



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 28, 2021 – 10:19 AM EST

PDB ID : 6X1T
Title : Structure of pHis Fab (SC50-3) in complex with pHis mimetic peptide
Authors : Kalagiri, R.; Stanfield, R.L.; Wilson, I.A.; Hunter, T.
Deposited on : 2020-05-19
Resolution : 2.34 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.16
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)	:	2.16

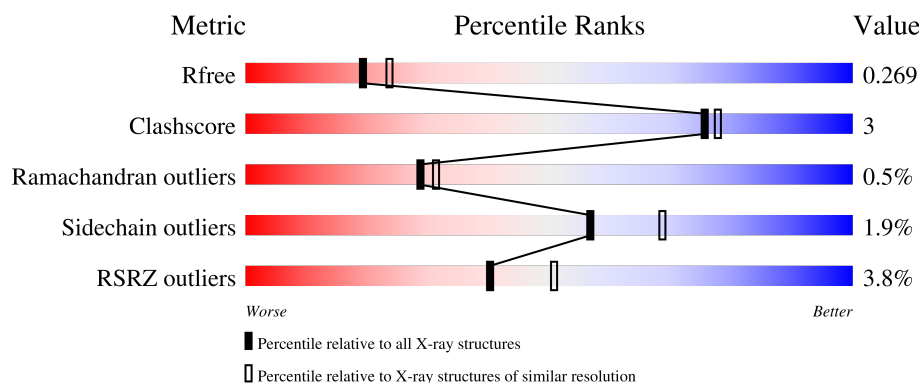
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.34 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	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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 ≥ 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	228	<div> <div>3%</div> <div>84%</div> <div>10%</div> <div>• •</div> </div>
1	C	228	<div> <div>3%</div> <div>83%</div> <div>12%</div> <div>• •</div> </div>
1	E	228	<div> <div>4%</div> <div>86%</div> <div>10%</div> <div>•</div> </div>
1	G	228	<div> <div>11%</div> <div>86%</div> <div>8%</div> <div>• 5%</div> </div>
1	H	228	<div> <div>0%</div> <div>82%</div> <div>14%</div> <div>• •</div> </div>

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Mol	Chain	Length	Quality of chain
1	J	228	
2	B	214	
2	D	214	
2	F	214	
2	I	214	
2	K	214	
2	L	214	
3	M	9	
3	N	9	
3	O	9	
3	P	9	
3	Q	9	
3	R	9	
4	S	2	
4	U	2	
4	V	2	
4	W	2	
5	T	3	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 20064 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 SC50-3 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	221	Total	C	N	O	S	0	4	0
			1640	1026	281	323	10			
1	A	221	Total	C	N	O	S	0	4	0
			1640	1026	281	323	10			
1	C	221	Total	C	N	O	S	0	4	0
			1640	1026	281	323	10			
1	E	221	Total	C	N	O	S	0	4	0
			1640	1026	281	323	10			
1	G	217	Total	C	N	O	S	0	4	0
			1612	1010	276	316	10			
1	J	219	Total	C	N	O	S	0	4	0
			1627	1019	279	320	9			

- Molecule 2 is a protein called SC50-3 Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	214	Total	C	N	O	S	0	1	0
			1593	993	258	333	9			
2	B	214	Total	C	N	O	S	0	1	0
			1593	993	258	333	9			
2	D	214	Total	C	N	O	S	0	1	0
			1593	993	258	333	9			
2	F	214	Total	C	N	O	S	0	1	0
			1593	993	258	333	9			
2	I	214	Total	C	N	O	S	0	1	0
			1593	993	258	333	9			
2	K	212	Total	C	N	O	S	0	1	0
			1579	986	256	328	9			

- Molecule 3 is a protein called NM23-1-pTza peptide.

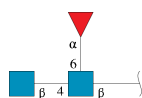
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	6	Total	C	N	O	P	0	0	0
			47	26	10	10	1			
3	N	6	Total	C	N	O	P	0	0	0
			44	25	9	9	1			
3	O	7	Total	C	N	O	P	0	0	0
			56	30	11	14	1			
3	P	5	Total	C	N	O	P	0	0	0
			39	22	8	8	1			
3	Q	7	Total	C	N	O	P	0	0	0
			56	30	11	14	1			
3	R	6	Total	C	N	O	P	0	0	0
			45	23	9	12	1			

- 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	S	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	U	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	V	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	W	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	T	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	H	1	Total	O	S	0	0
			5	4	1		
6	L	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		
6	F	1	Total	O	S	0	0
			5	4	1		
6	F	1	Total	O	S	0	0
			5	4	1		
6	F	1	Total	O	S	0	0
			5	4	1		
6	G	1	Total	O	S	0	0
			5	4	1		
6	G	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	H	36	Total	O	0	0
			36	36		
8	L	35	Total	O	0	0
			35	35		
8	A	25	Total	O	0	0
			25	25		
8	B	27	Total	O	0	0
			27	27		
8	C	25	Total	O	0	0
			25	25		
8	D	10	Total	O	0	0
			10	10		
8	E	11	Total	O	0	0
			11	11		
8	F	7	Total	O	0	0
			7	7		
8	G	24	Total	O	0	0
			24	24		
8	I	5	Total	O	0	0
			5	5		
8	J	5	Total	O	0	0
			5	5		

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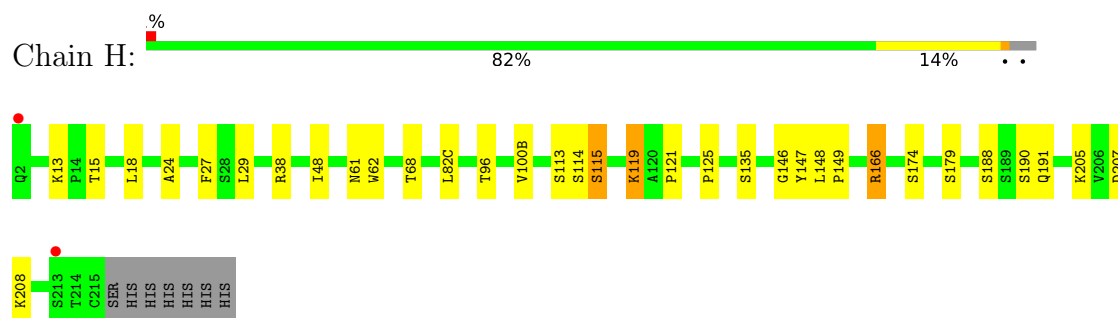
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	M	1	Total 1	O 1	0	0
8	N	1	Total 1	O 1	0	0
8	O	1	Total 1	O 1	0	0
8	P	1	Total 1	O 1	0	0
8	R	1	Total 1	O 1	0	0

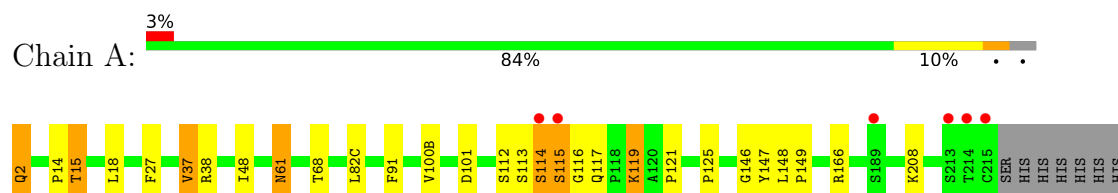
3 Residue-property plots [i](#)

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.

