



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 4, 2026 – 11:36 PM UTC

PDB ID : 9TJX / pdb\_00009tjx  
Title : Structure of factor VII Gla domain bound to EPCR  
Authors : Lopez-Sagasetta, J.  
Deposited on : 2025-12-08  
Resolution : 3.00 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  
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

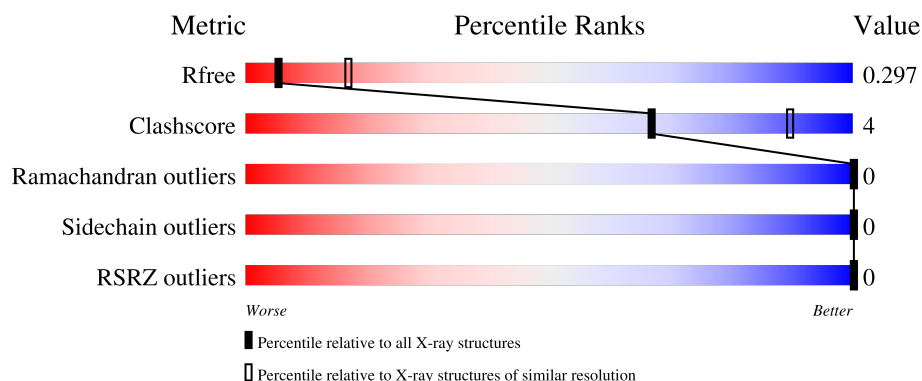
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	195	 78% 8% 13%
1	B	195	 79% 7% 13%
1	C	195	 69% 14% 16%
1	D	195	 76% 7% 17%
2	E	32	 66% 34%

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Mol	Chain	Length	Quality of chain
2	F	32	 72% 28%
2	L	32	 72% 25% .
2	R	32	 72% 28%
3	G	4	 25% 75%
4	H	2	 50% 50%
5	I	3	 33% 67%

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 6759 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 Endothelial protein C receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	169	Total	C	N	O	S	0	0	0
			1347	865	237	241	4			
1	B	169	Total	C	N	O	S	0	0	0
			1341	862	236	239	4			
1	C	163	Total	C	N	O	S	0	0	0
			1313	843	229	237	4			
1	D	162	Total	C	N	O	S	0	0	0
			1277	825	219	229	4			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q9UNN8
A	0	PRO	-	expression tag	UNP Q9UNN8
A	30	GLN	ASN	engineered mutation	UNP Q9UNN8
B	-1	GLY	-	expression tag	UNP Q9UNN8
B	0	PRO	-	expression tag	UNP Q9UNN8
B	30	GLN	ASN	engineered mutation	UNP Q9UNN8
C	-1	GLY	-	expression tag	UNP Q9UNN8
C	0	PRO	-	expression tag	UNP Q9UNN8
C	30	GLN	ASN	engineered mutation	UNP Q9UNN8
D	-1	GLY	-	expression tag	UNP Q9UNN8
D	0	PRO	-	expression tag	UNP Q9UNN8
D	30	GLN	ASN	engineered mutation	UNP Q9UNN8

- Molecule 2 is a protein called Factor VII light chain.

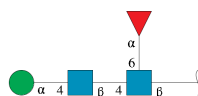
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	32	Total	C	N	O	S	0	0	0
			291	172	45	72	2			
2	E	32	Total	C	N	O	S	0	0	0
			287	169	44	72	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	32	Total	C	N	O	S	0	0	0
			283	167	43	71	2			
2	R	32	Total	C	N	O	S	0	0	0
			268	158	37	71	2			

- Molecule 3 is an oligosaccharide called alpha-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.



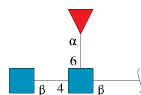
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	4	Total	C	N	O		0	0	0
			49	28	2	19				

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



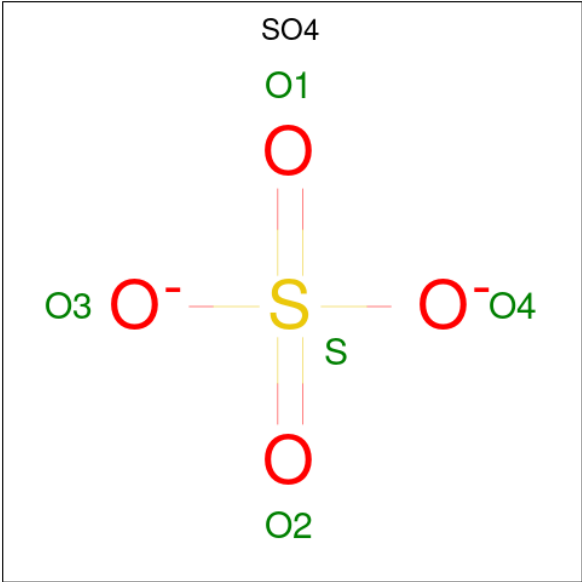
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	2	Total	C	N	O		0	0	0
			28	16	2	10				

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



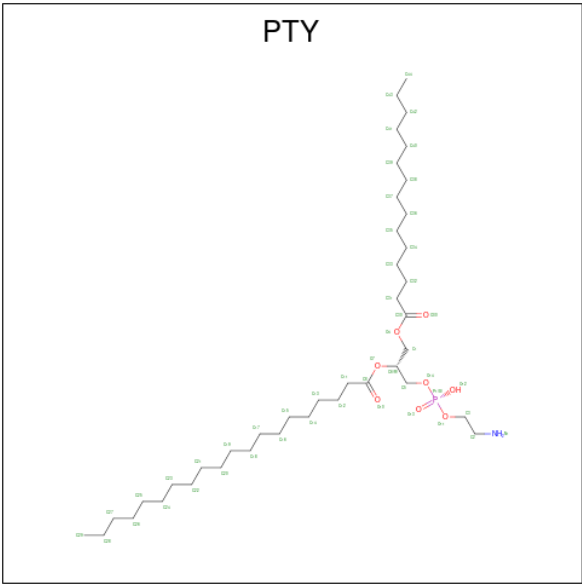
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	3	Total	C	N	O		0	0	0
			38	22	2	14				

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



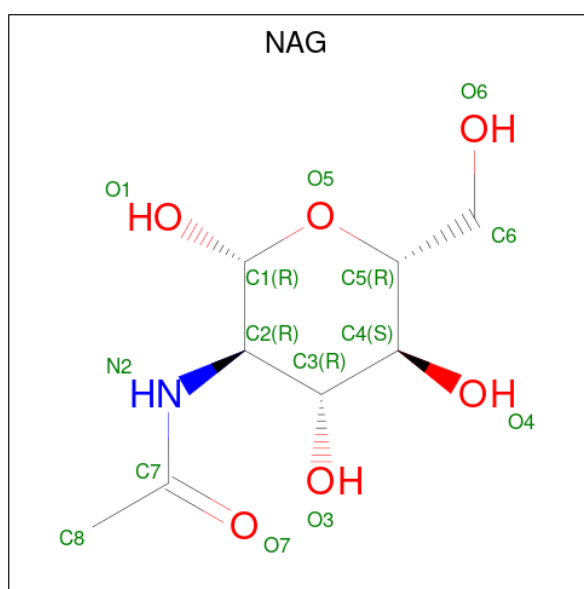
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: C<sub>40</sub>H<sub>80</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			50	40	1	8	1		
7	B	1	Total	C	N	O	P	0	0
			45	35	1	8	1		
7	C	1	Total	C	N	O	P	0	0
			50	40	1	8	1		
7	D	1	Total	C	N	O	P	0	0
			17	7	1	8	1		

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

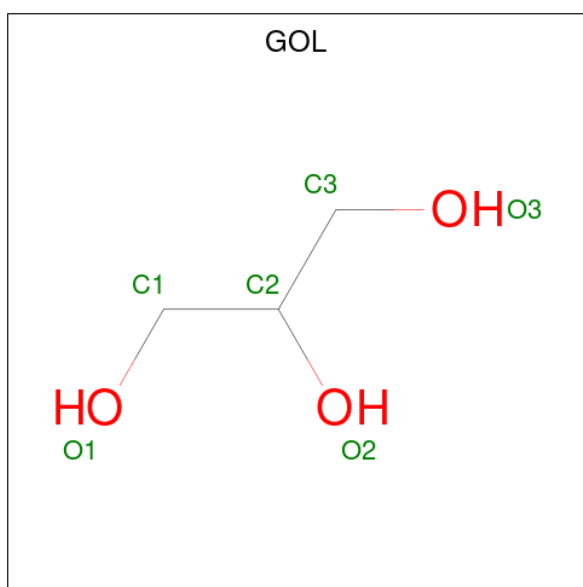
- Molecule 9 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	L	5	Total	Ca	0	0
			5	5		
9	E	5	Total	Ca	0	0
			5	5		
9	F	5	Total	Ca	0	0
			5	5		
9	R	5	Total	Ca	0	0
			5	5		

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	L	2	Total	Mg	0	0
			2	2		
10	E	2	Total	Mg	0	0
			2	2		
10	F	1	Total	Mg	0	0
			1	1		
10	R	2	Total	Mg	0	0
			2	2		

- Molecule 11 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 12 is water.

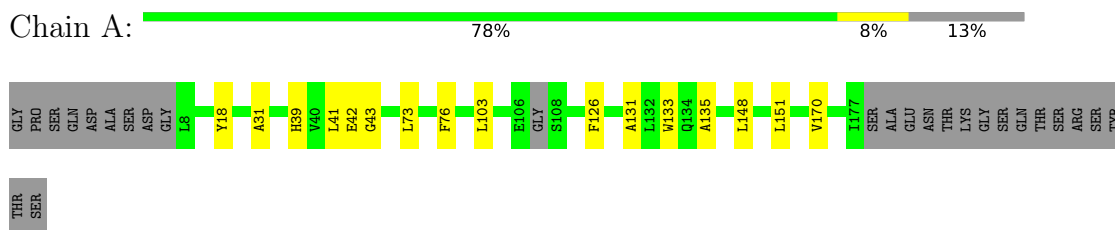
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	L	1	Total	O	0	0
			1	1		
12	E	2	Total	O	0	0
			2	2		



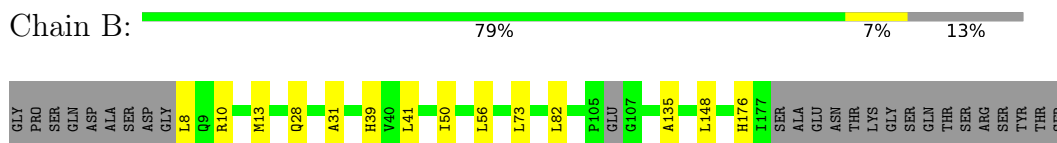
### 3 Residue-property plots

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.

