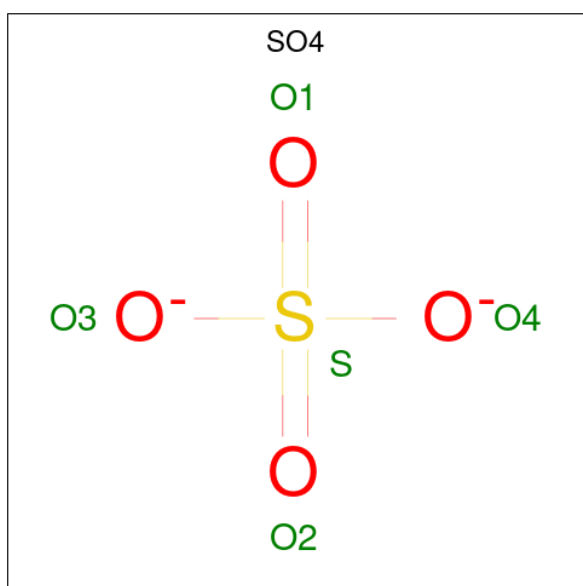
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	L	6	Total	C	N	O	0	0	0
			70	40	2	28			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

- Molecule 6 is SULFATE ION (CCD ID: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		

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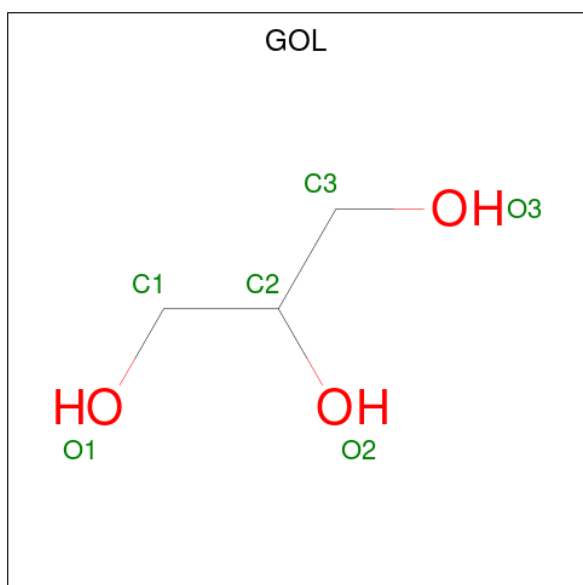
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			7	4	3		

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



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

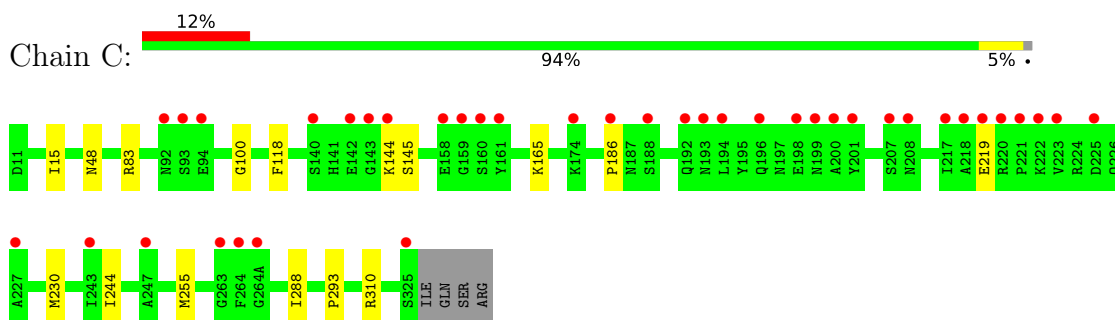
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	C	344	Total	O	0	0
			344	344		
9	D	224	Total	O	0	0
			224	224		
9	G	19	Total	O	0	0
			19	19		