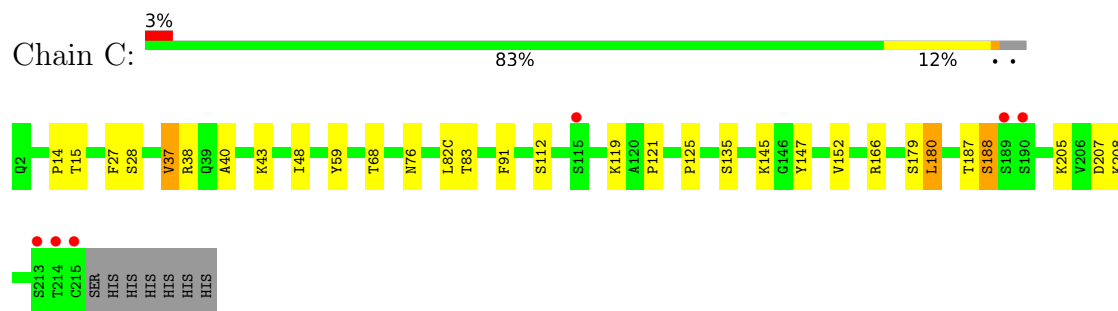
- Molecule 1: SC50-3 Heavy chain



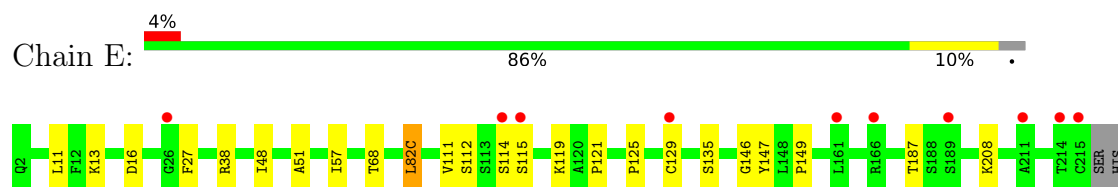
- Molecule 1: SC50-3 Heavy chain



- Molecule 1: SC50-3 Heavy chain




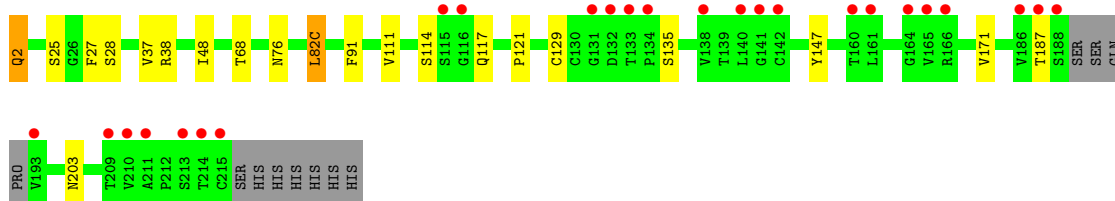
- Molecule 1: SC50-3 Heavy chain




HIS
HIS
HIS
HIS
HIS

• Molecule 1: SC50-3 Heavy chain

Chain G:  11% 86% 8% • 5%



• Molecule 1: SC50-3 Heavy chain

Chain J:  2% 84% 11% •



HIS
HIS
HIS
HIS
HIS

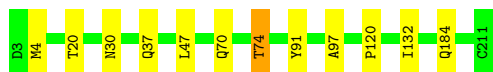
• Molecule 2: SC50-3 Light chain

Chain L:  94% 6%



• Molecule 2: SC50-3 Light chain

Chain B:  94% 5%



• Molecule 2: SC50-3 Light chain

Chain D:  95% 5%



• Molecule 2: SC50-3 Light chain

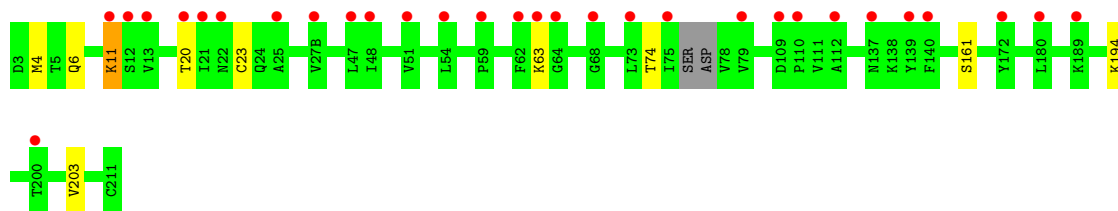
Chain F:  94% 6%



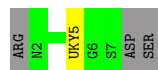
- Molecule 2: SC50-3 Light chain



- Molecule 2: SC50-3 Light chain



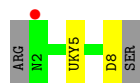
- Molecule 3: NM23-1-pTza peptide



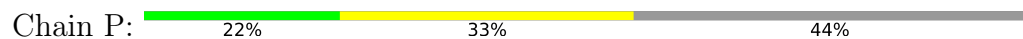
- Molecule 3: NM23-1-pTza peptide



- Molecule 3: NM23-1-pTza peptide

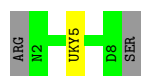


- Molecule 3: NM23-1-pTza peptide




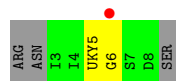
- Molecule 3: NM23-1-pTza peptide

Chain Q:  67% 11% 22%



- Molecule 3: NM23-1-pTza peptide

Chain R:  11% 44% 22% 33%



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

Chain S:  50% 50%



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

Chain U:  100%

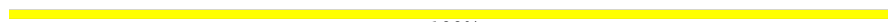


- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:  50% 50%



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

Chain W:  100%



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

Chain T:  33% 67%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	89.82Å 199.67Å 204.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.62 – 2.34 49.62 – 2.34	Depositor EDS
% Data completeness (in resolution range)	99.3 (49.62-2.34) 99.3 (49.62-2.34)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.244 , 0.269 0.244 , 0.269	Depositor DCC
R_{free} test set	7567 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	41.7	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 20.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.077 for -h,l,k	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	20064	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.01% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FUC, SO4, UKY, NAG

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	0.25	0/1690	0.50	0/2315
1	C	0.26	0/1690	0.49	0/2315
1	E	0.27	0/1690	0.52	0/2315
1	G	0.30	0/1660	0.49	0/2272
1	H	0.32	0/1690	0.51	0/2315
1	J	0.28	0/1677	0.52	0/2297
2	B	0.25	0/1628	0.48	0/2230
2	D	0.25	0/1628	0.48	0/2230
2	F	0.26	0/1628	0.49	0/2230
2	I	0.25	0/1628	0.49	0/2230
2	K	0.26	0/1613	0.49	0/2208
2	L	0.26	0/1628	0.49	0/2230
3	M	0.20	0/31	0.40	0/39
3	N	0.21	0/28	0.41	0/35
3	O	0.25	0/40	0.54	0/51
3	P	0.24	0/23	0.43	0/28
3	Q	0.23	0/40	0.38	0/51
3	R	0.26	0/29	0.47	0/36
All	All	0.27	0/20041	0.49	0/27427