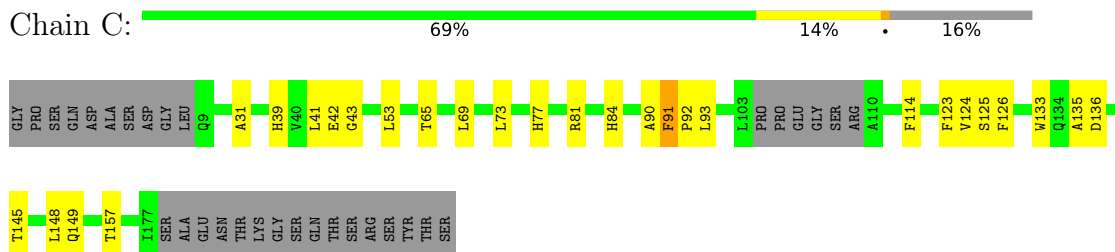
- Molecule 1: Endothelial protein C receptor



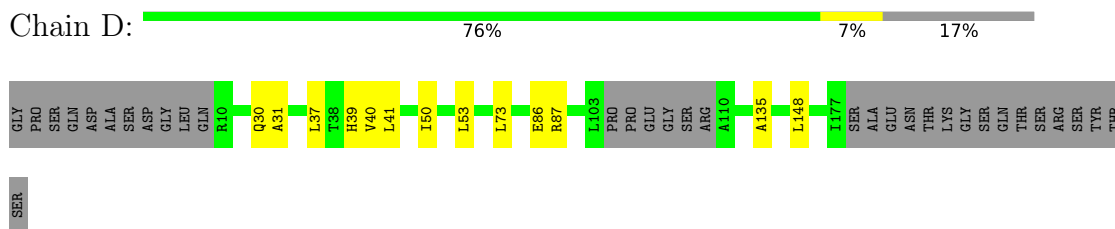
- Molecule 1: Endothelial protein C receptor



- Molecule 1: Endothelial protein C receptor



- Molecule 1: Endothelial protein C receptor



- Molecule 2: Factor VII light chain

Chain L:  72% 25%



- Molecule 2: Factor VII light chain

Chain E:  66% 34%



- Molecule 2: Factor VII light chain

Chain F:  72% 28%



- Molecule 2: Factor VII light chain

Chain R:  72% 28%



- Molecule 3: alpha-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:  25% 75%



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

Chain H:  50% 50%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  33% 67%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	278.41Å 44.22Å 111.25Å 90.00° 93.01° 90.00°	Depositor
Resolution (Å)	43.67 – 3.00 43.67 – 3.00	Depositor EDS
% Data completeness (in resolution range)	88.6 (43.67-3.00) 79.9 (43.67-3.00)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.86 (at 3.01Å)	Xtriage
Refinement program	PHENIX 2.0_5936	Depositor
R, $R_{free}$	0.242 , 0.295 0.241 , 0.297	Depositor DCC
$R_{free}$ test set	1249 reflections (4.48%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	52.4	Xtriage
Anisotropy	0.520	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 33.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6759	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.64% 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: FUC, NAG, MAN, PTY, SO4, CGU, CA, GOL, MG

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	0.10	0/1384	0.26	0/1888
1	B	0.09	0/1378	0.25	0/1881
1	C	0.10	0/1348	0.29	0/1837
1	D	0.10	0/1311	0.29	0/1790
2	E	0.10	0/176	0.29	0/224
2	F	0.09	0/172	0.27	0/219
2	L	0.10	0/180	0.31	0/228
2	R	0.10	0/157	0.28	0/201
All	All	0.10	0/6106	0.27	0/8268

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	C	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	91	PHE	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	1347	0	1268	10	0
1	B	1341	0	1263	9	0
1	C	1313	0	1246	20	0
1	D	1277	0	1203	9	0
2	E	287	0	220	1	0
2	F	283	0	214	0	0
2	L	291	0	231	1	0
2	R	268	0	183	0	0
3	G	49	0	43	0	0
4	H	28	0	25	0	0
5	I	38	0	34	2	0
6	A	10	0	0	0	0
6	B	10	0	0	0	0
6	F	5	0	0	0	0
7	A	50	0	79	1	0
7	B	45	0	66	1	0
7	C	50	0	79	3	0
7	D	17	0	11	0	0
8	C	14	0	13	2	0
9	E	5	0	0	0	0
9	F	5	0	0	0	0
9	L	5	0	0	0	0
9	R	5	0	0	0	0
10	E	2	0	0	0	0
10	F	1	0	0	0	0
10	L	2	0	0	0	0
10	R	2	0	0	0	0
11	R	6	0	8	0	0
12	E	2	0	0	0	0
12	L	1	0	0	0	0
All	All	6759	0	6186	48	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 4.

All (48) 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:42:GLU:HG2	1:C:42:GLU:HG2	1.59	0.84
1:D:41:LEU:HD11	1:D:73:LEU:HD11	1.76	0.66
5:I:1:NAG:H4	5:I:2:NAG:HN2	1.62	0.63
1:D:86:GLU:HB3	1:D:87:ARG:HH11	1.65	0.62
1:C:41:LEU:HD11	1:C:73:LEU:HD11	1.81	0.61
5:I:1:NAG:H4	5:I:2:NAG:N2	2.16	0.60
1:C:92:PRO:HG2	8:C:201:NAG:H5	1.84	0.60
1:D:30:GLN:HB3	1:D:37:LEU:HD11	1.84	0.60
1:B:8:LEU:HD23	1:B:10:ARG:HH21	1.66	0.59
1:C:124:VAL:HG12	1:C:133:TRP:HE3	1.71	0.56
1:A:135:ALA:HB2	1:A:148:LEU:HD11	1.89	0.55
1:C:69:LEU:HD11	7:C:202:PTY:H212	1.91	0.53
1:C:92:PRO:HG2	8:C:201:NAG:H3	1.90	0.52
1:C:90:ALA:O	1:C:93:LEU:HD23	2.10	0.52
1:D:86:GLU:C	1:D:87:ARG:HD2	2.35	0.52
1:B:41:LEU:HD11	1:B:73:LEU:HD11	1.92	0.51
1:C:145:THR:O	1:C:149:GLN:HG3	2.10	0.50
1:A:103:LEU:HD11	1:A:170:VAL:HG13	1.94	0.50
1:C:157:THR:HG22	7:C:202:PTY:H321	1.93	0.49
1:D:41:LEU:HD12	1:D:50:ILE:HG12	1.95	0.49
1:C:42:GLU:HG3	1:C:43:GLY:N	2.27	0.48
1:C:84:HIS:HB2	1:C:91:PHE:CE1	2.50	0.47
1:A:41:LEU:HD11	1:A:73:LEU:HD11	1.97	0.47
1:A:42:GLU:HG3	1:A:43:GLY:N	2.30	0.46
1:C:77:HIS:O	1:C:81:ARG:HG3	2.16	0.46
1:C:135:ALA:HB2	1:C:148:LEU:HD11	1.98	0.46
1:A:31:ALA:HB3	1:A:39:HIS:HB2	1.98	0.46
2:E:13:LEU:HA	2:E:30:ILE:HD13	1.98	0.45
1:B:41:LEU:HD12	1:B:50:ILE:HG12	1.97	0.45
1:B:135:ALA:HB2	1:B:148:LEU:HD11	1.97	0.45
1:B:13:MET:HB3	7:B:201:PTY:H361	1.99	0.44
1:C:31:ALA:HB3	1:C:39:HIS:HB2	1.99	0.44
1:D:40:VAL:HG23	1:D:53:LEU:HD21	1.99	0.44
1:B:31:ALA:HB3	1:B:39:HIS:HB2	1.99	0.44
1:B:28:GLN:NE2	1:D:30:GLN:HG3	2.33	0.43
1:D:135:ALA:HB2	1:D:148:LEU:HD11	2.00	0.43
1:A:18:TYR:CG	1:C:53:LEU:HD13	2.52	0.43
1:C:125:SER:HB3	1:C:136:ASP:OD2	2.19	0.43
1:A:133:TRP:CD2	1:A:151:LEU:HD13	2.54	0.43
1:C:123:PHE:CD2	1:C:124:VAL:HG23	2.55	0.42
1:C:84:HIS:HB2	1:C:91:PHE:HE1	1.83	0.42
1:C:65:THR:HG23	7:C:202:PTY:H271	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:PHE:CZ	1:A:131:ALA:HA	2.55	0.41
1:B:56:LEU:HB3	1:B:176:HIS:CD2	2.56	0.41
1:D:31:ALA:HB3	1:D:39:HIS:HB2	2.01	0.41
1:B:82:LEU:HD11	2:L:7:CGU:HB2	2.03	0.41
1:C:114:PHE:HB3	1:C:126:PHE:HB3	2.03	0.40
1:A:76:PHE:HD1	7:A:203:PTY:H361	1.86	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	A	165/195 (85%)	163 (99%)	2 (1%)	0	100	100
1	B	165/195 (85%)	163 (99%)	2 (1%)	0	100	100
1	C	159/195 (82%)	156 (98%)	3 (2%)	0	100	100
1	D	158/195 (81%)	156 (99%)	2 (1%)	0	100	100
2	E	21/32 (66%)	21 (100%)	0	0	100	100
2	F	21/32 (66%)	21 (100%)	0	0	100	100
2	L	21/32 (66%)	21 (100%)	0	0	100	100
2	R	21/32 (66%)	21 (100%)	0	0	100	100
All	All	731/908 (80%)	722 (99%)	9 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	140/172 (81%)	140 (100%)	0	100	100
1	B	139/172 (81%)	139 (100%)	0	100	100
1	C	139/172 (81%)	139 (100%)	0	100	100
1	D	132/172 (77%)	132 (100%)	0	100	100
2	E	18/19 (95%)	18 (100%)	0	100	100
2	F	17/19 (90%)	17 (100%)	0	100	100
2	L	19/19 (100%)	19 (100%)	0	100	100
2	R	14/19 (74%)	14 (100%)	0	100	100
All	All	618/764 (81%)	618 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	B	28	GLN
1	B	36	HIS
1	D	70	GLN
1	D	111	HIS
1	D	176	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

