



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:18 AM UTC

PDB ID : 4MBY / pdb_00004mby
Title : Structure of B-Lymphotropic Polyomavirus VP1 in complex with 3'-sialyllactose
Authors : Khan, Z.M.; Neu, U.; Stehle, T.
Deposited on : 2013-08-21
Resolution : 1.48 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

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>.

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
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

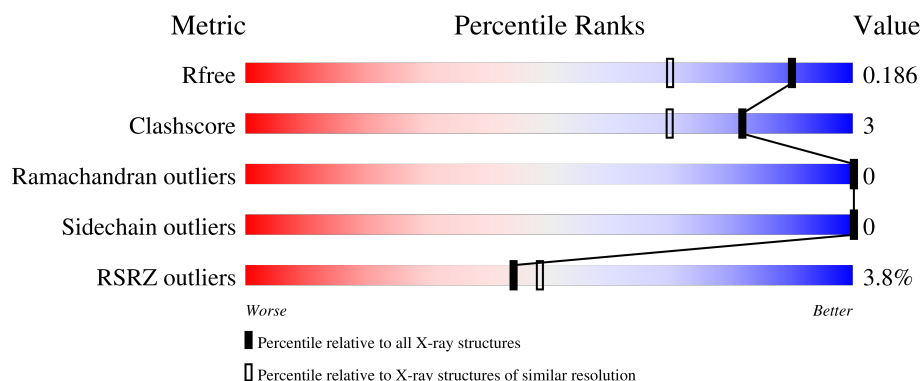
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.48 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.



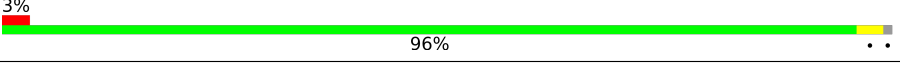
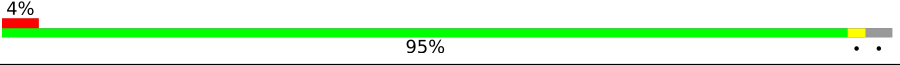
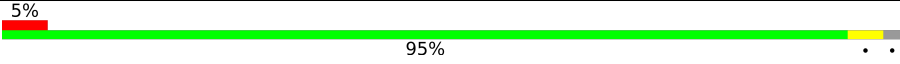
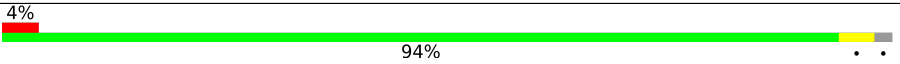
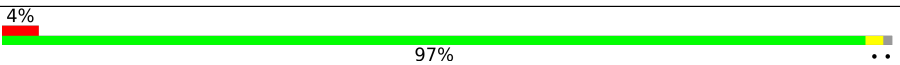
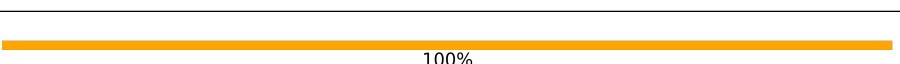
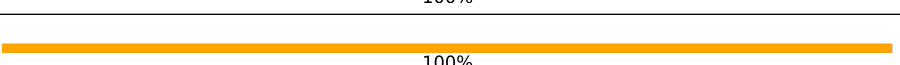
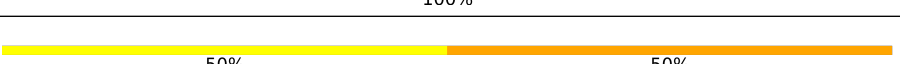
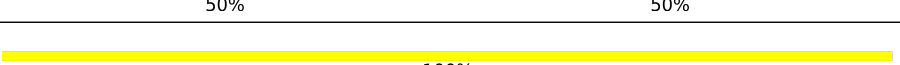
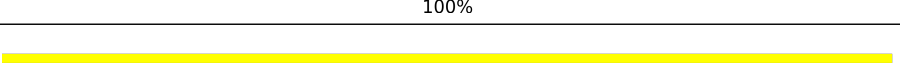
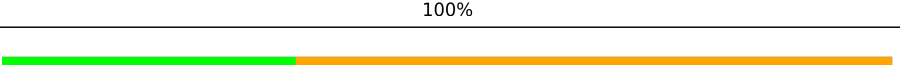
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6779 (1.50-1.46)
Clashscore	190562	7025 (1.50-1.46)
Ramachandran outliers	187476	6917 (1.50-1.46)
Sidechain outliers	187428	6914 (1.50-1.46)
RSRZ outliers	180081	6781 (1.50-1.46)

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	278	2% 94% 6%
1	B	278	5% 92% 6%
1	C	278	4% 93% 6%
1	D	278	5% 94% 5%
1	E	278	0% 95% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	278	
1	G	278	
1	H	278	
1	I	278	
1	J	278	
2	K	2	
2	L	2	
2	M	2	
2	N	2	
2	O	2	
2	P	2	
2	Q	2	
3	R	3	
3	S	3	

2 Entry composition [i](#)

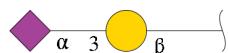
There are 8 unique types of molecules in this entry. The entry contains 24709 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Major Capsid Protein VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	277	Total	C	N	O	S	0	9	0
			2177	1374	357	433	13			
1	B	275	Total	C	N	O	S	0	12	0
			2173	1373	357	430	13			
1	C	275	Total	C	N	O	S	0	13	0
			2179	1377	360	429	13			
1	D	274	Total	C	N	O	S	0	10	0
			2146	1360	352	421	13			
1	E	277	Total	C	N	O	S	0	8	0
			2158	1363	354	428	13			
1	F	274	Total	C	N	O	S	0	7	0
			2119	1340	350	416	13			
1	G	270	Total	C	N	O	S	0	5	0
			2087	1322	345	407	13			
1	H	273	Total	C	N	O	S	0	7	0
			2117	1339	349	416	13			
1	I	273	Total	C	N	O	S	0	5	0
			2106	1330	348	415	13			
1	J	275	Total	C	N	O	S	0	5	0
			2125	1340	351	421	13			

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



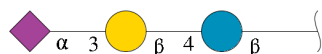
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	K	2	Total	C	N	O	0	0	0
			32	17	1	14			
2	L	2	Total	C	N	O	0	0	0
			32	17	1	14			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	M	2	Total	C	N	O	0	0	0
			32	17	1	14			
2	N	2	Total	C	N	O	0	0	0
			32	17	1	14			
2	O	2	Total	C	N	O	0	0	0
			32	17	1	14			
2	P	2	Total	C	N	O	0	0	0
			32	17	1	14			
2	Q	2	Total	C	N	O	0	0	0
			32	17	1	14			

- Molecule 3 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	R	3	Total	C	N	O	0	0	0
			43	23	1	19			
3	S	3	Total	C	N	O	0	0	0
			43	23	1	19			

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		
4	B	1	Total	Ca	0	0
			1	1		
4	C	1	Total	Ca	0	0
			1	1		
4	D	1	Total	Ca	0	0
			1	1		
4	E	1	Total	Ca	0	0
			1	1		
4	F	1	Total	Ca	0	0
			1	1		
4	G	1	Total	Ca	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	1	Total 1	Ca 1	0	0
4	I	1	Total 1	Ca 1	0	0
4	J	1	Total 1	Ca 1	0	0

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	Cl 1	0	0
5	B	1	Total 1	Cl 1	0	0
5	C	1	Total 1	Cl 1	0	0
5	D	1	Total 1	Cl 1	0	0
5	E	1	Total 1	Cl 1	0	0
5	F	1	Total 1	Cl 1	0	0
5	G	1	Total 1	Cl 1	0	0
5	H	1	Total 1	Cl 1	0	0
5	I	1	Total 1	Cl 1	0	0
5	J	1	Total 1	Cl 1	0	0

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



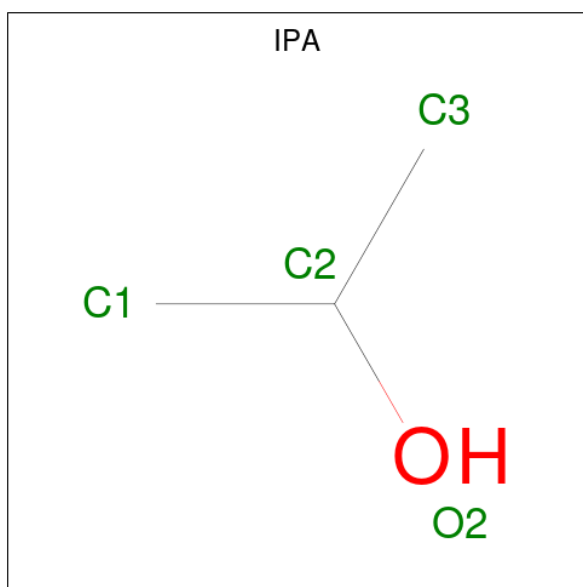
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		
6	E	1	Total	C	O	0	0
			4	2	2		
6	E	1	Total	C	O	0	0
			4	2	2		
6	E	1	Total	C	O	0	0
			4	2	2		
6	E	1	Total	C	O	0	0
			4	2	2		
6	F	1	Total	C	O	0	0
			4	2	2		
6	G	1	Total	C	O	0	0
			4	2	2		
6	G	1	Total	C	O	0	0
			4	2	2		
6	H	1	Total	C	O	0	0
			4	2	2		
6	H	1	Total	C	O	0	0
			4	2	2		
6	H	1	Total	C	O	0	0
			4	2	2		
6	I	1	Total	C	O	0	0
			4	2	2		
6	I	1	Total	C	O	0	0
			4	2	2		
6	J	1	Total	C	O	0	0
			4	2	2		
6	J	1	Total	C	O	0	0
			4	2	2		
6	J	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is ISOPROPYL ALCOHOL (CCD ID: IPA) (formula: C₃H₈O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 4 3 1	0	0
7	B	1	Total C O 4 3 1	0	0
7	C	1	Total C O 4 3 1	0	0
7	D	1	Total C O 4 3 1	0	0
7	E	1	Total C O 4 3 1	0	0
7	F	1	Total C O 4 3 1	0	0
7	G	1	Total C O 4 3 1	0	0
7	H	1	Total C O 4 3 1	0	0
7	I	1	Total C O 4 3 1	0	0
7	J	1	Total C O 4 3 1	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	349	Total O 349 349	0	0
8	B	323	Total O 323 323	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	315	Total 315	O 315	0	0
8	D	296	Total 296	O 296	0	0
8	E	329	Total 329	O 329	0	0
8	F	250	Total 250	O 250	0	0
8	G	225	Total 225	O 225	0	0
8	H	233	Total 233	O 233	0	0
8	I	249	Total 249	O 249	0	0
8	J	255	Total 255	O 255	0	0

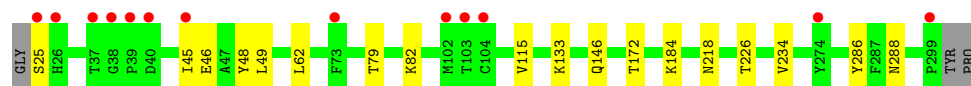
3 Residue-property plots [i](#)

