



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 10, 2020 – 05:29 AM BST

PDB ID : 2J3F
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

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 : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

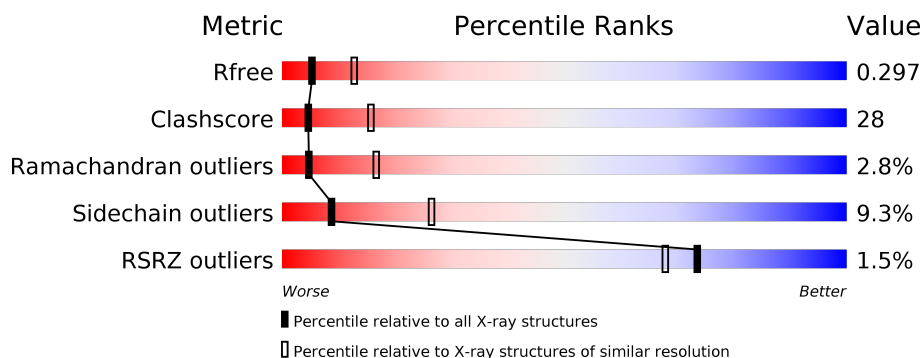
1 Overall quality at a glance

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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 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 $\leq 5\%$. 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	<div> <div>4%</div> <div> <div>32%</div> <div>58%</div> <div>8%</div> </div> </div>
1	B	219	<div> <div>70%</div> <div>26%</div> </div>
1	C	219	<div> <div>%</div> <div> <div>68%</div> <div>27%</div> </div> </div>
1	E	219	<div> <div>72%</div> <div>24%</div> </div>
1	F	219	<div> <div>70%</div> <div>24%</div> </div>
2	D	219	<div> <div>4%</div> <div> <div>44%</div> <div>44%</div> <div>10%</div> </div> </div>

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

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

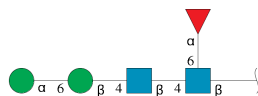
- Molecule 2 is a protein called FICOLIN-2.

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

There are 3 discrepancies between the modelled and reference sequences:

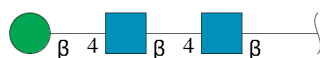
Chain	Residue	Modelled	Actual	Comment	Reference
D	168	THR	VAL	conflict	UNP Q15485
D	229	ASN	THR	conflict	UNP Q15485
D	247	THR	VAL	conflict	UNP Q15485

- 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
3	G	5	Total	C	N	O	0	0	0
			60	34	2	24			

- 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.



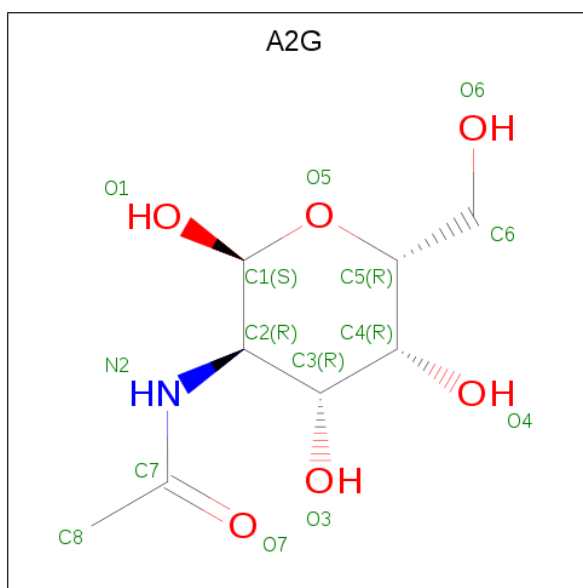
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

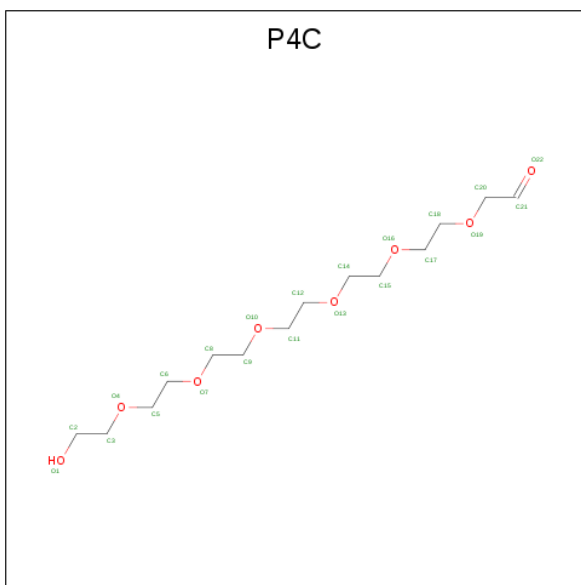
- Molecule 6 is 2-acetamido-2-deoxy-alpha-D-galactopyranose (three-letter code: A2G)

(formula: $C_8H_{15}NO_6$).



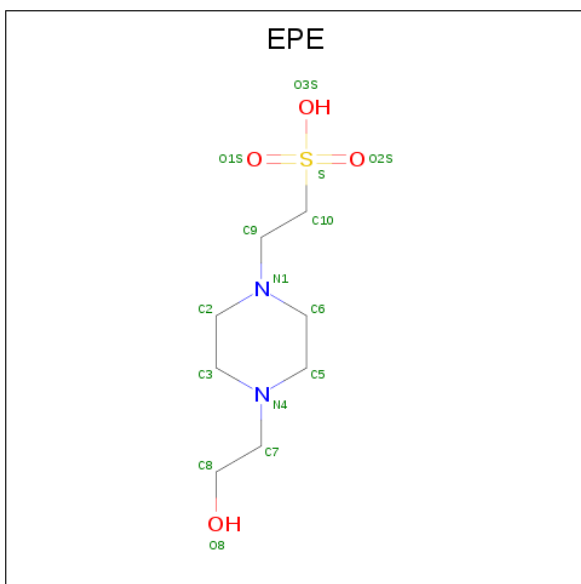
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	11	0
			15	8	1	6		
6	C	1	Total	C	N	O	0	0
			15	8	1	6		
6	E	1	Total	C	N	O	11	0
			15	8	1	6		
6	F	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 7 is O-ACETALDEHYDYL-HEXAETHYLENE GLYCOL (three-letter code: P4C) (formula: $C_{14}H_{28}O_8$).