36 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
2	CGU	E	7	9,2	9,11,12	1.59	2 (22%)	10,14,16	0.90	0
2	CGU	R	19	10,2	9,11,12	1.53	2 (22%)	10,14,16	0.78	0
2	CGU	E	19	10,2	9,11,12	1.58	2 (22%)	10,14,16	0.69	0
2	CGU	L	19	10,2	9,11,12	1.51	1 (11%)	10,14,16	0.83	0
2	CGU	L	14	10,2	9,11,12	1.56	2 (22%)	10,14,16	0.71	0
2	CGU	R	14	10,2	9,11,12	1.55	2 (22%)	10,14,16	0.79	0
2	CGU	E	14	10,2	9,11,12	1.50	2 (22%)	10,14,16	0.79	0
2	CGU	F	6	9,2	9,11,12	1.53	2 (22%)	10,14,16	0.87	0
2	CGU	F	29	9,10,2	9,11,12	1.58	2 (22%)	10,14,16	0.73	0
2	CGU	F	14	2	9,11,12	1.52	2 (22%)	10,14,16	0.81	0
2	CGU	F	26	9,2	9,11,12	1.58	2 (22%)	10,14,16	0.74	0
2	CGU	E	26	9,2	9,11,12	1.65	2 (22%)	10,14,16	0.64	0
2	CGU	E	6	9,2	9,11,12	1.59	2 (22%)	10,14,16	0.81	0
2	CGU	R	29	9,10,2	9,11,12	1.56	2 (22%)	10,14,16	0.72	0
2	CGU	L	29	9,10,2	9,11,12	1.63	2 (22%)	10,14,16	0.66	0
2	CGU	R	20	9,2	9,11,12	1.55	2 (22%)	10,14,16	0.71	0
2	CGU	R	25	10,2	9,11,12	1.56	2 (22%)	10,14,16	0.83	0
2	CGU	E	25	10,2	9,11,12	1.58	2 (22%)	10,14,16	0.88	0
2	CGU	L	7	9,2	9,11,12	1.54	2 (22%)	10,14,16	0.91	0
2	CGU	R	7	9,2	9,11,12	1.65	2 (22%)	10,14,16	0.80	0
2	CGU	F	20	9,2	9,11,12	1.57	2 (22%)	10,14,16	0.70	0
2	CGU	F	25	9,10,2	9,11,12	1.53	2 (22%)	10,14,16	0.77	0
2	CGU	L	20	9,2	9,11,12	1.63	2 (22%)	10,14,16	0.66	0
2	CGU	R	6	9,2	9,11,12	1.61	2 (22%)	10,14,16	0.74	0
2	CGU	F	16	9,2	9,11,12	1.59	2 (22%)	10,14,16	0.82	0
2	CGU	R	16	9,2	9,11,12	1.60	2 (22%)	10,14,16	0.78	0
2	CGU	F	7	9,2	9,11,12	1.53	2 (22%)	10,14,16	0.91	0
2	CGU	L	25	10,2	9,11,12	1.49	2 (22%)	10,14,16	0.87	0
2	CGU	E	29	9,10,2	9,11,12	1.58	2 (22%)	10,14,16	0.68	0
2	CGU	L	26	9,2	9,11,12	1.61	2 (22%)	10,14,16	0.68	0
2	CGU	R	26	9,2	9,11,12	1.61	2 (22%)	10,14,16	0.75	0
2	CGU	L	6	9,2	9,11,12	1.56	2 (22%)	10,14,16	0.81	0
2	CGU	E	16	9,2	9,11,12	1.58	2 (22%)	10,14,16	0.83	0
2	CGU	F	19	2	9,11,12	1.56	2 (22%)	10,14,16	0.80	0
2	CGU	E	20	9,2	9,11,12	1.54	2 (22%)	10,14,16	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	CGU	L	16	9,2	9,11,12	1.61	2 (22%)	10,14,16	0.85	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
2	CGU	E	7	9,2	-	4/13/14/16	-
2	CGU	R	19	10,2	-	1/13/14/16	-
2	CGU	E	19	10,2	-	0/13/14/16	-
2	CGU	L	19	10,2	-	0/13/14/16	-
2	CGU	L	14	10,2	-	3/13/14/16	-
2	CGU	R	14	10,2	-	2/13/14/16	-
2	CGU	E	14	10,2	-	3/13/14/16	-
2	CGU	F	6	9,2	-	2/13/14/16	-
2	CGU	F	29	9,10,2	-	1/13/14/16	-
2	CGU	F	14	2	-	2/13/14/16	-
2	CGU	F	26	9,2	-	3/13/14/16	-
2	CGU	E	26	9,2	-	3/13/14/16	-
2	CGU	E	6	9,2	-	5/13/14/16	-
2	CGU	R	29	9,10,2	-	0/13/14/16	-
2	CGU	L	29	9,10,2	-	0/13/14/16	-
2	CGU	R	20	9,2	-	0/13/14/16	-
2	CGU	R	25	10,2	-	0/13/14/16	-
2	CGU	E	25	10,2	-	0/13/14/16	-
2	CGU	L	7	9,2	-	3/13/14/16	-
2	CGU	R	7	9,2	-	3/13/14/16	-
2	CGU	F	20	9,2	-	0/13/14/16	-
2	CGU	F	25	9,10,2	-	0/13/14/16	-
2	CGU	L	20	9,2	-	0/13/14/16	-
2	CGU	R	6	9,2	-	5/13/14/16	-
2	CGU	F	16	9,2	-	2/13/14/16	-
2	CGU	R	16	9,2	-	2/13/14/16	-
2	CGU	F	7	9,2	-	3/13/14/16	-
2	CGU	L	25	10,2	-	0/13/14/16	-
2	CGU	E	29	9,10,2	-	1/13/14/16	-
2	CGU	L	26	9,2	-	3/13/14/16	-
2	CGU	R	26	9,2	-	3/13/14/16	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CGU	L	6	9,2	-	3/13/14/16	-
2	CGU	E	16	9,2	-	1/13/14/16	-
2	CGU	F	19	2	-	0/13/14/16	-
2	CGU	E	20	9,2	-	1/13/14/16	-
2	CGU	L	16	9,2	-	2/13/14/16	-

All (71) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	26	CGU	CG-CD1	2.93	1.55	1.52
2	L	29	CGU	CG-CD1	2.92	1.55	1.52
2	R	7	CGU	CG-CD1	2.83	1.55	1.52
2	R	6	CGU	CG-CD1	2.82	1.55	1.52
2	E	29	CGU	CG-CD1	2.79	1.55	1.52
2	L	20	CGU	CG-CD1	2.77	1.55	1.52
2	R	16	CGU	CG-CD1	2.77	1.55	1.52
2	L	26	CGU	CG-CD1	2.74	1.55	1.52
2	E	6	CGU	CG-CD1	2.74	1.55	1.52
2	E	25	CGU	CG-CD1	2.74	1.55	1.52
2	L	16	CGU	CG-CD1	2.73	1.55	1.52
2	E	19	CGU	CG-CD1	2.72	1.55	1.52
2	R	25	CGU	CG-CD1	2.71	1.55	1.52
2	R	26	CGU	CG-CD1	2.71	1.55	1.52
2	F	19	CGU	CG-CD1	2.67	1.55	1.52
2	E	7	CGU	CG-CD1	2.67	1.55	1.52
2	F	16	CGU	CG-CD1	2.66	1.55	1.52
2	E	16	CGU	CG-CD1	2.66	1.55	1.52
2	F	29	CGU	CG-CD1	2.65	1.55	1.52
2	F	26	CGU	CG-CD1	2.63	1.55	1.52
2	R	29	CGU	CG-CD1	2.62	1.55	1.52
2	L	14	CGU	CG-CD1	2.62	1.55	1.52
2	F	20	CGU	CG-CD1	2.62	1.55	1.52
2	L	6	CGU	CG-CD1	2.60	1.55	1.52
2	L	19	CGU	CG-CD1	2.59	1.55	1.52
2	R	19	CGU	CG-CD1	2.55	1.55	1.52
2	R	20	CGU	CG-CD1	2.51	1.55	1.52
2	F	14	CGU	CG-CD1	2.50	1.55	1.52
2	R	14	CGU	CG-CD1	2.50	1.55	1.52
2	F	6	CGU	CG-CD1	2.49	1.55	1.52
2	R	7	CGU	CG-CD2	2.47	1.55	1.52
2	E	20	CGU	CG-CD1	2.44	1.55	1.52
2	F	25	CGU	CG-CD1	2.44	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	16	CGU	CG-CD2	2.43	1.55	1.52
2	F	7	CGU	CG-CD1	2.43	1.55	1.52
2	L	20	CGU	CG-CD2	2.43	1.55	1.52
2	L	7	CGU	CG-CD1	2.42	1.55	1.52
2	F	16	CGU	CG-CD2	2.36	1.55	1.52
2	R	26	CGU	CG-CD2	2.35	1.55	1.52
2	E	16	CGU	CG-CD2	2.35	1.55	1.52
2	E	14	CGU	CG-CD1	2.35	1.55	1.52
2	R	16	CGU	CG-CD2	2.34	1.55	1.52
2	L	7	CGU	CG-CD2	2.29	1.55	1.52
2	E	7	CGU	CG-CD2	2.28	1.55	1.52
2	L	26	CGU	CG-CD2	2.28	1.55	1.52
2	F	29	CGU	CG-CD2	2.27	1.55	1.52
2	R	14	CGU	CG-CD2	2.26	1.55	1.52
2	L	29	CGU	CG-CD2	2.25	1.55	1.52
2	R	6	CGU	CG-CD2	2.25	1.55	1.52
2	E	26	CGU	CG-CD2	2.25	1.55	1.52
2	F	20	CGU	CG-CD2	2.25	1.55	1.52
2	F	26	CGU	CG-CD2	2.24	1.55	1.52
2	L	25	CGU	CG-CD1	2.22	1.55	1.52
2	E	19	CGU	CG-CD2	2.22	1.55	1.52
2	R	20	CGU	CG-CD2	2.21	1.55	1.52
2	E	6	CGU	CG-CD2	2.20	1.54	1.52
2	E	25	CGU	CG-CD2	2.18	1.54	1.52
2	L	25	CGU	CG-CD2	2.18	1.54	1.52
2	L	6	CGU	CG-CD2	2.18	1.54	1.52
2	E	20	CGU	CG-CD2	2.18	1.54	1.52
2	F	25	CGU	CG-CD2	2.17	1.54	1.52
2	F	6	CGU	CG-CD2	2.16	1.54	1.52
2	F	19	CGU	CG-CD2	2.16	1.54	1.52
2	F	7	CGU	CG-CD2	2.16	1.54	1.52
2	R	29	CGU	CG-CD2	2.14	1.54	1.52
2	E	29	CGU	CG-CD2	2.13	1.54	1.52
2	L	14	CGU	CG-CD2	2.11	1.54	1.52
2	E	14	CGU	CG-CD2	2.10	1.54	1.52
2	F	14	CGU	CG-CD2	2.09	1.54	1.52
2	R	19	CGU	CG-CD2	2.08	1.54	1.52
2	R	25	CGU	CG-CD2	2.07	1.54	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (61) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L	6	CGU	CA-CB-CG-CD1
2	L	6	CGU	CA-CB-CG-CD2
2	E	6	CGU	O-C-CA-CB
2	E	6	CGU	CA-CB-CG-CD1
2	E	6	CGU	CA-CB-CG-CD2
2	E	29	CGU	O-C-CA-CB
2	F	6	CGU	CA-CB-CG-CD1
2	F	6	CGU	CA-CB-CG-CD2
2	F	29	CGU	O-C-CA-CB
2	R	6	CGU	O-C-CA-CB
2	R	6	CGU	CA-CB-CG-CD1
2	R	6	CGU	CA-CB-CG-CD2
2	R	19	CGU	O-C-CA-CB
2	L	26	CGU	CA-CB-CG-CD1
2	F	26	CGU	CA-CB-CG-CD1
2	L	7	CGU	OE21-CD2-CG-CB
2	L	7	CGU	OE22-CD2-CG-CB
2	L	26	CGU	OE21-CD2-CG-CB
2	L	26	CGU	OE22-CD2-CG-CB
2	E	7	CGU	OE21-CD2-CG-CB
2	E	7	CGU	OE22-CD2-CG-CB
2	E	26	CGU	OE21-CD2-CG-CB
2	E	26	CGU	OE22-CD2-CG-CB
2	F	7	CGU	OE21-CD2-CG-CB
2	F	7	CGU	OE22-CD2-CG-CB
2	F	26	CGU	OE21-CD2-CG-CB
2	F	26	CGU	OE22-CD2-CG-CB
2	R	7	CGU	OE21-CD2-CG-CB
2	R	7	CGU	OE22-CD2-CG-CB
2	R	26	CGU	OE21-CD2-CG-CB
2	R	26	CGU	OE22-CD2-CG-CB
2	E	26	CGU	CA-CB-CG-CD1
2	R	26	CGU	CA-CB-CG-CD1
2	E	20	CGU	N-CA-CB-CG
2	L	14	CGU	OE11-CD1-CG-CB
2	L	14	CGU	OE12-CD1-CG-CB
2	E	14	CGU	OE11-CD1-CG-CB
2	E	14	CGU	OE12-CD1-CG-CB
2	F	14	CGU	OE11-CD1-CG-CB
2	F	14	CGU	OE12-CD1-CG-CB
2	R	14	CGU	OE11-CD1-CG-CB
2	R	14	CGU	OE12-CD1-CG-CB
2	L	6	CGU	OE22-CD2-CG-CD1

