



# wwPDB X-ray Structure Validation Summary Report

Dec 3, 2023 – 08:44 am GMT

PDB ID : 2W9L  
Title : CANINE ADENOVIRUS TYPE 2 FIBRE HEAD IN COMPLEX WITH CAR  
DOMAIN D1 AND SIALIC ACID  
Authors : Seiradake, E.; Henaff, D.; Wodrich, H.; Billet, O.; Perreau, M.; Hippert, C.;  
Mennechet, F.; Schoehn, G.; Lortat-Jacob, H.; Dreja, H.; Ibanes, S.; Kalatzis,  
V.; Wang, J.P.; Finberg, R.W.; Cusack, S.; Kremer, E.J.  
Deposited on : 2009-01-26  
Resolution : 2.91 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 : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

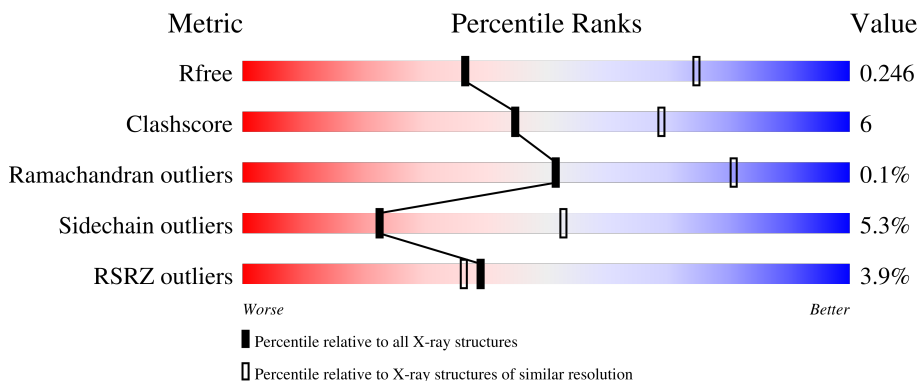
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.91 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	2307 (2.94-2.90)
Clashscore	141614	2531 (2.94-2.90)
Ramachandran outliers	138981	2462 (2.94-2.90)
Sidechain outliers	138945	2464 (2.94-2.90)
RSRZ outliers	127900	2248 (2.94-2.90)

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	124	 24% 74% 16% 6%
1	B	124	 23% 60% 31% 6%
1	G	124	 4% 78% 21% 6%
1	J	124	 7% 78% 20% 6%

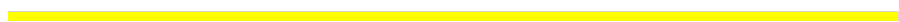


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Mol	Chain	Length	Quality of chain
1	K	124	 5% 72% 25% ..
1	O	124	 5% 71% 24% 5%
1	P	124	 7% 79% 18% ..
1	T	124	 2% 75% 17% . .
1	V	124	 15% 72% 23% ..
1	X	124	 3% 69% 27% ..
1	Y	124	 6% 77% 17% . .
1	Z	124	 10% 73% 19% . 6%
2	C	197	 79% 13% . 8%
2	D	197	 84% 8% 8%
2	E	197	 84% 8% . 8%
2	F	197	 83% 10% 8%
2	H	197	 82% 10% 8%
2	I	197	 84% 8% 8%
2	L	197	 81% 11% . 8%
2	M	197	 83% 9% . 8%
2	N	197	 82% 9% . 8%
2	Q	197	 83% 9% . 8%
2	R	197	 83% 9% 8%
2	S	197	 84% 9% 8%
3	U	2	 100%
3	W	2	 100%
3	a	2	 100%
3	c	2	 100%
3	d	2	 100%

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Mol	Chain	Length	Quality of chain
3	e	2	 100%
3	f	2	 100%
3	h	2	 100%
3	i	2	 100%
3	j	2	 100%
4	b	2	 100%
4	g	2	 100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GAL	U	1	X	-	-	-
3	GAL	W	1	X	-	-	X
3	GAL	d	1	X	-	-	-
3	GAL	e	1	X	-	-	-
3	GAL	f	1	X	-	-	-
3	GAL	h	1	X	-	-	-
3	GAL	i	1	X	-	-	-
3	GAL	j	1	X	-	-	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 28671 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 COXSACKIEVIRUS AND ADENOVIRUS RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	117	Total 914	C 581	N 147	O 183	S 3	0	0	0
1	B	117	Total 914	C 583	N 147	O 181	S 3	0	0	0
1	G	123	Total 959	C 611	N 156	O 189	S 3	0	0	0
1	J	123	Total 959	C 611	N 156	O 189	S 3	0	0	0
1	K	123	Total 963	C 615	N 156	O 189	S 3	0	0	0
1	O	118	Total 917	C 587	N 145	O 182	S 3	0	0	0
1	P	123	Total 959	C 611	N 156	O 189	S 3	0	0	0
1	T	119	Total 928	C 591	N 149	O 185	S 3	0	0	0
1	V	121	Total 944	C 600	N 154	O 187	S 3	0	0	0
1	X	123	Total 959	C 611	N 156	O 189	S 3	0	0	0
1	Y	119	Total 928	C 591	N 149	O 185	S 3	0	0	0
1	Z	117	Total 914	C 581	N 147	O 183	S 3	0	0	0

- Molecule 2 is a protein called FIBRE PROTEIN.

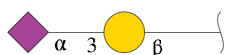
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	182	Total 1406	C 892	N 239	O 266	S 9	0	0	0
2	D	182	Total 1406	C 892	N 239	O 266	S 9	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	182	Total	C	N	O	S	0	0	0
			1406	892	239	266	9			
2	F	182	Total	C	N	O	S	0	0	0
			1406	892	239	266	9			
2	H	182	Total	C	N	O	S	0	0	0
			1406	892	239	266	9			
2	I	182	Total	C	N	O	S	0	0	0
			1406	892	239	266	9			
2	L	182	Total	C	N	O	S	0	0	0
			1406	892	239	266	9			
2	M	182	Total	C	N	O	S	0	0	0
			1406	892	239	266	9			
2	N	182	Total	C	N	O	S	0	0	0
			1406	892	239	266	9			
2	Q	182	Total	C	N	O	S	0	0	0
			1406	892	239	266	9			
2	R	182	Total	C	N	O	S	0	0	0
			1406	892	239	266	9			
2	S	182	Total	C	N	O	S	0	0	0
			1406	892	239	266	9			

- Molecule 3 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose.



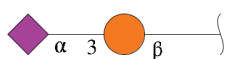
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	U	2	Total	C	N	O	0	0	0
			32	17	1	14			
3	W	2	Total	C	N	O	0	0	0
			32	17	1	14			
3	a	2	Total	C	N	O	0	0	0
			32	17	1	14			
3	c	2	Total	C	N	O	0	0	0
			32	17	1	14			
3	d	2	Total	C	N	O	0	0	0
			32	17	1	14			
3	e	2	Total	C	N	O	0	0	0
			32	17	1	14			
3	f	2	Total	C	N	O	0	0	0
			32	17	1	14			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	h	2	Total	C	N	O	0	0	0
			32	17	1	14			
3	i	2	Total	C	N	O	0	0	0
			32	17	1	14			
3	j	2	Total	C	N	O	0	0	0
			32	17	1	14			

- Molecule 4 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-gulopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	b	2	Total	C	N	O	0	0	0
			32	17	1	14			
4	g	2	Total	C	N	O	0	0	0
			32	17	1	14			

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	O	0	0
			2	2		
5	B	4	Total	O	0	0
			4	4		
5	C	5	Total	O	0	0
			5	5		
5	D	5	Total	O	0	0
			5	5		
5	E	4	Total	O	0	0
			4	4		
5	F	12	Total	O	0	0
			12	12		
5	G	9	Total	O	0	0
			9	9		
5	H	9	Total	O	0	0
			9	9		
5	I	10	Total	O	0	0
			10	10		
5	J	2	Total	O	0	0
			2	2		

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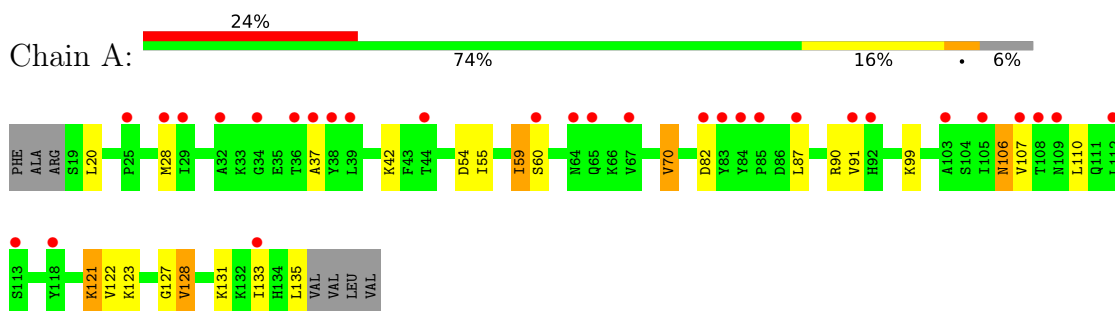
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
5	K	1	Total O 1 1	0	0
5	L	11	Total O 11 11	0	0
5	M	14	Total O 14 14	0	0
5	N	17	Total O 17 17	0	0
5	O	5	Total O 5 5	0	0
5	P	1	Total O 1 1	0	0
5	Q	13	Total O 13 13	0	0
5	R	10	Total O 10 10	0	0
5	S	7	Total O 7 7	0	0
5	T	5	Total O 5 5	0	0
5	V	1	Total O 1 1	0	0
5	X	3	Total O 3 3	0	0
5	Y	2	Total O 2 2	0	0
5	Z	5	Total O 5 5	0	0



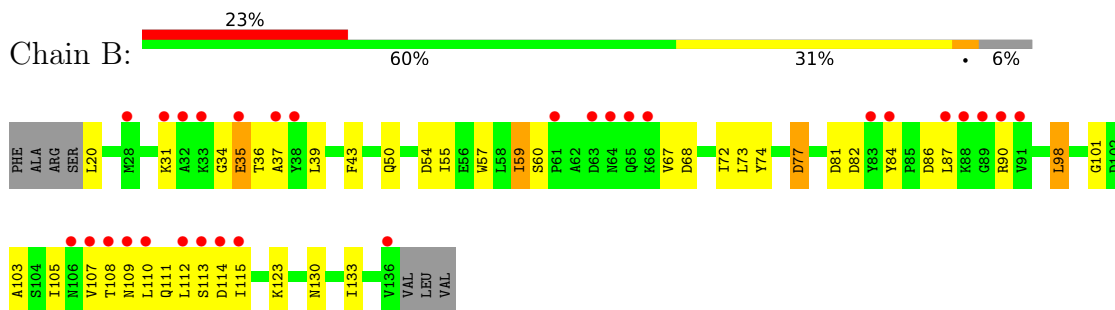
### 3 Residue-property plots [i](#)

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.