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1640	0	1625	23	0
1	C	1640	0	1625	21	0
1	E	1640	0	1625	11	0
1	G	1612	0	1599	11	0
1	H	1640	0	1625	23	0
1	J	1627	0	1615	13	0
2	B	1593	0	1540	6	0
2	D	1593	0	1540	7	0
2	F	1593	0	1540	8	0
2	I	1593	0	1540	8	0
2	K	1579	0	1530	5	0
2	L	1593	0	1540	9	0
3	M	47	0	32	0	0
3	N	44	0	28	0	0
3	O	56	0	39	0	0
3	P	39	0	26	1	0
3	Q	56	0	39	0	0
3	R	45	0	24	0	0
4	S	28	0	25	1	0
4	U	28	0	25	0	0
4	V	28	0	25	1	0
4	W	28	0	25	1	0
5	T	38	0	34	1	0
6	A	5	0	0	0	0
6	C	10	0	0	0	0
6	F	20	0	0	1	0
6	G	10	0	0	1	0
6	H	5	0	0	0	0
6	L	5	0	0	0	0
7	J	14	0	13	0	0
8	A	25	0	0	1	0
8	B	27	0	0	0	0
8	C	25	0	0	0	0
8	D	10	0	0	0	0
8	E	11	0	0	0	0
8	F	7	0	0	0	0
8	G	24	0	0	0	0
8	H	36	0	0	2	0
8	I	5	0	0	0	0
8	J	5	0	0	1	0
8	L	35	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	M	1	0	0	0	0
8	N	1	0	0	0	0
8	O	1	0	0	0	0
8	P	1	0	0	0	0
8	R	1	0	0	0	0
All	All	20064	0	19279	123	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 123 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:115:SER:OG	1:A:148:LEU:HD21	1.68	0.93
1:C:152:VAL:CG2	1:C:180:LEU:HD21	2.06	0.86
1:C:83:THR:HG21	1:J:113:SER:HB2	1.60	0.83
2:K:20:THR:HG22	2:K:74:THR:HG22	1.62	0.80
1:C:152:VAL:CG2	1:C:180:LEU:CD2	2.61	0.79

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	223/228 (98%)	218 (98%)	2 (1%)	3 (1%)	12	9
1	C	223/228 (98%)	218 (98%)	3 (1%)	2 (1%)	17	17
1	E	223/228 (98%)	219 (98%)	3 (1%)	1 (0%)	34	38
1	G	217/228 (95%)	213 (98%)	2 (1%)	2 (1%)	17	17
1	H	223/228 (98%)	219 (98%)	2 (1%)	2 (1%)	17	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	221/228 (97%)	216 (98%)	3 (1%)	2 (1%)	17	17
2	B	213/214 (100%)	207 (97%)	6 (3%)	0	100	100
2	D	213/214 (100%)	206 (97%)	7 (3%)	0	100	100
2	F	213/214 (100%)	207 (97%)	6 (3%)	0	100	100
2	I	213/214 (100%)	207 (97%)	6 (3%)	0	100	100
2	K	209/214 (98%)	202 (97%)	7 (3%)	0	100	100
2	L	213/214 (100%)	206 (97%)	7 (3%)	0	100	100
3	M	3/9 (33%)	2 (67%)	1 (33%)	0	100	100
3	N	3/9 (33%)	2 (67%)	1 (33%)	0	100	100
3	O	4/9 (44%)	3 (75%)	1 (25%)	0	100	100
3	P	2/9 (22%)	2 (100%)	0	0	100	100
3	Q	4/9 (44%)	3 (75%)	1 (25%)	0	100	100
3	R	3/9 (33%)	1 (33%)	1 (33%)	1 (33%)	0	0
All	All	2623/2706 (97%)	2551 (97%)	59 (2%)	13 (0%)	29	31

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	188	SER
1	A	116	GLY
1	C	188	SER
1	E	115	SER
1	H	15	THR

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	190/193 (98%)	181 (95%)	9 (5%)	26	33
1	C	190/193 (98%)	184 (97%)	6 (3%)	39	47
1	E	190/193 (98%)	186 (98%)	4 (2%)	53	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	186/193 (96%)	181 (97%)	5 (3%)	44	55
1	H	190/193 (98%)	183 (96%)	7 (4%)	34	43
1	J	188/193 (97%)	184 (98%)	4 (2%)	53	65
2	B	187/186 (100%)	184 (98%)	3 (2%)	62	74
2	D	187/186 (100%)	186 (100%)	1 (0%)	88	93
2	F	187/186 (100%)	186 (100%)	1 (0%)	88	93
2	I	187/186 (100%)	187 (100%)	0	100	100
2	K	185/186 (100%)	182 (98%)	3 (2%)	62	74
2	L	187/186 (100%)	186 (100%)	1 (0%)	88	93
3	M	3/7 (43%)	3 (100%)	0	100	100
3	N	2/7 (29%)	2 (100%)	0	100	100
3	O	5/7 (71%)	4 (80%)	1 (20%)	1	1
3	P	2/7 (29%)	2 (100%)	0	100	100
3	Q	5/7 (71%)	5 (100%)	0	100	100
3	R	3/7 (43%)	3 (100%)	0	100	100
All	All	2274/2316 (98%)	2229 (98%)	45 (2%)	57	66

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	27	PHE
1	C	180	LEU
2	K	4	MET
1	C	68	THR
2	D	63	LYS

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

Mol	Chain	Res	Type
1	A	61	ASN
1	C	173	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	UKY	O	5	3	9,14,15	1.03	0	9,20,22	2.01	1 (11%)
3	UKY	M	5	3	9,14,15	1.00	0	9,20,22	2.25	2 (22%)
3	UKY	P	5	3	9,14,15	1.00	0	9,20,22	1.99	1 (11%)
3	UKY	N	5	3	9,14,15	1.02	0	9,20,22	2.17	1 (11%)
3	UKY	R	5	3	9,14,15	1.00	0	9,20,22	2.30	2 (22%)
3	UKY	Q	5	3	9,14,15	1.03	0	9,20,22	2.05	1 (11%)

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	UKY	O	5	3	-	0/0/12/14	0/1/1/1
3	UKY	M	5	3	-	0/0/12/14	0/1/1/1
3	UKY	P	5	3	-	0/0/12/14	0/1/1/1
3	UKY	N	5	3	-	0/0/12/14	0/1/1/1
3	UKY	R	5	3	-	0/0/12/14	0/1/1/1
3	UKY	Q	5	3	-	0/0/12/14	0/1/1/1

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	5	UKY	CB-NG-ND2	5.92	125.36	116.67
3	M	5	UKY	CB-NG-ND2	5.76	125.12	116.67
3	N	5	UKY	CB-NG-ND2	5.54	124.80	116.67
3	Q	5	UKY	CB-NG-ND2	5.24	124.36	116.67
3	P	5	UKY	CB-NG-ND2	5.19	124.28	116.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

11 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	S	1	1,4	14,14,15	0.20	0	17,19,21	0.55	0
4	NAG	S	2	4	14,14,15	0.20	0	17,19,21	0.44	0
5	NAG	T	1	1,5	14,14,15	0.20	0	17,19,21	0.52	0
5	NAG	T	2	5	14,14,15	0.37	0	17,19,21	0.40	0
5	FUC	T	3	5	10,10,11	0.71	0	14,14,16	0.86	0
4	NAG	U	1	1,4	14,14,15	0.20	0	17,19,21	0.51	0
4	NAG	U	2	4	14,14,15	0.22	0	17,19,21	0.45	0
4	NAG	V	1	1,4	14,14,15	0.21	0	17,19,21	0.54	0
4	NAG	V	2	4	14,14,15	0.20	0	17,19,21	0.44	0
4	NAG	W	1	1,4	14,14,15	0.20	0	17,19,21	0.51	0
4	NAG	W	2	4	14,14,15	0.23	0	17,19,21	0.46	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	S	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	S	2	4	-	0/6/23/26	0/1/1/1
5	NAG	T	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	T	2	5	-	2/6/23/26	0/1/1/1
5	FUC	T	3	5	-	-	0/1/1/1
4	NAG	U	1	1,4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	U	2	4	-	0/6/23/26	0/1/1/1
4	NAG	V	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	V	2	4	-	0/6/23/26	0/1/1/1
4	NAG	W	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	W	2	4	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