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

- Molecule 8 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: 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		

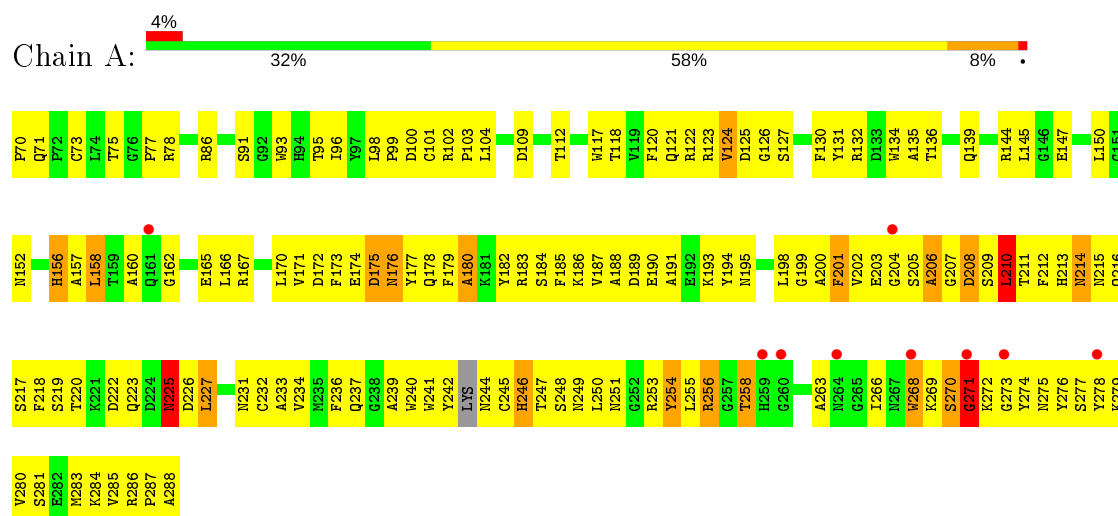
- Molecule 9 is water.

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

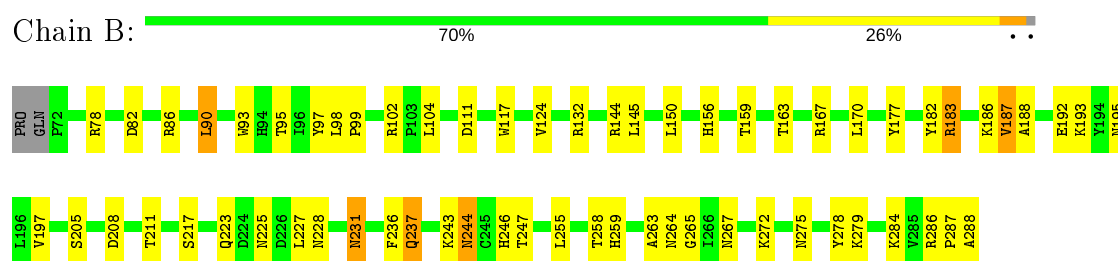
3 Residue-property plots

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 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.

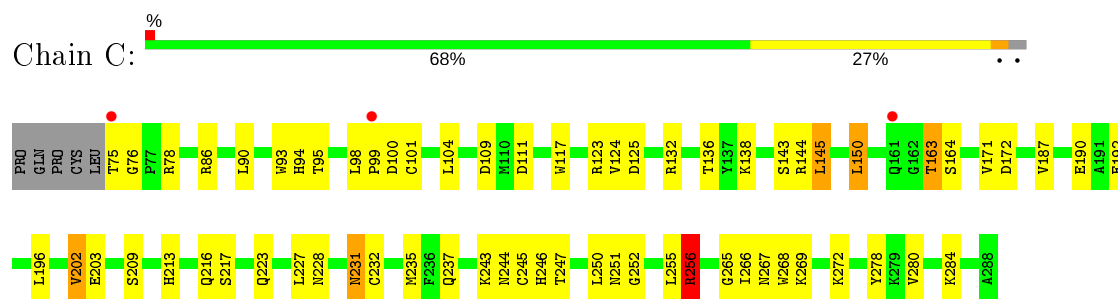
• Molecule 1: FICOLIN-2



• Molecule 1: FICOLIN-2

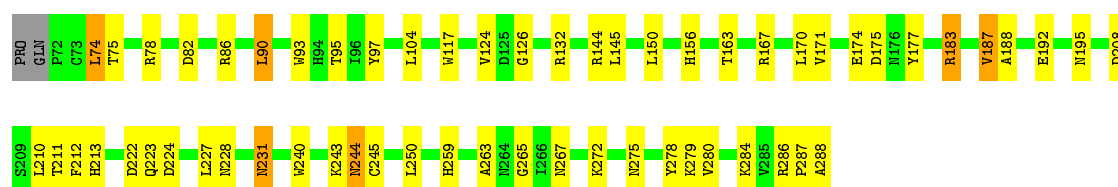


• Molecule 1: FICOLIN-2



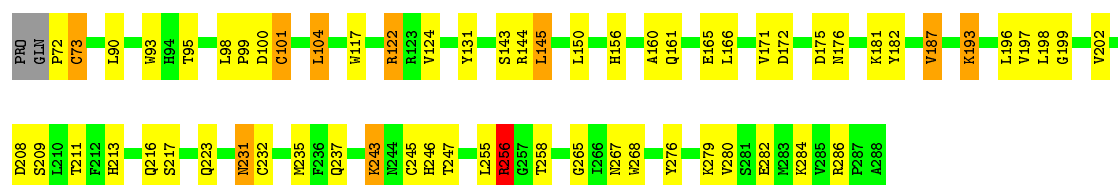
• Molecule 1: FICOLIN-2

Chain E:  72% 24% ..