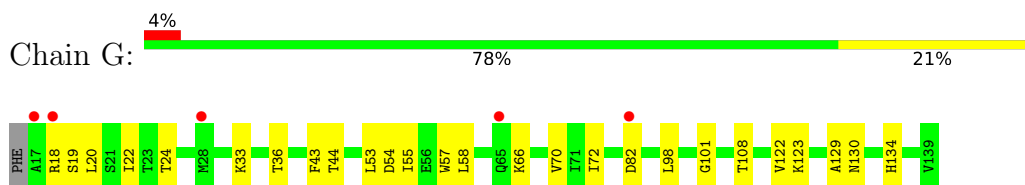
- Molecule 1: COXSACKIEVIRUS AND ADENOVIRUS RECEPTOR



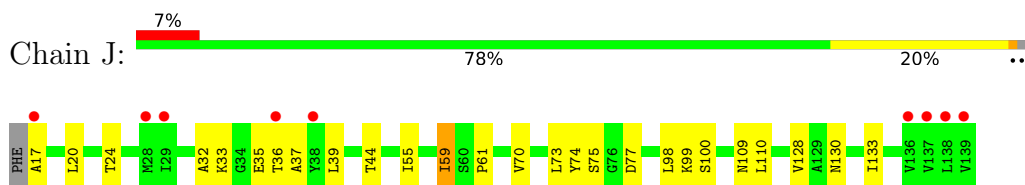
- Molecule 1: COXSACKIEVIRUS AND ADENOVIRUS RECEPTOR



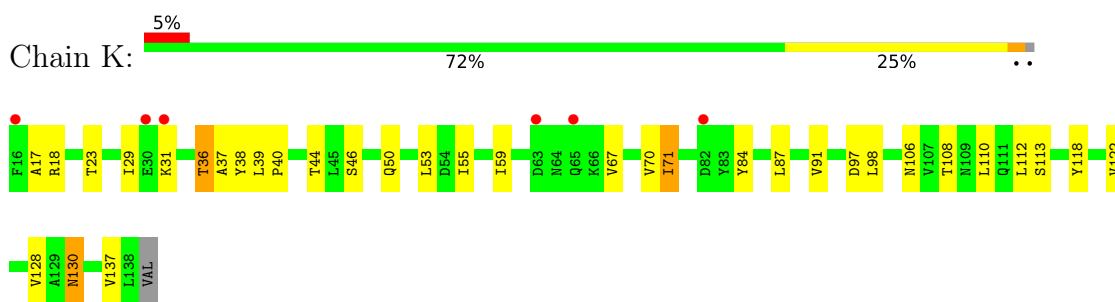
- Molecule 1: COXSACKIEVIRUS AND ADENOVIRUS RECEPTOR



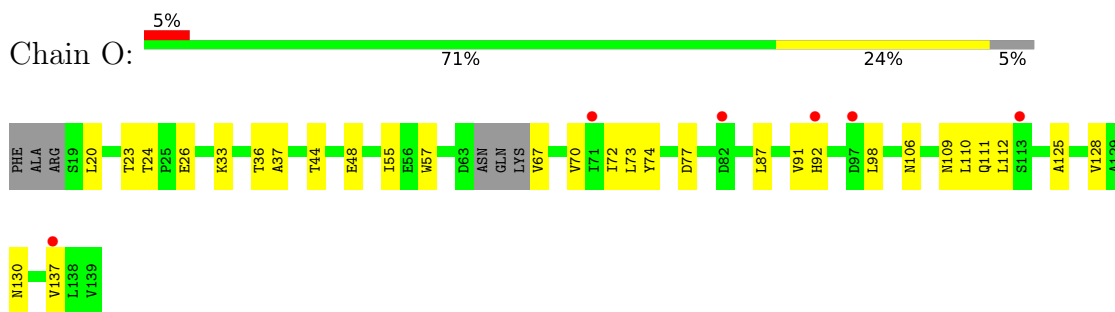
- Molecule 1: COXSACKIEVIRUS AND ADENOVIRUS RECEPTOR



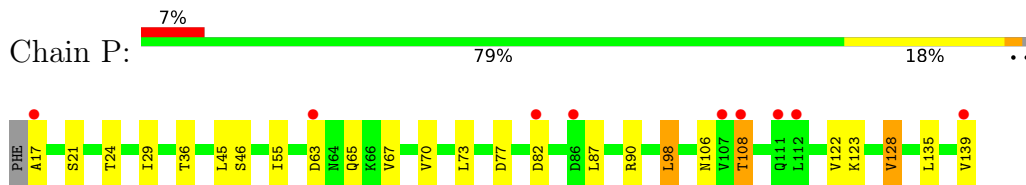
- Molecule 1: COXSACKIEVIRUS AND ADENOVIRUS RECEPTOR



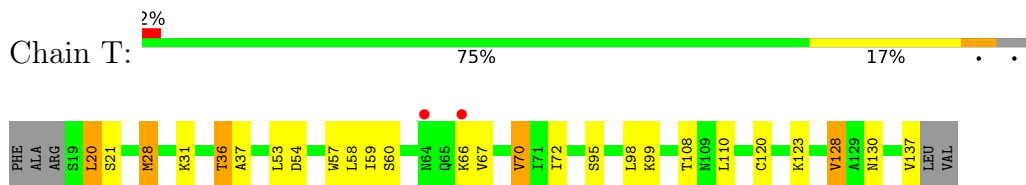
- Molecule 1: COXSACKIEVIRUS AND ADENOVIRUS RECEPTOR



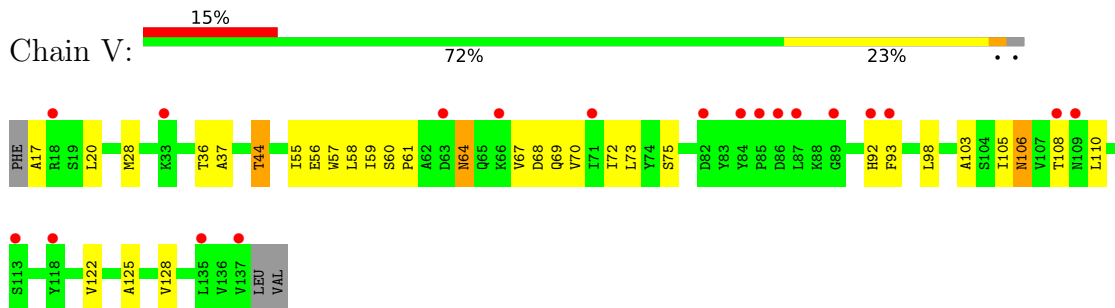
- Molecule 1: COXSACKIEVIRUS AND ADENOVIRUS RECEPTOR



- Molecule 1: COXSACKIEVIRUS AND ADENOVIRUS RECEPTOR



- Molecule 1: COXSACKIEVIRUS AND ADENOVIRUS RECEPTOR




- Molecule 1: COXSACKIEVIRUS AND ADENOVIRUS RECEPTOR






• Molecule 2: FIBRE PROTEIN

Chain F:  83% 10% 8%




• Molecule 2: FIBRE PROTEIN

Chain H:  82% 10% 8%




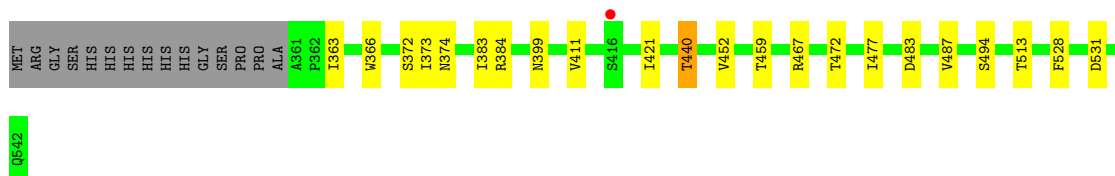
• Molecule 2: FIBRE PROTEIN

Chain I:  84% 8% 8%




• Molecule 2: FIBRE PROTEIN

Chain L:  81% 11% 8%




• Molecule 2: FIBRE PROTEIN

Chain M:  83% 9% 8%




• Molecule 2: FIBRE PROTEIN

Chain N:  82% 9% 8%



• Molecule 2: FIBRE PROTEIN

Chain Q:  83% 9% 8%



- Molecule 2: FIBRE PROTEIN

Chain R: 83% 9% 8%



- Molecule 2: FIBRE PROTEIN

Chain S: 84% 9% 8%



- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose

Chain U: 100%

GAL1  
SIA2

- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose

Chain W: 100%

GAL1  
SIA2

- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose

Chain a: 100%

GAL1  
SIA2

- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose

Chain c: 100%

GAL1  
SIA2

- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose

Chain d: 100%

GAL1  
SIA2

- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose

Chain e: 100%

GAL1  
SIA2

- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose

Chain f: 100%

GAL1  
SIA2

- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose

Chain h: 100%

GAL1  
SIA2

- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose

Chain i: 100%

GAL1  
SIA2

- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose

Chain j: 100%

GAL1  
SIA2

- Molecule 4: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-gulopyranose

Chain b: 100%

GL01  
SIA2

- Molecule 4: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-gulopyranose

Chain g: 100%

GL01  
SIA2

## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	221.15Å 221.15Å 391.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.63 – 2.91 49.61 – 2.91	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.63-2.91) 99.0 (49.61-2.91)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.15 (at 2.91Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.197 , 0.254 0.196 , 0.246	Depositor DCC
$R_{free}$ test set	1034 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.5	Xtrriage
Anisotropy	0.395	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 56.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	28671	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.13% 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: SIA, GL0, GAL

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	0.48	0/932	0.62	0/1264
1	B	0.56	0/932	0.75	0/1265
1	G	0.51	0/977	0.67	0/1326
1	J	0.49	0/977	0.66	0/1326
1	K	0.52	0/982	0.67	0/1332
1	O	0.52	0/934	0.61	0/1268
1	P	0.46	0/977	0.62	0/1326
1	T	0.45	0/946	0.64	0/1284
1	V	0.46	0/962	0.62	0/1305
1	X	0.49	0/977	0.63	0/1326
1	Y	0.53	0/946	0.63	0/1284
1	Z	0.49	0/932	0.63	0/1264
2	C	0.55	1/1441 (0.1%)	0.68	0/1964
2	D	0.49	0/1441	0.66	0/1964
2	E	0.49	0/1441	0.63	0/1964
2	F	0.53	0/1441	0.65	0/1964
2	H	0.52	0/1441	0.65	0/1964
2	I	0.48	0/1441	0.63	0/1964
2	L	0.50	0/1441	0.66	0/1964
2	M	0.52	0/1441	0.66	0/1964
2	N	0.54	0/1441	0.67	0/1964
2	Q	0.49	0/1441	0.65	0/1964
2	R	0.53	0/1441	0.66	0/1964
2	S	0.49	0/1441	0.65	0/1964
All	All	0.51	1/28766 (0.0%)	0.65	0/39138

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	G	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	388	CYS	CB-SG	-6.00	1.72	1.82

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	82	ASP	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	914	0	910	21	0
1	B	914	0	914	55	0
1	G	959	0	966	13	0
1	J	959	0	966	18	0
1	K	963	0	966	19	0
1	O	917	0	920	15	0
1	P	959	0	966	18	0
1	T	928	0	928	20	0
1	V	944	0	946	23	0
1	X	959	0	966	20	0
1	Y	928	0	928	13	0
1	Z	914	0	910	19	0
2	C	1406	0	1382	16	0
2	D	1406	0	1382	10	0
2	E	1406	0	1382	15	0
2	F	1406	0	1382	11	0
2	H	1406	0	1382	16	0
2	I	1406	0	1382	18	0
2	L	1406	0	1382	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	M	1406	0	1382	10	0
2	N	1406	0	1382	20	0
2	Q	1406	0	1382	13	0
2	R	1406	0	1382	14	0
2	S	1406	0	1382	16	0
3	U	32	0	27	0	0
3	W	32	0	27	0	0
3	a	32	0	28	0	0
3	c	32	0	28	0	0
3	d	32	0	27	0	0
3	e	32	0	27	0	0
3	f	32	0	27	0	0
3	h	32	0	27	0	0
3	i	32	0	27	0	0
3	j	32	0	27	0	0
4	b	32	0	27	0	0
4	g	32	0	28	0	0
5	A	2	0	0	0	0
5	B	4	0	0	1	0
5	C	5	0	0	0	0
5	D	5	0	0	2	0
5	E	4	0	0	2	0
5	F	12	0	0	3	0
5	G	9	0	0	3	0
5	H	9	0	0	1	0
5	I	10	0	0	1	0
5	J	2	0	0	1	0
5	K	1	0	0	1	0
5	L	11	0	0	3	0
5	M	14	0	0	0	0
5	N	17	0	0	4	0
5	O	5	0	0	0	0
5	P	1	0	0	0	0
5	Q	13	0	0	7	0
5	R	10	0	0	2	0
5	S	7	0	0	0	0
5	T	5	0	0	2	0
5	V	1	0	0	0	0
5	X	3	0	0	1	0
5	Y	2	0	0	0	0
5	Z	5	0	0	2	0
All	All	28671	0	28197	365	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 365 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:458:HIS:CD2	5:N:703:HOH:O	1.84	1.27
1:X:28:MET:HB3	5:X:203:HOH:O	1.48	1.14
1:B:90:ARG:HD2	1:B:108:THR:O	1.48	1.10
2:Q:467:ARG:HD2	5:Q:713:HOH:O	1.51	1.09
2:I:373:ILE:HD11	1:P:70:VAL:HG21	1.10	1.08