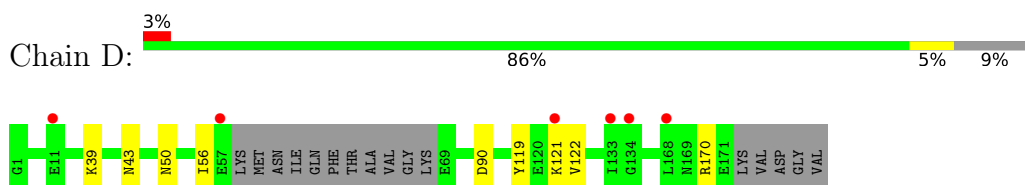
### 3 Residue-property plots [i](#)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

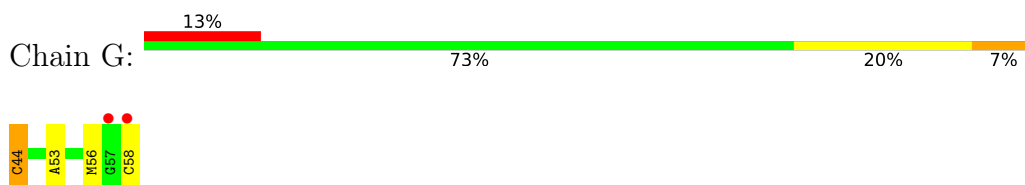
- Molecule 1: Hemagglutinin



- Molecule 2: Hemagglutinin HA2 chain



- Molecule 3: cyclic peptide CP141076



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.09Å 102.09Å 335.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.10 – 1.59 42.10 – 1.59	Depositor EDS
% Data completeness (in resolution range)	99.2 (42.10-1.59) 99.2 (42.10-1.59)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.40 (at 1.59Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.192 , 0.212 0.193 , 0.213	Depositor DCC
$R_{free}$ test set	4554 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.4	Xtriage
Anisotropy	0.426	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 42.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	4775	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, FUC, A1CRT, MAN, PEG, BMA, NAG, SO4

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	C	0.27	0/2708	0.49	0/3680
2	D	0.34	0/1367	0.55	0/1835
3	G	0.28	0/113	0.50	0/148
All	All	0.29	0/4188	0.51	0/5663

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2605	0	2582	12	0
2	D	1328	0	1262	12	0
3	G	129	0	110	2	0
4	L	70	0	61	0	0
5	C	28	0	26	0	0
6	C	15	0	0	0	0
7	C	7	0	10	1	0
8	C	6	0	8	0	0
9	C	344	0	0	3	0
9	D	224	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	G	19	0	0	0	0
All	All	4775	0	4059	22	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 3.

All (22) 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:D:121:LYS:HE3	9:D:375:HOH:O	1.90	0.71
2:D:170:ARG:NH2	9:D:201:HOH:O	2.25	0.66
3:G:44[B]:A1CRT:N	3:G:58[B]:CYS:SG	2.70	0.65
1:C:310:ARG:NH1	2:D:90:ASP:OD1	2.30	0.63
1:C:83:ARG:NH1	9:C:503:HOH:O	2.35	0.57
1:C:15:ILE:HD11	2:D:122:VAL:HG21	1.87	0.56
1:C:293:PRO:HD3	2:D:56:ILE:HG23	1.88	0.55
2:D:39:LYS:NZ	2:D:43[A]:ASN:HD21	2.05	0.55
2:D:39:LYS:HZ2	2:D:43[A]:ASN:HD21	1.56	0.54
3:G:53:ALA:HB1	3:G:56:MET:HE2	1.95	0.49
1:C:48:ASN:HD22	7:C:406:PEG:H32	1.77	0.48
1:C:255[B]:MET:HE3	9:C:528:HOH:O	2.14	0.47
2:D:50[B]:ASN:ND2	9:D:204:HOH:O	2.48	0.46
2:D:39:LYS:HD2	9:D:215:HOH:O	2.15	0.46
1:C:100:GLY:HA3	1:C:230:MET:O	2.16	0.46
1:C:186:PRO:O	1:C:219:GLU:HG2	2.19	0.42
1:C:144:LYS:HD2	1:C:145:SER:H	1.84	0.42
1:C:15:ILE:HG13	2:D:119:TYR:HA	2.02	0.42
1:C:83:ARG:NH1	9:C:516:HOH:O	2.52	0.41
2:D:56:ILE:HG22	2:D:56:ILE:O	2.21	0.41
2:D:121:LYS:NZ	9:D:205:HOH:O	2.51	0.40
1:C:165:LYS:HE2	1:C:244:ILE:HG21	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	C	333/326 (102%)	324 (97%)	9 (3%)	0	100	100
2	D	161/176 (92%)	156 (97%)	5 (3%)	0	100	100
3	G	14/15 (93%)	14 (100%)	0	0	100	100
All	All	508/517 (98%)	494 (97%)	14 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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	C	298/289 (103%)	295 (99%)	3 (1%)	68	50
2	D	144/151 (95%)	144 (100%)	0	100	100
3	G	11/9 (122%)	11 (100%)	0	100	100
All	All	453/449 (101%)	450 (99%)	3 (1%)	81	63

