



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 25, 2026 – 07:54 AM EDT

PDB ID : 2J3F / pdb\_00002j3f  
Title : L-ficolin complexed to N-acetyl-D-galactosamine  
Authors : Garlatti, V.; Gaboriaud, C.  
Deposited on : 2006-08-21  
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
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

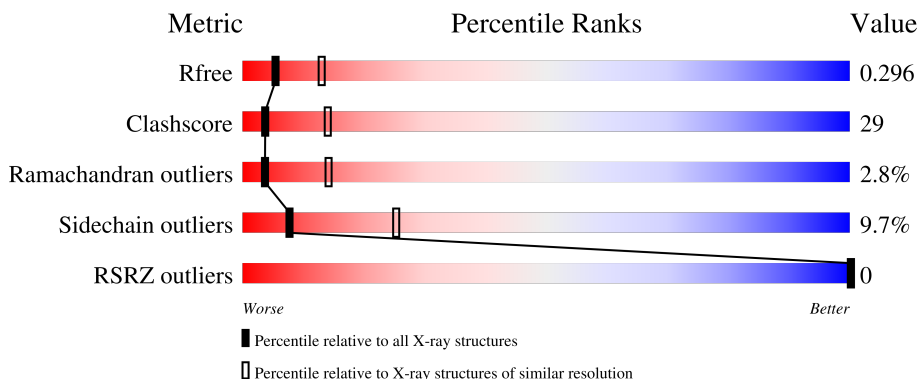
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	A	219	
1	B	219	
1	C	219	
1	E	219	
1	F	219	

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Mol	Chain	Length	Quality of chain
2	D	219	 43% 43% 12%
3	G	5	 20% 40% 40%
4	H	3	 33% 67%

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 10783 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 FICOLIN-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	218	Total 1744	C 1096	N 306	O 334	S 8	0	2	0
1	B	217	Total 1758	C 1107	N 310	O 332	S 9	0	2	0
1	C	214	Total 1741	C 1093	N 310	O 330	S 8	0	3	0
1	E	217	Total 1771	C 1116	N 311	O 335	S 9	0	2	0
1	F	217	Total 1746	C 1098	N 308	O 331	S 9	0	1	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	168	THR	VAL	conflict	UNP Q15485
A	247	THR	VAL	conflict	UNP Q15485
B	168	THR	VAL	conflict	UNP Q15485
B	247	THR	VAL	conflict	UNP Q15485
C	168	THR	VAL	conflict	UNP Q15485
C	247	THR	VAL	conflict	UNP Q15485
E	168	THR	VAL	conflict	UNP Q15485
E	247	THR	VAL	conflict	UNP Q15485
F	168	THR	VAL	conflict	UNP Q15485
F	247	THR	VAL	conflict	UNP Q15485

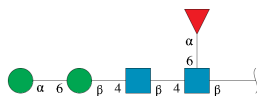
- Molecule 2 is a protein called FICOLIN-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	217	Total 1750	C 1100	N 309	O 332	S 9	0	2	0

There are 3 discrepancies between the modelled and reference sequences:

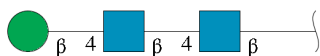
Chain	Residue	Modelled	Actual	Comment	Reference
D	168	THR	VAL	conflict	UNP Q15485
D	229	ASN	THR	conflict	UNP Q15485
D	247	THR	VAL	conflict	UNP Q15485

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-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
			Total	C	N	O			
3	G	5	60	34	2	24	0	0	0

- Molecule 4 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.



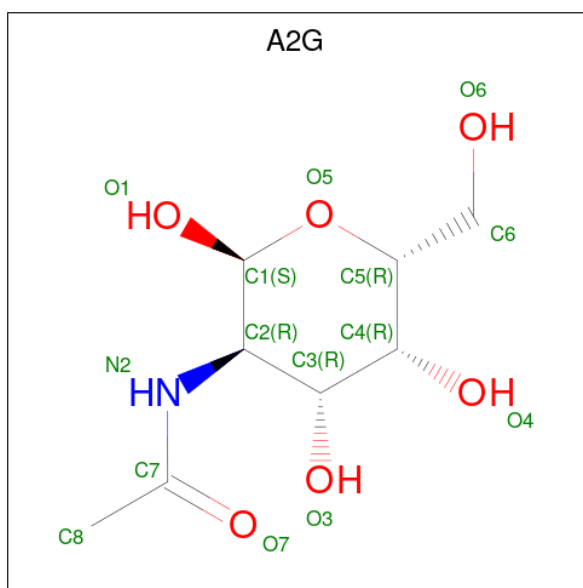
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	H	3	39	22	2	15	0	0	0

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Ca	0	0
			1	1		
5	B	1	Total	Ca	0	0
			1	1		
5	C	1	Total	Ca	0	0
			1	1		
5	E	1	Total	Ca	0	0
			1	1		
5	F	1	Total	Ca	0	0
			1	1		

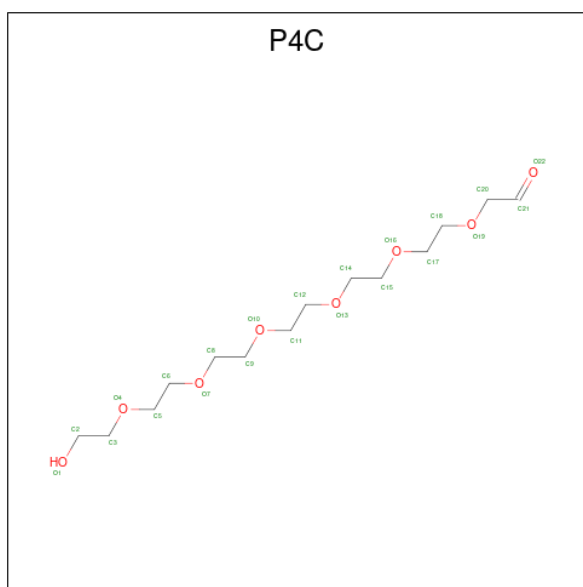
- Molecule 6 is 2-acetamido-2-deoxy-alpha-D-galactopyranose (CCD ID: A2G) (formula:

C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



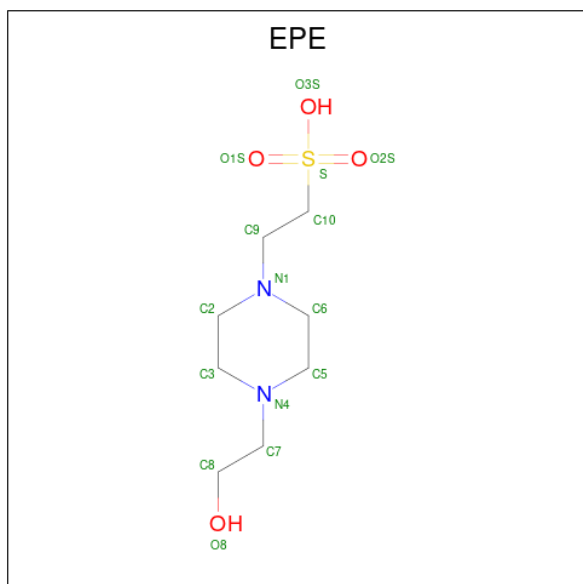
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	B	1	15	8	1	6	11	0
6	C	1	15	8	1	6	0	0
6	E	1	15	8	1	6	11	0
6	F	1	15	8	1	6	0	0

- Molecule 7 is O-ACETALDEHYDYL-HEXAETHYLENE GLYCOL (CCD ID: P4C) (formula: C<sub>14</sub>H<sub>28</sub>O<sub>8</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	4	0
			22	14	8		
7	E	1	Total	C	O	6	0
			22	14	8		

- Molecule 8 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula:  $C_8H_{18}N_2O_4S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	E	1	Total	C	N	O	S	0	0
			12	6	2	3	1		

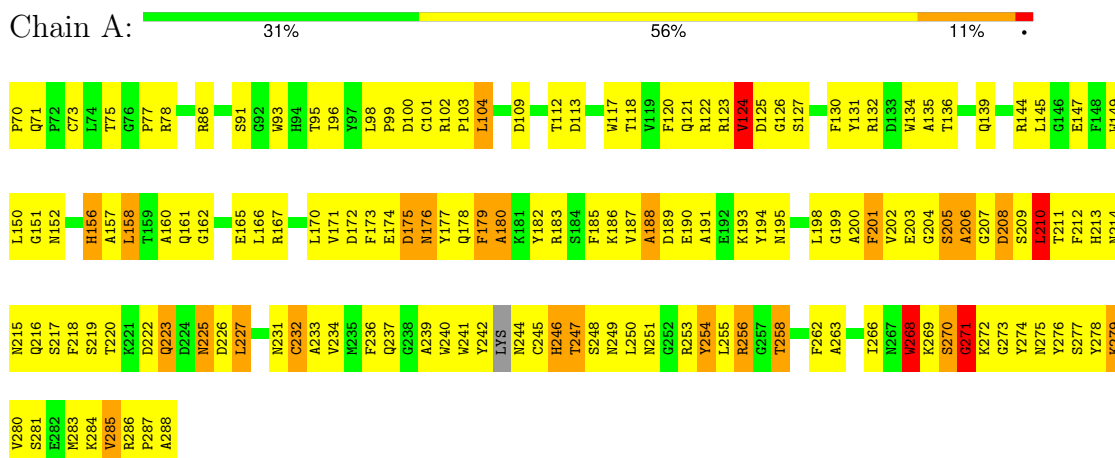
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	6	Total O 6 6	0	0
9	B	13	Total O 13 13	0	0
9	C	12	Total O 12 12	0	0
9	D	5	Total O 5 5	0	0
9	E	10	Total O 10 10	0	0
9	F	7	Total O 7 7	0	0

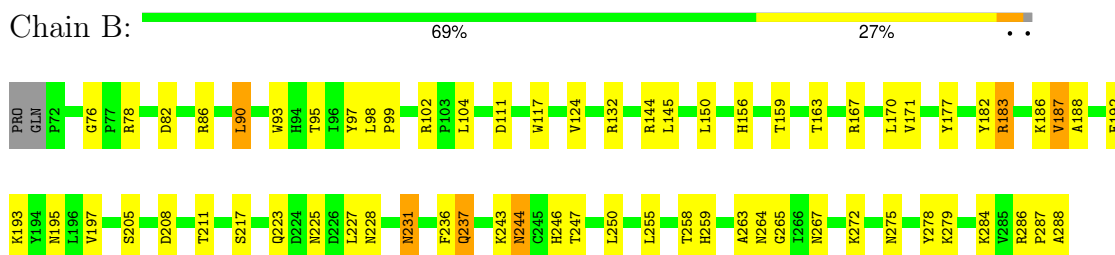
### 3 Residue-property plots [i](#)

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 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.

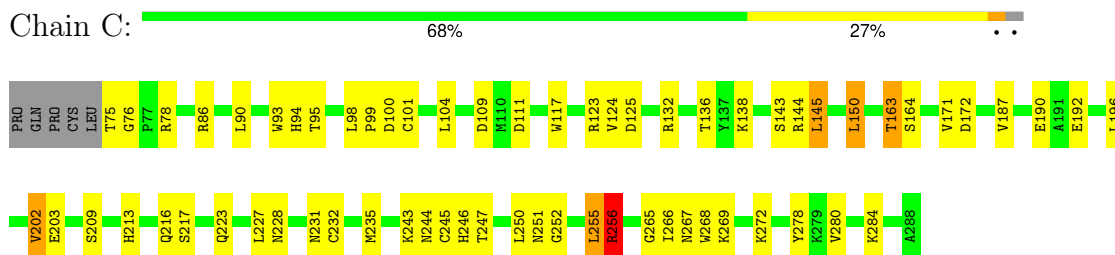
- Molecule 1: FICOLIN-2



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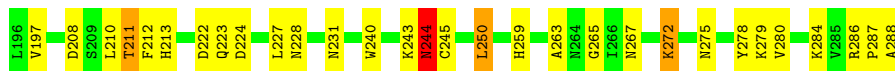