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Mol	Chain	Res	Type	Atoms
2	L	7	CGU	OE11-CD1-CG-CD2
2	L	14	CGU	OE11-CD1-CG-CD2
2	L	16	CGU	OE21-CD2-CG-CD1
2	L	16	CGU	OE22-CD2-CG-CD1
2	E	6	CGU	OE21-CD2-CG-CD1
2	E	6	CGU	OE22-CD2-CG-CD1
2	E	7	CGU	OE11-CD1-CG-CD2
2	E	7	CGU	OE12-CD1-CG-CD2
2	E	14	CGU	OE11-CD1-CG-CD2
2	E	16	CGU	OE21-CD2-CG-CD1
2	F	7	CGU	OE11-CD1-CG-CD2
2	F	16	CGU	OE21-CD2-CG-CD1
2	F	16	CGU	OE22-CD2-CG-CD1
2	R	6	CGU	OE21-CD2-CG-CD1
2	R	6	CGU	OE22-CD2-CG-CD1
2	R	7	CGU	OE11-CD1-CG-CD2
2	R	16	CGU	OE21-CD2-CG-CD1
2	R	16	CGU	OE22-CD2-CG-CD1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	7	CGU	1	0

## 5.5 Carbohydrates

9 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	0.70	0	17,19,21	1.04	1 (5%)
3	NAG	G	2	3	14,14,15	0.74	0	17,19,21	0.86	0
3	MAN	G	3	3	11,11,12	0.62	0	15,15,17	1.59	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	FUC	G	4	3	10,10,11	0.98	1 (10%)	14,14,16	1.21	1 (7%)
4	NAG	H	1	4,1	14,14,15	0.71	0	17,19,21	1.01	1 (5%)
4	NAG	H	2	4	14,14,15	0.74	0	17,19,21	0.92	0
5	NAG	I	1	5,1	14,14,15	0.76	0	17,19,21	1.24	2 (11%)
5	NAG	I	2	5	14,14,15	0.95	1 (7%)	17,19,21	2.62	5 (29%)
5	FUC	I	3	5	10,10,11	0.69	0	14,14,16	2.07	5 (35%)

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
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	MAN	G	3	3	-	2/2/19/22	1/1/1/1
3	FUC	G	4	3	-	-	0/1/1/1
4	NAG	H	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	H	2	4	-	0/6/23/26	0/1/1/1
5	NAG	I	1	5,1	-	4/6/23/26	0/1/1/1
5	NAG	I	2	5	-	1/6/23/26	0/1/1/1
5	FUC	I	3	5	-	-	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	2	NAG	C1-C2	2.83	1.56	1.52
3	G	4	FUC	O5-C1	-2.43	1.39	1.43

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	2	NAG	C2-N2-C7	8.12	133.78	122.90
3	G	3	MAN	C1-O5-C5	4.95	118.82	112.19
5	I	3	FUC	C1-O5-C5	4.32	123.16	112.97
5	I	2	NAG	C1-C2-N2	4.02	116.77	110.43
5	I	3	FUC	C1-C2-C3	3.87	115.28	109.64
5	I	2	NAG	O5-C1-C2	-3.33	106.14	111.29
5	I	1	NAG	C2-N2-C7	2.85	126.72	122.90
5	I	2	NAG	O7-C7-N2	2.81	126.94	121.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	3	FUC	C3-C4-C5	-2.71	105.69	109.81
3	G	1	NAG	C1-O5-C5	2.54	115.58	112.19
5	I	2	NAG	C1-O5-C5	2.51	115.55	112.19
5	I	3	FUC	O5-C5-C4	2.43	113.93	109.55
5	I	3	FUC	O4-C4-C5	2.38	114.98	109.74
3	G	4	FUC	O5-C5-C4	2.20	113.52	109.55
4	H	1	NAG	C2-N2-C7	2.17	125.81	122.90
5	I	1	NAG	O4-C4-C3	-2.03	105.60	110.38

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	I	2	NAG	C3-C2-N2-C7
5	I	1	NAG	O5-C5-C6-O6
3	G	3	MAN	O5-C5-C6-O6
3	G	3	MAN	C4-C5-C6-O6
5	I	1	NAG	C4-C5-C6-O6
4	H	1	NAG	C8-C7-N2-C2
4	H	1	NAG	O7-C7-N2-C2
5	I	1	NAG	C8-C7-N2-C2
5	I	1	NAG	O7-C7-N2-C2
3	G	1	NAG	O5-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6

All (1) ring outliers are listed below:

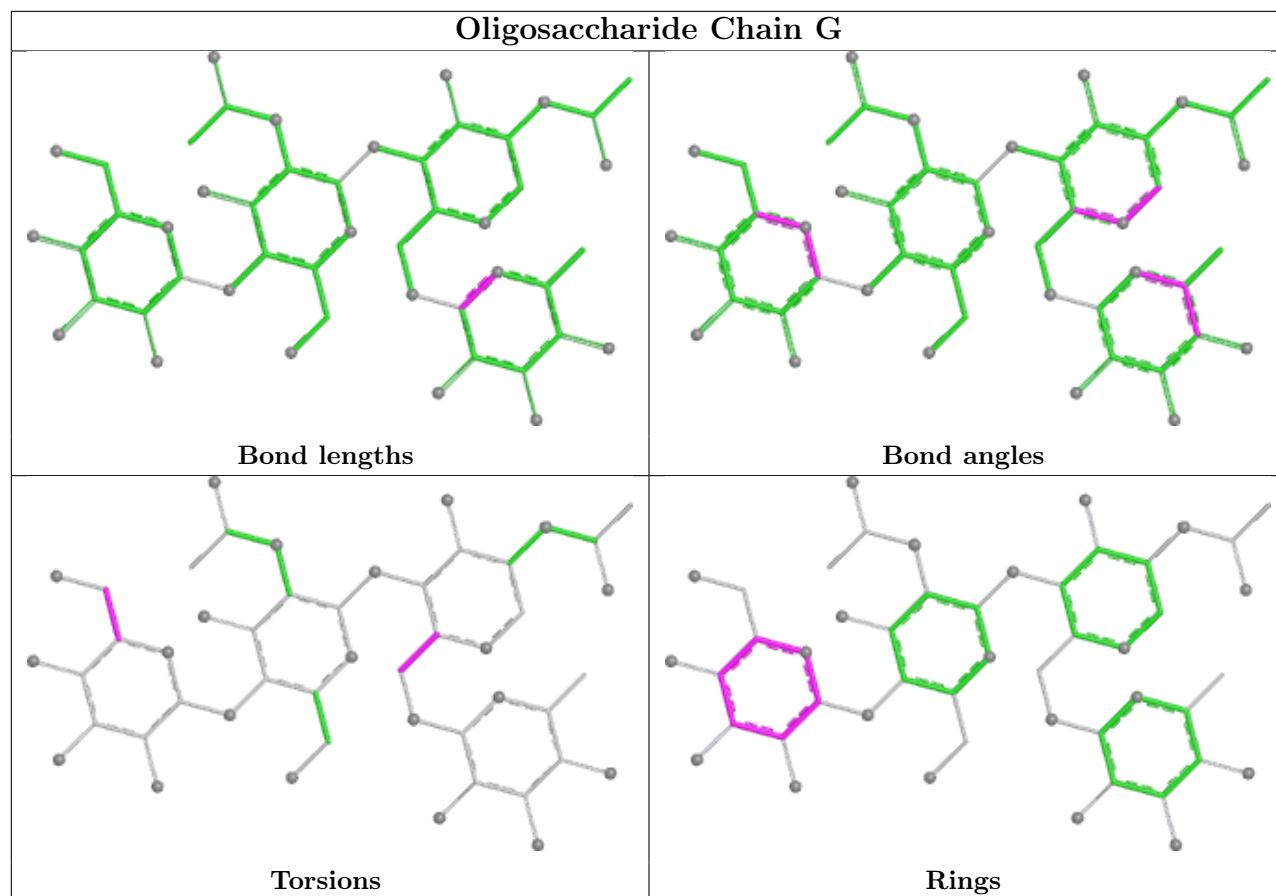
Mol	Chain	Res	Type	Atoms
3	G	3	MAN	C1-C2-C3-C4-C5-O5