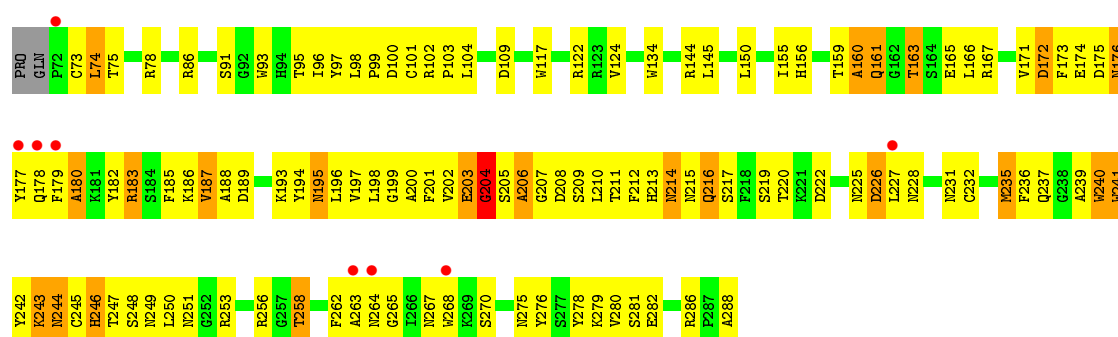
• Molecule 1: FICOLIN-2

Chain F:  70% 24% ..




• Molecule 2: FICOLIN-2

Chain D:  4% 44% 44% 10% .



• 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

Chain G:  20% 40% 40%



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

Chain H:  33% 67%



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	96.83Å 96.83Å 141.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 2.80 19.91 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (15.00-2.80) 99.1 (19.91-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.89 (at 2.79Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.222 , 0.277 0.233 , 0.297	Depositor DCC
R_{free} test set	1814 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	46.7	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 22.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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	0.91	EDS
Total number of atoms	10783	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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, CA, P4C, FUC, A2G, EPE, 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	0.85	1/1795 (0.1%)	0.77	0/2429
1	B	0.60	0/1807	0.68	0/2443
1	C	0.65	0/1789	0.69	0/2419
1	E	0.58	0/1821	0.67	0/2463
1	F	0.66	1/1795 (0.1%)	0.71	1/2428 (0.0%)
2	D	0.73	0/1799	0.72	2/2433 (0.1%)
All	All	0.68	2/10806 (0.0%)	0.71	3/14615 (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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	271	GLY	N-CA	9.33	1.60	1.46
1	F	232	CYS	CB-SG	-5.05	1.73	1.81

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	204	GLY	N-CA-C	5.97	128.03	113.10
2	D	161	GLN	N-CA-C	5.34	125.43	111.00
1	F	256	ARG	N-CA-C	5.14	124.88	111.00

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 ⓘ

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	187	0
1	B	1758	0	1626	52	1
1	C	1741	0	1604	58	0
1	E	1771	0	1635	47	1
1	F	1746	0	1613	53	0
2	D	1750	0	1607	183	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	5	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	580	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 28.

The worst 5 of 580 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	3
1	B	217/219 (99%)	200 (92%)	17 (8%)	0	100	100
1	C	215/219 (98%)	193 (90%)	18 (8%)	4 (2%)	8	26
1	E	218/219 (100%)	197 (90%)	21 (10%)	0	100	100
1	F	216/219 (99%)	191 (88%)	21 (10%)	4 (2%)	8	26
2	D	217/219 (99%)	175 (81%)	28 (13%)	14 (6%)	1	3
All	All	1299/1314 (99%)	1126 (87%)	136 (10%)	37 (3%)	5	17

5 of 37 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	175	ASP
1	A	254	TYR

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

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	A	182/184 (99%)	166 (91%)	16 (9%)	10	29
1	B	184/184 (100%)	168 (91%)	16 (9%)	10	30
1	C	181/184 (98%)	161 (89%)	20 (11%)	6	19
1	E	185/184 (100%)	172 (93%)	13 (7%)	15	40
1	F	183/184 (100%)	165 (90%)	18 (10%)	8	24
2	D	182/184 (99%)	163 (90%)	19 (10%)	7	21
All	All	1097/1104 (99%)	995 (91%)	102 (9%)	9	26

5 of 102 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	223	GLN
2	D	145	LEU
1	F	187	VAL
1	C	231	ASN
1	C	256[B]	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	244	ASN
2	D	195	ASN
1	F	156	HIS
1	C	267	ASN
2	D	139	GLN

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 ⓘ

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	1,3	14,14,15	0.64	0	17,19,21	1.42	3 (17%)
3	NAG	G	2	3	14,14,15	0.51	0	17,19,21	0.92	0
3	BMA	G	3	3	11,11,12	0.57	0	15,15,17	1.98	5 (33%)
3	MAN	G	4	3	11,11,12	0.64	0	15,15,17	1.04	0
3	FUC	G	5	3	10,10,11	0.87	0	14,14,16	1.73	4 (28%)
4	NAG	H	1	1,4	14,14,15	0.54	0	17,19,21	1.63	3 (17%)
4	NAG	H	2	4	14,14,15	0.63	0	17,19,21	1.36	1 (5%)
4	BMA	H	3	4	11,11,12	0.52	0	15,15,17	2.03	6 (40%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	H	1	1,4	-	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 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	3	BMA	O5-C5-C6	5.15	115.28	107.20
4	H	3	BMA	O5-C1-C2	-3.85	104.83	110.77
4	H	3	BMA	O5-C5-C6	3.82	113.19	107.20
3	G	5	FUC	O2-C2-C3	-3.63	102.86	110.14
4	H	1	NAG	C2-N2-C7	3.36	127.69	122.90