- Molecule 1: FICOLIN-2

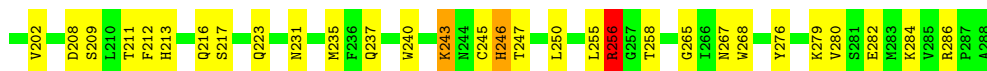
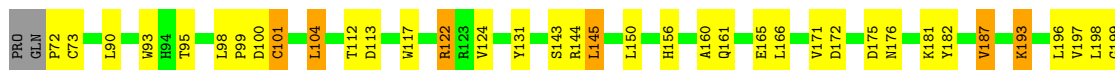


- Molecule 1: FICOLIN-2

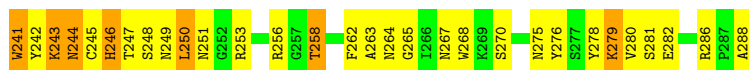




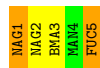
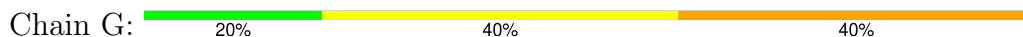
- Molecule 1: FICOLIN-2



- Molecule 2: FICOLIN-2



- Molecule 3: alpha-D-mannopyranose-(1-6)-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



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.83Å 96.83Å 141.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 2.80 15.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (15.00-2.80) 99.2 (15.00-2.80)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.89 (at 2.79Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.222 , 0.277 0.233 , 0.296	Depositor DCC
$R_{free}$ test set	1814 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.7	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 25.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.033 for -h,-k,l 0.460 for h,-h-k,-l 0.034 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	10783	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% 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: NAG, EPE, CA, A2G, FUC, BMA, P4C, MAN

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	0.95	1/1795 (0.1%)	1.06	10/2429 (0.4%)
1	B	0.70	0/1807	0.95	4/2443 (0.2%)
1	C	0.81	1/1789 (0.1%)	0.96	2/2419 (0.1%)
1	E	0.67	0/1821	0.90	1/2463 (0.0%)
1	F	0.78	0/1795	0.96	3/2428 (0.1%)
2	D	0.85	0/1799	0.95	5/2433 (0.2%)
All	All	0.80	2/10806 (0.0%)	0.96	25/14615 (0.2%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	271	GLY	N-CA	10.12	1.60	1.45
1	C	255	LEU	C-O	-5.37	1.15	1.23

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	232	CYS	N-CA-C	-8.05	102.50	111.28
1	A	268	TRP	N-CA-C	-7.67	100.98	110.41
1	B	244	ASN	N-CA-C	7.66	119.45	110.41
2	D	171	VAL	N-CA-C	7.29	118.64	107.78
1	A	179	PHE	N-CA-C	7.08	117.37	108.45

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	270	SER	Peptide

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1744	0	1595	191	0
1	B	1758	0	1626	53	1
1	C	1741	0	1604	59	0
1	E	1771	0	1635	49	1
1	F	1746	0	1613	57	0
2	D	1750	0	1607	186	0
3	G	60	0	52	4	0
4	H	39	0	34	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
6	B	15	0	12	3	0
6	C	15	0	12	0	0
6	E	15	0	12	1	0
6	F	15	0	12	1	0
7	B	22	0	24	6	0
7	E	22	0	27	6	0
8	E	12	0	13	4	0
9	A	6	0	0	3	0
9	B	13	0	0	0	0
9	C	12	0	0	0	0
9	D	5	0	0	3	0
9	E	10	0	0	2	0
9	F	7	0	0	0	0
All	All	10783	0	9878	595	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 29.

The worst 5 of 595 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)
1:A:266:ILE:HG22	1:A:278:TYR:CE1	1.59	1.36
1:A:247:THR:HG23	1:A:269:LYS:CD	1.61	1.30
2:D:236:PHE:CD2	2:D:246:HIS:CE1	2.20	1.30
1:A:266:ILE:HG21	1:A:278:TYR:CZ	1.71	1.26
2:D:236:PHE:CD2	2:D:246:HIS:HE1	1.54	1.25

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:B:193:LYS:NZ	1:E:224:ASP:O[1_554]	2.13	0.07

## 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	216/219 (99%)	170 (79%)	31 (14%)	15 (7%)	1	2
1	B	217/219 (99%)	200 (92%)	17 (8%)	0	100	100
1	C	215/219 (98%)	193 (90%)	18 (8%)	4 (2%)	6	22
1	E	218/219 (100%)	197 (90%)	21 (10%)	0	100	100
1	F	216/219 (99%)	191 (88%)	21 (10%)	4 (2%)	6	22
2	D	217/219 (99%)	175 (81%)	28 (13%)	14 (6%)	1	3
All	All	1299/1314 (99%)	1126 (87%)	136 (10%)	37 (3%)	4	14

5 of 37 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	175	ASP

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Mol	Chain	Res	Type
1	A	254	TYR
1	A	256	ARG
1	A	271	GLY
2	D	206	ALA

### 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	182/184 (99%)	164 (90%)	18 (10%)	7	24
1	B	184/184 (100%)	168 (91%)	16 (9%)	9	30
1	C	181/184 (98%)	163 (90%)	18 (10%)	7	24
1	E	185/184 (100%)	170 (92%)	15 (8%)	11	33
1	F	183/184 (100%)	166 (91%)	17 (9%)	8	27
2	D	182/184 (99%)	160 (88%)	22 (12%)	5	16
All	All	1097/1104 (99%)	991 (90%)	106 (10%)	8	25