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	118	PHE
1	C	288[A]	ILE
1	C	288[B]	ILE

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

Mol	Chain	Res	Type
1	C	95	ASN
2	D	154	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	A1CRT	G	44[A]	3	10,12,13	1.29	1 (10%)	10,14,16	1.85	2 (20%)
3	A1CRT	G	44[B]	3	10,12,13	1.34	1 (10%)	10,14,16	1.72	1 (10%)

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	A1CRT	G	44[A]	3	-	6/11/13/15	-
3	A1CRT	G	44[B]	3	-	7/11/13/15	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	44[A]	A1CRT	O3-C4	-3.20	1.31	1.40
3	G	44[B]	A1CRT	O3-C4	-3.20	1.31	1.40

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	44[A]	A1CRT	C3-C2-C1	3.67	122.29	112.49
3	G	44[B]	A1CRT	C3-C2-C1	3.67	122.29	112.49
3	G	44[A]	A1CRT	CA-CB-SG	-2.90	110.89	114.16

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	44[A]	A1CRT	C2-C3-C4-O3
3	G	44[A]	A1CRT	O-C-CA-CB
3	G	44[B]	A1CRT	C2-C3-C4-O3
3	G	44[B]	A1CRT	O-C-CA-CB
3	G	44[B]	A1CRT	N-CA-CB-SG
3	G	44[B]	A1CRT	C2-C3-C4-N
3	G	44[A]	A1CRT	CB-CA-N-C4
3	G	44[A]	A1CRT	C2-C3-C4-N
3	G	44[B]	A1CRT	C-CA-CB-SG
3	G	44[A]	A1CRT	O1-C1-C2-C3
3	G	44[A]	A1CRT	O2-C1-C2-C3
3	G	44[B]	A1CRT	O1-C1-C2-C3
3	G	44[B]	A1CRT	O2-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	44[B]	A1CRT	1	0

## 5.5 Carbohydrates ⓘ

6 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	L	1	1,4	14,14,15	0.42	0	17,19,21	0.53	0
4	NAG	L	2	4	14,14,15	0.34	0	17,19,21	0.66	0
4	BMA	L	3	4	11,11,12	0.71	0	15,15,17	0.73	0
4	MAN	L	4	4	11,11,12	0.68	0	15,15,17	1.16	2 (13%)
4	FUC	L	5	4	10,10,11	0.87	1 (10%)	14,14,16	0.96	1 (7%)
4	FUC	L	6	4	10,10,11	1.06	1 (10%)	14,14,16	0.56	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	L	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	L	2	4	-	2/6/23/26	0/1/1/1
4	BMA	L	3	4	-	0/2/19/22	0/1/1/1
4	MAN	L	4	4	-	0/2/19/22	0/1/1/1
4	FUC	L	5	4	-	-	0/1/1/1
4	FUC	L	6	4	-	-	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	6	FUC	C2-C3	2.14	1.55	1.52
4	L	5	FUC	C1-C2	2.08	1.57	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	4	MAN	C1-O5-C5	3.18	116.44	112.19
4	L	4	MAN	O3-C3-C2	2.06	114.27	110.05
4	L	5	FUC	C1-O5-C5	2.01	117.70	112.97

There are no chirality outliers.