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

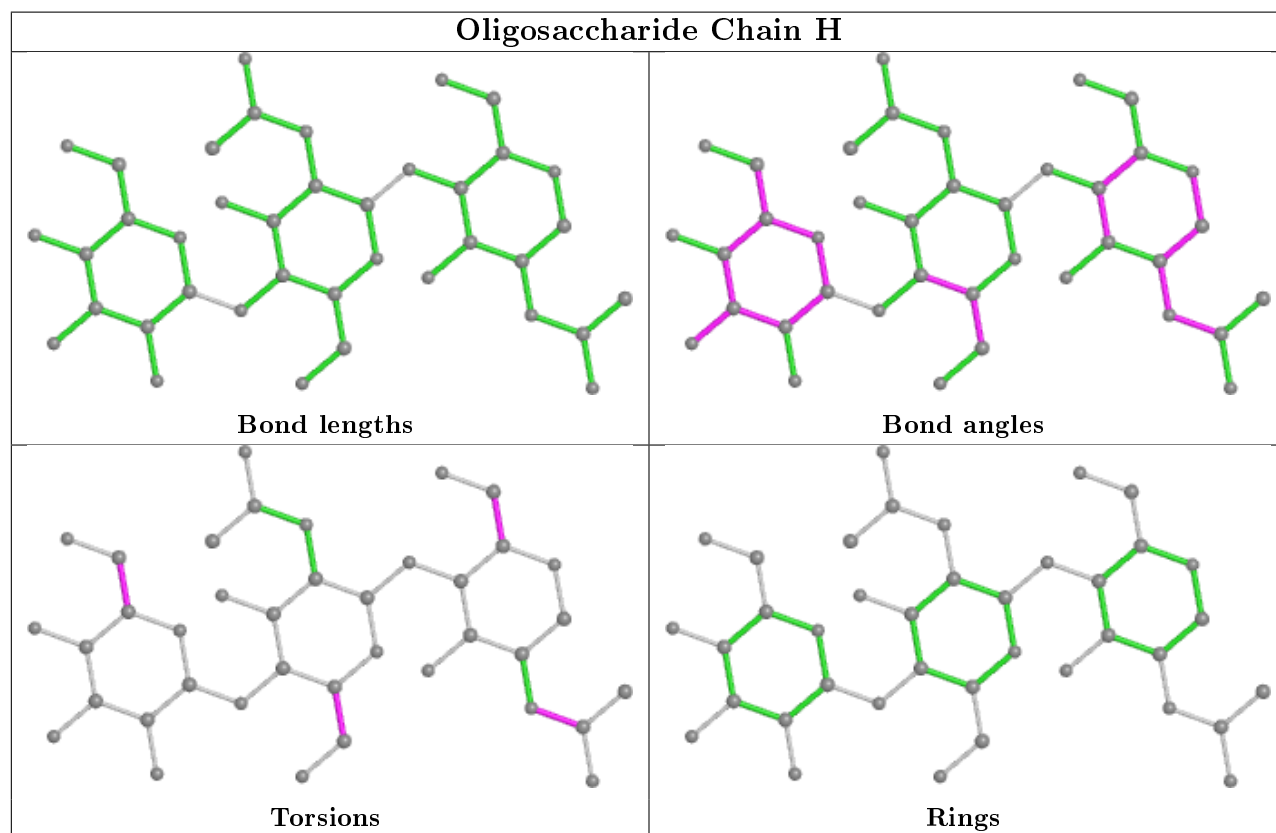
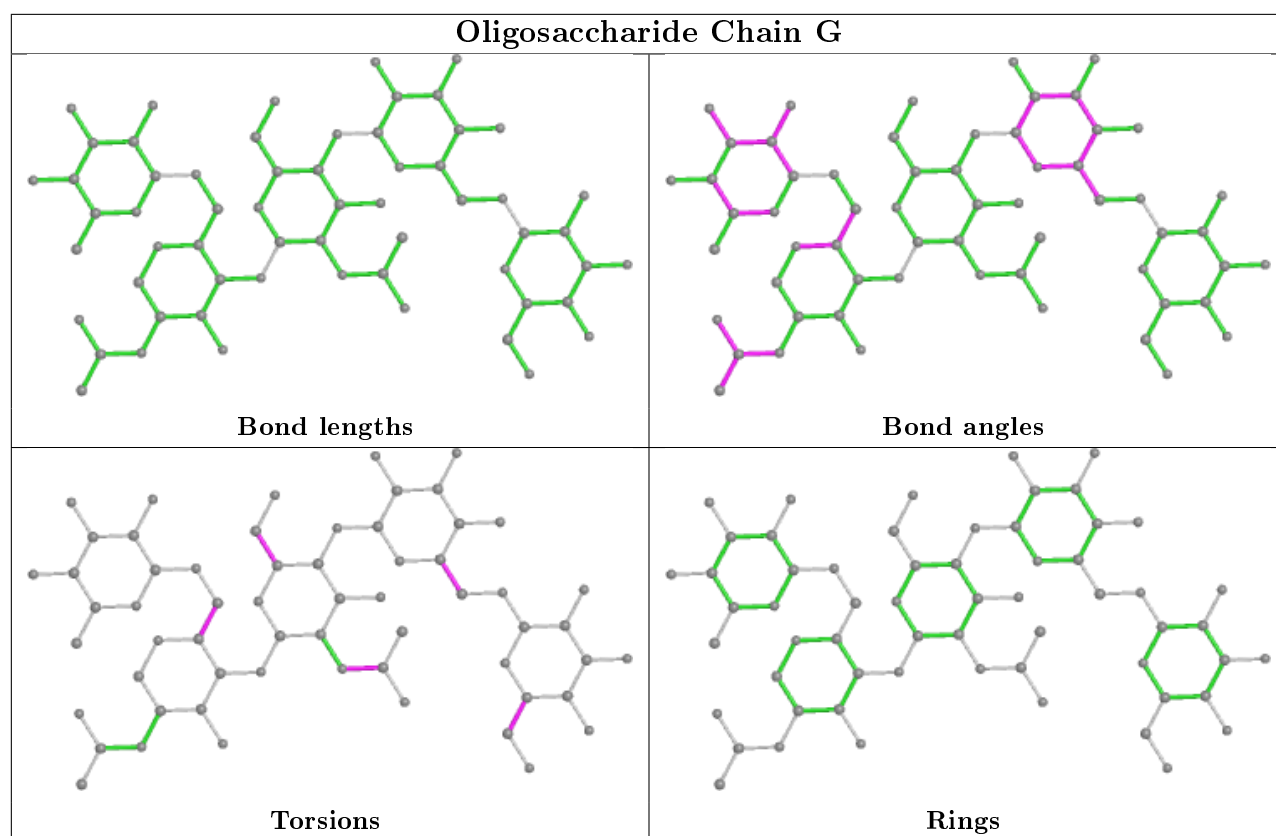
Mol	Chain	Res	Type	Atoms
3	G	2	NAG	O5-C5-C6-O6
3	G	4	MAN	O5-C5-C6-O6
4	H	2	NAG	C4-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
4	H	2	NAG	O5-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 5 short contacts:

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

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	1.00	1 (8%)	14,16,20	1.86	5 (35%)
6	A2G	C	1289	-	15,15,15	0.78	0	21,21,21	3.99	5 (23%)
6	A2G	E	1289	-	15,15,15	2.88	1 (6%)	21,21,21	3.13	5 (23%)
7	P4C	E	1294	-	21,21,21	5.30	4 (19%)	20,20,20	2.60	2 (10%)
7	P4C	B	1296	-	21,21,21	3.35	3 (14%)	20,20,20	5.73	4 (20%)
6	A2G	B	1289	-	15,15,15	2.01	2 (13%)	21,21,21	2.85	7 (33%)
6	A2G	F	1289	-	15,15,15	0.76	0	21,21,21	1.74	6 (28%)

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	EPE	E	1295	-	-	4/6/14/19	0/1/1/1
6	A2G	C	1289	-	-	3/6/26/26	0/1/1/1
6	A2G	E	1289	-	-	1/6/26/26	0/1/1/1
7	P4C	E	1294	-	-	14/18/19/19	-
7	P4C	B	1296	-	-	12/18/19/19	-
6	A2G	B	1289	-	-	3/6/26/26	0/1/1/1
6	A2G	F	1289	-	-	2/6/26/26	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	23.23	2.42	1.42
7	B	1296	P4C	O4-C5	-13.67	0.82	1.42
6	E	1289	A2G	C2-N2	-10.75	1.28	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1289	A2G	C2-N2	5.51	1.54	1.45
6	B	1289	A2G	O1-C1	-4.87	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	-21.00	22.28	113.29
6	C	1289	A2G	O1-C1-C2	16.23	142.94	109.22
7	B	1296	P4C	O4-C5-C6	13.29	170.33	110.39
6	E	1289	A2G	C1-C2-N2	-9.83	99.34	110.73
7	E	1294	P4C	C17-O16-C15	8.99	152.23	113.29

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	F	1289	A2G	O7-C7-N2-C2
6	F	1289	A2G	C8-C7-N2-C2
8	E	1295	EPE	S-C10-C9-N1
8	E	1295	EPE	C9-C10-S-O2S
8	E	1295	EPE	C9-C10-S-O3S

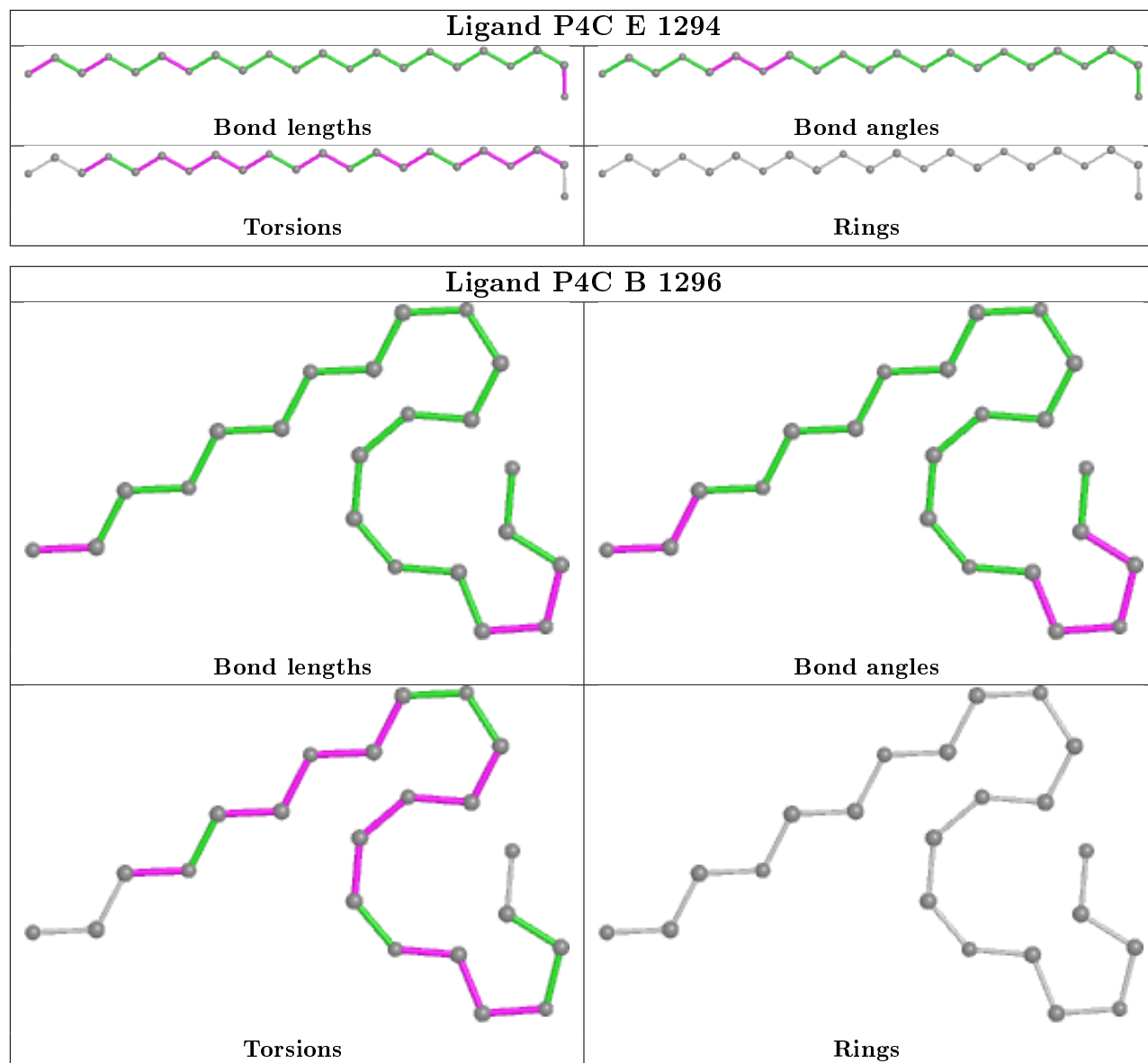
There are no ring outliers.