5 of 106 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	124	VAL
2	D	258	THR
1	F	193	LYS
2	D	150	LEU
2	D	214	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	231	ASN
1	E	178	GLN
2	D	237	GLN
1	E	139	GLN

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Mol	Chain	Res	Type
1	E	231	ASN

### 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](#)

8 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	G	1	3,1	14,14,15	0.64	0	17,19,21	1.32	3 (17%)
3	NAG	G	2	3	14,14,15	0.50	0	17,19,21	0.86	0
3	BMA	G	3	3	11,11,12	0.56	0	15,15,17	1.72	4 (26%)
3	MAN	G	4	3	11,11,12	0.63	0	15,15,17	0.94	0
3	FUC	G	5	3	10,10,11	0.87	0	14,14,16	1.63	4 (28%)
4	NAG	H	1	4,1	14,14,15	0.55	0	17,19,21	1.65	3 (17%)
4	NAG	H	2	4	14,14,15	0.63	0	17,19,21	1.33	1 (5%)
4	BMA	H	3	4	11,11,12	0.51	0	15,15,17	1.69	5 (33%)

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	G	1	3,1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	G	2	3	-	4/6/23/26	0/1/1/1
3	BMA	G	3	3	-	2/2/19/22	0/1/1/1
3	MAN	G	4	3	-	2/2/19/22	0/1/1/1
3	FUC	G	5	3	-	-	0/1/1/1
4	NAG	H	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	H	2	4	-	2/6/23/26	0/1/1/1
4	BMA	H	3	4	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	3	BMA	O5-C5-C6	3.91	115.28	107.66
4	H	1	NAG	C2-N2-C7	3.57	127.69	122.90
3	G	5	FUC	O2-C2-C3	-3.52	102.86	110.15
4	H	3	BMA	O5-C5-C6	2.84	113.19	107.66
4	H	1	NAG	C3-C4-C5	-2.83	105.10	110.23

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	2	NAG	O5-C5-C6-O6
3	G	4	MAN	O5-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
4	H	2	NAG	C4-C5-C6-O6
4	H	2	NAG	O5-C5-C6-O6

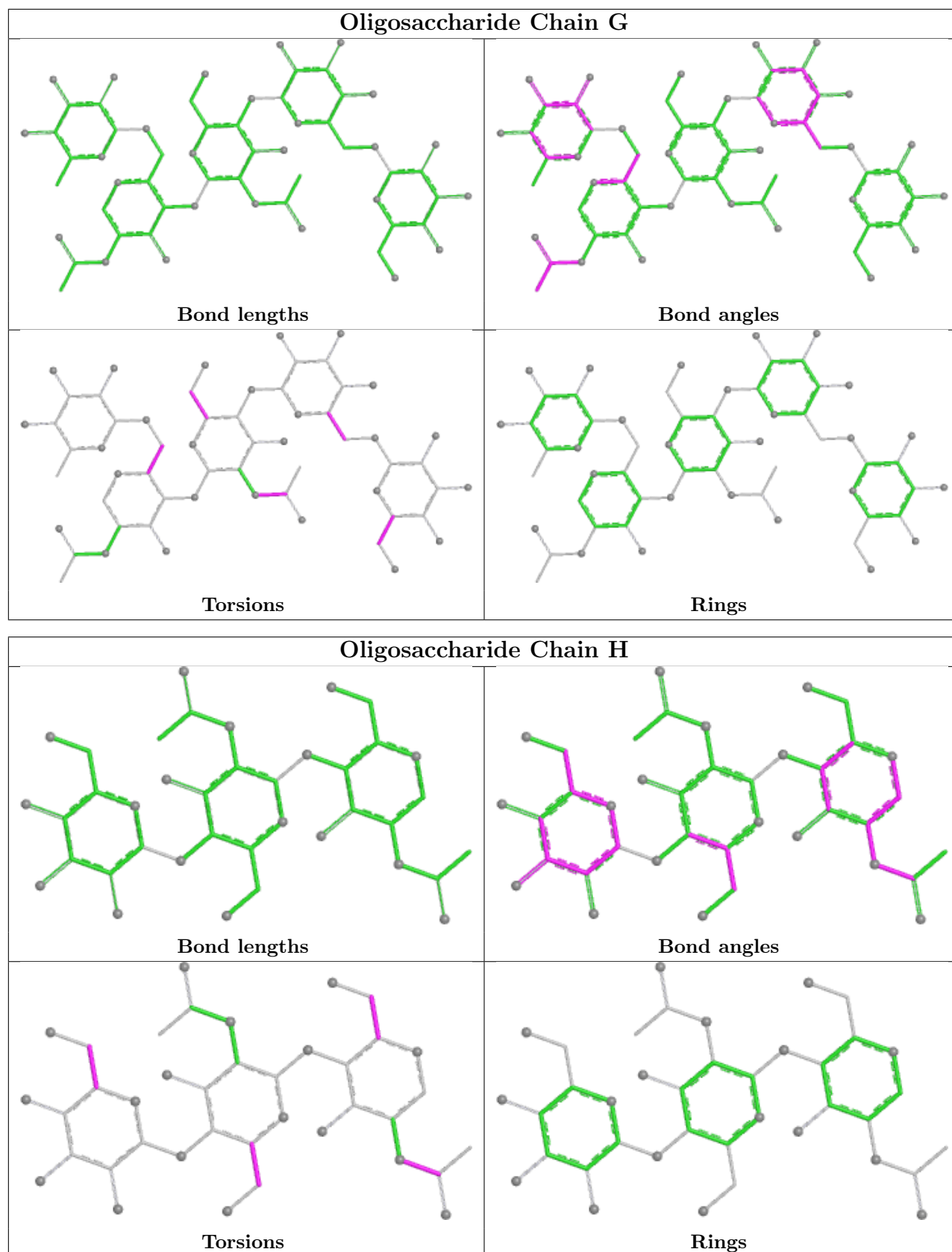
There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	2	NAG	2	0
3	G	5	FUC	2	0
4	H	2	NAG	1	0
4	H	1	NAG	1	0
3	G	1	NAG	2	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)