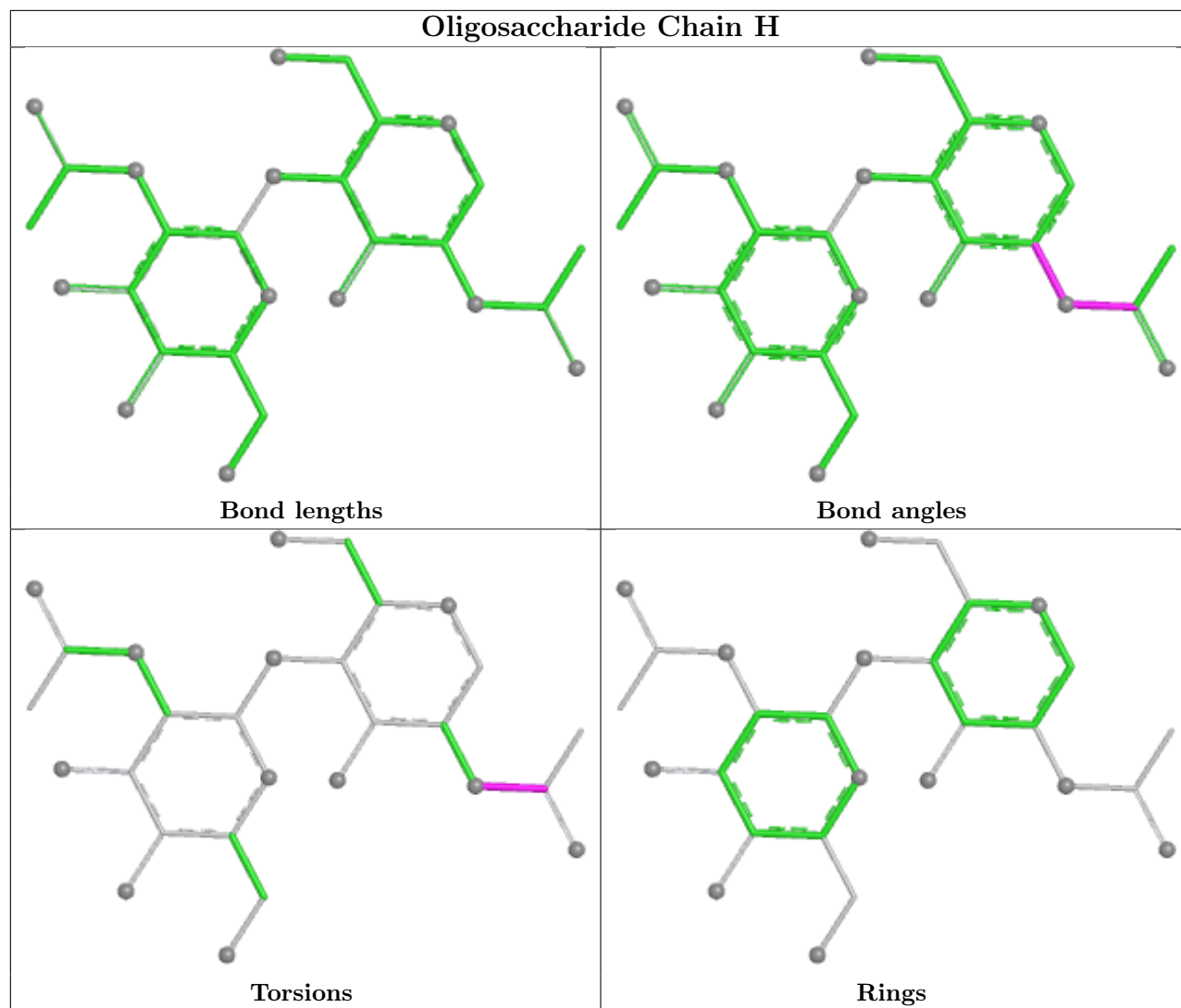
2 monomers are involved in 2 short contacts:

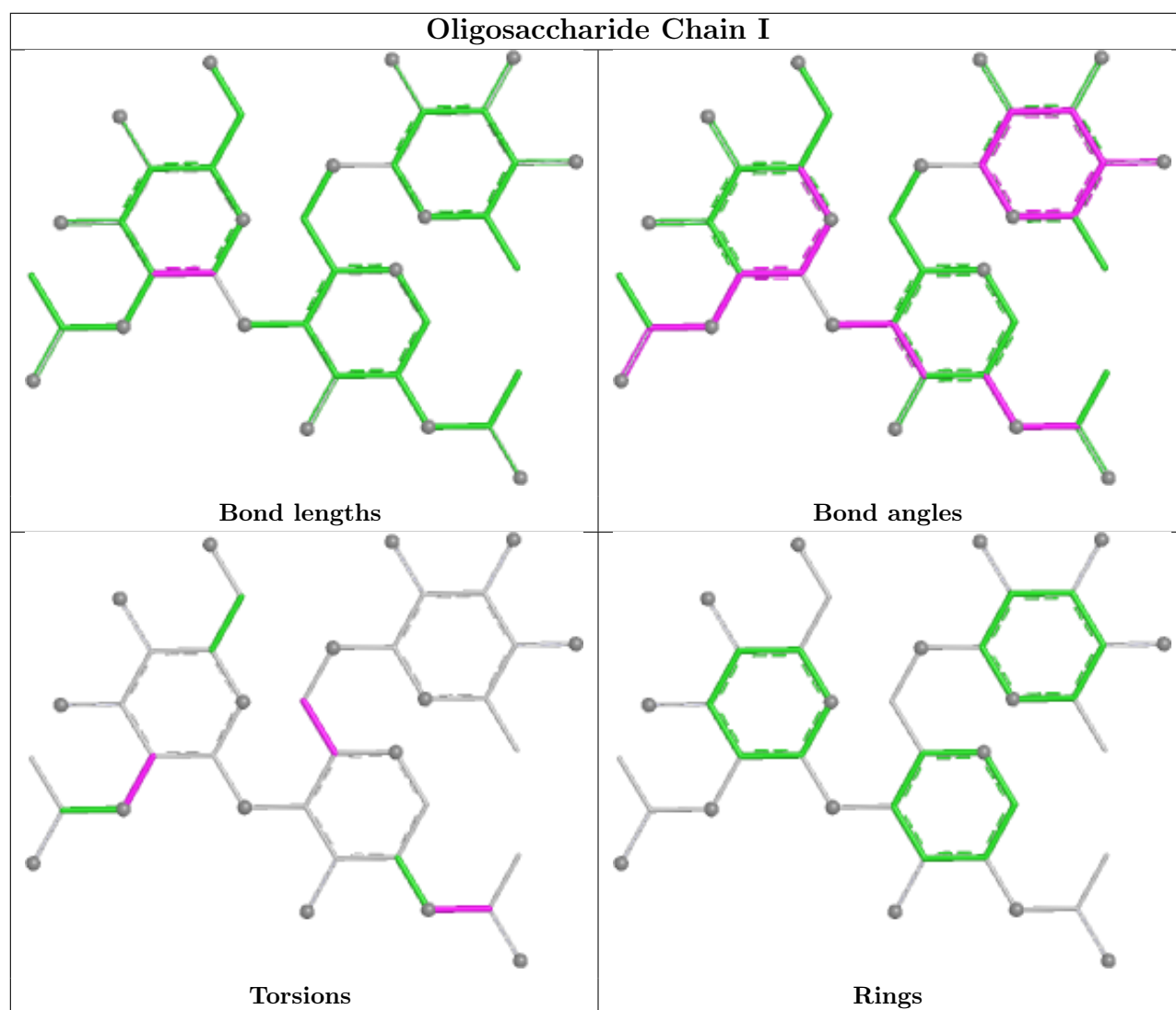
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	I	1	NAG	2	0
5	I	2	NAG	2	0

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 [i](#)

Of 38 ligands modelled in this entry, 27 are monoatomic - leaving 11 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	NAG	C	201	1	14,14,15	0.74	0	17,19,21	1.02	1 (5%)
6	SO4	A	201	-	4,4,4	0.67	0	6,6,6	0.05	0
7	PTY	B	201	-	44,44,49	0.50	0	47,49,54	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	PTY	D	201	-	16,16,49	0.82	1 (6%)	15,19,54	0.79	0
6	SO4	B	202	-	4,4,4	0.67	0	6,6,6	0.11	0
7	PTY	A	203	-	49,49,49	0.47	0	52,54,54	0.39	0
6	SO4	A	202	-	4,4,4	0.67	0	6,6,6	0.10	0
7	PTY	C	202	-	49,49,49	0.46	0	52,54,54	0.40	0
6	SO4	F	106	-	4,4,4	0.67	0	6,6,6	0.08	0
6	SO4	B	203	-	4,4,4	0.67	0	6,6,6	0.04	0
11	GOL	R	101	-	5,5,5	0.34	0	5,5,5	0.37	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	NAG	C	201	1	-	0/6/23/26	0/1/1/1
7	PTY	D	201	-	-	12/18/18/53	-
7	PTY	B	201	-	-	24/48/48/53	-
7	PTY	A	203	-	-	25/53/53/53	-
7	PTY	C	202	-	-	22/53/53/53	-
11	GOL	R	101	-	-	3/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	201	PTY	O7-C6	-2.04	1.43	1.46

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	201	NAG	C1-O5-C5	2.75	115.86	112.19

There are no chirality outliers.