6 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	E	1295	EPE	4	0
6	E	1289	A2G	1	0
7	E	1294	P4C	6	0
7	B	1296	P4C	5	0
6	B	1289	A2G	3	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, 95th 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 ²)	Q<0.9
1	A	218/219 (99%)	0.24	9 (4%) 37 27	31, 43, 51, 54	2 (0%)
1	B	217/219 (99%)	-0.29	0 100 100	26, 37, 39, 44	0
1	C	214/219 (97%)	-0.25	3 (1%) 75 70	28, 36, 43, 49	0
1	E	217/219 (99%)	-0.30	0 100 100	27, 37, 40, 42	0
1	F	217/219 (99%)	-0.29	0 100 100	30, 37, 43, 47	0
2	D	217/219 (99%)	0.17	8 (3%) 41 31	33, 39, 49, 52	0
All	All	1300/1314 (98%)	-0.12	20 (1%) 73 68	26, 37, 48, 54	2 (0%)

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	204	GLY	6.0
1	A	278	TYR	4.5
1	A	271	GLY	4.3
1	A	268	TRP	3.8
2	D	263	ALA	3.7

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

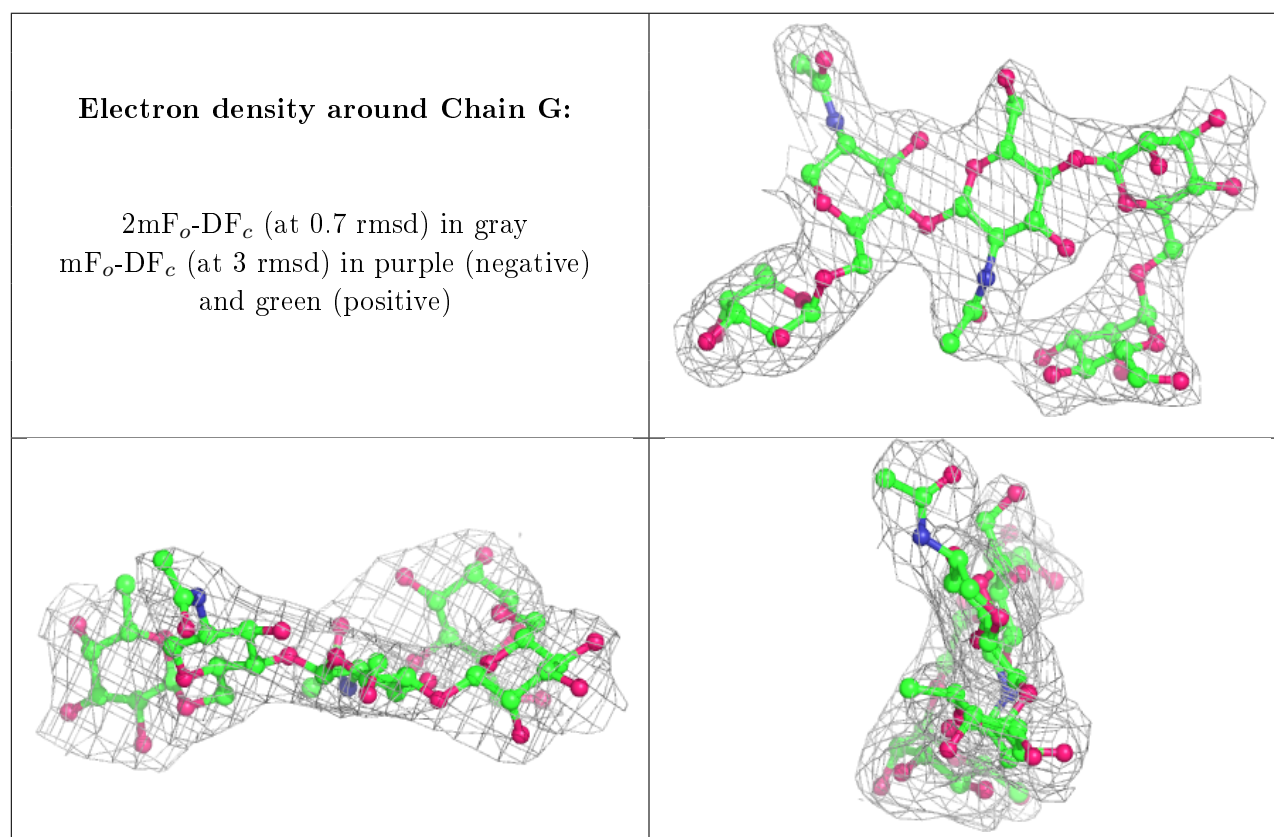
There are no non-standard protein/DNA/RNA residues in this entry.