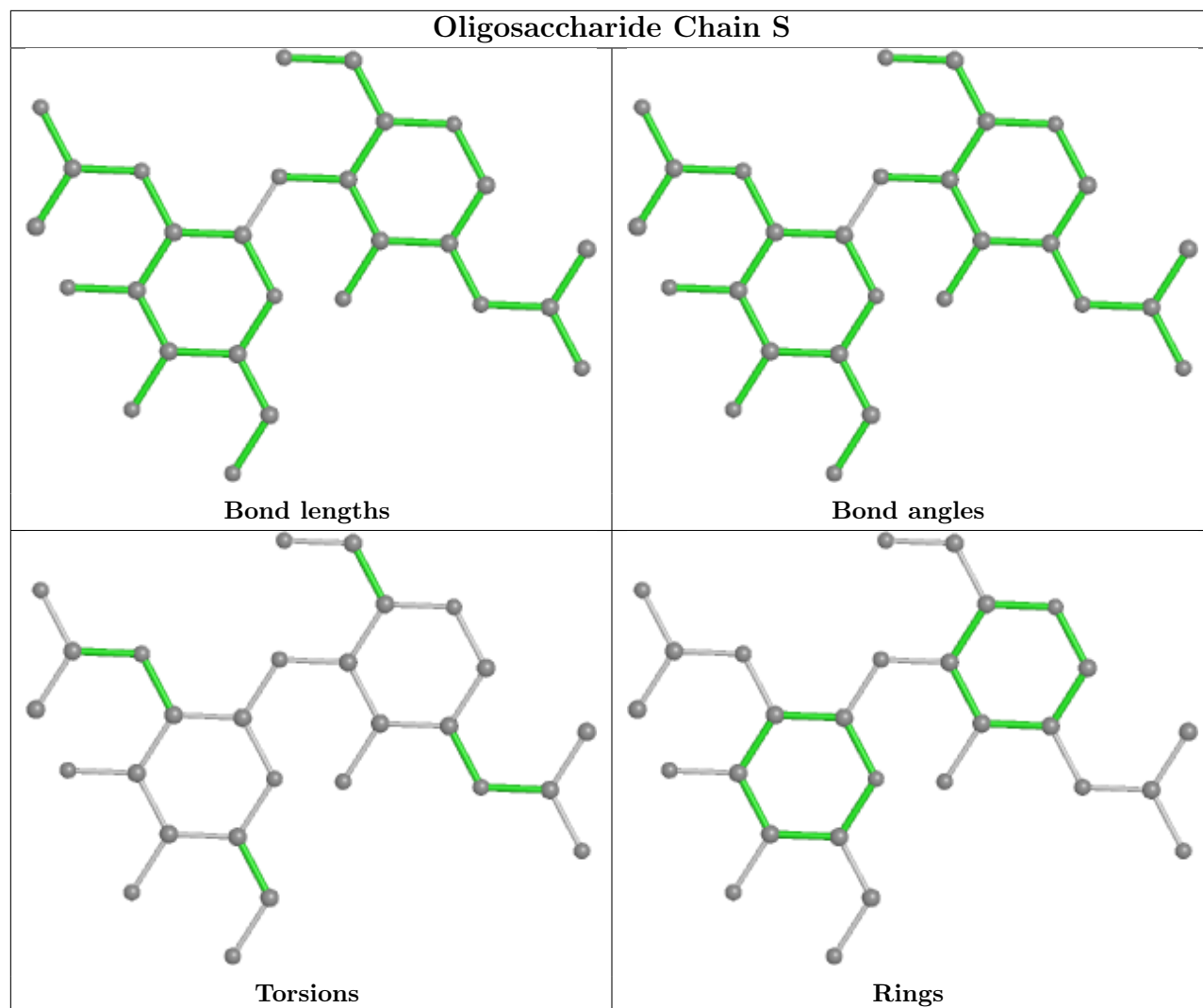
Mol	Chain	Res	Type	Atoms
4	W	2	NAG	C8-C7-N2-C2
4	W	2	NAG	O7-C7-N2-C2
5	T	2	NAG	C1-C2-N2-C7
4	W	2	NAG	O5-C5-C6-O6
5	T	2	NAG	C3-C2-N2-C7

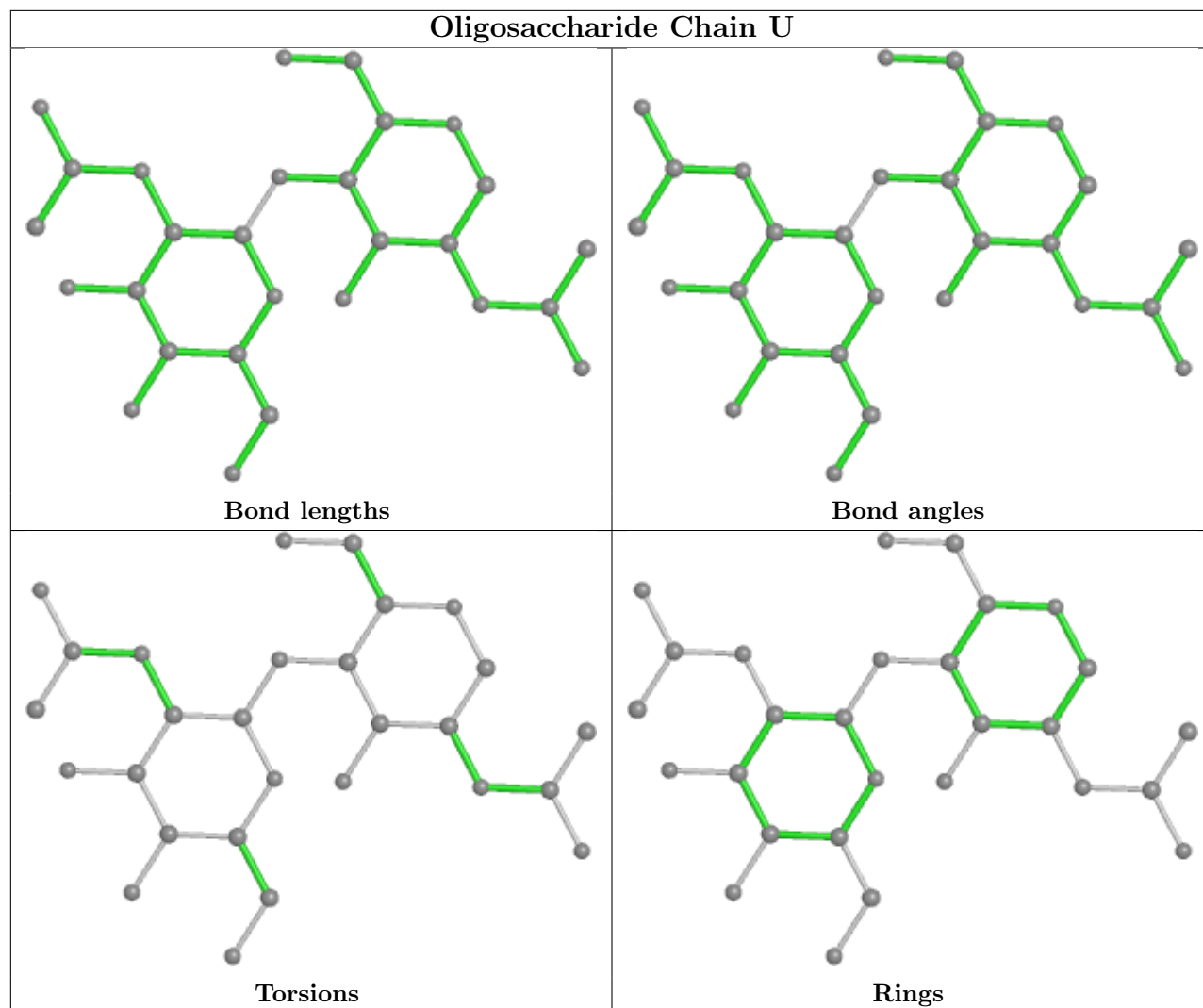
There are no ring outliers.