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	115/124 (93%)	104 (90%)	11 (10%)	0	100	100
1	B	115/124 (93%)	104 (90%)	10 (9%)	1 (1%)	17	46
1	G	121/124 (98%)	110 (91%)	11 (9%)	0	100	100
1	J	121/124 (98%)	113 (93%)	8 (7%)	0	100	100
1	K	121/124 (98%)	107 (88%)	14 (12%)	0	100	100
1	O	114/124 (92%)	106 (93%)	8 (7%)	0	100	100
1	P	121/124 (98%)	111 (92%)	8 (7%)	2 (2%)	9	29
1	T	117/124 (94%)	104 (89%)	13 (11%)	0	100	100
1	V	119/124 (96%)	113 (95%)	6 (5%)	0	100	100
1	X	121/124 (98%)	116 (96%)	5 (4%)	0	100	100
1	Y	117/124 (94%)	113 (97%)	4 (3%)	0	100	100
1	Z	115/124 (93%)	104 (90%)	10 (9%)	1 (1%)	17	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	180/197 (91%)	171 (95%)	9 (5%)	0	100	100
2	D	180/197 (91%)	172 (96%)	8 (4%)	0	100	100
2	E	180/197 (91%)	171 (95%)	9 (5%)	0	100	100
2	F	180/197 (91%)	169 (94%)	11 (6%)	0	100	100
2	H	180/197 (91%)	170 (94%)	10 (6%)	0	100	100
2	I	180/197 (91%)	172 (96%)	8 (4%)	0	100	100
2	L	180/197 (91%)	171 (95%)	9 (5%)	0	100	100
2	M	180/197 (91%)	170 (94%)	10 (6%)	0	100	100
2	N	180/197 (91%)	171 (95%)	9 (5%)	0	100	100
2	Q	180/197 (91%)	171 (95%)	9 (5%)	0	100	100
2	R	180/197 (91%)	170 (94%)	10 (6%)	0	100	100
2	S	180/197 (91%)	170 (94%)	10 (6%)	0	100	100
All	All	3577/3852 (93%)	3353 (94%)	220 (6%)	4 (0%)	51	81

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	35	GLU
1	P	63	ASP
1	Z	65	GLN
1	P	24	THR

### 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	104/110 (94%)	95 (91%)	9 (9%)	10	29
1	B	104/110 (94%)	98 (94%)	6 (6%)	20	48
1	G	109/110 (99%)	103 (94%)	6 (6%)	21	51
1	J	109/110 (99%)	101 (93%)	8 (7%)	14	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	109/110 (99%)	96 (88%)	13 (12%)	5	14
1	O	105/110 (96%)	95 (90%)	10 (10%)	8	24
1	P	109/110 (99%)	99 (91%)	10 (9%)	9	26
1	T	106/110 (96%)	97 (92%)	9 (8%)	10	30
1	V	107/110 (97%)	101 (94%)	6 (6%)	21	50
1	X	109/110 (99%)	100 (92%)	9 (8%)	11	30
1	Y	106/110 (96%)	99 (93%)	7 (7%)	16	42
1	Z	104/110 (94%)	95 (91%)	9 (9%)	10	29
2	C	159/171 (93%)	150 (94%)	9 (6%)	20	49
2	D	159/171 (93%)	154 (97%)	5 (3%)	40	72
2	E	159/171 (93%)	153 (96%)	6 (4%)	33	65
2	F	159/171 (93%)	151 (95%)	8 (5%)	24	55
2	H	159/171 (93%)	156 (98%)	3 (2%)	57	83
2	I	159/171 (93%)	157 (99%)	2 (1%)	69	89
2	L	159/171 (93%)	152 (96%)	7 (4%)	28	60
2	M	159/171 (93%)	150 (94%)	9 (6%)	20	49
2	N	159/171 (93%)	153 (96%)	6 (4%)	33	65
2	Q	159/171 (93%)	155 (98%)	4 (2%)	47	77
2	R	159/171 (93%)	155 (98%)	4 (2%)	47	77
2	S	159/171 (93%)	156 (98%)	3 (2%)	57	83
All	All	3189/3372 (95%)	3021 (95%)	168 (5%)	22	53

5 of 168 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	108	THR
1	X	23	THR
2	Q	416	SER
1	T	36	THR
1	X	98	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
1	O	50	GLN
2	Q	429	GLN
1	X	134	HIS
1	O	111	GLN
1	P	65	GLN

### 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](#)

24 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	GAL	U	1	3	12,12,12	0.83	0	17,17,17	2.50	5 (29%)
3	SIA	U	2	3	20,20,21	0.68	0	24,28,31	1.32	3 (12%)
3	GAL	W	1	3	12,12,12	0.82	0	17,17,17	2.41	4 (23%)
3	SIA	W	2	3	20,20,21	0.67	0	24,28,31	1.26	3 (12%)
3	GAL	a	1	3	12,12,12	0.72	0	17,17,17	1.11	1 (5%)
3	SIA	a	2	3	20,20,21	0.73	0	24,28,31	1.58	6 (25%)
4	GL0	b	1	4	12,12,12	1.10	1 (8%)	17,17,17	2.96	5 (29%)
4	SIA	b	2	4	20,20,21	0.61	0	24,28,31	1.17	1 (4%)
3	GAL	c	1	3	12,12,12	0.50	0	17,17,17	1.23	1 (5%)
3	SIA	c	2	3	20,20,21	0.69	0	24,28,31	1.30	3 (12%)
3	GAL	d	1	3	12,12,12	0.69	0	17,17,17	2.06	4 (23%)
3	SIA	d	2	3	20,20,21	0.62	0	24,28,31	1.36	3 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GAL	e	1	3	12,12,12	0.97	0	17,17,17	2.85	3 (17%)
3	SIA	e	2	3	20,20,21	0.90	0	24,28,31	1.21	3 (12%)
3	GAL	f	1	3	12,12,12	0.86	0	17,17,17	2.38	6 (35%)
3	SIA	f	2	3	20,20,21	0.83	1 (5%)	24,28,31	1.58	5 (20%)
4	GL0	g	1	4	12,12,12	0.76	0	17,17,17	2.39	5 (29%)
4	SIA	g	2	4	20,20,21	0.76	0	24,28,31	1.55	5 (20%)
3	GAL	h	1	3	12,12,12	0.73	0	17,17,17	2.40	5 (29%)
3	SIA	h	2	3	20,20,21	0.78	1 (5%)	24,28,31	1.31	3 (12%)
3	GAL	i	1	3	12,12,12	0.76	0	17,17,17	2.56	4 (23%)
3	SIA	i	2	3	20,20,21	0.78	1 (5%)	24,28,31	1.52	4 (16%)
3	GAL	j	1	3	12,12,12	0.98	1 (8%)	17,17,17	2.33	5 (29%)
3	SIA	j	2	3	20,20,21	0.76	1 (5%)	24,28,31	1.17	3 (12%)

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	GAL	U	1	3	1/1/5/5	2/2/22/22	0/1/1/1
3	SIA	U	2	3	-	3/18/34/38	0/1/1/1
3	GAL	W	1	3	1/1/5/5	0/2/22/22	0/1/1/1
3	SIA	W	2	3	-	3/18/34/38	0/1/1/1
3	GAL	a	1	3	-	2/2/22/22	0/1/1/1
3	SIA	a	2	3	-	3/18/34/38	0/1/1/1
4	GL0	b	1	4	-	0/2/22/22	0/1/1/1
4	SIA	b	2	4	-	0/18/34/38	0/1/1/1
3	GAL	c	1	3	-	2/2/22/22	0/1/1/1
3	SIA	c	2	3	-	4/18/34/38	0/1/1/1
3	GAL	d	1	3	1/1/5/5	2/2/22/22	0/1/1/1
3	SIA	d	2	3	-	0/18/34/38	0/1/1/1
3	GAL	e	1	3	1/1/5/5	2/2/22/22	0/1/1/1
3	SIA	e	2	3	-	3/18/34/38	0/1/1/1
3	GAL	f	1	3	1/1/5/5	2/2/22/22	0/1/1/1
3	SIA	f	2	3	-	1/18/34/38	0/1/1/1
4	GL0	g	1	4	-	2/2/22/22	0/1/1/1
4	SIA	g	2	4	-	5/18/34/38	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GAL	h	1	3	1/1/5/5	2/2/22/22	0/1/1/1
3	SIA	h	2	3	-	0/18/34/38	0/1/1/1
3	GAL	i	1	3	1/1/5/5	0/2/22/22	0/1/1/1
3	SIA	i	2	3	-	5/18/34/38	0/1/1/1
3	GAL	j	1	3	1/1/5/5	1/2/22/22	0/1/1/1
3	SIA	j	2	3	-	3/18/34/38	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	j	1	GAL	O3-C3	2.49	1.48	1.43
3	h	2	SIA	C2-C1	-2.38	1.50	1.52
3	f	2	SIA	C4-C5	-2.29	1.51	1.53
3	j	2	SIA	C2-C1	-2.17	1.50	1.52
4	b	1	GL0	O3-C3	-2.15	1.37	1.43

The worst 5 of 90 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	e	1	GAL	O3-C3-C4	8.95	131.04	110.35
4	b	1	GL0	O3-C3-C2	8.03	128.91	110.35
3	W	1	GAL	O3-C3-C4	7.27	127.15	110.35
3	U	1	GAL	O3-C3-C4	6.48	125.33	110.35
3	h	1	GAL	O3-C3-C2	6.37	125.07	110.35

5 of 8 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	U	1	GAL	C3
3	W	1	GAL	C3
3	d	1	GAL	C3
3	e	1	GAL	C3
3	f	1	GAL	C3

5 of 47 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	a	2	SIA	O8-C8-C9-O9
3	c	2	SIA	O1A-C1-C2-O6
3	e	2	SIA	O1A-C1-C2-O6
3	i	2	SIA	O1A-C1-C2-O6