Of 12 ligands modelled in this entry, 5 are monoatomic - leaving 7 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
8	EPE	E	1295	-	12,12,15	0.99	1 (8%)	15,16,20	1.55	5 (33%)
6	A2G	E	1289	-	15,15,15	2.94	1 (6%)	21,21,21	3.14	5 (23%)
6	A2G	B	1289	-	15,15,15	2.05	2 (13%)	21,21,21	2.86	7 (33%)
7	P4C	E	1294	-	21,21,21	5.30	4 (19%)	20,20,20	2.57	2 (10%)
7	P4C	B	1296	-	21,21,21	3.36	3 (14%)	20,20,20	5.68	4 (20%)
6	A2G	F	1289	-	15,15,15	0.77	0	21,21,21	1.75	6 (28%)
6	A2G	C	1289	-	15,15,15	0.78	0	21,21,21	4.00	5 (23%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	EPE	E	1295	-	-	4/6/14/19	0/1/1/1
6	A2G	E	1289	-	-	1/6/26/26	0/1/1/1
6	A2G	B	1289	-	-	3/6/26/26	0/1/1/1
7	P4C	E	1294	-	-	13/18/19/19	-
7	P4C	B	1296	-	-	12/18/19/19	-
6	A2G	F	1289	-	-	2/6/26/26	0/1/1/1
6	A2G	C	1289	-	-	3/6/26/26	0/1/1/1

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	1294	P4C	O16-C17	23.29	2.42	1.42
7	B	1296	P4C	O4-C5	-13.73	0.82	1.42
6	E	1289	A2G	C2-N2	-11.00	1.28	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1289	A2G	C2-N2	5.64	1.54	1.45
6	B	1289	A2G	O1-C1	-4.95	1.24	1.39

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	1296	P4C	C5-O4-C3	-20.79	22.28	113.26
6	C	1289	A2G	O1-C1-C2	16.23	142.94	109.22
7	B	1296	P4C	O4-C5-C6	13.16	170.33	110.35
6	E	1289	A2G	C1-C2-N2	-9.83	99.34	110.73
7	E	1294	P4C	C17-O16-C15	8.91	152.23	113.26

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	1289	A2G	O7-C7-N2-C2
6	B	1289	A2G	C8-C7-N2-C2
6	C	1289	A2G	O7-C7-N2-C2
6	C	1289	A2G	C8-C7-N2-C2
6	F	1289	A2G	O7-C7-N2-C2

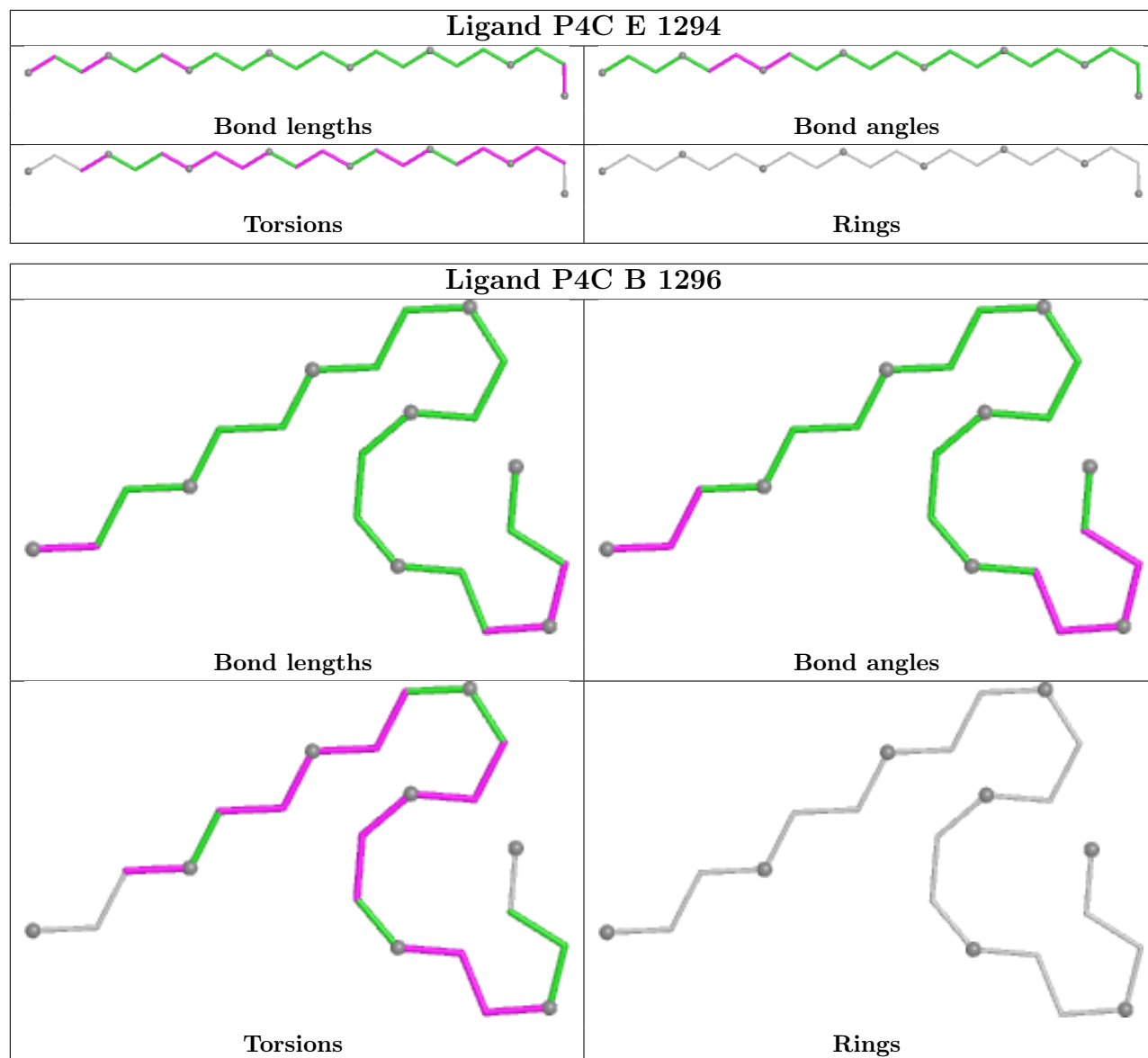
There are no ring outliers.