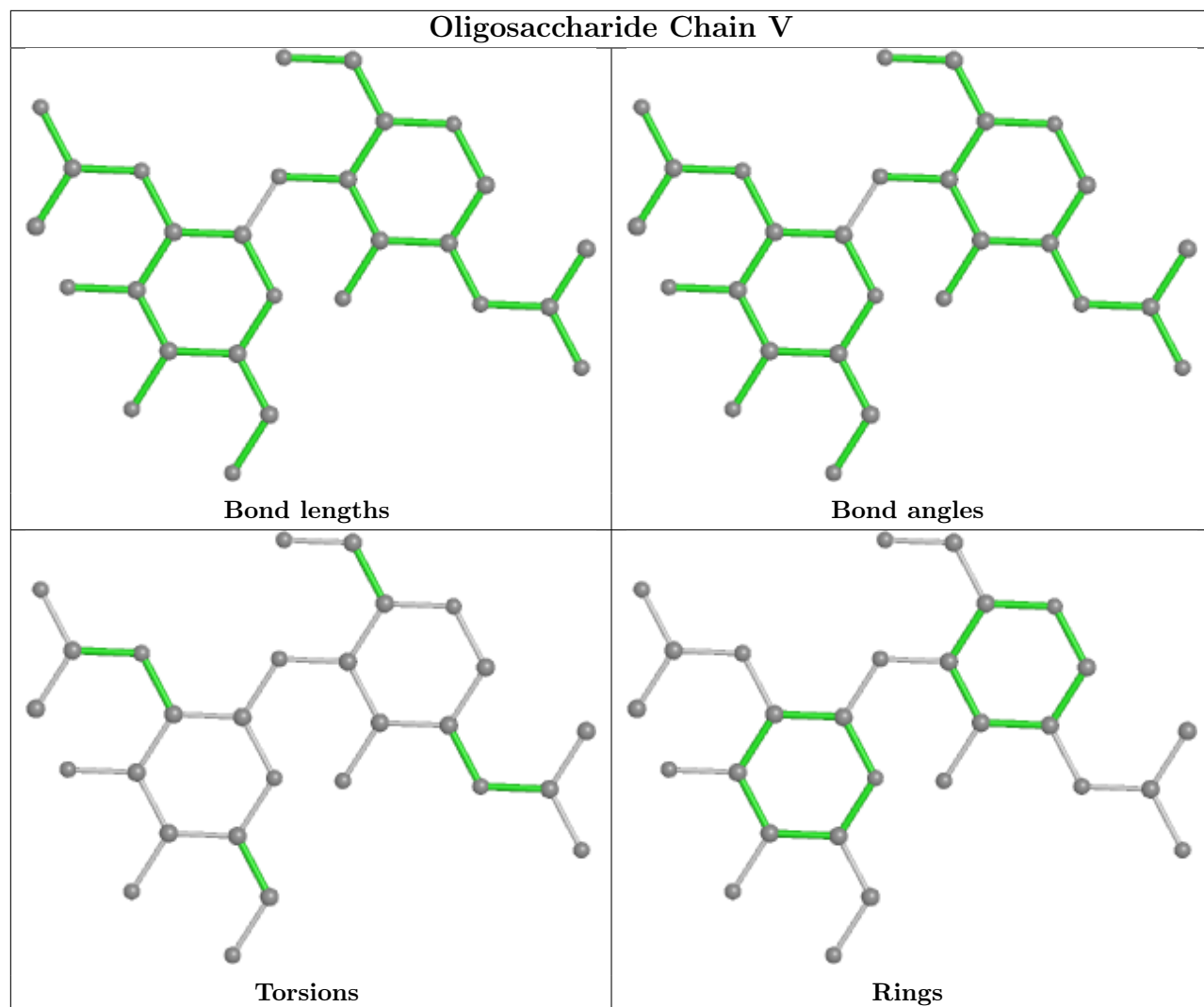
6 monomers are involved in 4 short contacts:

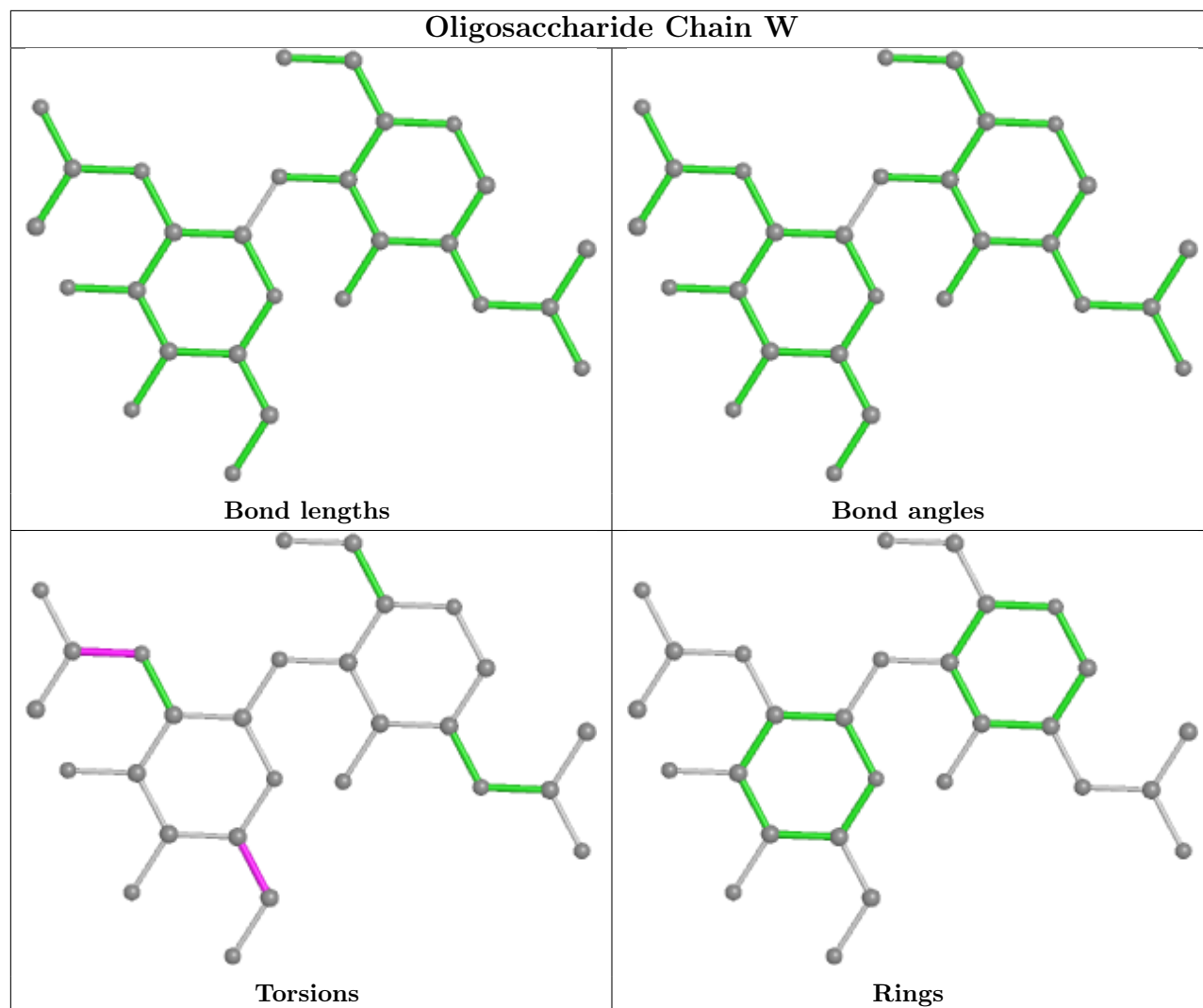
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	W	1	NAG	1	0
5	T	1	NAG	1	0
4	S	1	NAG	1	0
4	V	2	NAG	1	0
5	T	2	NAG	1	0
4	W	2	NAG	1	0