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: Major Capsid Protein VP1



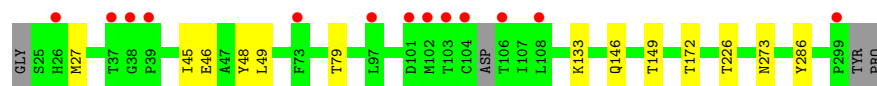
- Molecule 1: Major Capsid Protein VP1



- Molecule 1: Major Capsid Protein VP1



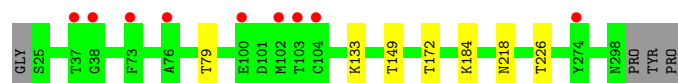
- Molecule 1: Major Capsid Protein VP1



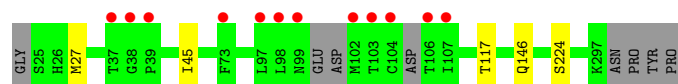
- Molecule 1: Major Capsid Protein VP1



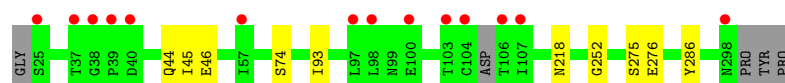
- Molecule 1: Major Capsid Protein VP1



- Molecule 1: Major Capsid Protein VP1



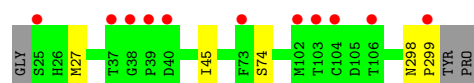
- Molecule 1: Major Capsid Protein VP1



- Molecule 1: Major Capsid Protein VP1



- Molecule 1: Major Capsid Protein VP1



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



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



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

Chain M:  100%

GAL1
SIA2

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

Chain N:  50% 50%

GAL1
SIA2

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

Chain O:  50% 50%

GAL1
SIA2

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

Chain P:  100%

GAL1
SIA2

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

Chain Q:  100%

GAL1
SIA2

- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain R:  33% 67%

BGC1
GAL2
SIA3

- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain S:  67% 33%

BGC1
GAL2
SIA3

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	150.53Å 97.21Å 234.66Å 90.00° 96.25° 90.00°	Depositor
Resolution (Å)	48.82 – 1.48 48.82 – 1.48	Depositor EDS
% Data completeness (in resolution range)	98.6 (48.82-1.48) 98.6 (48.82-1.48)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 1.48Å)	Xtriage
Refinement program	REFMAC 5.8.0025	Depositor
R, R_{free}	0.165 , 0.186 0.166 , 0.186	Depositor DCC
R_{free} test set	27599 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	16.4	Xtriage
Anisotropy	0.365	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 36.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	24709	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.93% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IPA, GAL, CA, CL, SIA, EDO, BGC

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	0.63	0/2233	0.72	0/3045
1	B	0.63	0/2232	0.70	0/3043
1	C	0.62	0/2241	0.69	0/3052
1	D	0.62	0/2208	0.70	0/3010
1	E	0.62	0/2219	0.72	0/3025
1	F	0.59	0/2183	0.68	0/2974
1	G	0.58	0/2138	0.70	0/2909
1	H	0.59	0/2177	0.69	0/2963
1	I	0.58	0/2160	0.70	0/2941
1	J	0.58	0/2178	0.68	0/2968
All	All	0.60	0/21969	0.70	0/29930

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

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	2177	0	2129	14	0
1	B	2173	0	2147	17	0
1	C	2179	0	2165	17	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2146	0	2129	11	0
1	E	2158	0	2127	11	0
1	F	2119	0	2110	6	0
1	G	2087	0	2063	5	0
1	H	2117	0	2101	9	0
1	I	2106	0	2078	10	0
1	J	2125	0	2089	4	0
2	K	32	0	28	2	0
2	L	32	0	28	3	0
2	M	32	0	28	1	0
2	N	32	0	28	3	0
2	O	32	0	28	2	0
2	P	32	0	28	1	0
2	Q	32	0	28	2	0
3	R	43	0	37	2	0
3	S	43	0	37	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	1	0
5	C	1	0	0	1	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
5	I	1	0	0	0	0
5	J	1	0	0	0	0
6	A	20	0	30	8	0
6	B	24	0	36	6	0
6	C	12	0	18	2	0
6	D	8	0	12	0	0
6	E	16	0	24	4	0
6	F	4	0	6	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	G	8	0	12	1	0
6	H	12	0	18	4	0
6	I	8	0	12	1	0
6	J	16	0	24	0	0
7	A	4	0	8	0	0
7	B	4	0	8	0	0
7	C	4	0	8	1	0
7	D	4	0	8	0	0
7	E	4	0	8	0	0
7	F	4	0	8	0	0
7	G	4	0	8	1	0
7	H	4	0	8	0	0
7	I	4	0	8	0	0
7	J	4	0	8	0	0
8	A	349	0	0	7	0
8	B	323	0	0	4	0
8	C	315	0	0	5	0
8	D	296	0	0	2	0
8	E	329	0	0	4	0
8	F	250	0	0	2	0
8	G	225	0	0	1	0
8	H	233	0	0	1	0
8	I	249	0	0	1	0
8	J	255	0	0	0	0
All	All	24709	0	21680	111	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.

All (111) 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)
6:A:404:EDO:H11	8:A:706:HOH:O	1.70	0.92
1:C:193[B]:LYS:HA	1:C:193[B]:LYS:HE2	1.52	0.91
1:B:288:ASN:O	6:B:403:EDO:H22	1.72	0.90
1:B:226[B]:THR:HG23	8:B:745:HOH:O	1.72	0.89
1:A:226[B]:THR:HG23	8:A:612:HOH:O	1.75	0.86
1:E:226[B]:THR:HG23	8:E:712:HOH:O	1.78	0.82
1:I:74:SER:HB2	2:Q:1:GAL:H2	1.64	0.80
1:A:79[B]:THR:HG22	1:A:172:THR:HB	1.66	0.78
1:B:79[B]:THR:HG22	1:B:172:THR:HB	1.67	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:226[B]:THR:HG23	8:D:629:HOH:O	1.88	0.72
1:F:226[B]:THR:HG23	8:F:662:HOH:O	1.89	0.72
1:C:226[B]:THR:HG23	8:C:592:HOH:O	1.88	0.72
6:A:403:EDO:H12	8:A:828:HOH:O	1.91	0.71
1:C:79[B]:THR:HG22	1:C:172:THR:HB	1.71	0.70
6:E:404:EDO:H21	8:E:759:HOH:O	1.91	0.70
1:E:46[B]:GLU:OE2	1:E:286:TYR:OH	2.10	0.68
1:E:79[B]:THR:HG22	1:E:172:THR:HB	1.75	0.67
1:D:79[B]:THR:HG22	1:D:172:THR:HB	1.77	0.66
1:I:113[B]:VAL:HG22	8:I:548:HOH:O	1.96	0.65
1:H:45[A]:ILE:C	1:H:45[A]:ILE:HD12	2.21	0.65
1:C:288:ASN:O	6:C:403:EDO:H22	1.97	0.64
5:B:402:CL:CL	8:B:738:HOH:O	2.52	0.63
1:E:79[B]:THR:HG21	8:E:732:HOH:O	1.97	0.62
1:A:79[B]:THR:HG21	8:A:837:HOH:O	1.98	0.62
6:A:404:EDO:H12	8:A:619:HOH:O	2.00	0.60
1:D:46[C]:GLU:OE1	1:D:286:TYR:OH	2.22	0.58
1:H:252:GLY:O	6:H:405:EDO:H11	2.03	0.58
1:A:175:ASP:HA	6:A:404:EDO:H21	1.87	0.57
1:B:46[B]:GLU:OE2	1:B:286:TYR:OH	2.22	0.57
1:C:136:TYR:CE1	1:D:133:LYS:HE2	2.41	0.56
1:B:82[B]:LYS:HG2	6:B:408:EDO:H11	1.87	0.56
1:H:45[A]:ILE:HD12	1:H:45[A]:ILE:O	2.06	0.56
6:E:406:EDO:H12	1:G:27:MET:HG3	1.88	0.55
1:F:149:THR:HG1	1:F:226[B]:THR:HG1	1.52	0.55
1:I:39:PRO:HG2	1:I:42:ILE:HD12	1.89	0.54
1:G:224[B]:SER:OG	7:G:405:IPA:H31	2.09	0.53
1:C:193[B]:LYS:HE2	1:C:193[B]:LYS:CA	2.34	0.53
1:J:74:SER:HB2	3:R:2:GAL:H2	1.91	0.52
2:L:1:GAL:H4	2:L:2:SIA:C1	2.40	0.52
1:F:79[B]:THR:HG22	1:F:172:THR:HB	1.91	0.52
1:I:74:SER:CB	2:Q:1:GAL:H2	2.38	0.52
6:H:404:EDO:H12	8:H:697:HOH:O	2.09	0.52
1:B:62:LEU:HD11	2:L:2:SIA:H91	1.91	0.52
1:A:251:VAL:HG12	6:A:405:EDO:H11	1.92	0.51
1:H:44:GLN:C	1:H:45[B]:ILE:HD12	2.36	0.51
1:E:115:VAL:HA	6:E:403:EDO:H22	1.92	0.51
1:H:218:ASN:OD1	6:H:405:EDO:H12	2.11	0.51
1:F:184:LYS:HE3	8:F:608:HOH:O	2.10	0.51
6:B:405:EDO:H12	1:J:27:MET:HG3	1.91	0.51
1:F:218:ASN:OD1	6:F:403:EDO:H22	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:177:VAL:O	6:E:404:EDO:H22	2.12	0.49
1:B:45:ILE:HD12	1:B:45:ILE:C	2.38	0.49
1:H:74:SER:HB2	2:P:1:GAL:H2	1.95	0.49
1:C:115:VAL:HA	6:C:403:EDO:H11	1.95	0.49
1:B:46[B]:GLU:CD	1:B:286:TYR:HH	2.19	0.48
1:C:149:THR:HG1	1:C:226[B]:THR:HG1	1.61	0.48
1:F:133[B]:LYS:HE3	1:F:133[B]:LYS:HB2	1.55	0.47
1:D:149:THR:HG1	1:D:226[B]:THR:HG1	1.62	0.47
1:C:46[A]:GLU:OE2	1:C:286:TYR:OH	2.31	0.47
6:B:406:EDO:H12	1:I:29:GLY:N	2.30	0.47
1:B:115:VAL:HA	6:B:403:EDO:H11	1.98	0.46
1:A:146:GLN:HA	8:A:572:HOH:O	2.16	0.46
1:A:290:THR:OG1	6:A:403:EDO:O1	2.28	0.46
1:B:218:ASN:OD1	6:B:405:EDO:H11	2.16	0.46
1:A:27:MET:HG3	6:F:403:EDO:H21	1.97	0.46
1:C:234:VAL:HG22	1:D:226[B]:THR:HG22	1.97	0.46
1:D:146:GLN:HA	8:D:569:HOH:O	2.16	0.46
2:M:1:GAL:H4	2:M:2:SIA:C1	2.45	0.46
1:A:136:TYR:CE1	1:B:133:LYS:HE2	2.51	0.45
1:B:146:GLN:HA	8:B:600:HOH:O	2.16	0.45
1:D:48:TYR:C	1:D:49:LEU:HD12	2.42	0.45
1:B:234:VAL:HG22	1:C:226[B]:THR:HG22	1.98	0.45
1:A:48:TYR:C	1:A:49:LEU:HD12	2.42	0.44
1:A:273:ASN:HB3	2:K:2:SIA:O1A	2.16	0.44
1:C:224[B]:SER:OG	7:C:406:IPA:H31	2.18	0.44
1:E:74:SER:HB2	2:N:1:GAL:H2	1.98	0.44
1:I:117:THR:HG23	6:I:404:EDO:H22	2.00	0.44
1:A:218:ASN:HA	6:A:405:EDO:H21	2.00	0.44
1:C:146:GLN:HA	8:C:560:HOH:O	2.16	0.44
1:B:45:ILE:HD12	1:B:45:ILE:O	2.18	0.44
5:C:402:CL:CL	8:C:666:HOH:O	2.59	0.43
1:E:146:GLN:HA	8:E:570:HOH:O	2.18	0.43
2:O:1:GAL:H4	2:O:2:SIA:C1	2.49	0.43
1:H:46[B]:GLU:OE2	1:H:286:TYR:OH	2.35	0.43
1:B:25:SER:HB3	1:I:37:THR:HG22	2.00	0.43
1:G:45:ILE:HD12	1:G:45:ILE:C	2.44	0.43
1:B:184:LYS:HE2	8:B:693:HOH:O	2.17	0.43
1:H:45[B]:ILE:HG21	1:H:93:ILE:HG21	2.01	0.43
1:C:74:SER:HB2	2:L:1:GAL:H2	2.00	0.43
2:N:1:GAL:H4	2:N:2:SIA:C1	2.49	0.43
1:I:48:TYR:C	1:I:49:LEU:HD12	2.44	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:146:GLN:HA	8:G:531:HOH:O	2.20	0.42
1:H:275:SER:O	1:H:276:GLU:HB2	2.20	0.42
1:I:273:ASN:HB3	3:R:3:SIA:O1A	2.20	0.42
1:A:46[C]:GLU:OE2	1:A:286:TYR:OH	2.33	0.42
6:A:405:EDO:H12	8:A:845:HOH:O	2.20	0.42
1:D:45:ILE:C	1:D:45:ILE:HD12	2.45	0.41
1:B:48:TYR:C	1:B:49:LEU:HD12	2.46	0.41
1:C:79[B]:THR:HG21	8:C:616:HOH:O	2.20	0.41
1:E:273:ASN:HB3	2:O:2:SIA:O1A	2.20	0.41
1:G:117:THR:HG23	6:G:403:EDO:H22	2.02	0.41
1:D:273:ASN:HB3	2:N:2:SIA:O1A	2.21	0.41
1:J:45:ILE:HD12	1:J:45:ILE:C	2.47	0.41
1:C:45:ILE:HD12	1:C:45:ILE:C	2.46	0.40
1:A:133:LYS:HE2	1:E:136:TYR:CE1	2.56	0.40
1:E:92:VAL:HG22	1:E:261:PHE:CE1	2.57	0.40
1:C:184[B]:LYS:HG2	8:C:645:HOH:O	2.21	0.40
1:I:45:ILE:C	1:I:45:ILE:HD12	2.47	0.40
1:J:298:ASN:HA	1:J:299:PRO:HD2	1.97	0.40
1:D:27:MET:HG3	6:H:405:EDO:H22	2.03	0.40
2:K:1:GAL:H4	2:K:2:SIA:C1	2.51	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	284/278 (102%)	277 (98%)	7 (2%)	0	100	100
1	B	285/278 (102%)	278 (98%)	7 (2%)	0	100	100
1	C	286/278 (103%)	278 (97%)	8 (3%)	0	100	100
1	D	280/278 (101%)	273 (98%)	7 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	283/278 (102%)	276 (98%)	7 (2%)	0	100	100
1	F	279/278 (100%)	272 (98%)	7 (2%)	0	100	100
1	G	269/278 (97%)	263 (98%)	6 (2%)	0	100	100
1	H	276/278 (99%)	268 (97%)	8 (3%)	0	100	100
1	I	274/278 (99%)	268 (98%)	6 (2%)	0	100	100
1	J	278/278 (100%)	272 (98%)	6 (2%)	0	100	100
All	All	2794/2780 (100%)	2725 (98%)	69 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	246/237 (104%)	246 (100%)	0	100	100
1	B	247/237 (104%)	247 (100%)	0	100	100
1	C	248/237 (105%)	248 (100%)	0	100	100
1	D	244/237 (103%)	244 (100%)	0	100	100
1	E	245/237 (103%)	245 (100%)	0	100	100
1	F	241/237 (102%)	241 (100%)	0	100	100
1	G	235/237 (99%)	235 (100%)	0	100	100
1	H	240/237 (101%)	240 (100%)	0	100	100
1	I	238/237 (100%)	238 (100%)	0	100	100
1	J	240/237 (101%)	240 (100%)	0	100	100
All	All	2424/2370 (102%)	2424 (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 (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	182	ASN
1	C	44	GLN
1	C	55	ASN
1	C	67	ASN
1	C	182	ASN
1	C	249	ASN
1	G	249	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