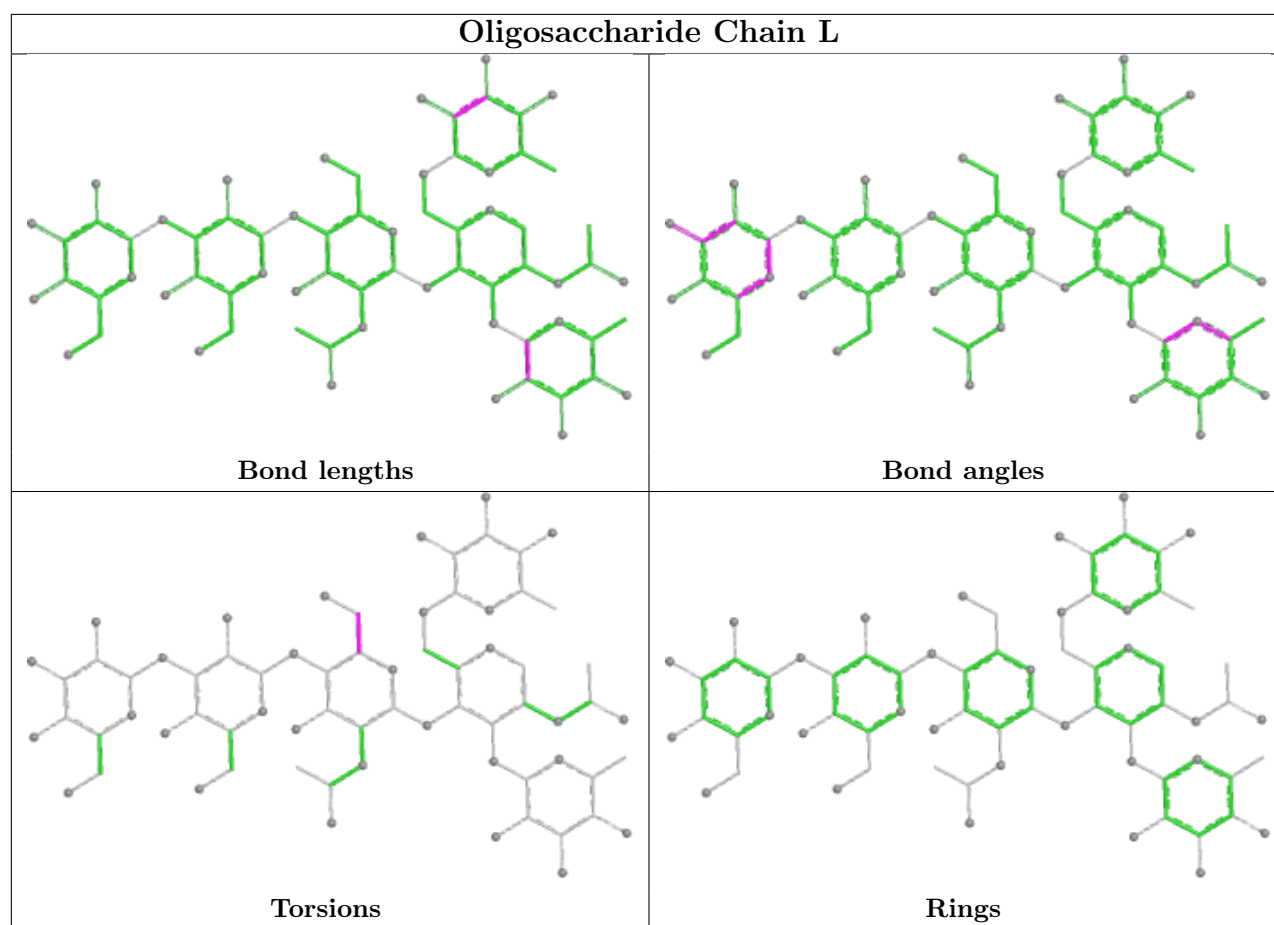
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	2	NAG	C4-C5-C6-O6
4	L	2	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