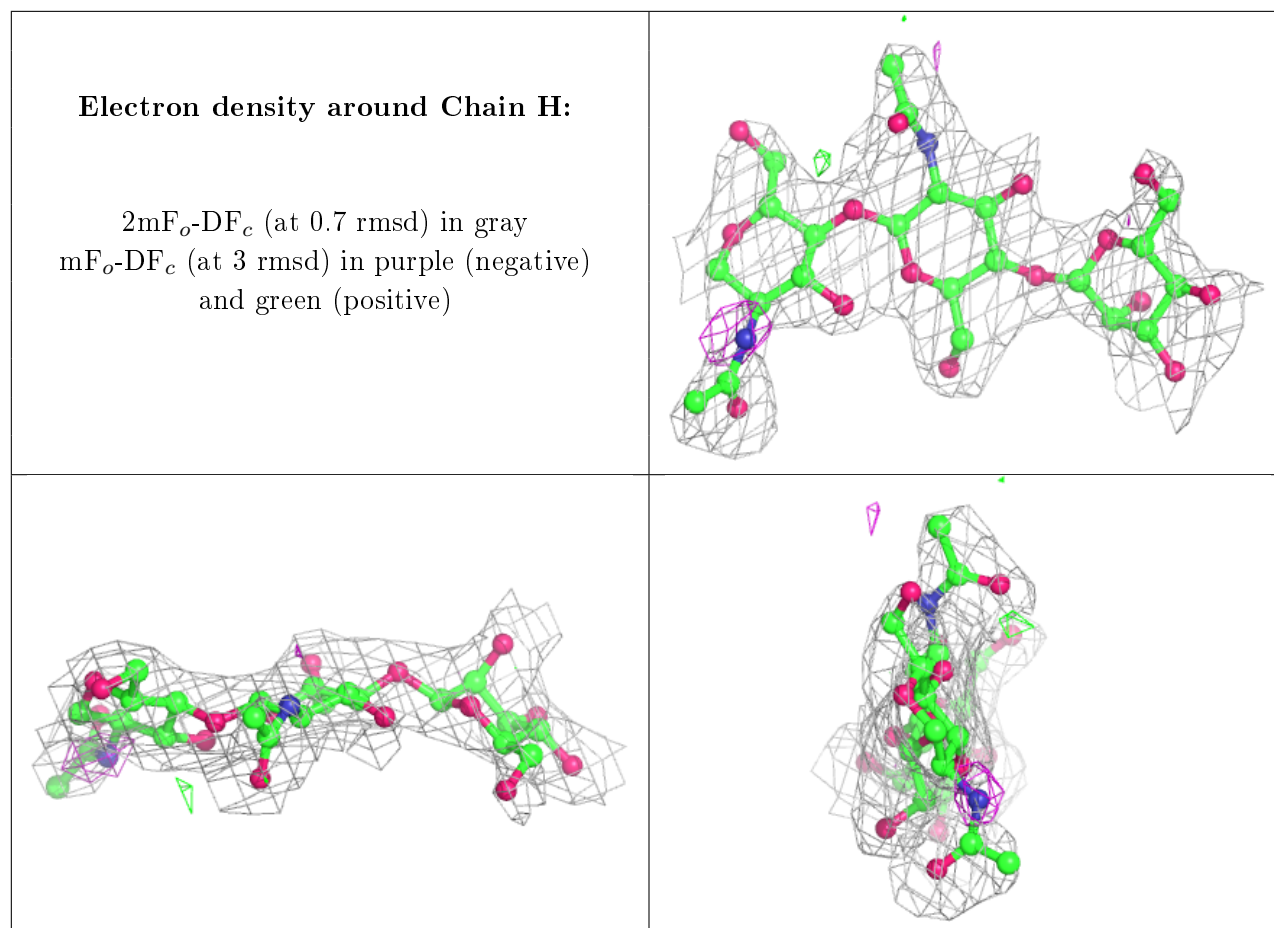
6.3 Carbohydrates [i](#)

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, 95th 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(\AA^2)	Q<0.9
4	BMA	H	3	11/12	0.78	0.26	42,44,45,45	0
4	NAG	H	2	14/15	0.90	0.24	38,39,42,42	0
4	NAG	H	1	14/15	0.91	0.24	36,39,40,42	0
3	MAN	G	4	11/12	0.94	0.17	45,46,46,47	0
3	FUC	G	5	10/11	0.95	0.22	39,41,41,43	0
3	BMA	G	3	11/12	0.95	0.13	43,44,45,46	0
3	NAG	G	1	14/15	0.97	0.11	36,37,41,43	0
3	NAG	G	2	14/15	0.97	0.17	37,39,40,41	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.