All (86) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	203	PTY	N1-C2-C3-O11
7	A	203	PTY	C3-O11-P1-O12
7	A	203	PTY	C3-O11-P1-O14
7	A	203	PTY	C5-O14-P1-O12

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Mol	Chain	Res	Type	Atoms
7	A	203	PTY	C5-O14-P1-O13
7	B	201	PTY	C3-O11-P1-O12
7	B	201	PTY	C3-O11-P1-O14
7	B	201	PTY	C5-O14-P1-O11
7	B	201	PTY	C5-O14-P1-O12
7	B	201	PTY	C5-O14-P1-O13
7	C	202	PTY	C3-O11-P1-O13
7	D	201	PTY	O10-C8-O7-C6
7	D	201	PTY	C3-O11-P1-O12
7	D	201	PTY	C3-O11-P1-O13
7	D	201	PTY	C3-O11-P1-O14
7	D	201	PTY	C5-O14-P1-O11
7	D	201	PTY	C5-O14-P1-O12
7	D	201	PTY	C5-O14-P1-O13
7	B	201	PTY	C31-C30-O4-C1
7	B	201	PTY	O30-C30-O4-C1
11	R	101	GOL	O1-C1-C2-C3
7	A	203	PTY	C34-C35-C36-C37
7	C	202	PTY	C24-C25-C26-C27
7	A	203	PTY	C32-C33-C34-C35
7	C	202	PTY	C36-C37-C38-C39
7	A	203	PTY	C23-C24-C25-C26
7	C	202	PTY	C23-C24-C25-C26
7	B	201	PTY	C31-C32-C33-C34
7	C	202	PTY	C31-C32-C33-C34
7	B	201	PTY	C17-C18-C19-C20
7	D	201	PTY	O14-C5-C6-C1
7	C	202	PTY	C20-C21-C22-C23
7	B	201	PTY	O4-C1-C6-C5
7	C	202	PTY	C35-C36-C37-C38
7	B	201	PTY	C13-C14-C15-C16
7	C	202	PTY	C16-C17-C18-C19
7	A	203	PTY	C36-C37-C38-C39
7	A	203	PTY	C31-C32-C33-C34
7	A	203	PTY	C40-C41-C42-C43
7	A	203	PTY	O14-C5-C6-C1
7	C	202	PTY	O14-C5-C6-O7
7	D	201	PTY	O14-C5-C6-O7
11	R	101	GOL	O1-C1-C2-O2
7	C	202	PTY	O14-C5-C6-C1
7	C	202	PTY	O4-C1-C6-C5
7	C	202	PTY	C17-C18-C19-C20

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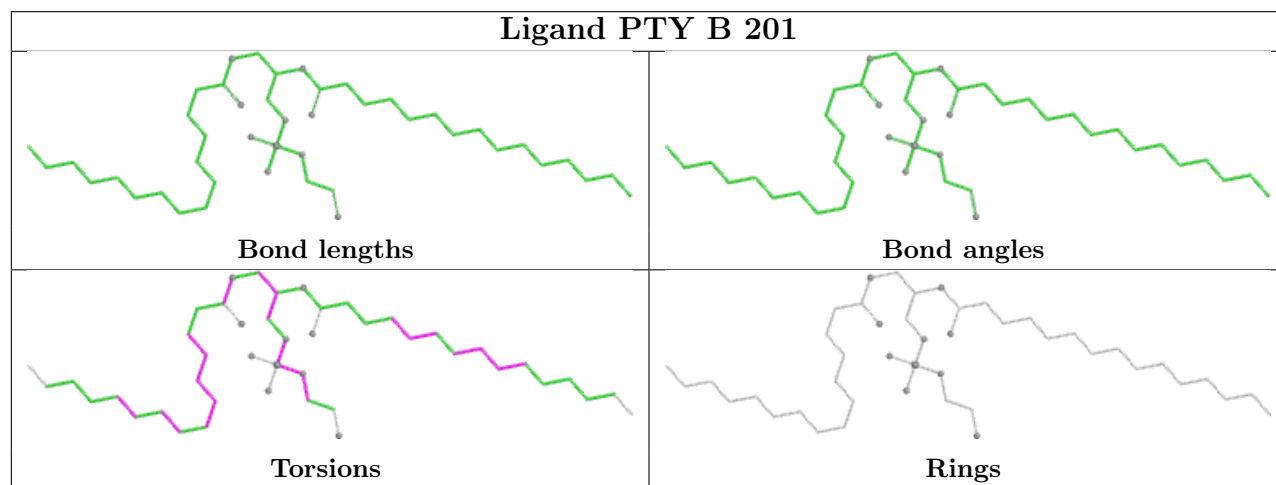
Mol	Chain	Res	Type	Atoms
7	A	203	PTY	C35-C36-C37-C38
7	B	201	PTY	C32-C33-C34-C35
7	A	203	PTY	C2-C3-O11-P1
7	B	201	PTY	C2-C3-O11-P1
7	A	203	PTY	C20-C21-C22-C23
7	C	202	PTY	C14-C15-C16-C17
7	C	202	PTY	C40-C41-C42-C43
7	B	201	PTY	C12-C13-C14-C15
7	B	201	PTY	O14-C5-C6-C1
7	C	202	PTY	C19-C20-C21-C22
7	A	203	PTY	C17-C18-C19-C20
7	A	203	PTY	O14-C5-C6-O7
7	B	201	PTY	O14-C5-C6-O7
7	A	203	PTY	C11-C12-C13-C14
7	A	203	PTY	C5-O14-P1-O11
7	B	201	PTY	C3-O11-P1-O13
7	C	202	PTY	C5-O14-P1-O13
7	D	201	PTY	O30-C30-O4-C1
7	C	202	PTY	C6-C5-O14-P1
7	C	202	PTY	C15-C16-C17-C18
7	C	202	PTY	C25-C26-C27-C28
7	A	203	PTY	C24-C25-C26-C27
7	B	201	PTY	O4-C1-C6-O7
7	B	201	PTY	C16-C17-C18-C19
7	B	201	PTY	C15-C16-C17-C18
7	C	202	PTY	C26-C27-C28-C29
7	A	203	PTY	C19-C20-C21-C22
7	A	203	PTY	C18-C19-C20-C21
11	R	101	GOL	C1-C2-C3-O3
7	C	202	PTY	O4-C1-C6-O7
7	C	202	PTY	C39-C40-C41-C42
7	D	201	PTY	C1-C6-O7-C8
7	D	201	PTY	C5-C6-O7-C8
7	A	203	PTY	C22-C23-C24-C25
7	B	201	PTY	C34-C35-C36-C37
7	B	201	PTY	C36-C37-C38-C39
7	A	203	PTY	O4-C30-C31-C32
7	B	201	PTY	C38-C39-C40-C41
7	A	203	PTY	O30-C30-C31-C32
7	B	201	PTY	C33-C34-C35-C36

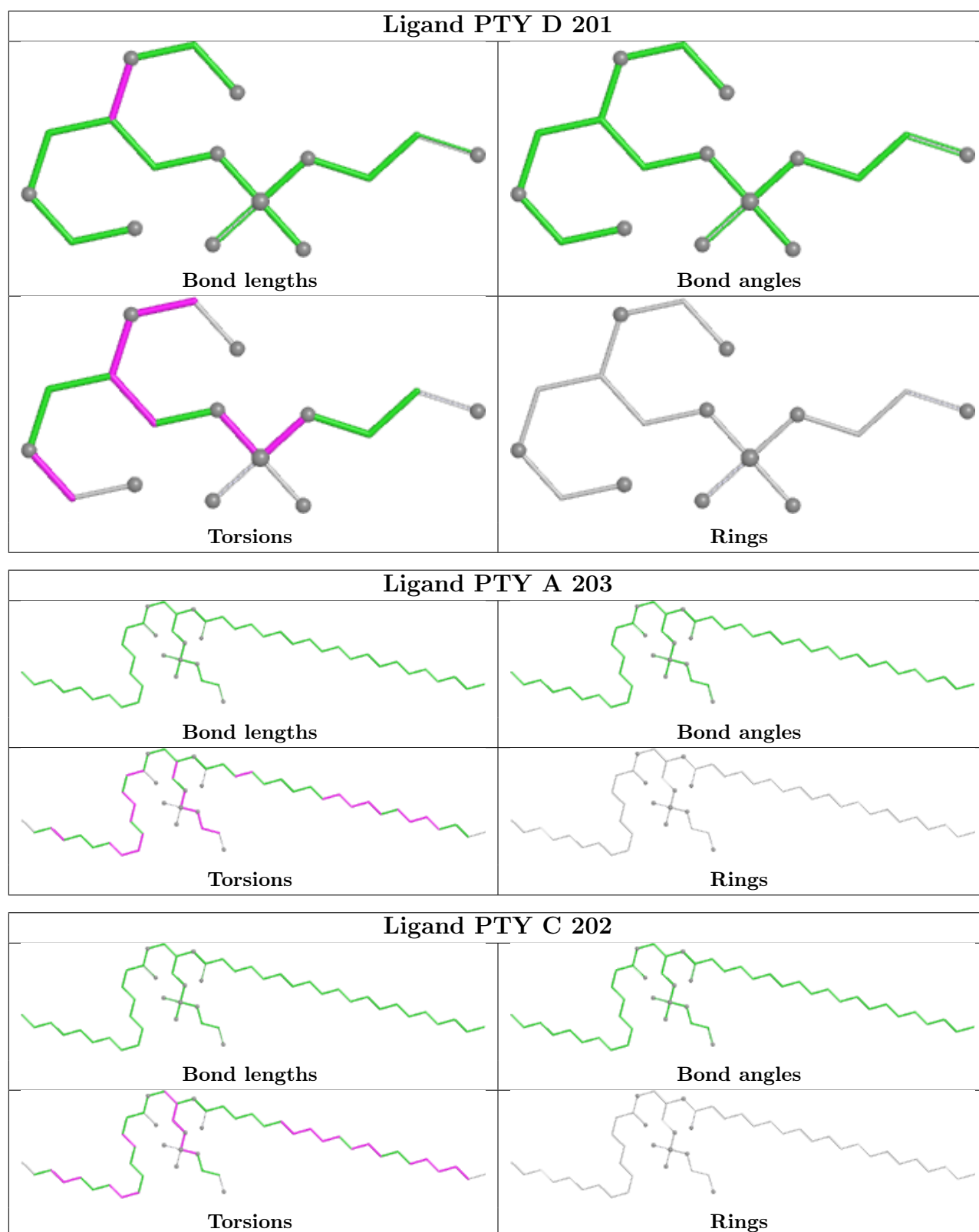
There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	201	NAG	2	0
7	B	201	PTY	1	0
7	A	203	PTY	1	0
7	C	202	PTY	3	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 ⓘ

There are no such residues in this entry.



## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

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

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

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	169/195 (86%)	-1.44	0 100 100	34, 50, 77, 103	0
1	B	169/195 (86%)	-1.47	0 100 100	31, 49, 77, 105	0
1	C	163/195 (83%)	-1.37	0 100 100	39, 65, 89, 102	0
1	D	162/195 (83%)	-1.40	0 100 100	32, 59, 87, 111	0
2	E	23/32 (71%)	-1.47	0 100 100	35, 41, 59, 66	0
2	F	23/32 (71%)	-1.08	0 100 100	58, 69, 84, 93	0
2	L	23/32 (71%)	-1.43	0 100 100	31, 39, 57, 62	0
2	R	23/32 (71%)	-1.24	0 100 100	58, 81, 96, 114	0
All	All	755/908 (83%)	-1.41	0 100 100	31, 55, 88, 114	0

There are no RSRZ outliers to report.