6 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	E	1295	EPE	4	0
6	E	1289	A2G	1	0
6	B	1289	A2G	3	0
7	E	1294	P4C	6	0
7	B	1296	P4C	6	0
6	F	1289	A2G	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 than 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.



## 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 [i](#)

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

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	A	218/219 (99%)	-1.63	0 100 100	19, 43, 51, 54	4 (1%)
1	B	217/219 (99%)	-1.75	0 100 100	18, 37, 39, 44	2 (0%)
1	C	214/219 (97%)	-1.73	0 100 100	18, 36, 43, 49	3 (1%)
1	E	217/219 (99%)	-1.75	0 100 100	12, 37, 40, 42	2 (0%)
1	F	217/219 (99%)	-1.73	0 100 100	18, 37, 43, 47	1 (0%)
2	D	217/219 (99%)	-1.62	0 100 100	19, 39, 49, 52	2 (0%)
All	All	1300/1314 (98%)	-1.70	0 100 100	12, 37, 48, 54	14 (1%)

There are no RSRZ outliers to report.

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

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

### 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.

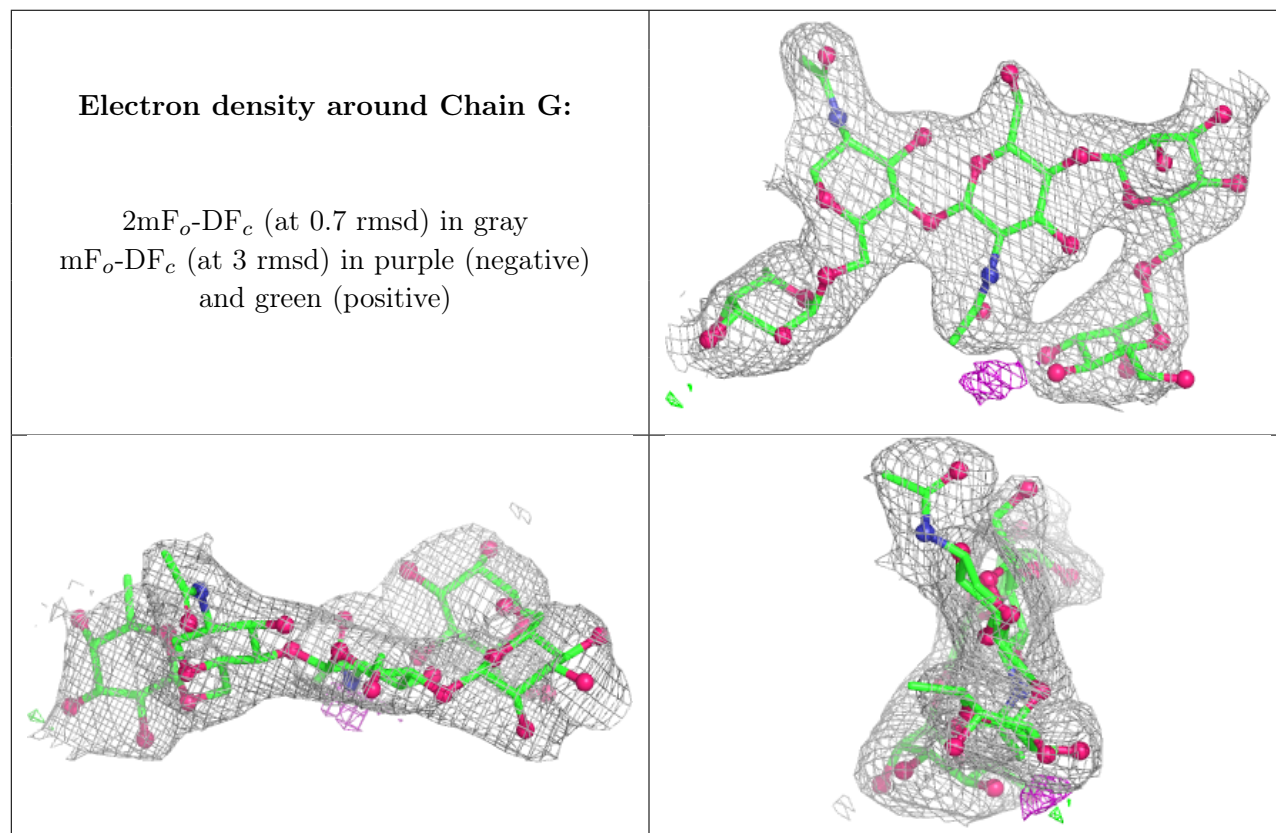
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	BMA	H	3	11/12	0.98	0.04	42,44,45,45	0
3	NAG	G	2	14/15	0.99	0.03	37,39,40,41	0
3	BMA	G	3	11/12	0.99	0.03	43,44,45,46	0
3	MAN	G	4	11/12	0.99	0.04	45,46,46,47	0
3	FUC	G	5	10/11	0.99	0.03	39,41,41,43	0
4	NAG	H	1	14/15	0.99	0.03	36,39,40,42	0