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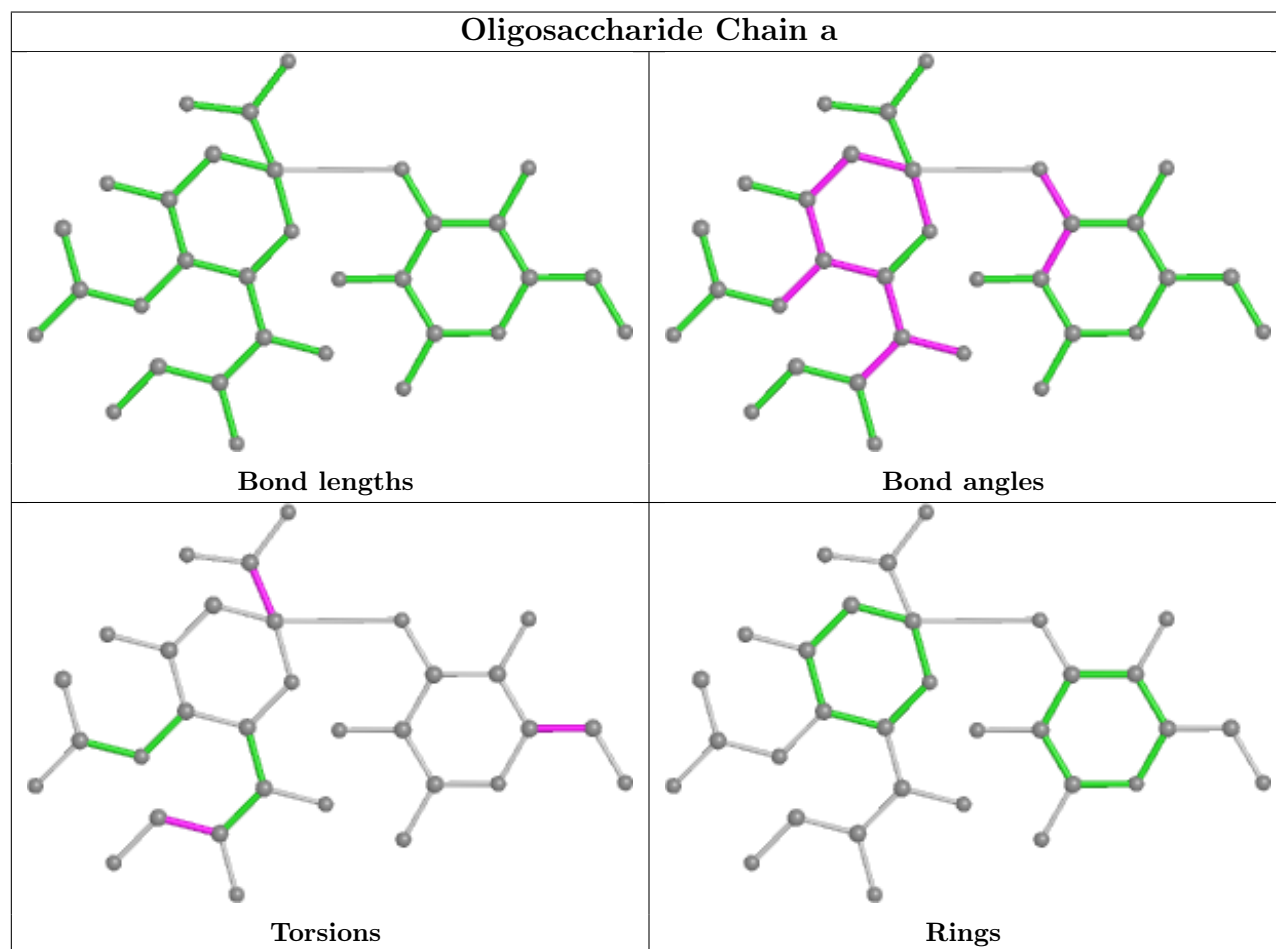
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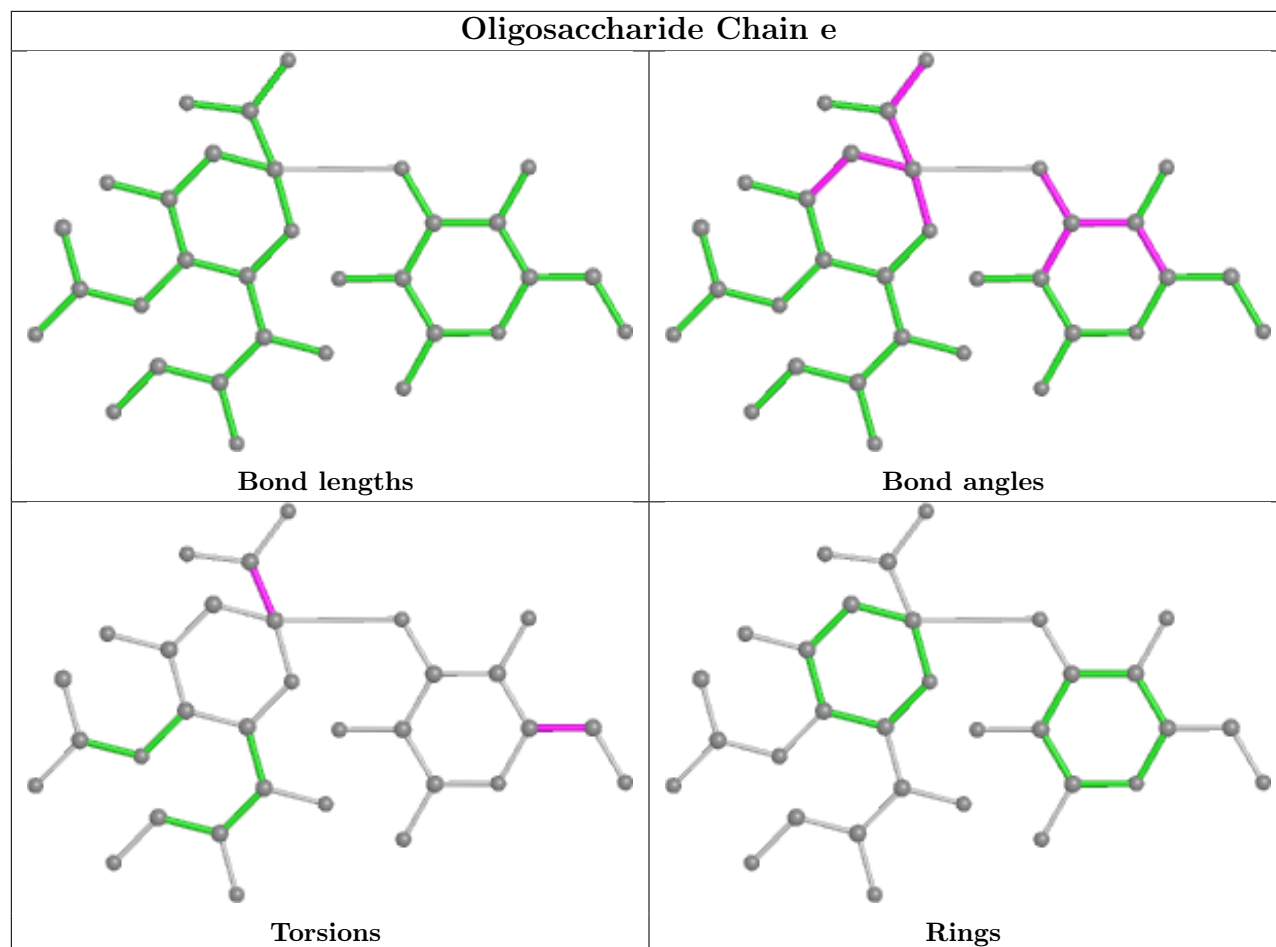
Mol	Chain	Res	Type	Atoms
3	j	2	SIA	O1A-C1-C2-C3

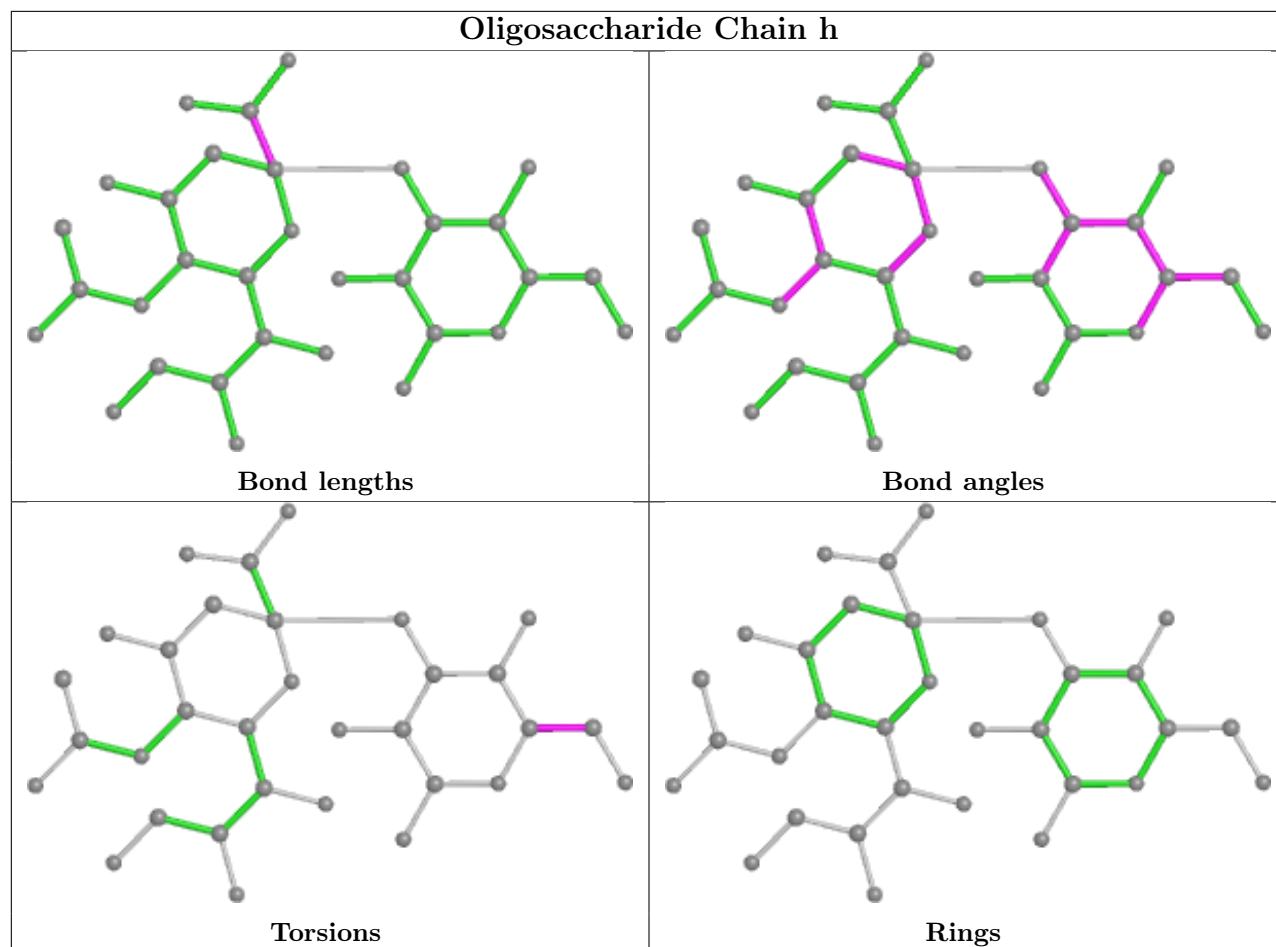
There are no ring outliers.

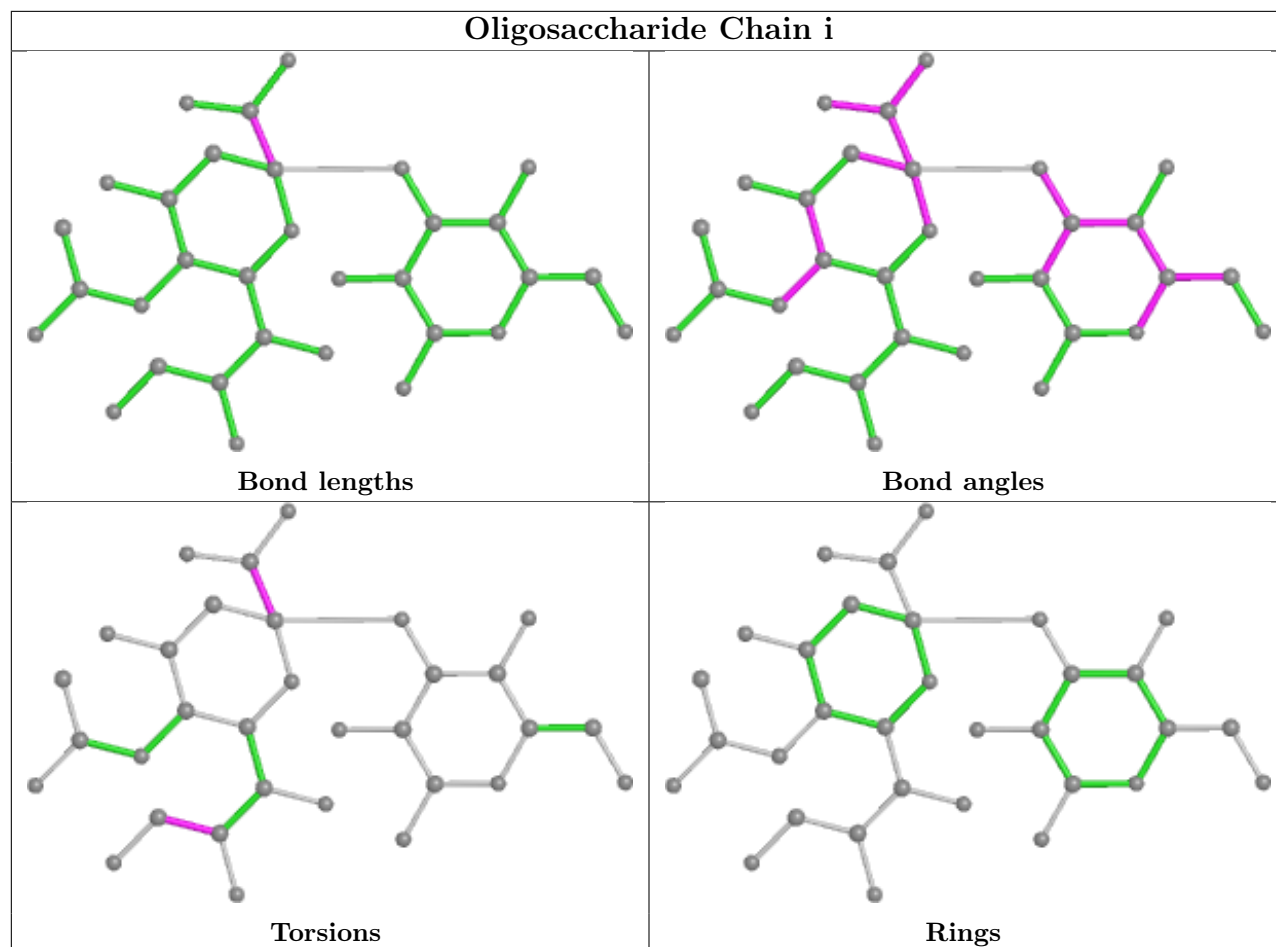
No monomer is involved in short contacts.