20 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	$\# Z > 2$
2	GAL	K	1	2	12,12,12	0.46	0	17,17,17	0.74	0
2	SIA	K	2	2	20,20,21	0.58	0	21,28,31	1.41	3 (14%)
2	GAL	L	1	2	12,12,12	0.46	0	17,17,17	0.88	1 (5%)
2	SIA	L	2	2	20,20,21	0.58	0	21,28,31	1.47	3 (14%)
2	GAL	M	1	2	12,12,12	0.48	0	17,17,17	0.87	1 (5%)
2	SIA	M	2	2	20,20,21	0.52	0	21,28,31	1.44	3 (14%)
2	GAL	N	1	2	12,12,12	0.48	0	17,17,17	0.73	0
2	SIA	N	2	2	20,20,21	0.59	0	21,28,31	1.39	3 (14%)
2	GAL	O	1	2	12,12,12	0.46	0	17,17,17	0.74	0
2	SIA	O	2	2	20,20,21	0.56	0	21,28,31	1.38	3 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GAL	P	1	2	12,12,12	0.47	0	17,17,17	0.70	0
2	SIA	P	2	2	20,20,21	0.57	0	21,28,31	1.22	3 (14%)
2	GAL	Q	1	2	12,12,12	0.53	0	17,17,17	0.68	0
2	SIA	Q	2	2	20,20,21	0.53	0	21,28,31	1.08	2 (9%)
3	BGC	R	1	3	12,12,12	0.51	0	17,17,17	0.69	0
3	GAL	R	2	3	11,11,12	0.55	0	15,15,17	1.20	2 (13%)
3	SIA	R	3	3	20,20,21	0.61	0	21,28,31	1.23	3 (14%)
3	BGC	S	1	3	12,12,12	0.55	0	17,17,17	0.79	0
3	GAL	S	2	3	11,11,12	0.51	0	15,15,17	0.94	0
3	SIA	S	3	3	20,20,21	0.57	0	21,28,31	1.32	3 (14%)

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	GAL	K	1	2	-	1/2/22/22	0/1/1/1
2	SIA	K	2	2	-	0/18/34/38	0/1/1/1
2	GAL	L	1	2	-	2/2/22/22	0/1/1/1
2	SIA	L	2	2	-	0/18/34/38	0/1/1/1
2	GAL	M	1	2	-	1/2/22/22	0/1/1/1
2	SIA	M	2	2	-	2/18/34/38	0/1/1/1
2	GAL	N	1	2	-	2/2/22/22	0/1/1/1
2	SIA	N	2	2	-	2/18/34/38	0/1/1/1
2	GAL	O	1	2	-	1/2/22/22	0/1/1/1
2	SIA	O	2	2	-	2/18/34/38	0/1/1/1
2	GAL	P	1	2	-	1/2/22/22	0/1/1/1
2	SIA	P	2	2	-	0/18/34/38	0/1/1/1
2	GAL	Q	1	2	-	1/2/22/22	0/1/1/1
2	SIA	Q	2	2	-	6/18/34/38	0/1/1/1
3	BGC	R	1	3	-	0/2/22/22	0/1/1/1
3	GAL	R	2	3	-	1/2/19/22	0/1/1/1
3	SIA	R	3	3	-	0/18/34/38	0/1/1/1
3	BGC	S	1	3	-	0/2/22/22	0/1/1/1
3	GAL	S	2	3	-	1/2/19/22	0/1/1/1
3	SIA	S	3	3	-	2/18/34/38	0/1/1/1

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	2	SIA	O1B-C1-C2	3.75	122.47	112.71
2	L	2	SIA	O1A-C1-C2	-3.73	114.80	122.85
2	M	2	SIA	O1B-C1-C2	3.61	122.09	112.71
2	M	2	SIA	O6-C2-C1	3.54	114.41	107.72
2	O	2	SIA	O6-C2-C1	3.50	114.33	107.72
2	K	2	SIA	O6-C2-C1	3.45	114.24	107.72
2	M	2	SIA	O1A-C1-C2	-3.42	115.47	122.85
2	N	2	SIA	O6-C2-C1	3.36	114.06	107.72
2	N	2	SIA	O1B-C1-C2	3.35	121.42	112.71
2	L	2	SIA	O6-C2-C1	3.25	113.85	107.72
2	P	2	SIA	O1B-C1-C2	3.21	121.07	112.71
2	K	2	SIA	O1B-C1-C2	3.20	121.04	112.71
3	S	3	SIA	O1B-C1-C2	3.16	120.93	112.71
2	K	2	SIA	O1A-C1-C2	-3.12	116.10	122.85
2	Q	2	SIA	O1B-C1-C2	3.10	120.77	112.71
3	R	3	SIA	O1B-C1-C2	3.05	120.64	112.71
3	S	3	SIA	O6-C2-C1	3.04	113.45	107.72
2	O	2	SIA	O1B-C1-C2	3.03	120.58	112.71
3	R	2	GAL	C1-O5-C5	2.93	116.11	112.19
2	N	2	SIA	O1A-C1-C2	-2.90	116.59	122.85
3	R	2	GAL	C1-C2-C3	2.85	113.80	109.64
2	P	2	SIA	O6-C2-C1	2.67	112.76	107.72
2	O	2	SIA	O1A-C1-C2	-2.63	117.17	122.85
2	Q	2	SIA	O1A-C1-C2	-2.61	117.22	122.85
2	P	2	SIA	O1A-C1-C2	-2.53	117.38	122.85
3	S	3	SIA	O1A-C1-C2	-2.51	117.43	122.85
2	M	1	GAL	C1-O5-C5	2.43	118.34	113.65
3	R	3	SIA	O1A-C1-C2	-2.33	117.82	122.85
3	R	3	SIA	O6-C2-C1	2.30	112.06	107.72
2	L	1	GAL	C1-O5-C5	2.11	117.73	113.65

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	Q	2	SIA	C6-C7-C8-C9
2	Q	2	SIA	O7-C7-C8-C9
3	S	3	SIA	C7-C8-C9-O9
3	S	3	SIA	O8-C8-C9-O9
2	Q	2	SIA	C6-C7-C8-O8
2	Q	2	SIA	O7-C7-C8-O8

Continued on next page...

Continued from previous page...