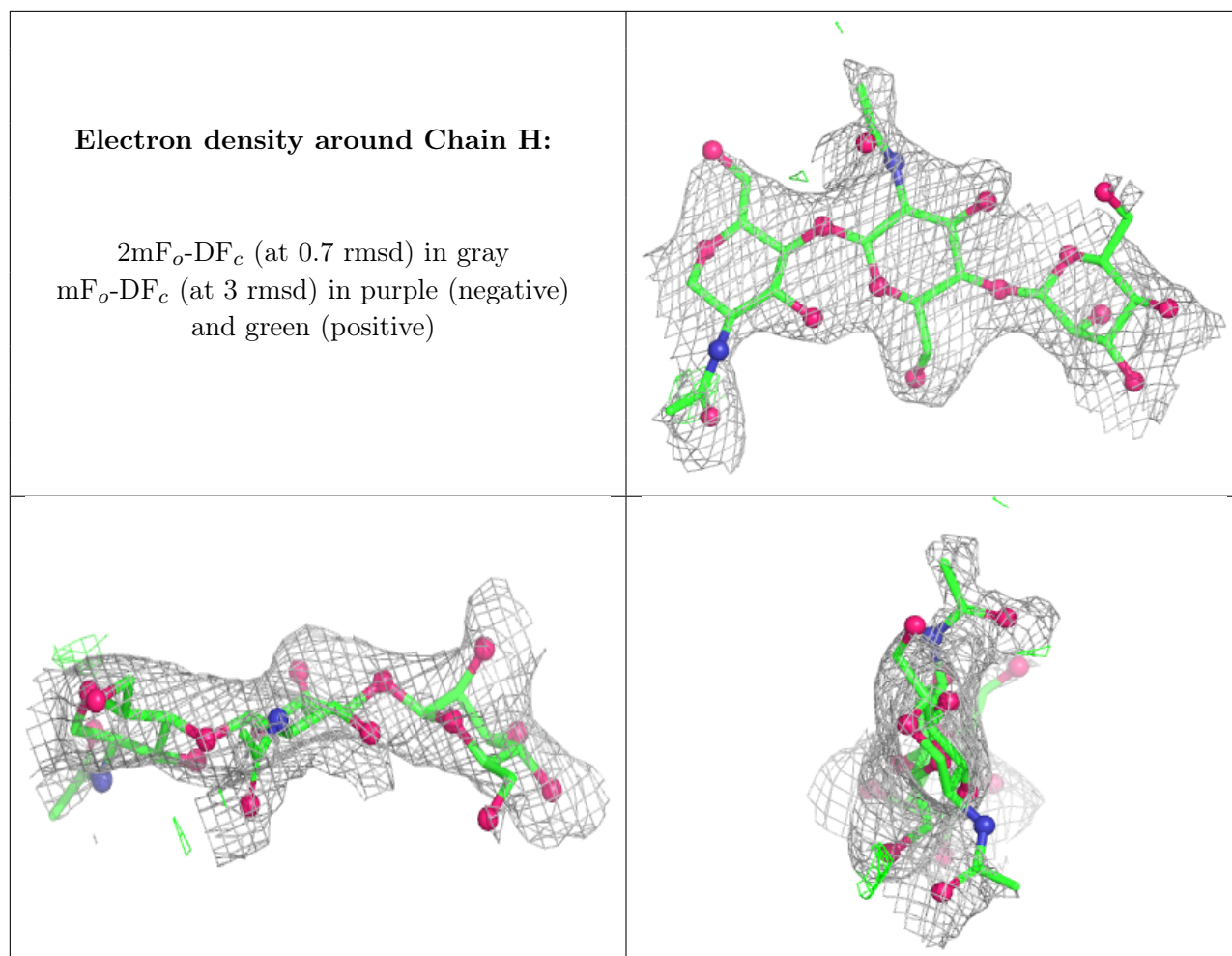
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	H	2	14/15	0.99	0.04	38,39,42,42	0
3	NAG	G	1	14/15	0.99	0.02	36,37,41,43	0

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.

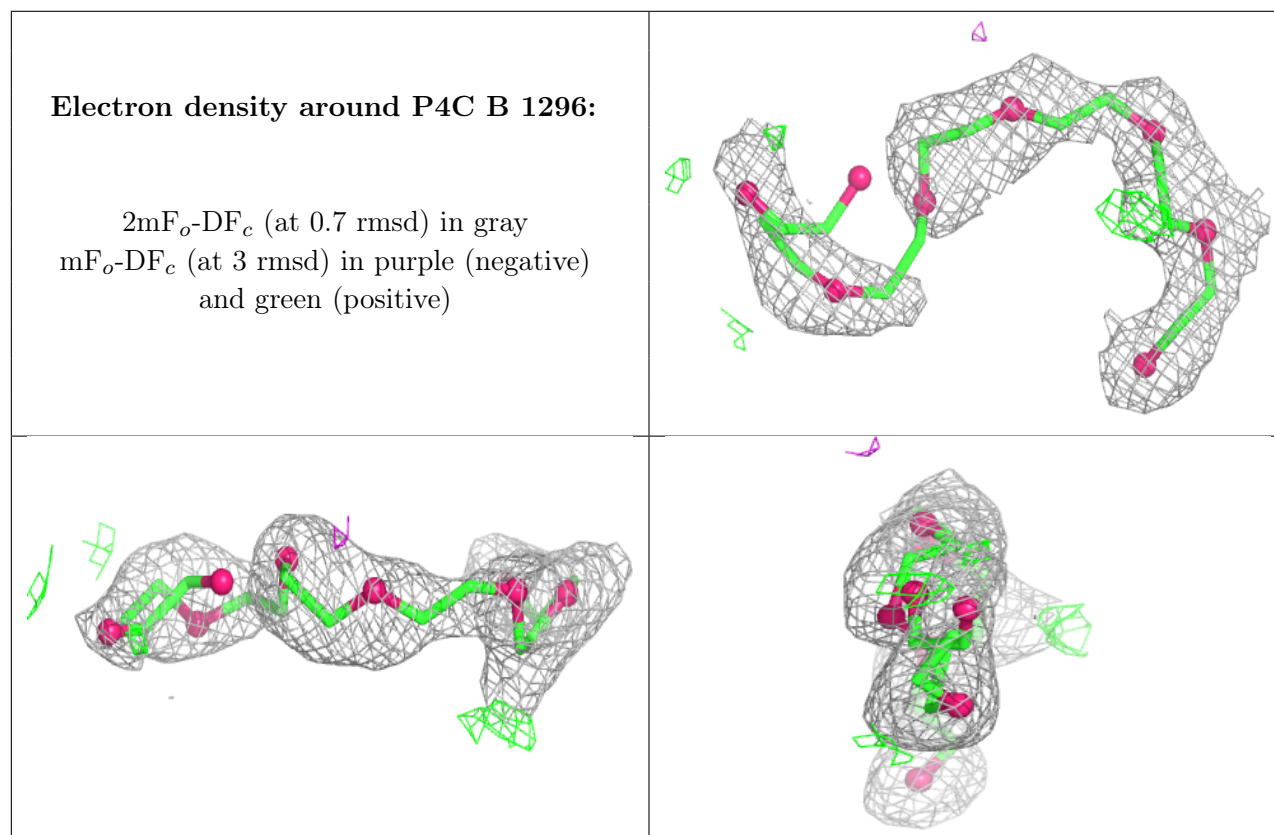
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	A2G	E	1289	15/15	0.98	0.03	20,20,32,33	11
7	P4C	B	1296	22/22	0.98	0.04	39,41,74,74	4
6	A2G	B	1289	15/15	0.99	0.03	20,20,25,27	11
6	A2G	C	1289	15/15	0.99	0.04	20,26,27,28	11
5	CA	A	1289	1/1	0.99	0.01	58,58,58,58	0
6	A2G	F	1289	15/15	0.99	0.04	20,26,30,31	11
5	CA	B	1290	1/1	0.99	0.03	30,30,30,30	0
7	P4C	E	1294	22/22	0.99	0.03	20,42,45,45	6
8	EPE	E	1295	12/15	0.99	0.06	39,40,42,43	12
5	CA	E	1290	1/1	1.00	0.03	33,33,33,33	0