### 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
2	CGU	R	29	12/13	0.98	0.04	48,69,78,79	0
2	CGU	L	7	12/13	0.99	0.03	28,44,61,63	0
2	CGU	L	14	12/13	0.99	0.04	29,32,42,44	0
2	CGU	L	19	12/13	0.99	0.04	33,46,66,68	0
2	CGU	L	20	12/13	0.99	0.04	35,46,52,53	0
2	CGU	L	25	12/13	0.99	0.03	32,44,47,47	0
2	CGU	L	26	12/13	0.99	0.04	23,35,42,43	0
2	CGU	L	29	12/13	0.99	0.03	29,39,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CGU	E	6	12/13	0.99	0.04	24,40,44,54	0
2	CGU	E	7	12/13	0.99	0.03	26,35,65,67	0
2	CGU	E	14	12/13	0.99	0.04	24,41,50,52	0
2	CGU	E	16	12/13	0.99	0.03	34,40,65,67	0
2	CGU	E	19	12/13	0.99	0.05	34,52,66,67	0
2	CGU	E	20	12/13	0.99	0.03	21,44,54,58	0
2	CGU	E	25	12/13	0.99	0.04	36,52,59,70	0
2	CGU	E	26	12/13	0.99	0.03	23,44,59,61	0
2	CGU	E	29	12/13	0.99	0.03	35,46,57,88	0
2	CGU	F	6	12/13	0.99	0.04	52,73,87,92	0
2	CGU	F	7	12/13	0.99	0.04	59,78,84,87	0
2	CGU	F	14	12/13	0.99	0.04	60,79,93,104	0
2	CGU	F	16	12/13	0.99	0.06	67,81,89,89	0
2	CGU	F	19	12/13	0.99	0.03	53,70,85,97	0
2	CGU	F	20	12/13	0.99	0.03	64,78,93,98	0
2	CGU	F	25	12/13	0.99	0.03	50,66,80,95	0
2	CGU	F	26	12/13	0.99	0.03	44,60,65,73	0
2	CGU	F	29	12/13	0.99	0.04	57,69,79,80	0
2	CGU	R	6	12/13	0.99	0.03	65,79,91,104	0
2	CGU	R	7	12/13	0.99	0.05	82,86,97,99	0
2	CGU	R	14	12/13	0.99	0.04	68,81,88,96	0
2	CGU	R	16	12/13	0.99	0.03	71,84,95,95	0
2	CGU	R	19	12/13	0.99	0.04	72,100,113,114	0
2	CGU	R	20	12/13	0.99	0.04	77,93,101,105	0
2	CGU	R	25	12/13	0.99	0.04	62,78,86,103	0
2	CGU	L	6	12/13	0.99	0.04	36,48,61,72	0
2	CGU	R	26	12/13	1.00	0.03	49,74,84,84	0
2	CGU	L	16	12/13	1.00	0.04	30,43,66,72	0

## 6.3 Carbohydrates

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.

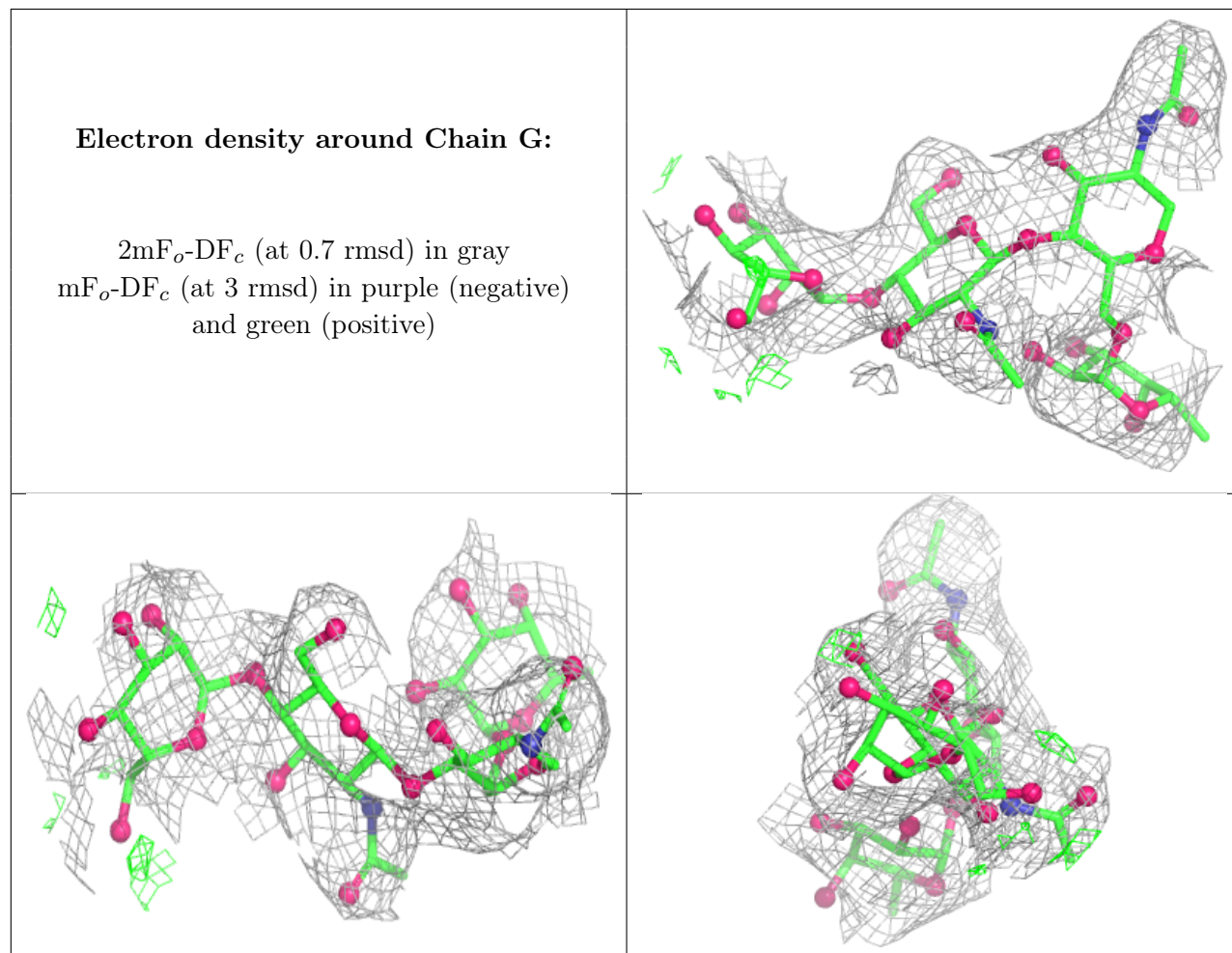
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	G	1	14/15	-	-	40,71,83,86	0
3	NAG	G	2	14/15	-	-	56,74,79,81	0
3	MAN	G	3	11/12	-	-	73,86,99,100	0
3	FUC	G	4	10/11	-	-	93,108,110,124	0
4	NAG	H	1	14/15	-	-	42,55,61,61	0

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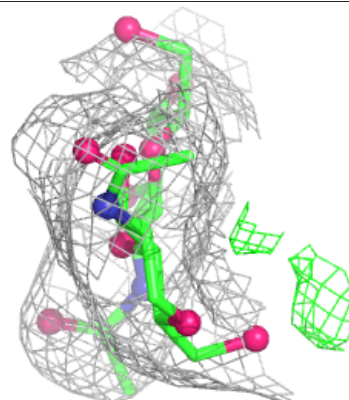
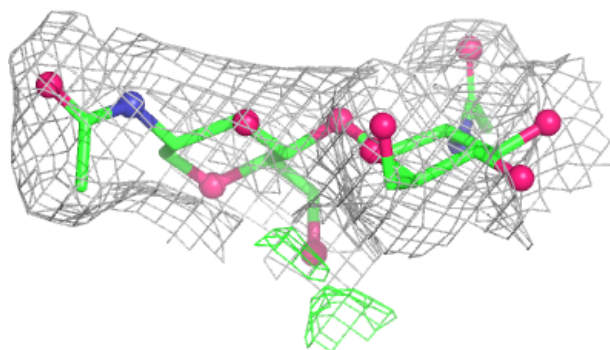
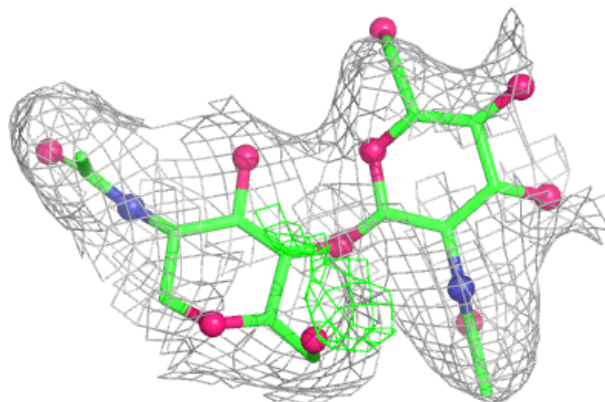
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	H	2	14/15	-	-	43,65,90,103	0
5	NAG	I	1	14/15	0.99	0.04	48,62,88,93	0
5	NAG	I	2	14/15	0.99	0.04	89,107,129,135	0
5	FUC	I	3	10/11	-	-	52,79,100,101	0