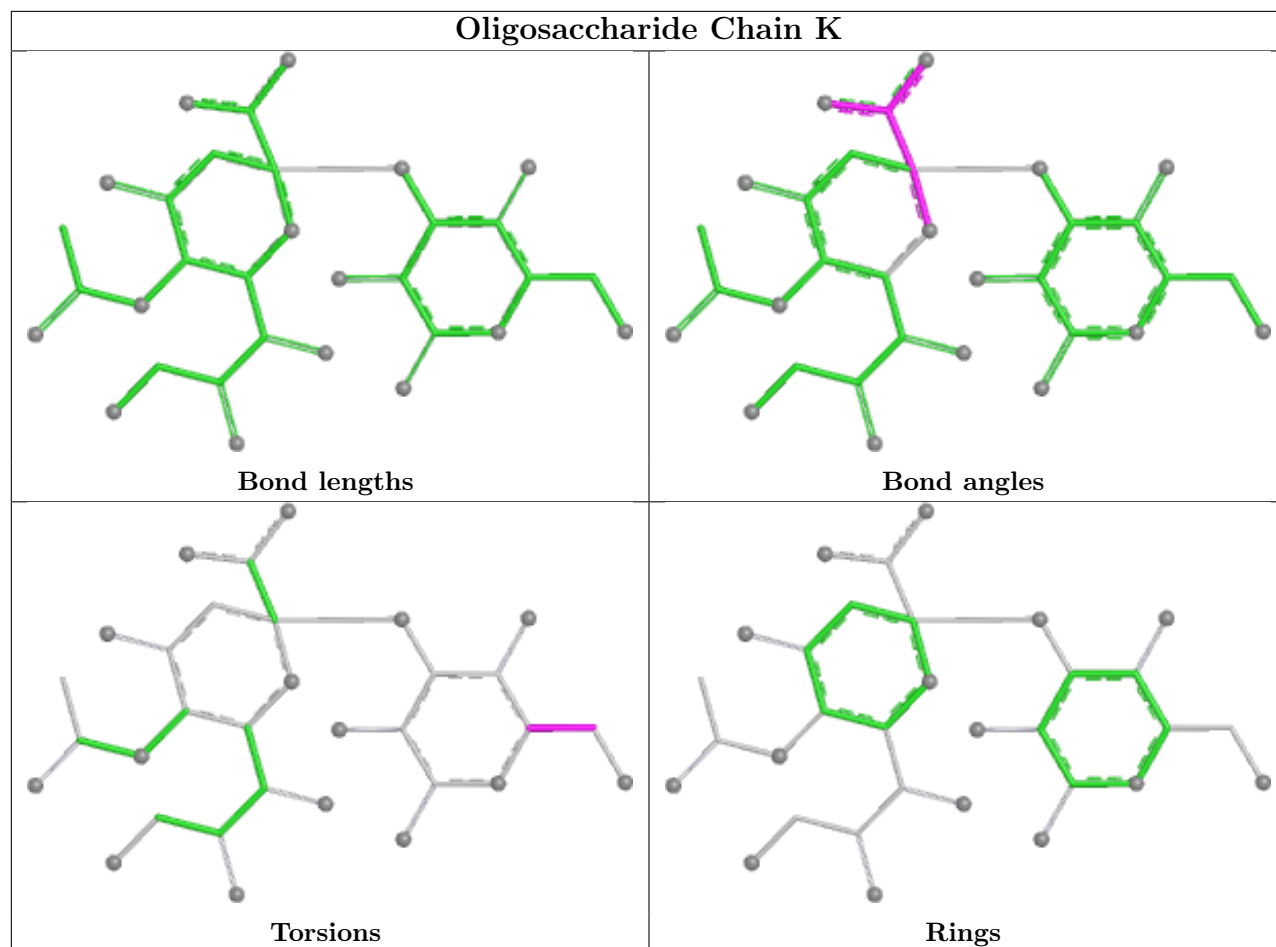
Mol	Chain	Res	Type	Atoms
2	N	1	GAL	O5-C5-C6-O6
2	L	1	GAL	O5-C5-C6-O6
2	N	2	SIA	C7-C8-C9-O9
2	Q	1	GAL	O5-C5-C6-O6
2	N	2	SIA	O8-C8-C9-O9
2	M	1	GAL	O5-C5-C6-O6
2	O	1	GAL	O5-C5-C6-O6
3	S	2	GAL	O5-C5-C6-O6
2	P	1	GAL	O5-C5-C6-O6
2	K	1	GAL	O5-C5-C6-O6
3	R	2	GAL	O5-C5-C6-O6
2	Q	2	SIA	O8-C8-C9-O9
2	M	2	SIA	C7-C8-C9-O9
2	N	1	GAL	C4-C5-C6-O6
2	M	2	SIA	O8-C8-C9-O9
2	O	2	SIA	C6-C7-C8-O8
2	L	1	GAL	C4-C5-C6-O6
2	O	2	SIA	O7-C7-C8-C9
2	Q	2	SIA	C7-C8-C9-O9

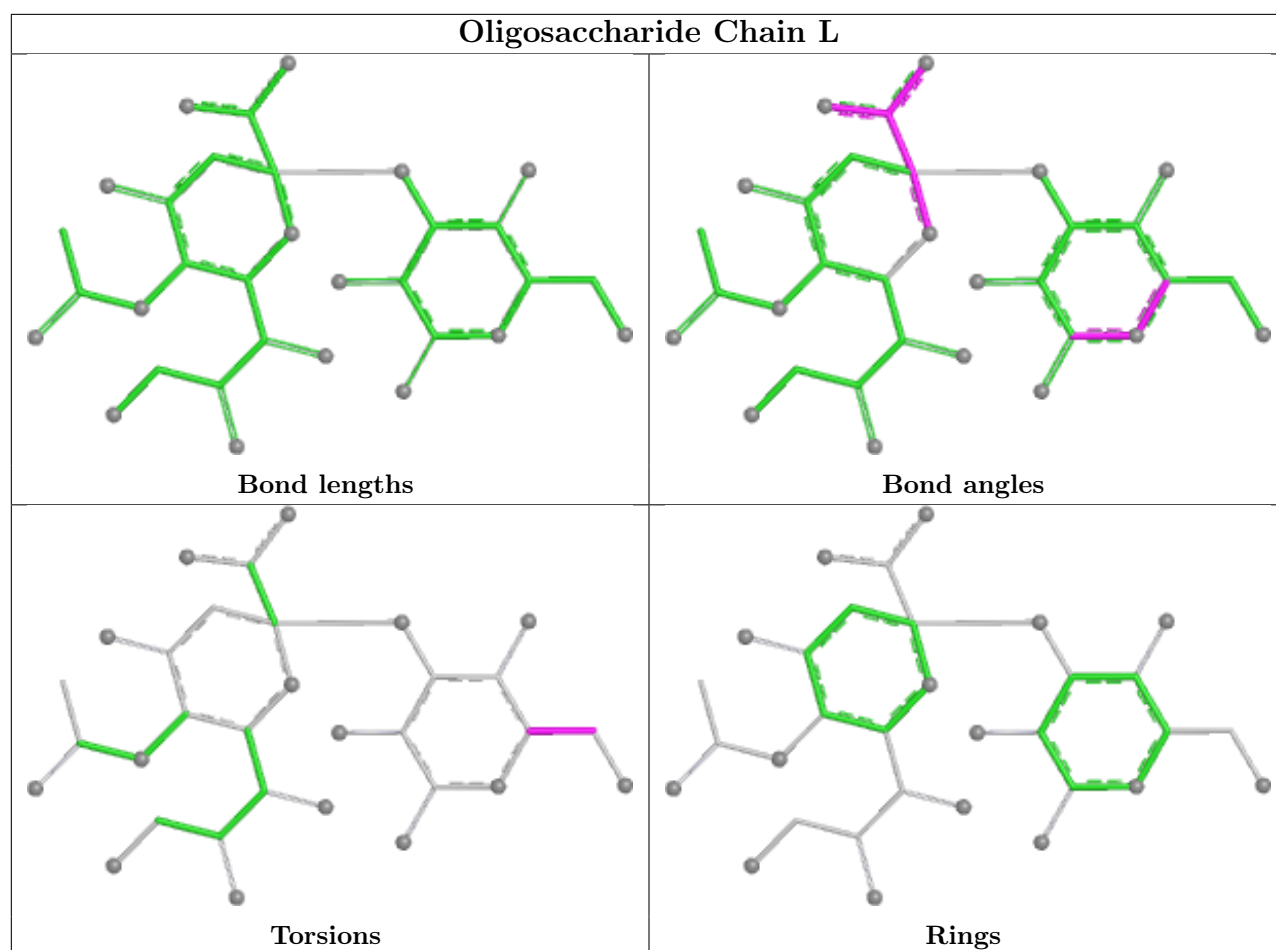
There are no ring outliers.

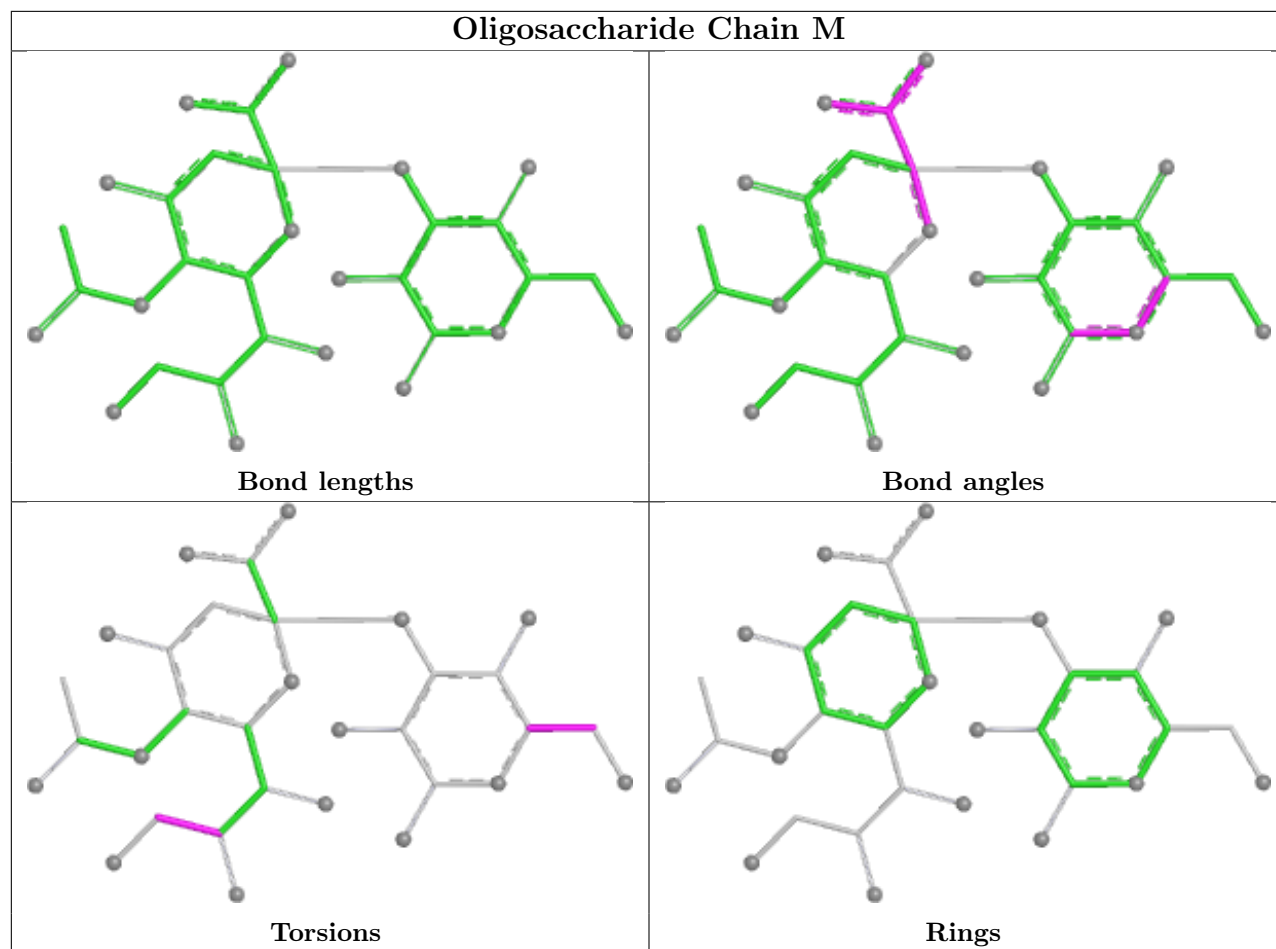
14 monomers are involved in 16 short contacts:

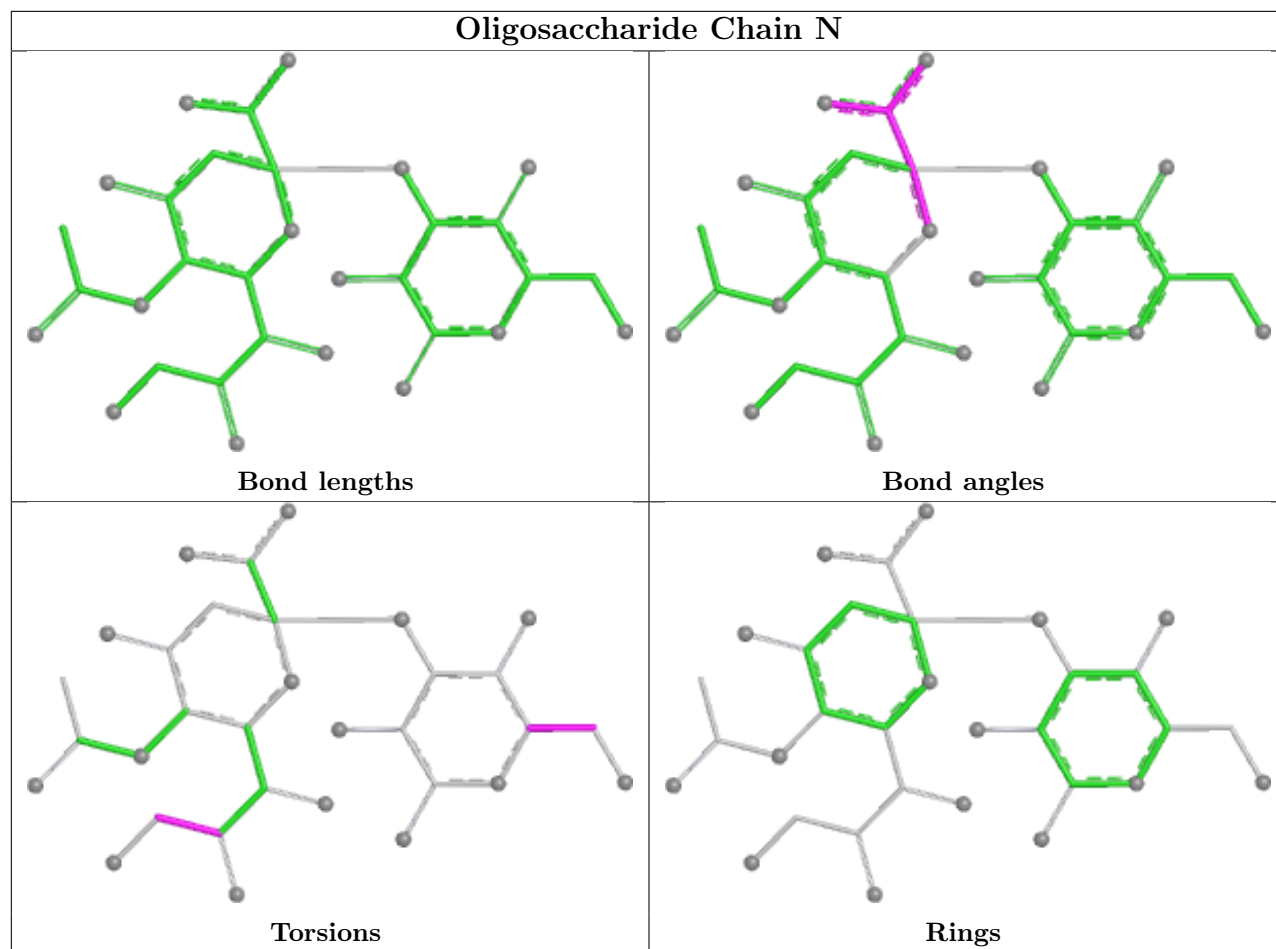
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	O	2	SIA	2	0
2	K	2	SIA	2	0
2	M	2	SIA	1	0
2	N	1	GAL	2	0
2	Q	1	GAL	2	0
2	O	1	GAL	1	0
2	N	2	SIA	2	0
2	P	1	GAL	1	0
2	M	1	GAL	1	0
2	K	1	GAL	1	0
3	R	3	SIA	1	0
2	L	2	SIA	2	0
2	L	1	GAL	2	0
3	R	2	GAL	1	0

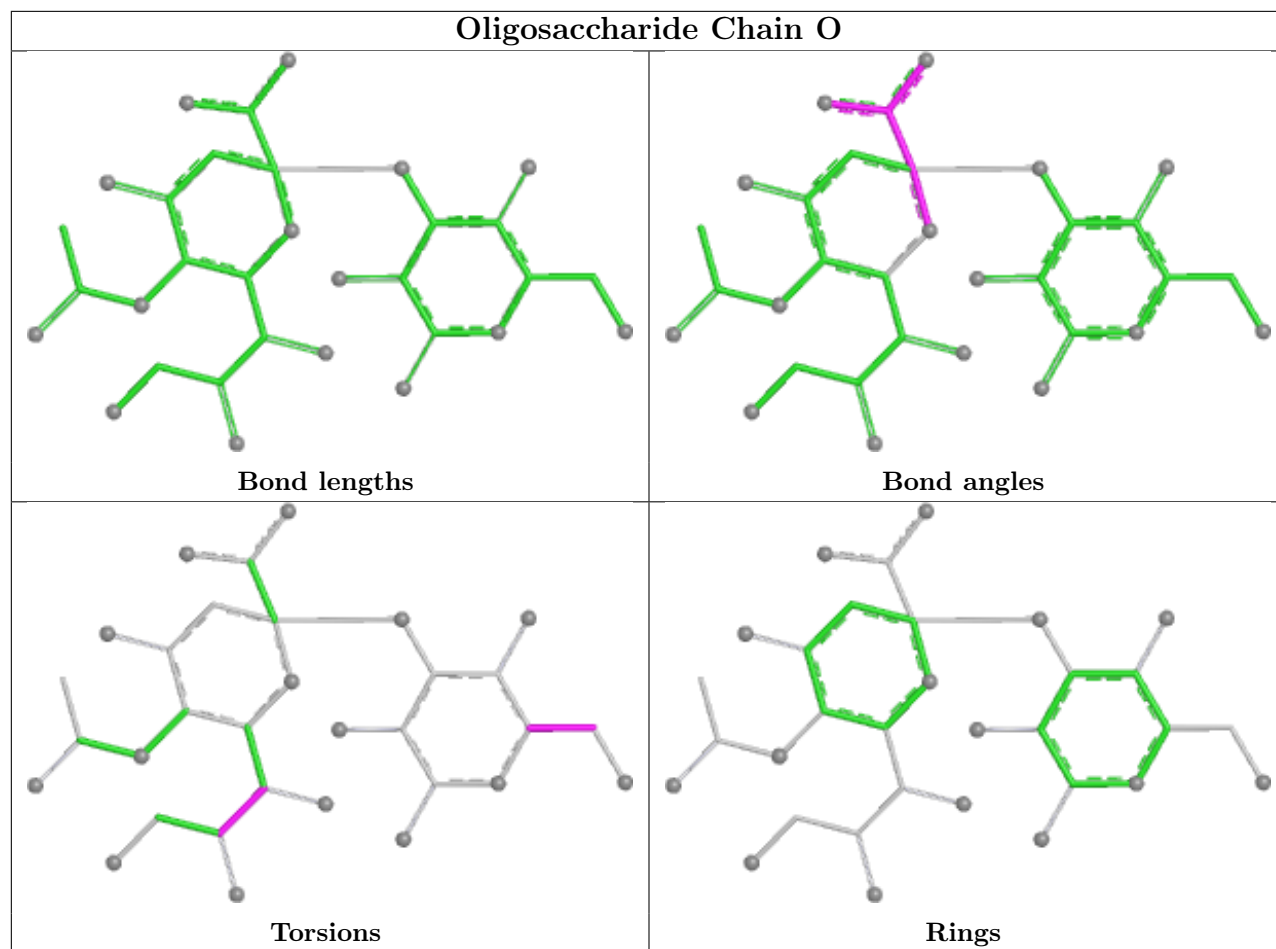
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