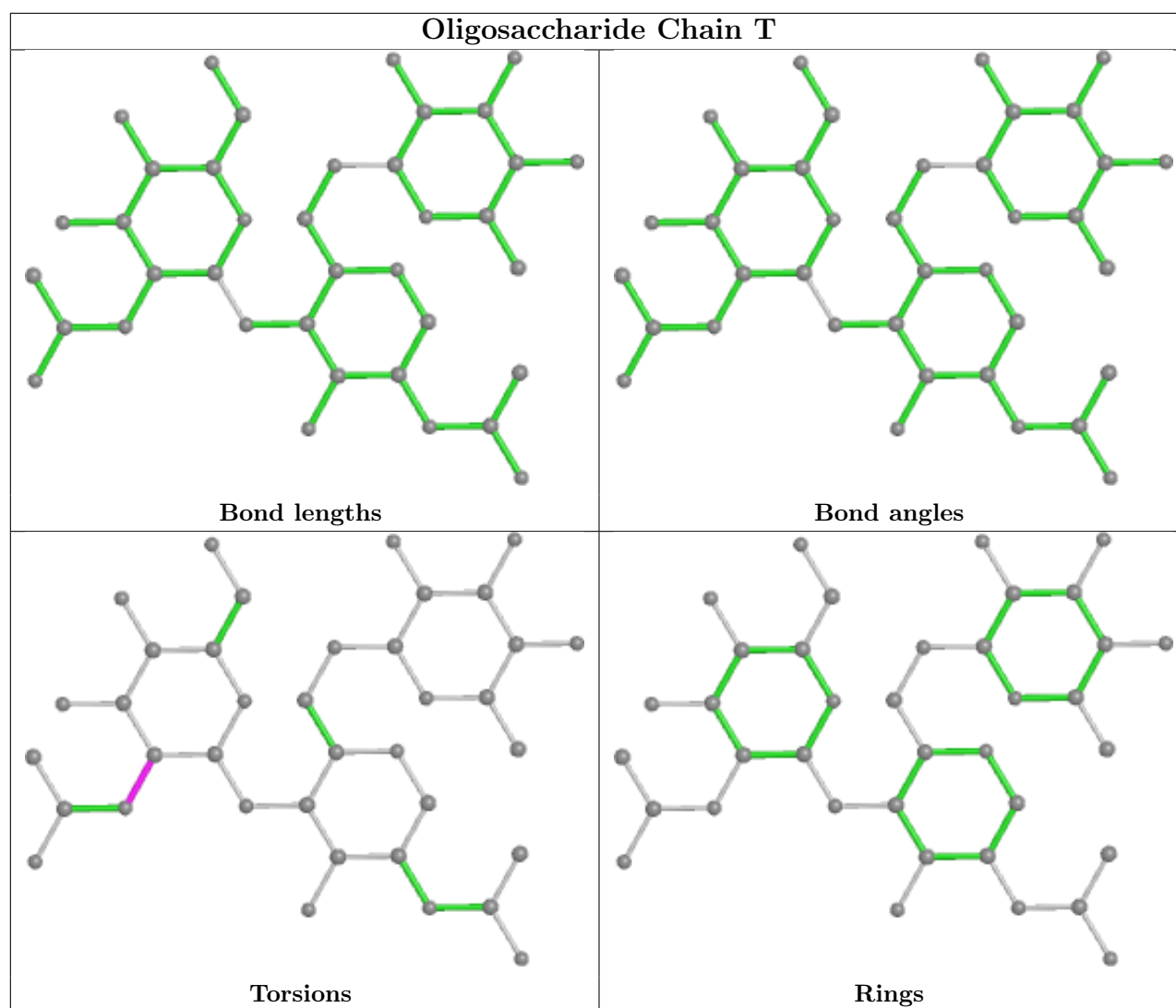
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	SO4	F	301	-	4,4,4	0.14	0	6,6,6	0.05	0
6	SO4	L	301	-	4,4,4	0.14	0	6,6,6	0.06	0
6	SO4	F	304	-	4,4,4	0.14	0	6,6,6	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	SO4	H	303	-	4,4,4	0.14	0	6,6,6	0.06	0
6	SO4	F	303	-	4,4,4	0.15	0	6,6,6	0.05	0
6	SO4	G	303	-	4,4,4	0.14	0	6,6,6	0.08	0
6	SO4	G	304	-	4,4,4	0.14	0	6,6,6	0.05	0
6	SO4	C	303	-	4,4,4	0.14	0	6,6,6	0.05	0
6	SO4	A	304	-	4,4,4	0.14	0	6,6,6	0.10	0
6	SO4	C	304	-	4,4,4	0.14	0	6,6,6	0.06	0
6	SO4	F	302	-	4,4,4	0.14	0	6,6,6	0.06	0
7	NAG	J	301	1	14,14,15	0.21	0	17,19,21	0.49	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	J	301	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	304	SO4	1	0
6	G	304	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	221/228 (96%)	-0.00	6 (2%) 54 64	26, 40, 62, 92	0
1	C	221/228 (96%)	0.16	6 (2%) 54 64	26, 39, 70, 119	0
1	E	221/228 (96%)	0.27	10 (4%) 33 44	32, 50, 82, 111	0
1	G	217/228 (95%)	0.67	25 (11%) 4 8	24, 47, 98, 126	0
1	H	221/228 (96%)	-0.04	2 (0%) 84 89	22, 35, 59, 72	0
1	J	219/228 (96%)	0.41	5 (2%) 60 69	35, 54, 80, 92	0
2	B	214/214 (100%)	-0.10	0 100 100	25, 38, 49, 64	0
2	D	214/214 (100%)	-0.03	0 100 100	30, 44, 67, 88	0
2	F	214/214 (100%)	-0.02	1 (0%) 91 95	32, 47, 64, 77	0
2	I	214/214 (100%)	0.61	14 (6%) 18 26	34, 61, 83, 97	0
2	K	212/214 (99%)	1.03	30 (14%) 2 4	42, 74, 90, 100	0
2	L	214/214 (100%)	-0.14	0 100 100	22, 34, 53, 62	0
3	M	5/9 (55%)	-0.19	0 100 100	38, 45, 49, 57	0
3	N	5/9 (55%)	0.45	0 100 100	52, 53, 60, 67	0
3	O	6/9 (66%)	1.28	1 (16%) 1 2	56, 62, 78, 82	0
3	P	4/9 (44%)	1.30	0 100 100	68, 72, 74, 78	0
3	Q	6/9 (66%)	0.61	0 100 100	57, 64, 68, 70	0
3	R	5/9 (55%)	1.52	1 (20%) 1 2	57, 61, 72, 77	0
All	All	2633/2706 (97%)	0.24	101 (3%) 40 51	22, 46, 82, 126	0

The worst 5 of 101 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	215	CYS	9.4
1	G	186	VAL	8.3
1	C	215	CYS	8.0

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Mol	Chain	Res	Type	RSRZ
1	C	189	SER	7.4
1	C	214	THR	7.1