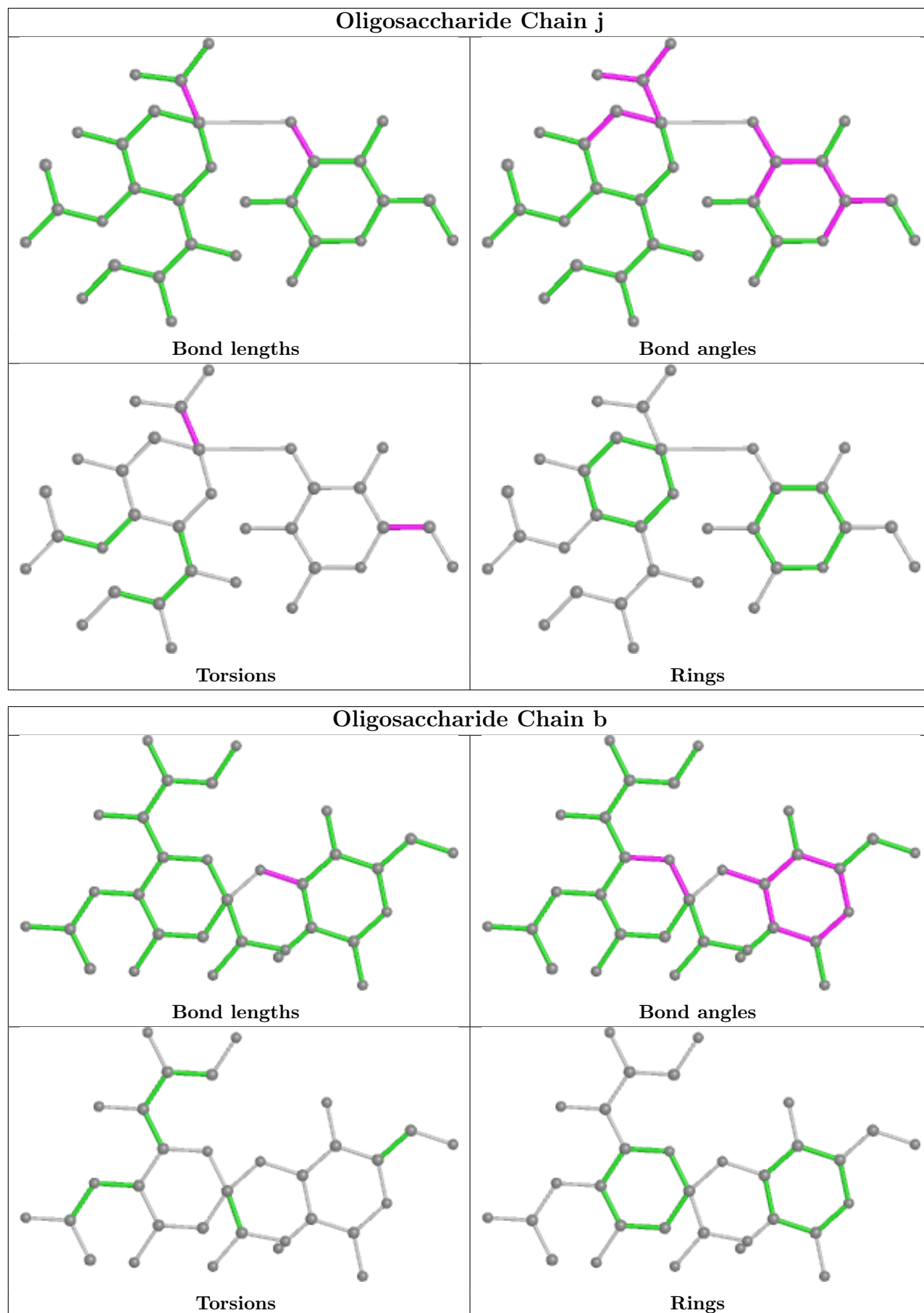
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

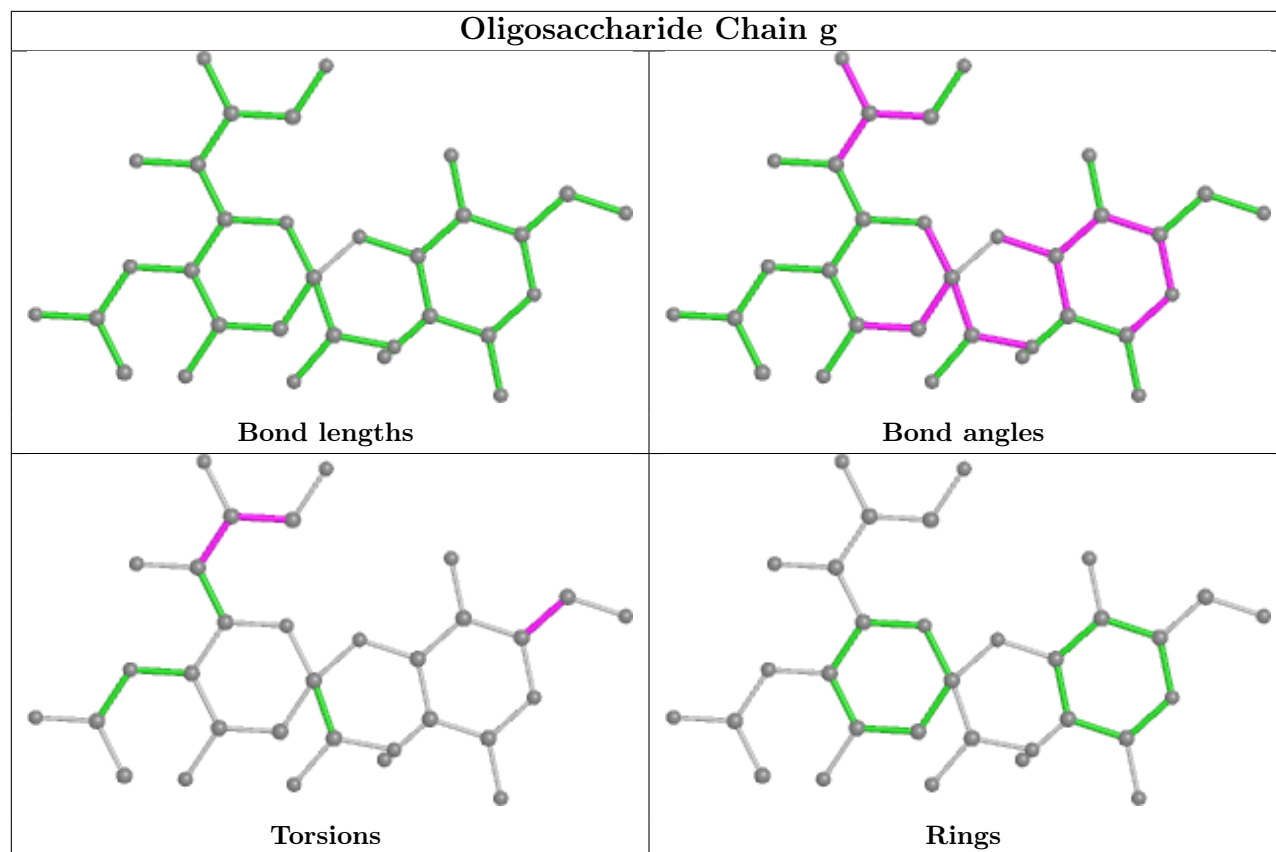












## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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	117/124 (94%)	1.27	30 (25%) 0 0	36, 40, 43, 44	0
1	B	117/124 (94%)	1.23	29 (24%) 0 0	27, 34, 40, 42	0
1	G	123/124 (99%)	0.26	5 (4%) 37 34	35, 40, 44, 47	0
1	J	123/124 (99%)	0.54	9 (7%) 15 12	35, 40, 44, 47	0
1	K	123/124 (99%)	0.44	6 (4%) 29 26	35, 40, 44, 48	0
1	O	118/124 (95%)	0.58	6 (5%) 28 24	37, 40, 43, 43	0
1	P	123/124 (99%)	0.79	9 (7%) 15 12	36, 40, 43, 46	0
1	T	119/124 (95%)	0.53	2 (1%) 70 70	37, 40, 43, 45	0
1	V	121/124 (97%)	0.75	19 (15%) 2 1	36, 40, 43, 47	0
1	X	123/124 (99%)	0.41	4 (3%) 46 42	36, 40, 44, 47	0
1	Y	119/124 (95%)	0.52	8 (6%) 17 14	35, 40, 43, 45	0
1	Z	117/124 (94%)	0.76	13 (11%) 5 4	37, 40, 43, 44	0
2	C	182/197 (92%)	-0.11	0 100 100	38, 40, 42, 46	0
2	D	182/197 (92%)	-0.13	0 100 100	39, 40, 42, 44	0
2	E	182/197 (92%)	-0.18	0 100 100	38, 40, 42, 44	0
2	F	182/197 (92%)	-0.21	0 100 100	39, 40, 42, 47	0
2	H	182/197 (92%)	-0.17	0 100 100	39, 40, 42, 46	0
2	I	182/197 (92%)	-0.17	0 100 100	39, 40, 42, 44	0
2	L	182/197 (92%)	-0.06	1 (0%) 91 91	39, 40, 42, 45	0
2	M	182/197 (92%)	-0.15	0 100 100	39, 40, 41, 44	0
2	N	182/197 (92%)	-0.21	0 100 100	39, 40, 42, 47	0
2	Q	182/197 (92%)	-0.05	0 100 100	39, 40, 42, 45	0
2	R	182/197 (92%)	-0.19	0 100 100	39, 40, 42, 45	0
2	S	182/197 (92%)	-0.12	0 100 100	39, 40, 42, 45	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	3627/3852 (94%)	0.18	141 (3%) 39 36	27, 40, 43, 48	0

The worst 5 of 141 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	109	ASN	8.2
1	B	32	ALA	6.1
1	B	136	VAL	6.0
1	B	65	GLN	5.1
1	B	112	LEU	5.0