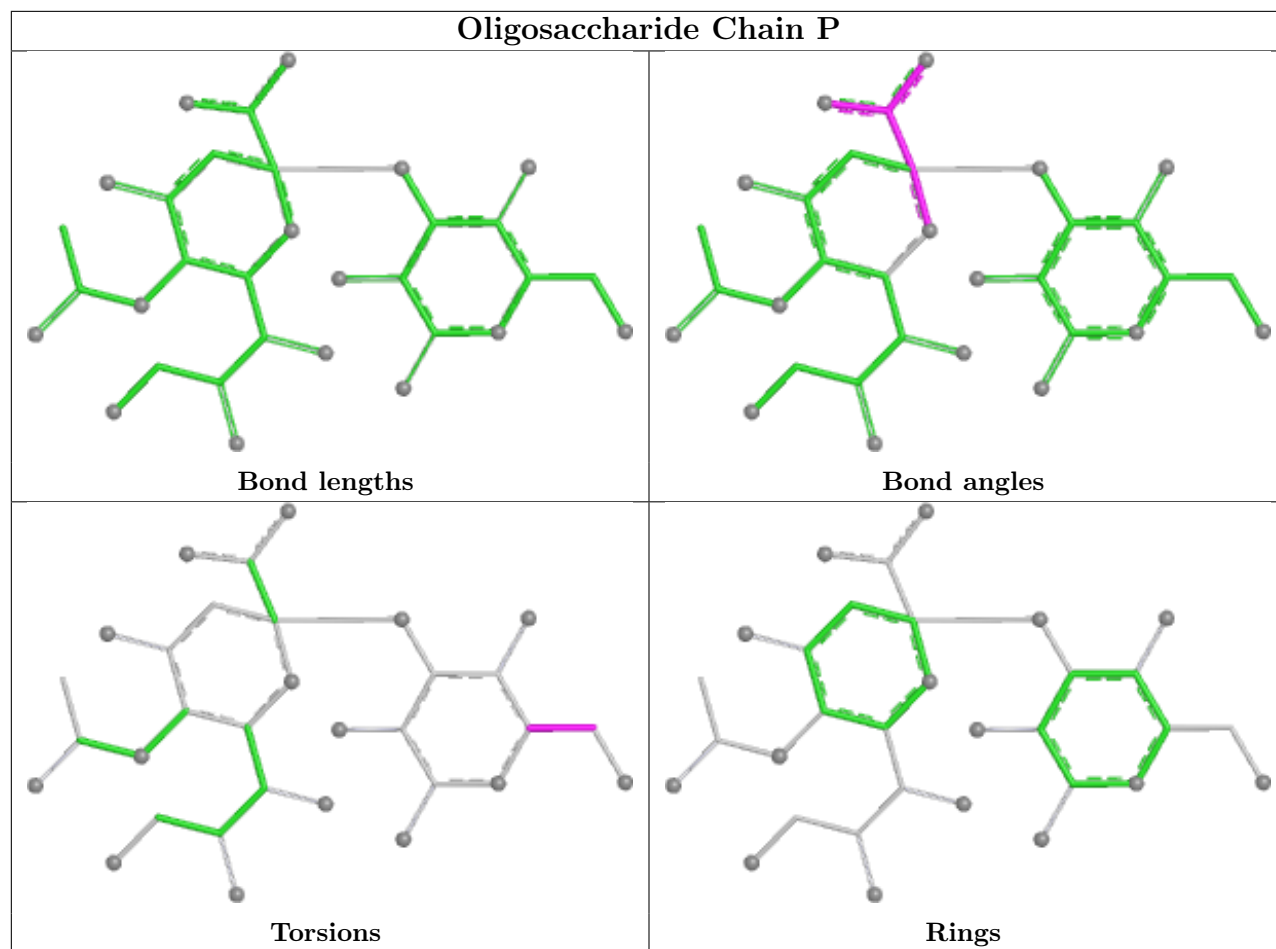


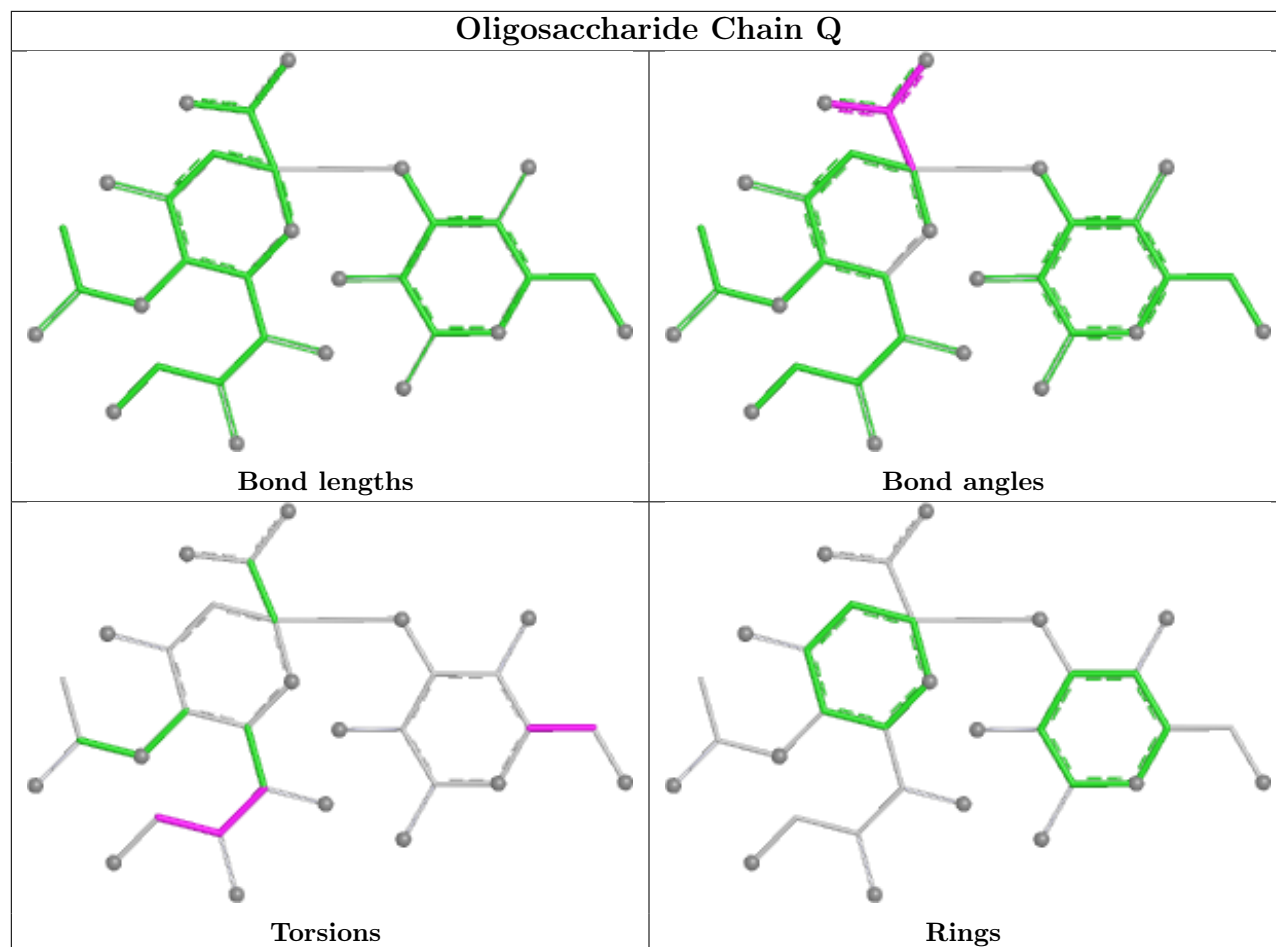


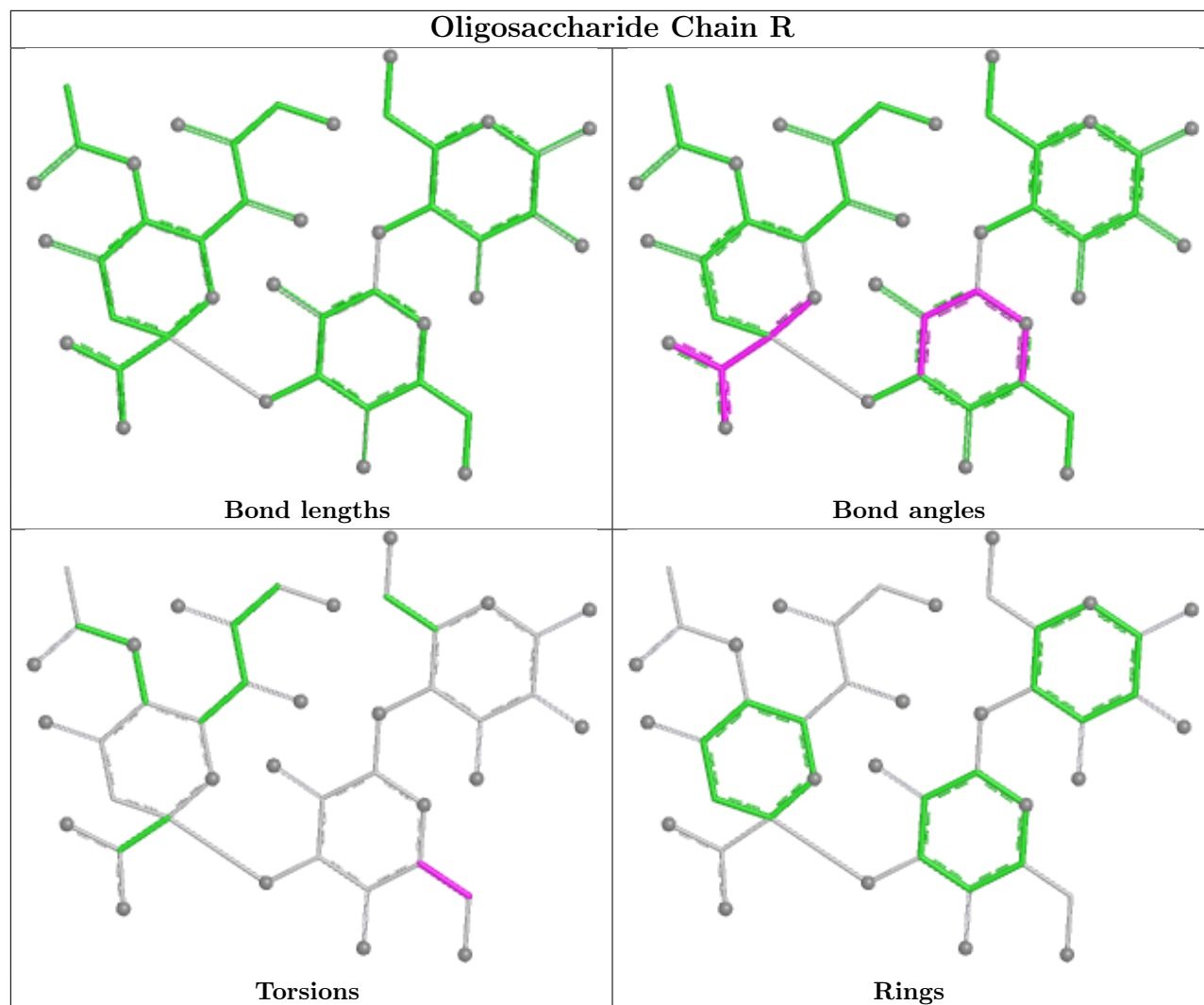


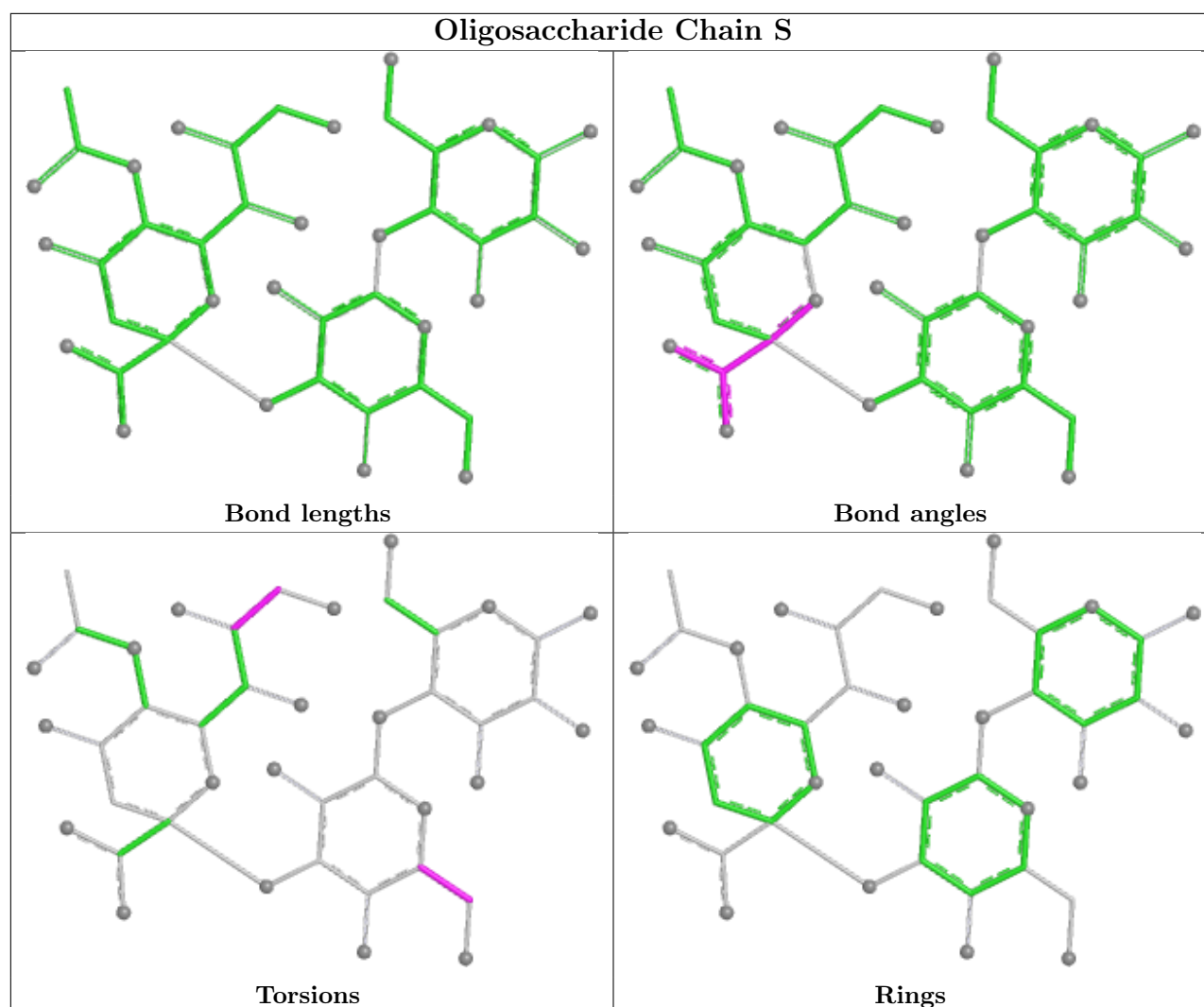












5.6 Ligand geometry [i](#)

Of 62 ligands modelled in this entry, 20 are monoatomic - leaving 42 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	$\# Z > 2$
6	EDO	E	403	-	3,3,3	0.26	0	2,2,2	1.05	0
7	IPA	F	404	-	3,3,3	0.50	0	3,3,3	0.25	0
6	EDO	B	407	-	3,3,3	0.46	0	2,2,2	0.34	0
7	IPA	J	407	-	3,3,3	0.44	0	3,3,3	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	EDO	A	407	-	3,3,3	0.42	0	2,2,2	0.43	0
6	EDO	B	406	-	3,3,3	0.44	0	2,2,2	0.46	0
6	EDO	G	403	-	3,3,3	0.51	0	2,2,2	0.12	0
6	EDO	D	403	-	3,3,3	0.46	0	2,2,2	0.23	0
6	EDO	F	403	-	3,3,3	0.52	0	2,2,2	0.06	0
6	EDO	E	406	-	3,3,3	0.55	0	2,2,2	0.10	0
7	IPA	G	405	-	3,3,3	0.42	0	3,3,3	0.37	0
6	EDO	J	403	-	3,3,3	0.28	0	2,2,2	0.62	0
7	IPA	D	405	-	3,3,3	0.44	0	3,3,3	0.26	0
6	EDO	A	406	-	3,3,3	0.41	0	2,2,2	0.42	0
7	IPA	I	405	-	3,3,3	0.49	0	3,3,3	0.24	0
6	EDO	A	405	-	3,3,3	0.28	0	2,2,2	0.66	0
6	EDO	J	404	-	3,3,3	0.44	0	2,2,2	0.29	0
6	EDO	H	405	-	3,3,3	0.39	0	2,2,2	0.50	0
7	IPA	H	406	-	3,3,3	0.51	0	3,3,3	0.34	0
7	IPA	A	408	-	3,3,3	0.48	0	3,3,3	0.23	0
6	EDO	H	404	-	3,3,3	0.45	0	2,2,2	0.37	0
6	EDO	C	403	-	3,3,3	0.22	0	2,2,2	0.40	0
6	EDO	E	405	-	3,3,3	0.46	0	2,2,2	0.23	0
6	EDO	A	403	-	3,3,3	0.27	0	2,2,2	0.10	0
6	EDO	I	403	-	3,3,3	0.42	0	2,2,2	0.37	0
6	EDO	J	406	-	3,3,3	0.52	0	2,2,2	0.16	0
6	EDO	B	408	-	3,3,3	0.49	0	2,2,2	0.34	0
6	EDO	A	404	-	3,3,3	0.67	0	2,2,2	0.30	0
6	EDO	D	404	-	3,3,3	0.49	0	2,2,2	0.31	0
6	EDO	G	404	-	3,3,3	0.50	0	2,2,2	0.19	0
6	EDO	B	404	-	3,3,3	0.44	0	2,2,2	0.40	0
6	EDO	H	403	-	3,3,3	0.46	0	2,2,2	0.45	0
6	EDO	E	404	-	3,3,3	0.44	0	2,2,2	0.19	0
7	IPA	E	407	-	3,3,3	0.44	0	3,3,3	0.34	0
6	EDO	B	403	-	3,3,3	0.22	0	2,2,2	0.63	0
6	EDO	C	405	-	3,3,3	0.42	0	2,2,2	0.36	0
6	EDO	C	404	-	3,3,3	0.42	0	2,2,2	0.57	0
6	EDO	B	405	-	3,3,3	0.54	0	2,2,2	0.21	0
6	EDO	I	404	-	3,3,3	0.39	0	2,2,2	0.35	0
7	IPA	B	409	-	3,3,3	0.45	0	3,3,3	0.28	0
7	IPA	C	406	-	3,3,3	0.47	0	3,3,3	0.32	0
6	EDO	J	405	-	3,3,3	0.39	0	2,2,2	0.36	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
6	EDO	E	403	-	-	1/1/1/1	-
6	EDO	B	407	-	-	1/1/1/1	-
6	EDO	A	407	-	-	0/1/1/1	-
6	EDO	B	406	-	-	0/1/1/1	-
6	EDO	G	403	-	-	1/1/1/1	-
6	EDO	D	403	-	-	1/1/1/1	-
6	EDO	F	403	-	-	1/1/1/1	-
6	EDO	E	406	-	-	1/1/1/1	-
6	EDO	J	403	-	-	1/1/1/1	-
6	EDO	A	406	-	-	1/1/1/1	-
6	EDO	A	405	-	-	0/1/1/1	-
6	EDO	J	404	-	-	1/1/1/1	-
6	EDO	H	405	-	-	0/1/1/1	-
6	EDO	H	404	-	-	1/1/1/1	-
6	EDO	C	403	-	-	1/1/1/1	-
6	EDO	E	405	-	-	1/1/1/1	-
6	EDO	A	403	-	-	1/1/1/1	-
6	EDO	I	403	-	-	1/1/1/1	-
6	EDO	J	406	-	-	1/1/1/1	-
6	EDO	B	408	-	-	0/1/1/1	-
6	EDO	A	404	-	-	1/1/1/1	-
6	EDO	D	404	-	-	0/1/1/1	-
6	EDO	G	404	-	-	0/1/1/1	-
6	EDO	B	404	-	-	0/1/1/1	-
6	EDO	H	403	-	-	0/1/1/1	-
6	EDO	E	404	-	-	1/1/1/1	-
6	EDO	B	403	-	-	1/1/1/1	-
6	EDO	C	405	-	-	0/1/1/1	-
6	EDO	C	404	-	-	0/1/1/1	-
6	EDO	B	405	-	-	1/1/1/1	-
6	EDO	I	404	-	-	0/1/1/1	-
6	EDO	J	405	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	403	EDO	O1-C1-C2-O2
6	A	404	EDO	O1-C1-C2-O2
6	B	407	EDO	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	E	403	EDO	O1-C1-C2-O2
6	E	404	EDO	O1-C1-C2-O2
6	H	404	EDO	O1-C1-C2-O2