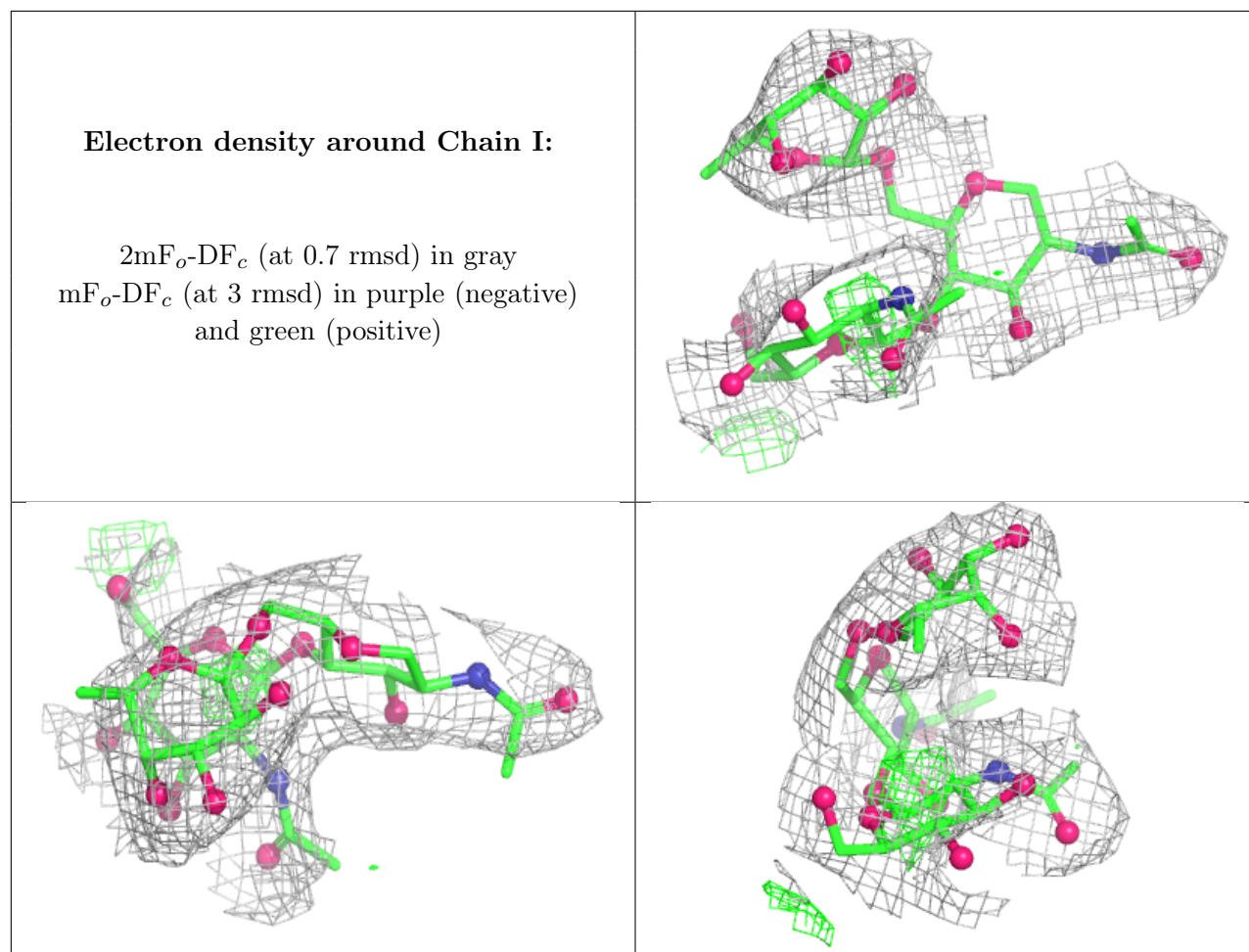
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



**Electron density around Chain H:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 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
11	GOL	R	101	6/6	0.97	0.07	49,57,70,84	0
8	NAG	C	201	14/15	0.98	0.04	49,61,79,81	0
10	MG	R	108	1/1	0.98	0.03	75,75,75,75	0
6	SO4	B	203	5/5	0.98	0.05	88,101,109,122	0
6	SO4	F	106	5/5	0.99	0.03	95,97,117,118	0
7	PTY	A	203	50/50	0.99	0.06	15,49,70,106	0
7	PTY	B	201	45/50	0.99	0.05	21,44,71,75	0
7	PTY	C	202	50/50	0.99	0.06	28,57,81,98	0
7	PTY	D	201	17/50	0.99	0.04	28,54,83,87	0
6	SO4	A	202	5/5	0.99	0.06	74,77,123,132	0
9	CA	L	102	1/1	0.99	0.02	39,39,39,39	0

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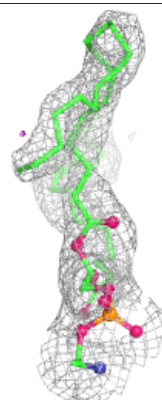
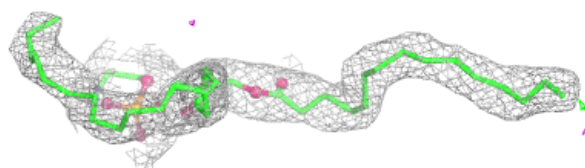
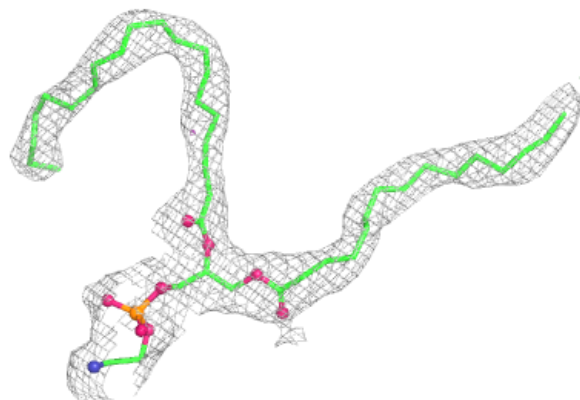
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
9	CA	F	104	1/1	0.99	0.02	69,69,69,69	0
9	CA	R	105	1/1	0.99	0.02	75,75,75,75	0
10	MG	E	107	1/1	0.99	0.02	25,25,25,25	0
6	SO4	B	202	5/5	0.99	0.04	48,50,63,75	0
6	SO4	A	201	5/5	0.99	0.04	36,43,58,72	0
9	CA	E	102	1/1	1.00	0.01	43,43,43,43	0
9	CA	E	103	1/1	1.00	0.01	43,43,43,43	0
9	CA	E	104	1/1	1.00	0.02	51,51,51,51	0
9	CA	E	105	1/1	1.00	0.01	37,37,37,37	0
9	CA	F	101	1/1	1.00	0.02	69,69,69,69	0
9	CA	F	102	1/1	1.00	0.01	63,63,63,63	0
9	CA	F	103	1/1	1.00	0.01	60,60,60,60	0
9	CA	L	101	1/1	1.00	0.01	51,51,51,51	0
9	CA	F	105	1/1	1.00	0.02	65,65,65,65	0
9	CA	R	102	1/1	1.00	0.01	68,68,68,68	0
9	CA	R	103	1/1	1.00	0.01	61,61,61,61	0
9	CA	R	104	1/1	1.00	0.02	64,64,64,64	0
9	CA	L	103	1/1	1.00	0.02	39,39,39,39	0
9	CA	R	106	1/1	1.00	0.01	86,86,86,86	0
10	MG	L	106	1/1	1.00	0.02	31,31,31,31	0
10	MG	L	107	1/1	1.00	0.02	35,35,35,35	0
10	MG	E	106	1/1	1.00	0.02	35,35,35,35	0
9	CA	L	104	1/1	1.00	0.01	40,40,40,40	0
10	MG	F	107	1/1	1.00	0.01	64,64,64,64	0
10	MG	R	107	1/1	1.00	0.02	54,54,54,54	0
9	CA	L	105	1/1	1.00	0.01	42,42,42,42	0
9	CA	E	101	1/1	1.00	0.03	39,39,39,39	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.

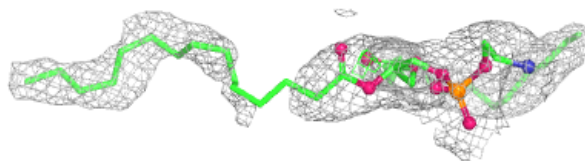
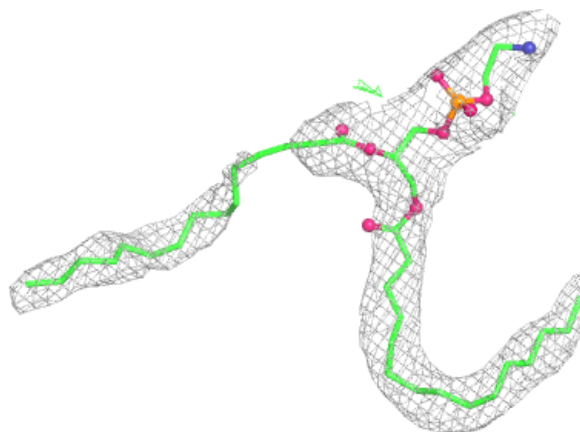


**Electron density around PTY A 203:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around PTY B 201:**

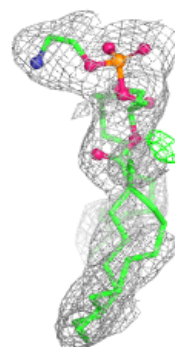
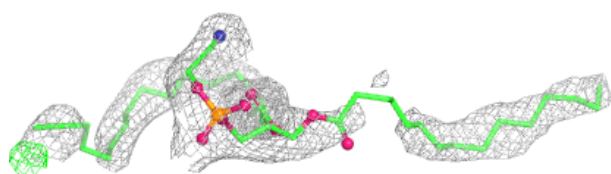
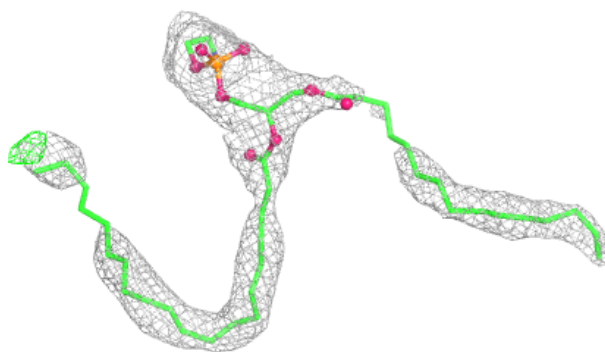
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



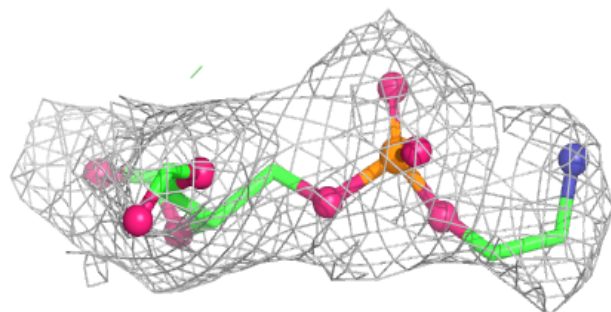
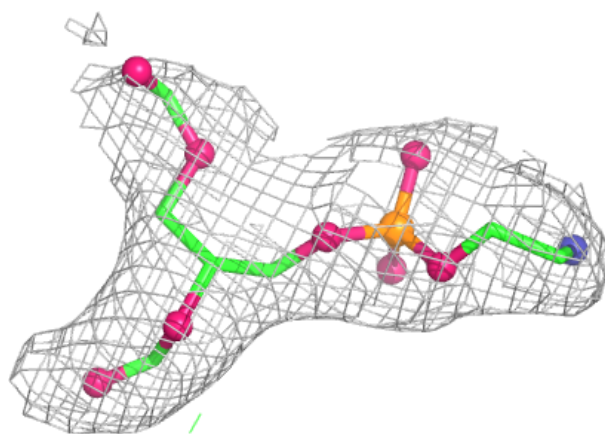


**Electron density around PTY C 202:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around PTY D 201:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.