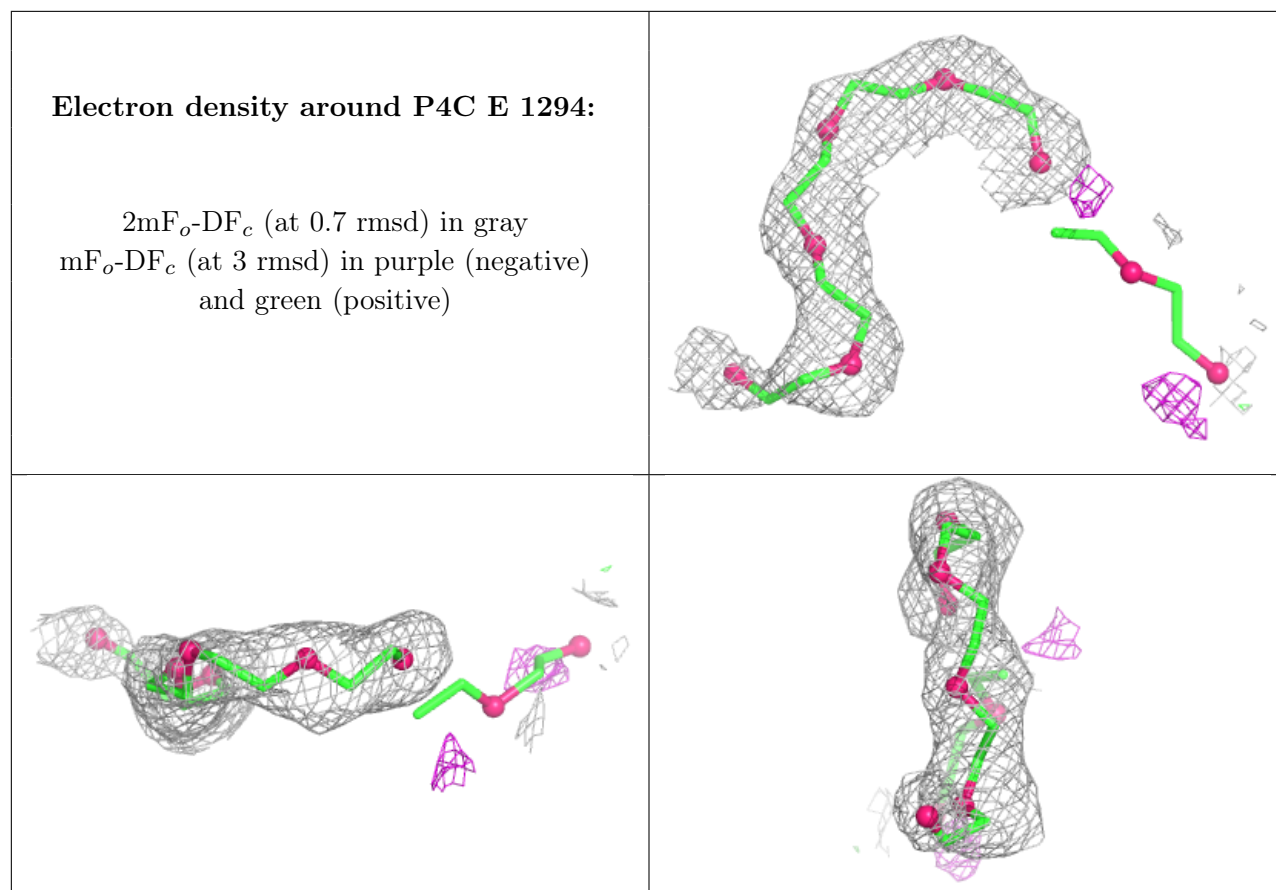
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	CA	F	1290	1/1	1.00	0.01	37,37,37,37	0
5	CA	C	1290	1/1	1.00	0.01	37,37,37,37	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.