6	B	403	EDO	O1-C1-C2-O2
6	C	403	EDO	O1-C1-C2-O2
6	J	403	EDO	O1-C1-C2-O2
6	E	406	EDO	O1-C1-C2-O2
6	J	404	EDO	O1-C1-C2-O2
6	A	406	EDO	O1-C1-C2-O2
6	B	405	EDO	O1-C1-C2-O2
6	G	403	EDO	O1-C1-C2-O2
6	I	403	EDO	O1-C1-C2-O2
6	D	403	EDO	O1-C1-C2-O2
6	E	405	EDO	O1-C1-C2-O2
6	F	403	EDO	O1-C1-C2-O2
6	J	406	EDO	O1-C1-C2-O2

There are no ring outliers.

18 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	403	EDO	1	0
6	B	406	EDO	1	0
6	G	403	EDO	1	0
6	F	403	EDO	2	0
6	E	406	EDO	1	0
7	G	405	IPA	1	0
6	A	405	EDO	3	0
6	H	405	EDO	3	0
6	H	404	EDO	1	0
6	C	403	EDO	2	0
6	A	403	EDO	2	0
6	B	408	EDO	1	0
6	A	404	EDO	3	0
6	E	404	EDO	2	0
6	B	403	EDO	2	0
6	B	405	EDO	2	0
6	I	404	EDO	1	0
7	C	406	IPA	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	277/278 (99%)	-0.27	5 (1%) 67 72	6, 14, 29, 71	9 (3%)
1	B	275/278 (98%)	-0.24	13 (4%) 36 40	5, 14, 34, 78	12 (4%)
1	C	275/278 (98%)	-0.22	12 (4%) 39 43	7, 15, 39, 78	13 (4%)
1	D	274/278 (98%)	-0.10	13 (4%) 36 40	6, 17, 42, 83	10 (3%)
1	E	277/278 (99%)	-0.27	4 (1%) 73 77	7, 16, 29, 73	8 (2%)
1	F	274/278 (98%)	0.19	9 (3%) 49 53	12, 20, 38, 90	7 (2%)
1	G	270/278 (97%)	0.24	12 (4%) 39 43	12, 21, 39, 87	5 (1%)
1	H	273/278 (98%)	0.25	14 (5%) 33 36	11, 22, 45, 82	7 (2%)
1	I	273/278 (98%)	0.09	11 (4%) 42 46	11, 21, 45, 92	5 (1%)
1	J	275/278 (98%)	0.03	11 (4%) 42 46	11, 20, 37, 85	5 (1%)
All	All	2743/2780 (98%)	-0.03	104 (3%) 44 48	5, 18, 40, 92	81 (2%)

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	73[A]	PHE	8.3
1	D	299	PRO	5.3
1	G	103	THR	5.2
1	D	39	PRO	5.2
1	G	104	CYS	5.0
1	I	104	CYS	4.7
1	D	103	THR	4.7
1	C	39	PRO	4.4
1	H	98	LEU	4.3
1	B	39	PRO	4.3
1	F	37	THR	4.3
1	H	104	CYS	4.2
1	F	38	GLY	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	38	GLY	4.2
1	H	103	THR	4.1
1	I	38	GLY	4.1
1	A	37	THR	4.0
1	I	73	PHE	4.0
1	B	37	THR	4.0
1	G	39	PRO	3.9
1	H	39	PRO	3.9
1	D	104	CYS	3.9
1	C	103	THR	3.7
1	F	73	PHE	3.5
1	J	104	CYS	3.5
1	G	107	ILE	3.5
1	J	299	PRO	3.5
1	A	38	GLY	3.5
1	I	102	MET	3.5
1	F	274	TYR	3.4
1	I	37	THR	3.4
1	E	38	GLY	3.3
1	D	73	PHE	3.3
1	H	97	LEU	3.3
1	D	37	THR	3.3
1	C	37	THR	3.2
1	J	37	THR	3.2
1	J	38	GLY	3.2
1	F	103	THR	3.2
1	H	100	GLU	3.1
1	H	298	ASN	3.1
1	B	73	PHE	3.1
1	B	38	GLY	3.1
1	B	103	THR	3.0
1	F	100	GLU	3.0
1	G	106	THR	3.0
1	J	73	PHE	3.0
1	I	40	ASP	2.9
1	F	104	CYS	2.9
1	J	103	THR	2.9
1	C	38	GLY	2.8
1	H	107	ILE	2.8
1	B	25	SER	2.8
1	I	105	ASP	2.8
1	G	97	LEU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	45	ILE	2.8
1	H	38	GLY	2.7
1	E	37	THR	2.7
1	C	299	PRO	2.7
1	G	37	THR	2.7
1	F	76	ALA	2.7
1	J	25	SER	2.7
1	G	102	MET	2.7
1	I	39	PRO	2.7
1	J	102	MET	2.6
1	J	39	PRO	2.6
1	C	73	PHE	2.6
1	I	298	ASN	2.6
1	B	299	PRO	2.5
1	C	35	VAL	2.5
1	C	25	SER	2.5
1	D	38	GLY	2.5
1	J	106	THR	2.5
1	E	73	PHE	2.4
1	I	175	ASP	2.4
1	C	26	HIS	2.4
1	G	99	ASN	2.4
1	D	101	ASP	2.4
1	B	274	TYR	2.4
1	H	106	THR	2.4
1	C	102	MET	2.4
1	D	108	LEU	2.4
1	G	98	LEU	2.4
1	C	274	TYR	2.4
1	B	102	MET	2.4
1	F	102	MET	2.4
1	A	40	ASP	2.3
1	B	26	HIS	2.3
1	H	37	THR	2.3
1	C	104	CYS	2.2
1	E	274	TYR	2.2
1	I	101	ASP	2.2
1	B	104	CYS	2.2
1	H	25	SER	2.2
1	H	40	ASP	2.1
1	D	106	THR	2.1
1	B	40	ASP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	57	ILE	2.1
1	D	102	MET	2.1
1	A	39	PRO	2.1
1	J	40	ASP	2.1
1	A	300	TYR	2.1
1	D	26	HIS	2.1
1	D	97	LEU	2.0