## 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
3	GAL	W	1	12/12	0.65	0.42	58,68,69,69	0
3	GAL	e	1	12/12	0.70	0.29	50,59,60,61	0
3	GAL	i	1	12/12	0.80	0.25	48,57,59,60	0
3	GAL	h	1	12/12	0.81	0.26	53,61,64,65	0
3	GAL	d	1	12/12	0.82	0.28	50,60,64,65	0
3	GAL	f	1	12/12	0.82	0.21	45,52,56,56	0
3	GAL	j	1	12/12	0.82	0.25	54,62,63,64	0
3	GAL	U	1	12/12	0.86	0.26	45,53,54,55	0
3	GAL	a	1	12/12	0.88	0.29	48,53,54,54	0
4	GL0	b	1	12/12	0.88	0.29	51,60,63,63	0
4	GL0	g	1	12/12	0.88	0.19	43,51,56,58	0
3	GAL	c	1	12/12	0.89	0.23	46,51,53,54	0
3	SIA	W	2	20/21	0.94	0.27	41,46,54,54	0
3	SIA	f	2	20/21	0.95	0.19	31,34,39,40	0
3	SIA	j	2	20/21	0.95	0.19	42,44,49,49	0
3	SIA	e	2	20/21	0.95	0.24	36,39,43,44	0
3	SIA	c	2	20/21	0.95	0.20	33,38,41,41	0

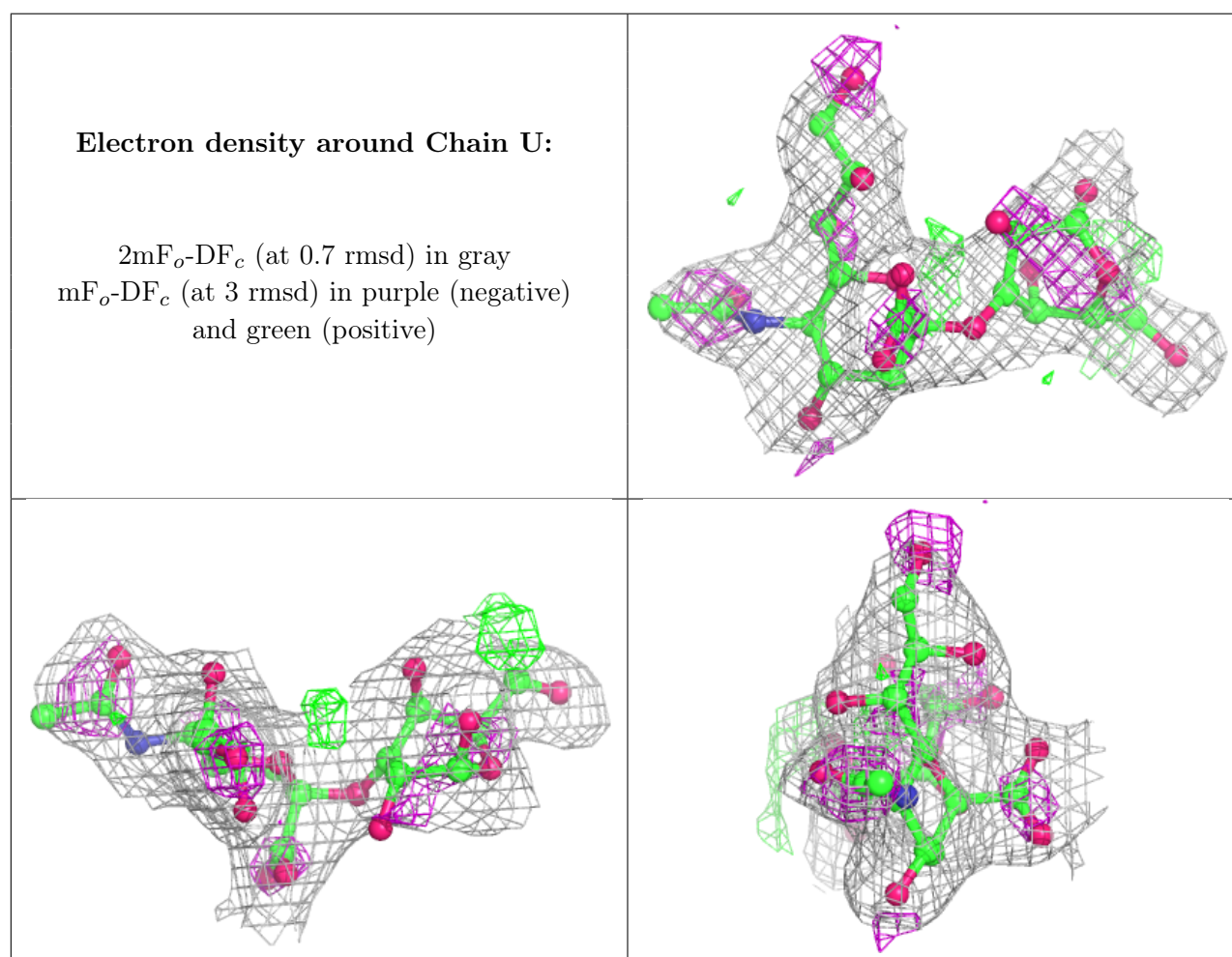
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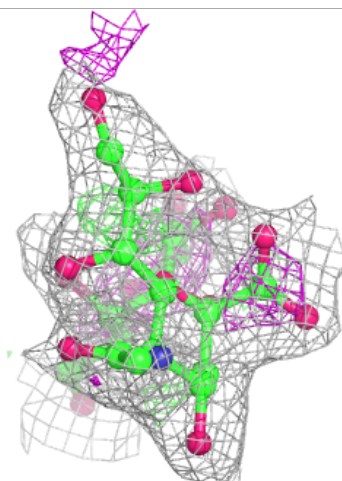
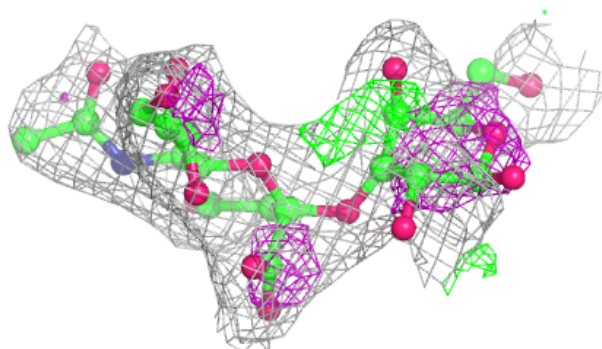
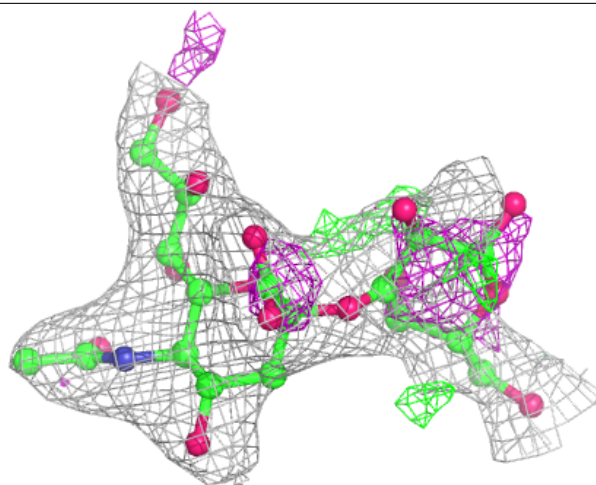
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	SIA	g	2	20/21	0.95	0.14	31,35,38,38	0
3	SIA	a	2	20/21	0.96	0.20	32,40,42,42	0
3	SIA	U	2	20/21	0.96	0.22	34,37,39,39	0
3	SIA	h	2	20/21	0.96	0.20	38,42,48,48	0
4	SIA	b	2	20/21	0.96	0.20	36,40,45,45	0
3	SIA	d	2	20/21	0.96	0.18	31,36,43,43	0
3	SIA	i	2	20/21	0.96	0.14	31,37,43,45	0

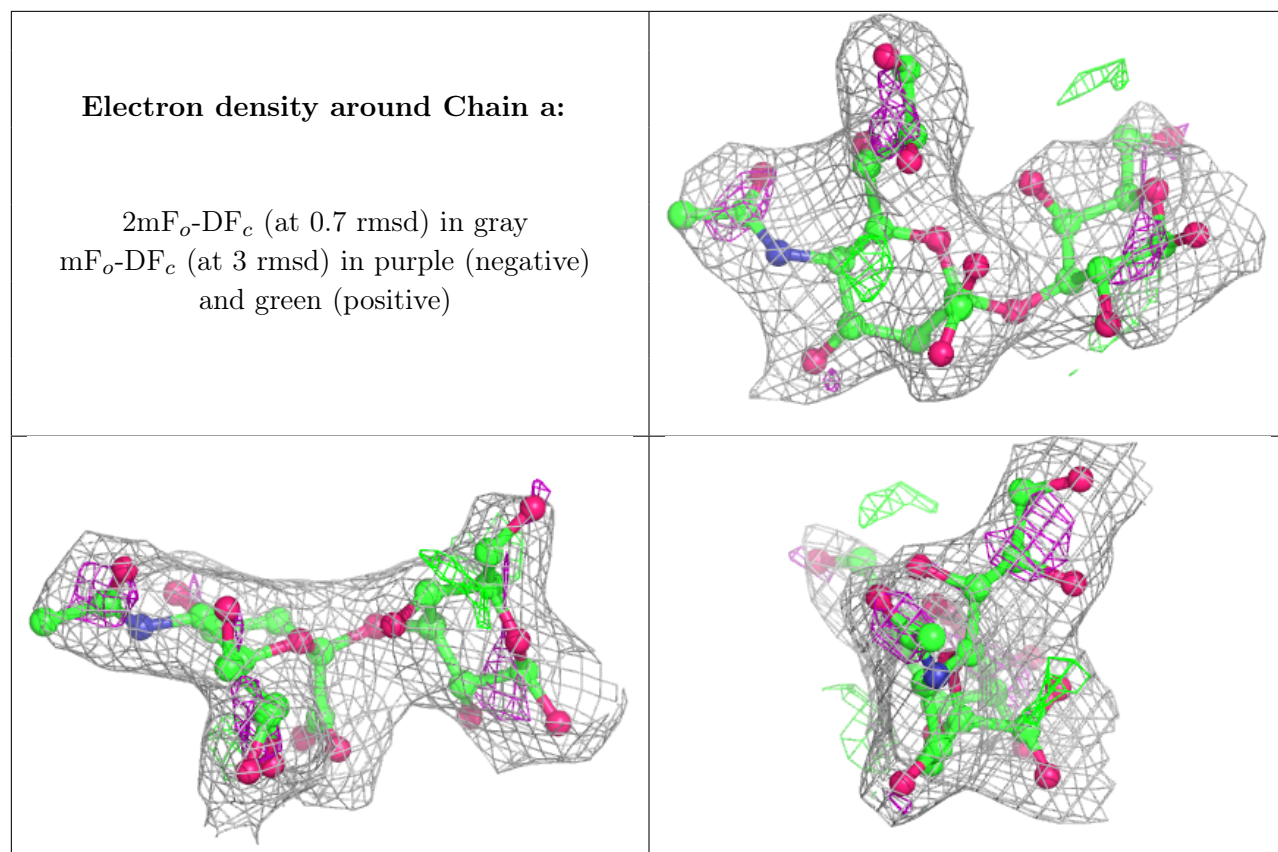
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