## 5.6 Ligand geometry [i](#)

7 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	$\# Z  > 2$
6	SO4	C	404	-	4,4,4	0.38	0	6,6,6	0.40	0
8	GOL	C	407	-	5,5,5	0.74	0	5,5,5	1.11	0
7	PEG	C	406	-	6,6,6	0.14	0	5,5,5	0.08	0
5	NAG	C	402	1	14,14,15	0.30	0	17,19,21	0.58	0
6	SO4	C	403	-	4,4,4	0.24	0	6,6,6	0.08	0
6	SO4	C	405	-	4,4,4	0.24	0	6,6,6	0.08	0
5	NAG	C	401	1	14,14,15	0.18	0	17,19,21	0.46	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
7	PEG	C	406	-	-	3/4/4/4	-
5	NAG	C	402	1	-	0/6/23/26	0/1/1/1
5	NAG	C	401	1	-	2/6/23/26	0/1/1/1
8	GOL	C	407	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	407	GOL	O1-C1-C2-C3
5	C	401	NAG	O5-C5-C6-O6
5	C	401	NAG	C4-C5-C6-O6
7	C	406	PEG	O2-C3-C4-O4
7	C	406	PEG	O1-C1-C2-O2
8	C	407	GOL	O1-C1-C2-O2
8	C	407	GOL	O2-C2-C3-O3
7	C	406	PEG	C4-C3-O2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	406	PEG	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	C	322/326 (98%)	0.71	39 (12%) <b>8</b> <b>8</b>	10, 26, 51, 74	13 (4%)
2	D	160/176 (90%)	0.28	6 (3%) 44 46	7, 18, 39, 63	6 (3%)
3	G	14/15 (93%)	0.83	2 (14%) <b>6</b> <b>5</b>	12, 19, 29, 38	2 (14%)
All	All	496/517 (95%)	0.58	47 (9%) <b>14</b> <b>14</b>	7, 23, 48, 74	21 (4%)

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	221	PRO	5.9
1	C	218	ALA	5.6
2	D	168	LEU	4.7
1	C	223	VAL	4.4
1	C	325	SER	4.2
1	C	159	GLY	4.1
2	D	133[A]	ILE	4.1
1	C	144	LYS	3.7
1	C	264	PHE	3.6
2	D	57[A]	GLU	3.6
1	C	160	SER	3.6
1	C	143	GLY	3.4
1	C	94	GLU	3.4
1	C	207	SER	3.1
3	G	58[A]	CYS	3.1
1	C	142	GLU	2.9
1	C	193	ASN	2.9
2	D	134	GLY	2.8
1	C	227	ALA	2.8
2	D	11	GLU	2.6
1	C	199	ASN	2.6
1	C	208	ASN	2.6
3	G	57	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	92	ASN	2.5
1	C	263	GLY	2.5
1	C	196	GLN	2.5
1	C	217	ILE	2.4
1	C	222	LYS	2.4
1	C	219	GLU	2.4
1	C	93	SER	2.4
1	C	201	TYR	2.4
1	C	158	GLU	2.4
1	C	225	ASP	2.3
1	C	192	GLN	2.3
1	C	220	ARG	2.3
2	D	121	LYS	2.3
1	C	188	SER	2.2
1	C	140	SER	2.2
1	C	264(A)	GLY	2.2
1	C	174	LYS	2.2
1	C	194	LEU	2.1
1	C	186	PRO	2.1
1	C	161	TYR	2.1
1	C	198	GLU	2.1
1	C	243	ILE	2.1
1	C	200	ALA	2.0
1	C	247	ALA	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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(Å <sup>2</sup> )	Q<0.9
3	A1CRT	G	44[A]	13/14	0.95	0.08	18,23,29,31	6
3	A1CRT	G	44[B]	13/14	0.95	0.08	18,22,31,40	6