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	UKY	P	5	14/15	0.94	0.11	47,68,73,75	0
3	UKY	O	5	14/15	0.95	0.12	29,50,57,57	0
3	UKY	R	5	14/15	0.95	0.13	35,64,70,72	0
3	UKY	N	5	14/15	0.97	0.11	41,48,54,60	0
3	UKY	Q	5	14/15	0.97	0.11	34,53,62,64	0
3	UKY	M	5	14/15	0.98	0.11	27,35,44,49	0

6.3 Carbohydrates [i](#)

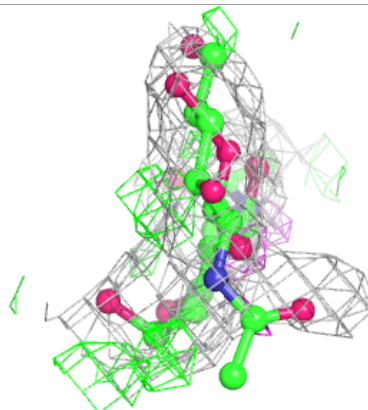
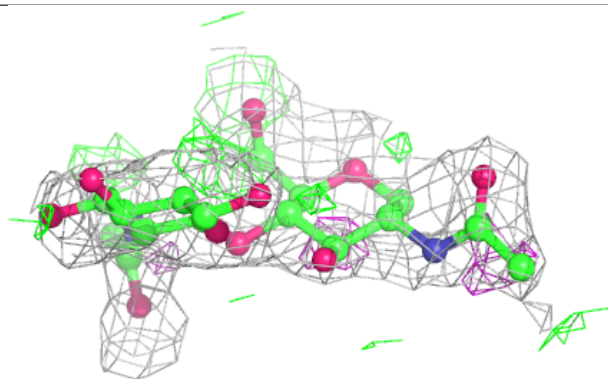
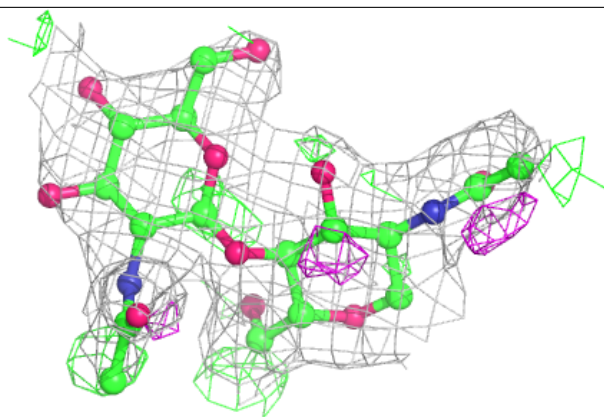
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	FUC	T	3	10/11	0.59	0.29	64,92,102,106	0
4	NAG	W	2	14/15	0.76	0.34	113,120,125,127	0
5	NAG	T	2	14/15	0.77	0.32	69,99,114,130	0
4	NAG	S	2	14/15	0.77	0.24	62,78,83,86	0
4	NAG	W	1	14/15	0.78	0.20	61,88,103,111	0
4	NAG	U	2	14/15	0.79	0.29	79,92,95,98	0
4	NAG	V	2	14/15	0.81	0.26	83,94,99,101	0
4	NAG	V	1	14/15	0.84	0.15	53,69,84,89	0
4	NAG	U	1	14/15	0.84	0.12	46,67,77,87	0
4	NAG	S	1	14/15	0.85	0.17	35,48,71,79	0
5	NAG	T	1	14/15	0.87	0.17	44,58,87,91	0

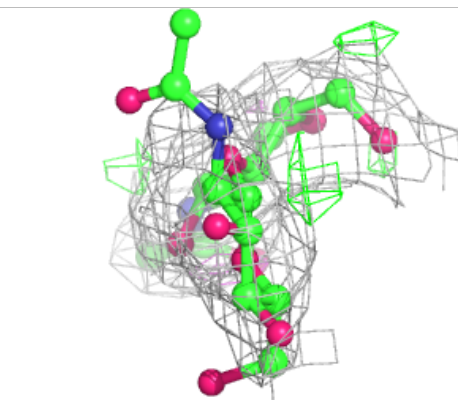
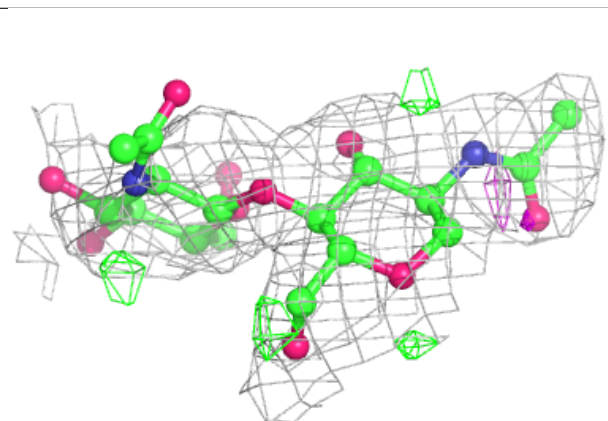
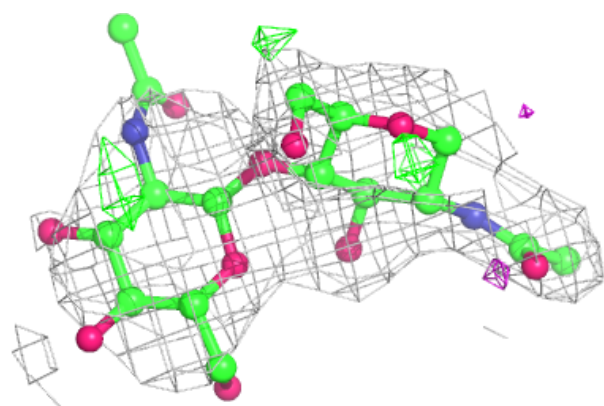
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain S:

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

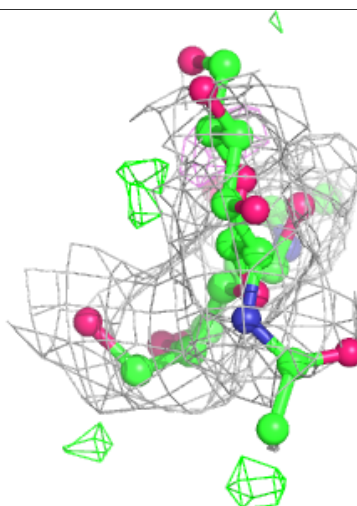
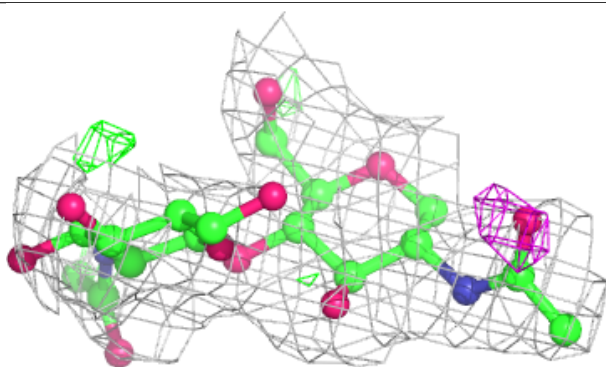
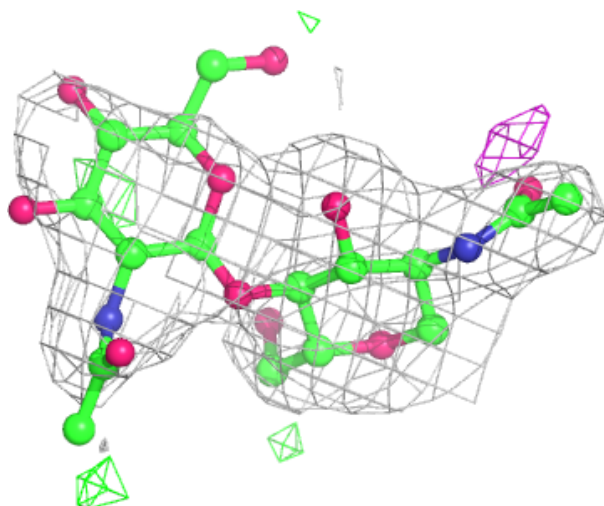
**Electron density around Chain U:**