**Electron density around Chain W:**

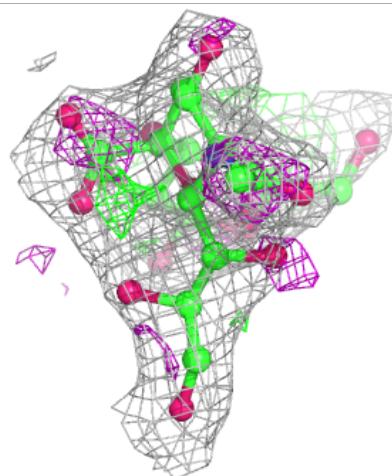
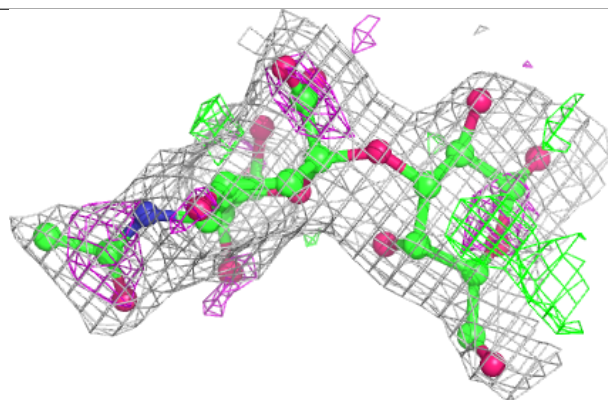
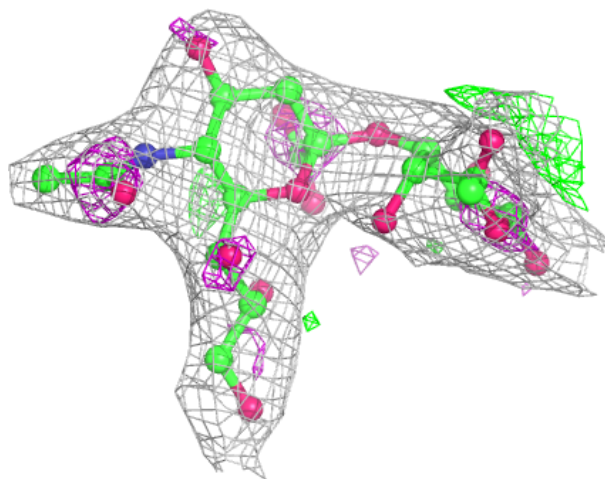
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





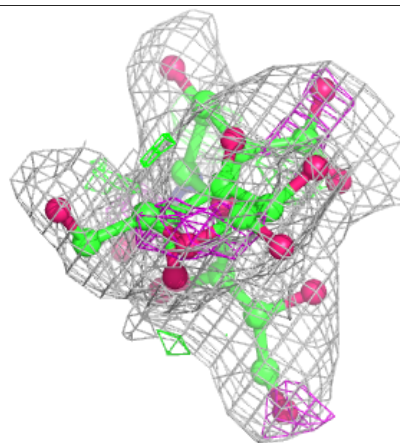
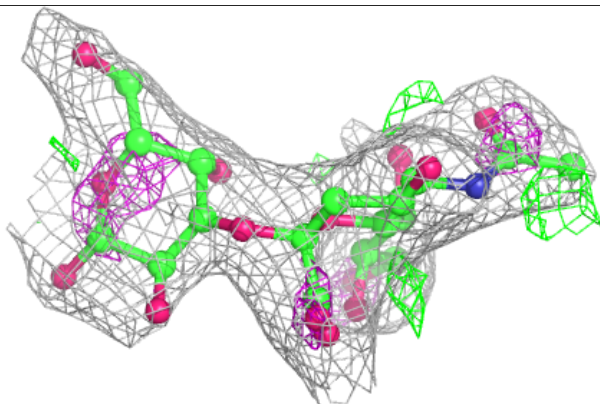
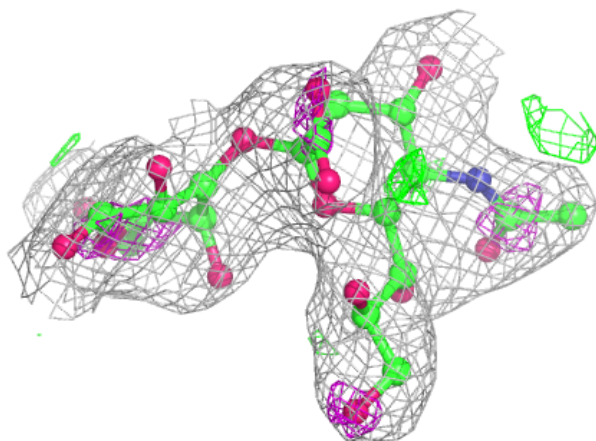
**Electron density around Chain c:**

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



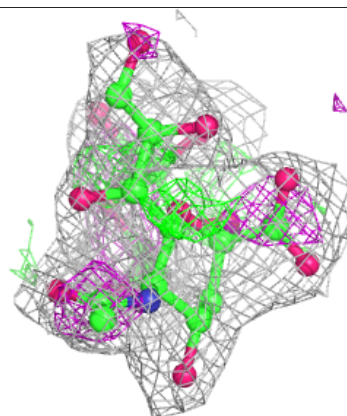
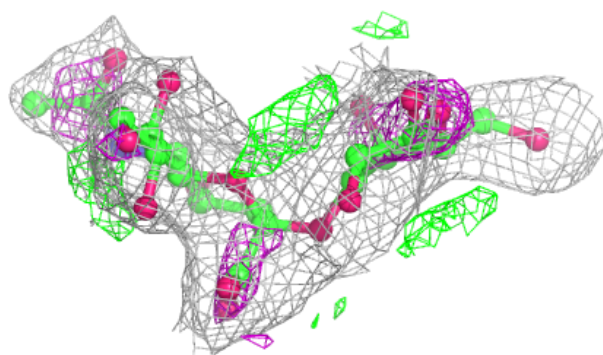
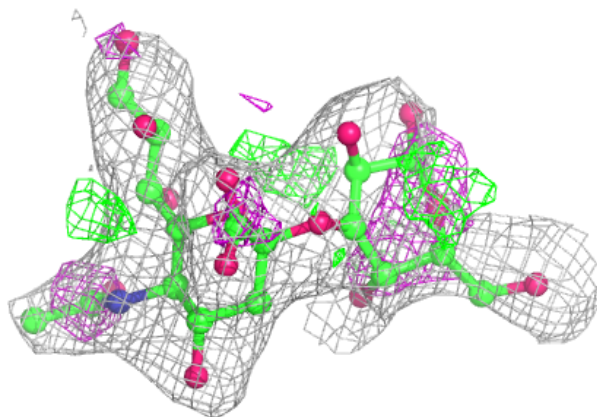
**Electron density around Chain d:**

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



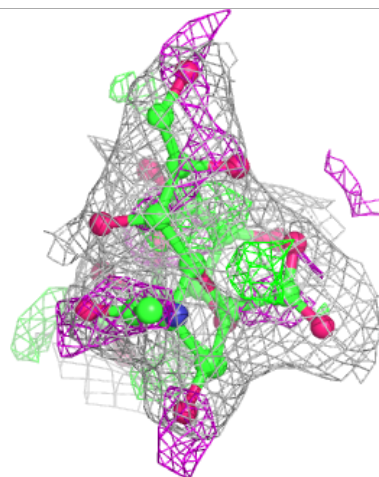
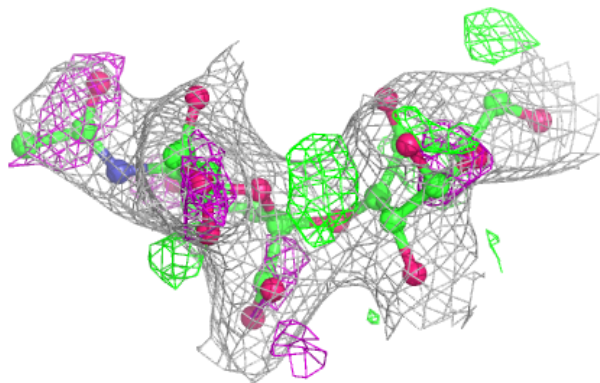
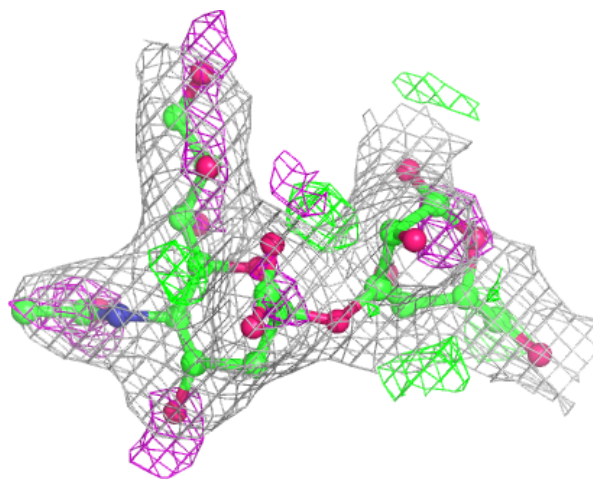
**Electron density around Chain e:**

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



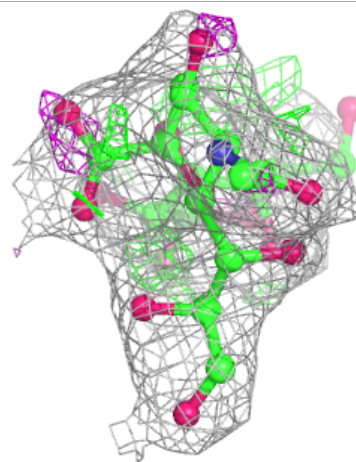
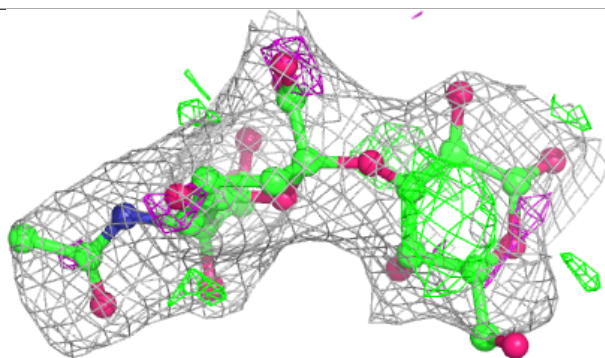
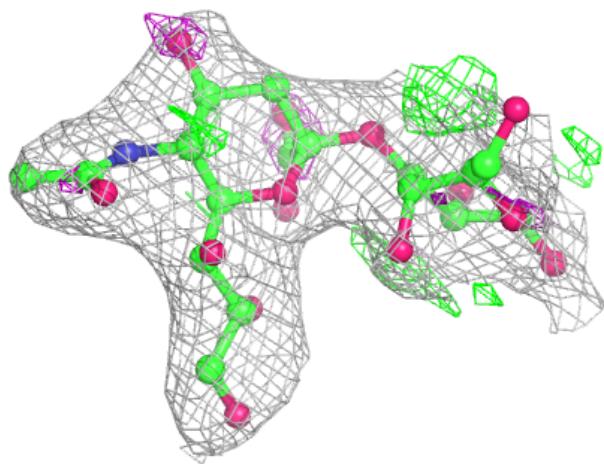
**Electron density around Chain f:**