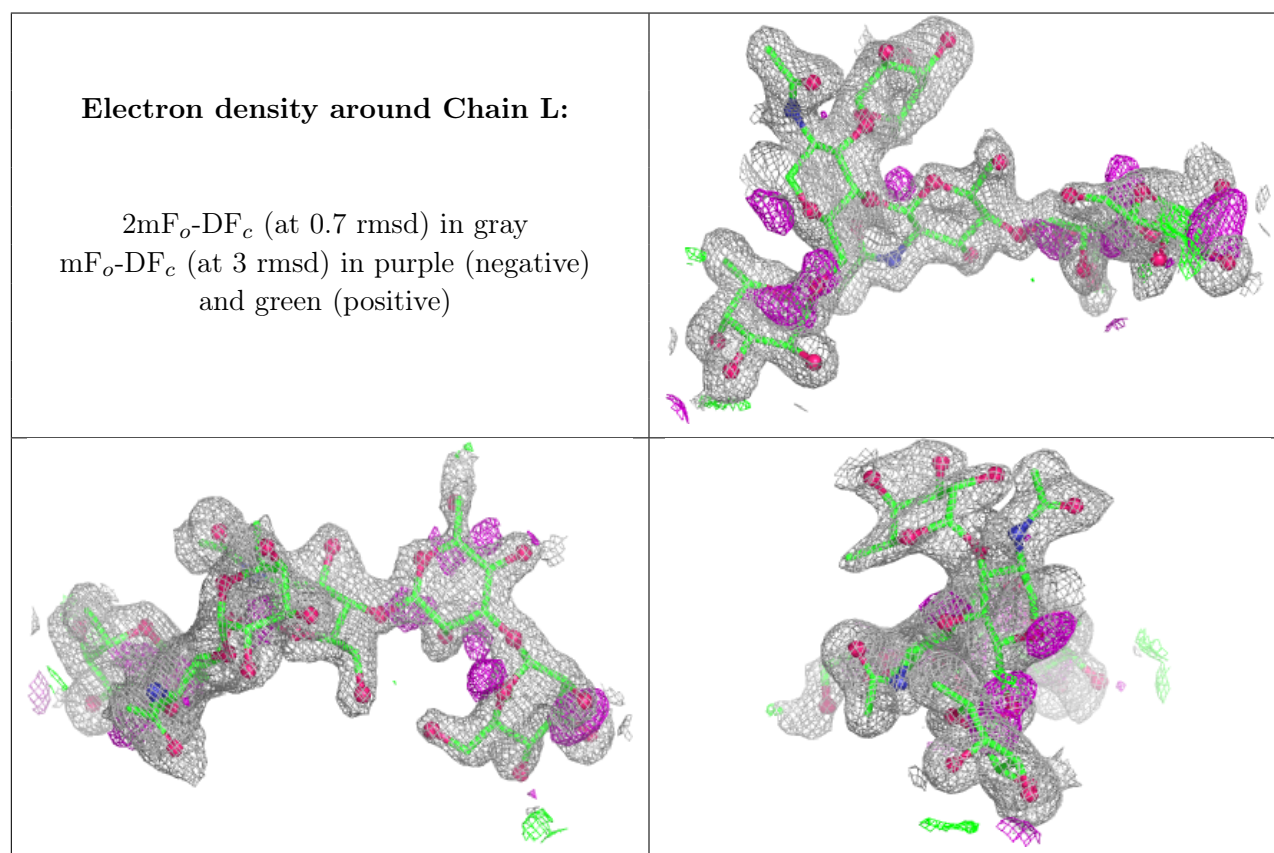
## 6.3 Carbohydrates [i](#)

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
4	NAG	L	1	14/15	-	-	31,39,49,52	0
4	NAG	L	2	14/15	-	-	33,41,49,54	0
4	BMA	L	3	11/12	-	-	38,45,49,54	0
4	MAN	L	4	11/12	-	-	26,43,52,53	0
4	FUC	L	5	10/11	-	-	64,75,80,85	0
4	FUC	L	6	10/11	-	-	23,28,30,31	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



## 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
5	NAG	C	401	14/15	0.68	0.15	54,64,67,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NAG	C	402	14/15	0.72	0.15	51,63,72,78	0
6	SO4	C	403	5/5	0.75	0.12	89,90,92,101	0
6	SO4	C	405	5/5	0.76	0.15	44,46,54,56	0
8	GOL	C	407	6/6	0.79	0.17	38,42,48,57	0
7	PEG	C	406	7/7	0.81	0.17	51,56,57,58	0
6	SO4	C	404	5/5	0.96	0.16	18,23,26,26	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.