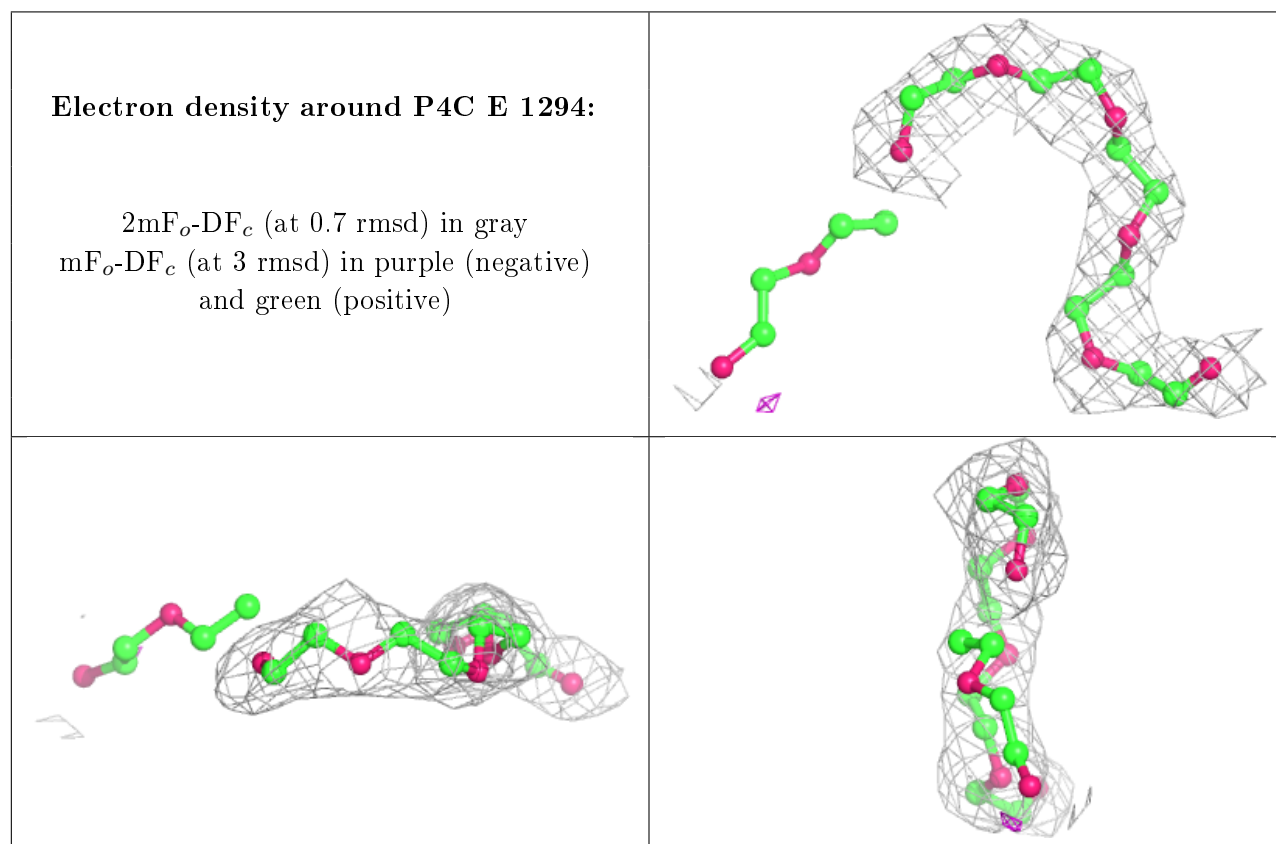


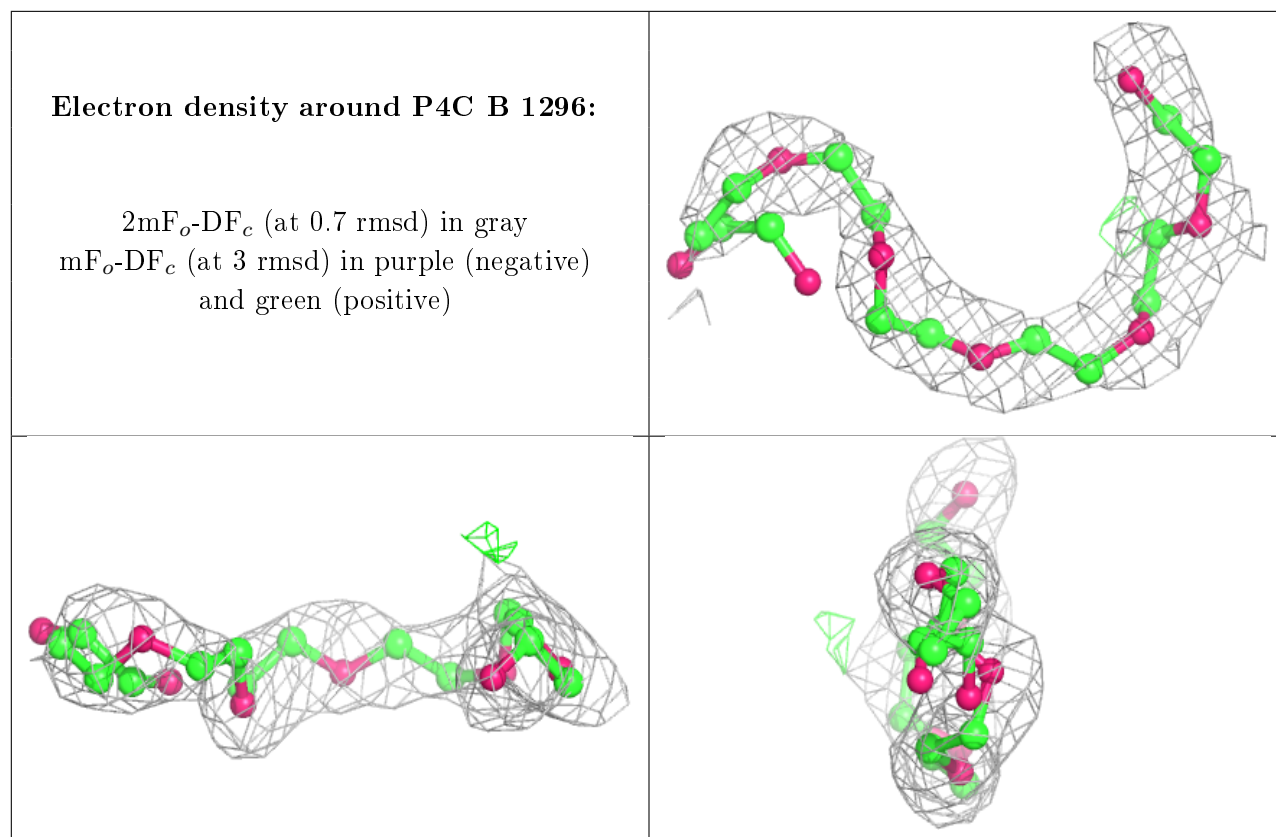
6.4 Ligands ⓘ

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, 95th 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(\AA^2)	Q<0.9
5	CA	A	1289	1/1	0.59	0.12	58,58,58,58	0
6	A2G	F	1289	15/15	0.80	0.26	20,26,30,31	11
6	A2G	C	1289	15/15	0.86	0.24	20,26,27,28	11
8	EPE	E	1295	12/15	0.88	0.33	39,40,42,43	12
6	A2G	E	1289	15/15	0.91	0.21	20,20,32,33	11
7	P4C	E	1294	22/22	0.92	0.22	20,42,45,45	6
7	P4C	B	1296	22/22	0.92	0.23	39,41,74,74	4
5	CA	E	1290	1/1	0.92	0.26	33,33,33,33	0
5	CA	F	1290	1/1	0.94	0.11	37,37,37,37	0
6	A2G	B	1289	15/15	0.94	0.17	20,20,25,27	11
5	CA	B	1290	1/1	0.95	0.19	30,30,30,30	0
5	CA	C	1290	1/1	0.95	0.12	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.