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

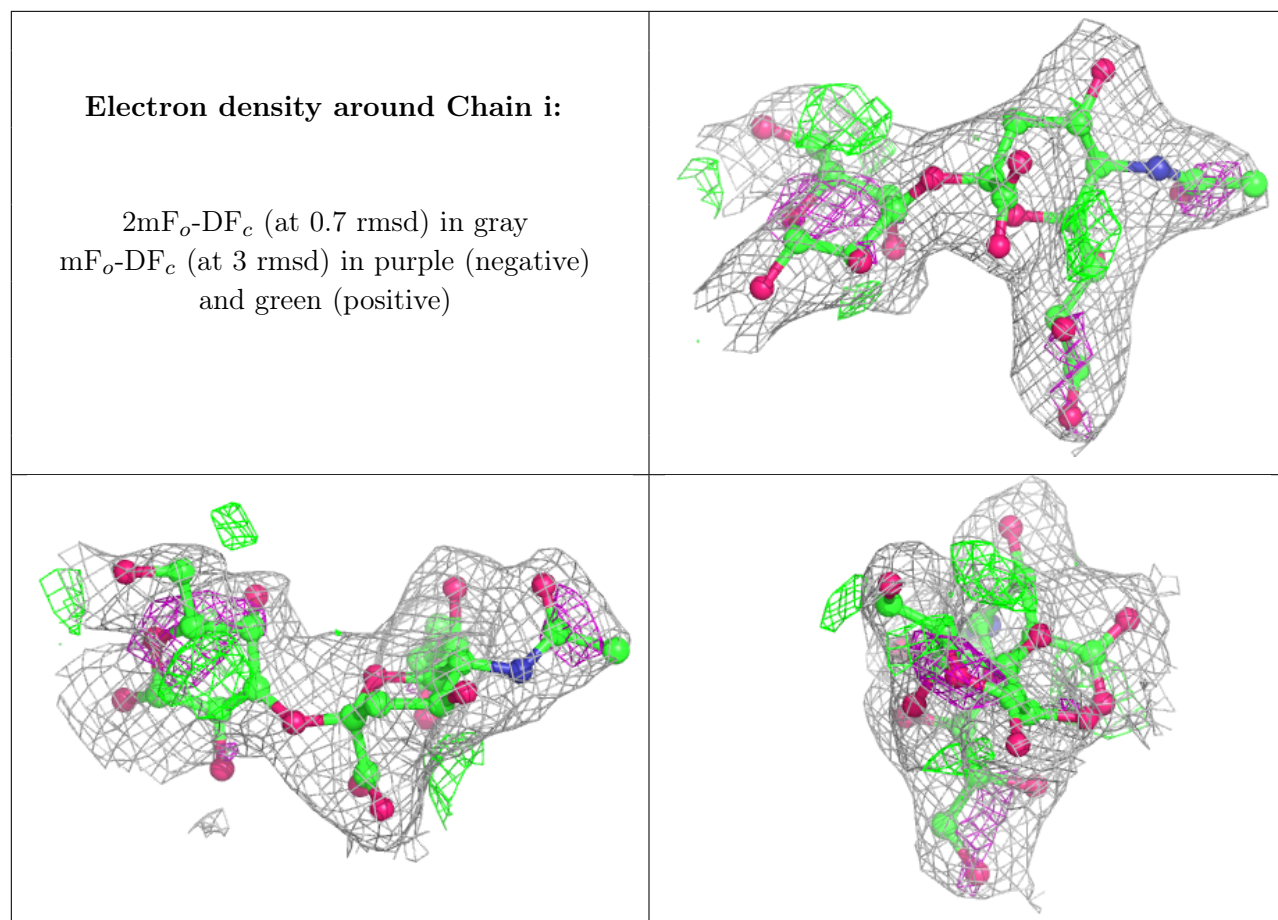


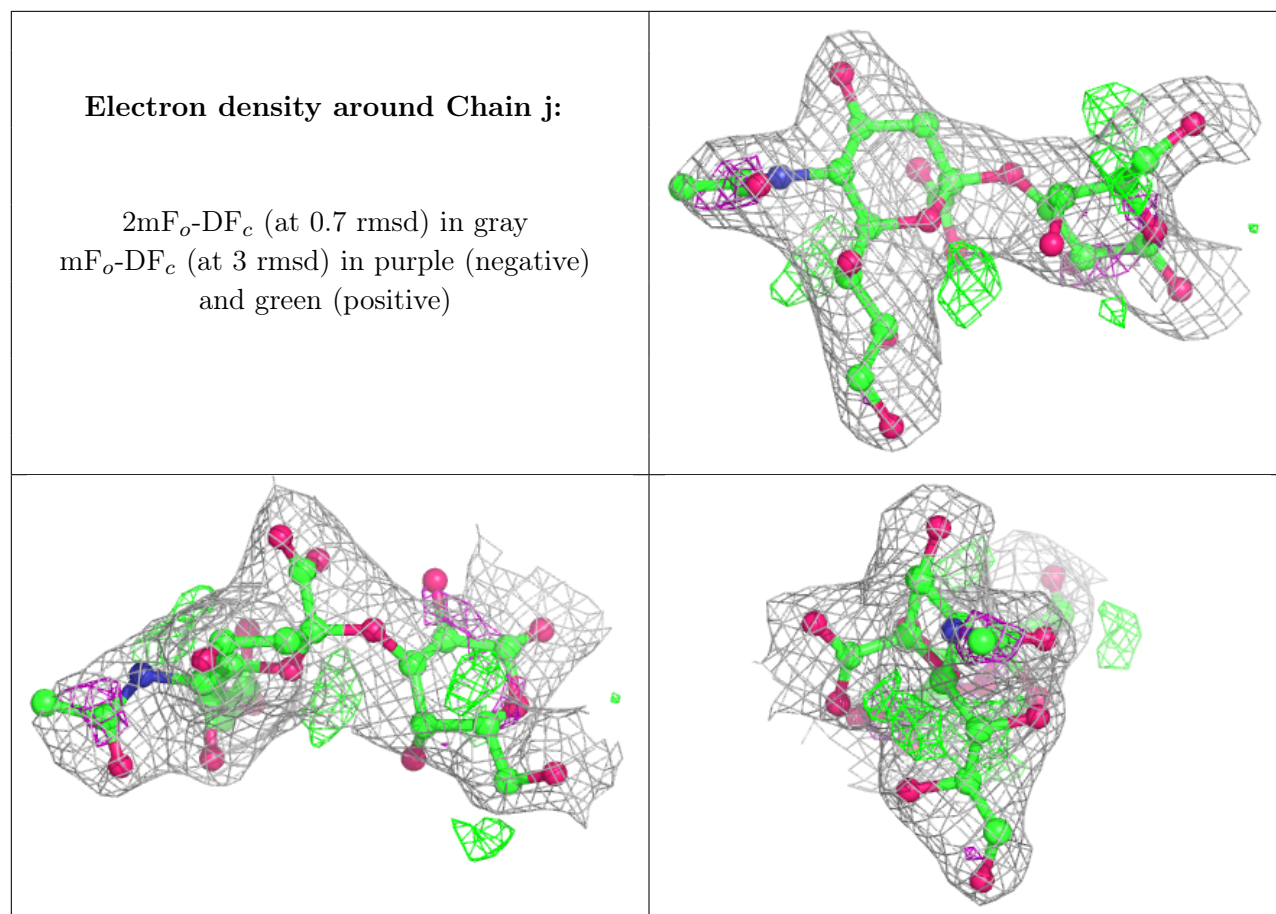
**Electron density around Chain h:**

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



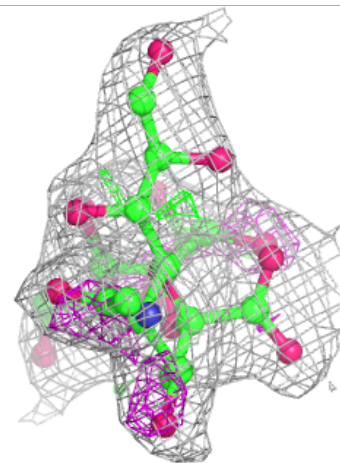
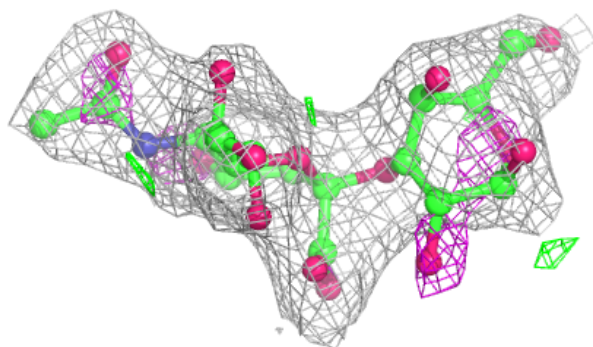
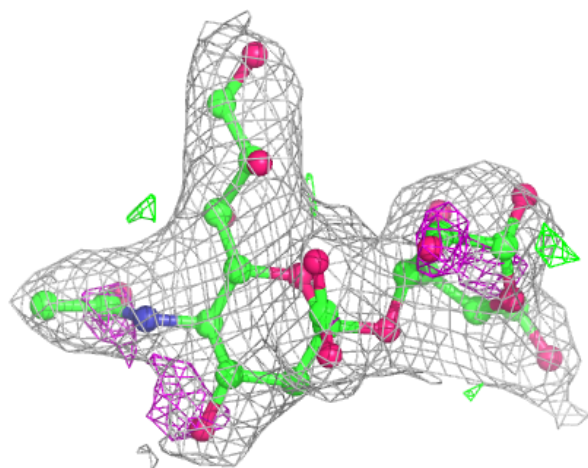


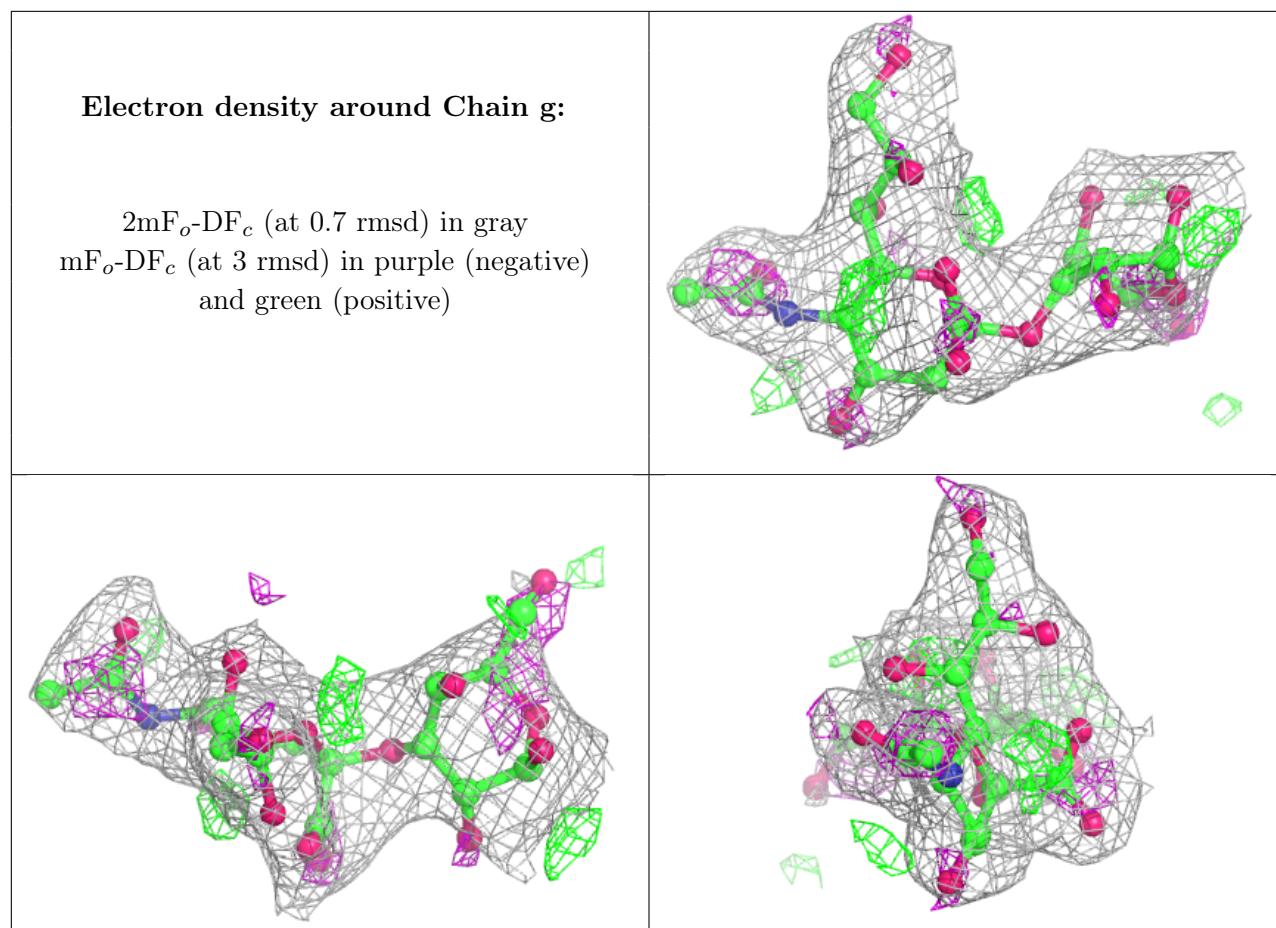




**Electron density around Chain b:**

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





## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.