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



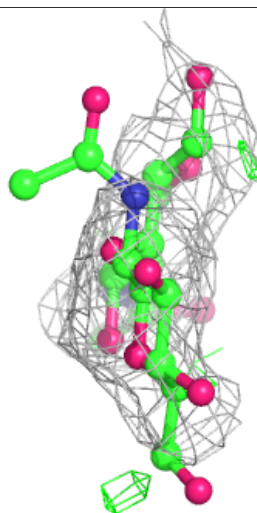
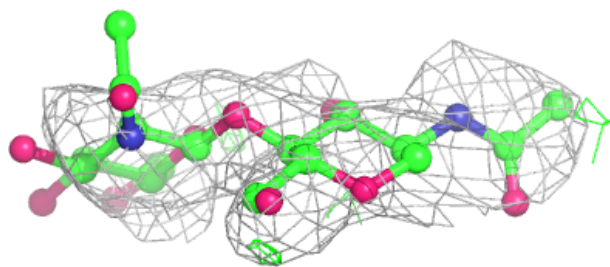
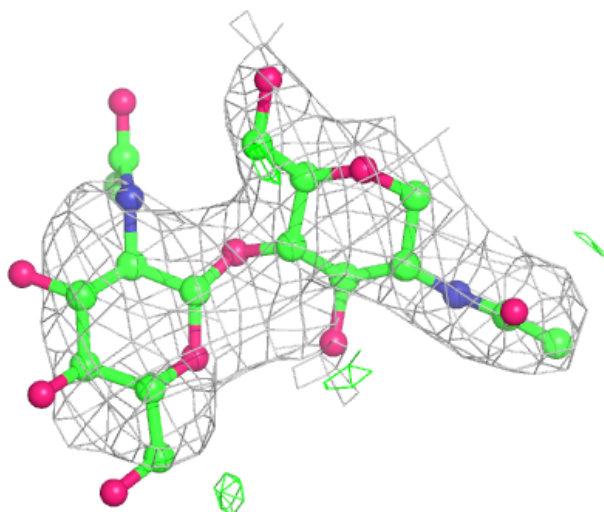
Electron density around Chain V:

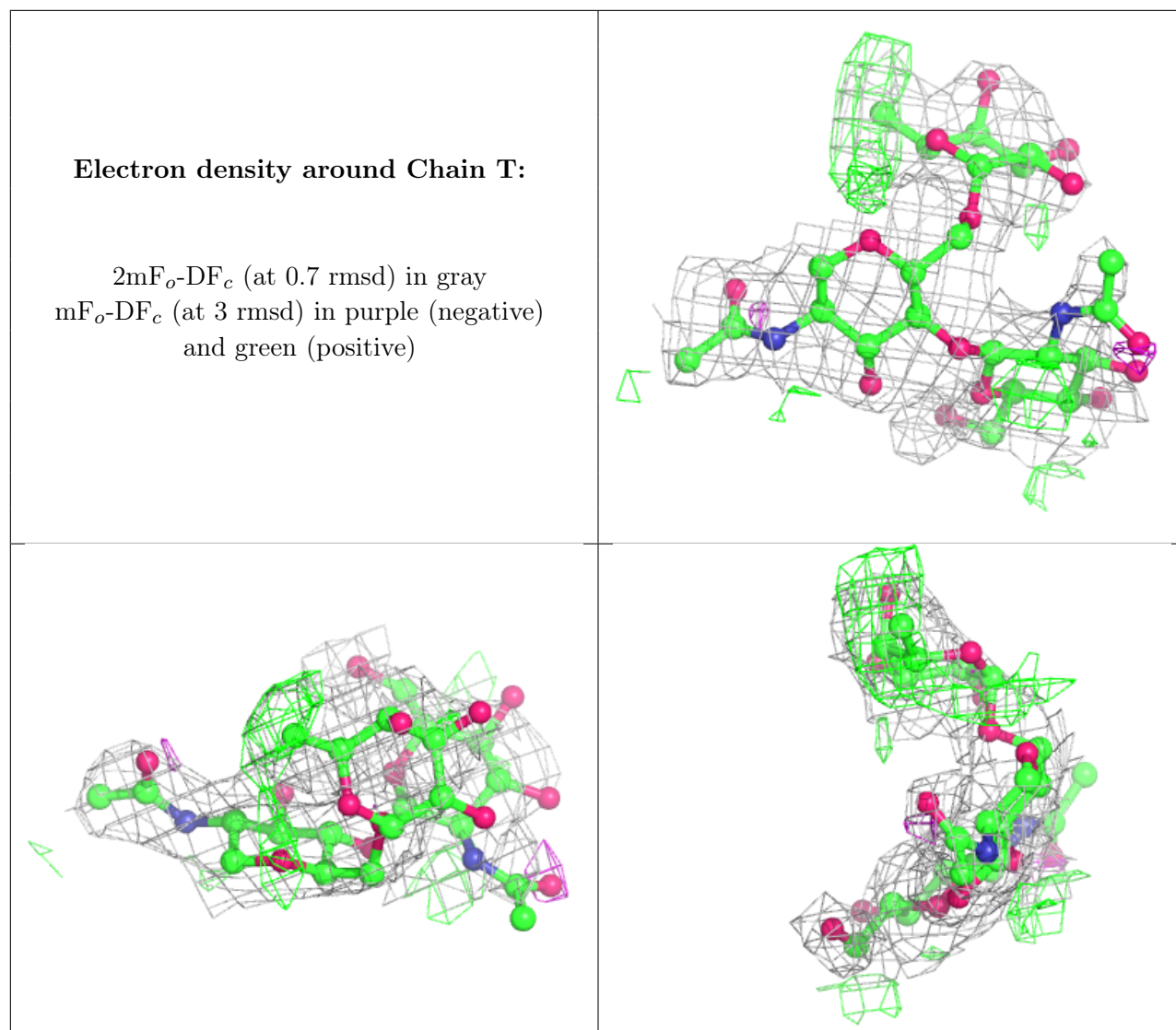
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain W:

$2mF_o-DF_c$ (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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	NAG	J	301	14/15	0.79	0.20	69,82,88,94	0
6	SO4	H	303	5/5	0.84	0.22	60,67,82,94	0
6	SO4	A	304	5/5	0.88	0.23	39,42,63,68	0
6	SO4	G	303	5/5	0.90	0.30	26,44,65,70	0
6	SO4	G	304	5/5	0.91	0.10	60,82,83,94	0
6	SO4	C	303	5/5	0.93	0.14	59,76,81,84	0
6	SO4	F	304	5/5	0.93	0.14	75,88,91,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	SO4	C	304	5/5	0.94	0.20	64,75,88,95	0
6	SO4	F	302	5/5	0.94	0.13	76,83,91,96	0
6	SO4	L	301	5/5	0.94	0.15	42,60,69,73	0
6	SO4	F	303	5/5	0.95	0.09	59,68,87,88	0
6	SO4	F	301	5/5	0.95	0.17	78,87,98,104	0

6.5 Other polymers [i](#)

There are no such residues in this entry.