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

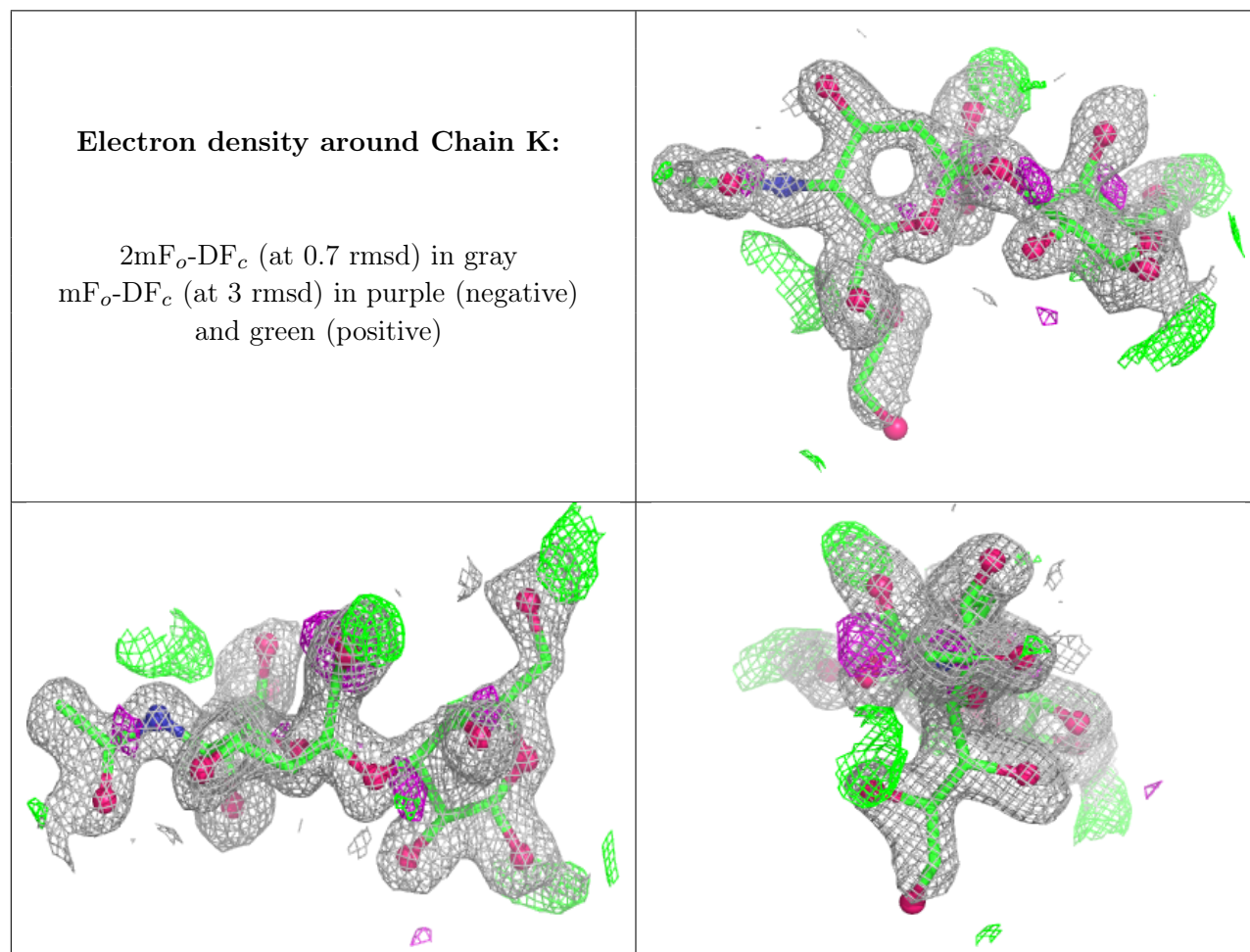
There are no non-standard protein/DNA/RNA residues in this entry.

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, 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.

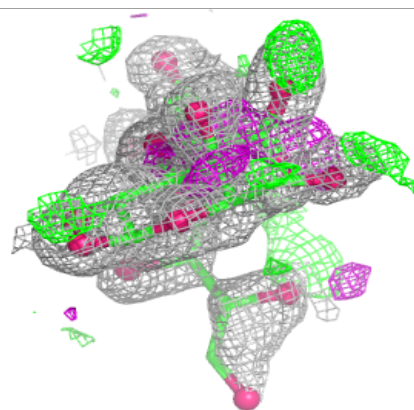
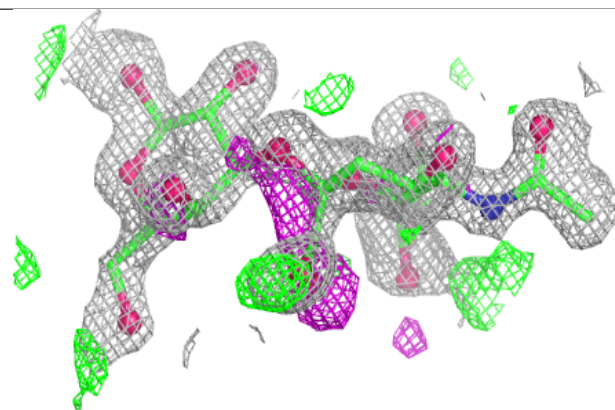
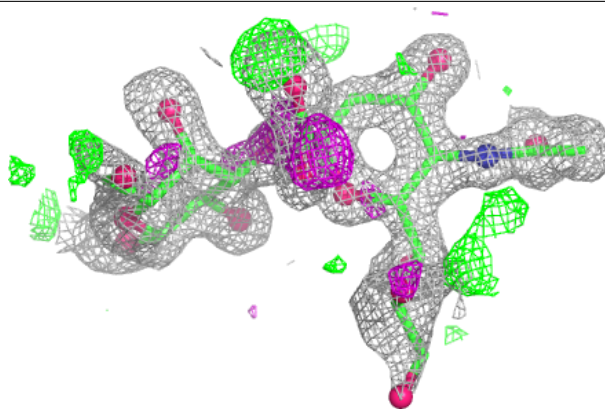
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	BGC	R	1	12/12	0.71	0.14	39,51,64,69	0
2	GAL	M	1	12/12	0.75	0.16	30,31,35,38	12
2	GAL	Q	1	12/12	0.77	0.16	34,39,43,44	12
2	SIA	L	2	20/21	0.80	0.15	22,29,42,50	20
2	GAL	P	1	12/12	0.81	0.16	27,30,38,45	12
3	BGC	S	1	12/12	0.81	0.13	33,43,49,52	0
2	SIA	P	2	20/21	0.82	0.16	24,29,42,48	20
2	SIA	M	2	20/21	0.82	0.15	21,29,41,41	20
2	GAL	N	1	12/12	0.82	0.13	30,34,41,43	0
2	GAL	L	1	12/12	0.82	0.13	27,31,36,37	12
2	GAL	O	1	12/12	0.83	0.13	27,29,39,39	0
2	GAL	K	1	12/12	0.84	0.13	25,28,32,33	12
2	SIA	N	2	20/21	0.85	0.13	24,30,45,46	0
2	SIA	K	2	20/21	0.86	0.13	22,25,37,47	20
2	SIA	Q	2	20/21	0.86	0.14	27,32,42,49	20
3	GAL	R	2	11/12	0.87	0.11	30,34,40,40	0
2	SIA	O	2	20/21	0.89	0.12	20,25,44,50	0
3	SIA	R	3	20/21	0.90	0.12	24,29,50,51	0
3	GAL	S	2	11/12	0.91	0.10	26,29,33,39	0
3	SIA	S	3	20/21	0.91	0.10	21,25,37,49	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.



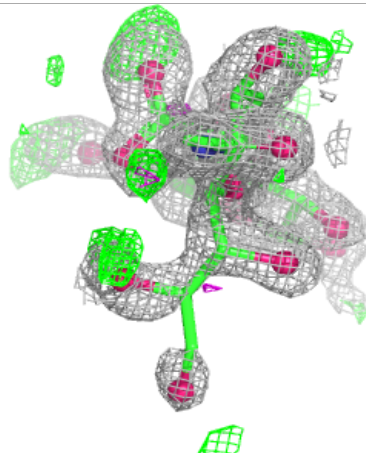
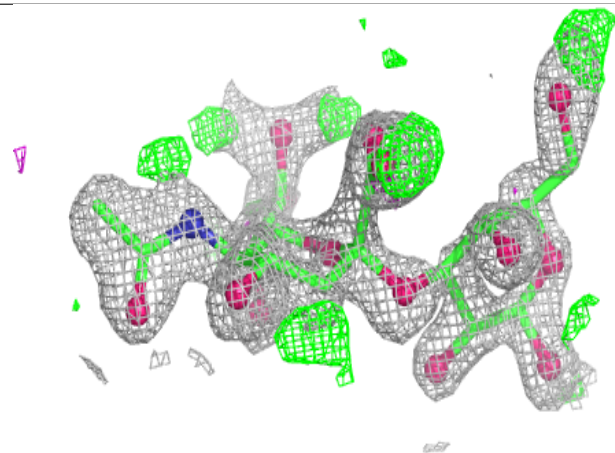
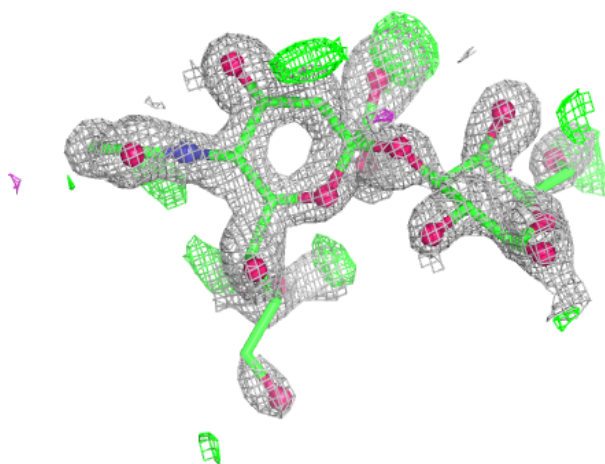
Electron density around Chain L:

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



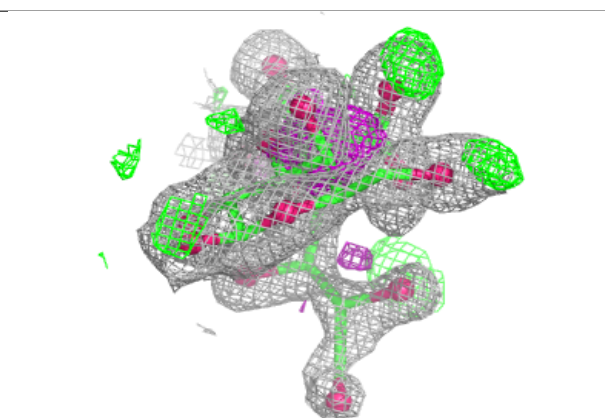
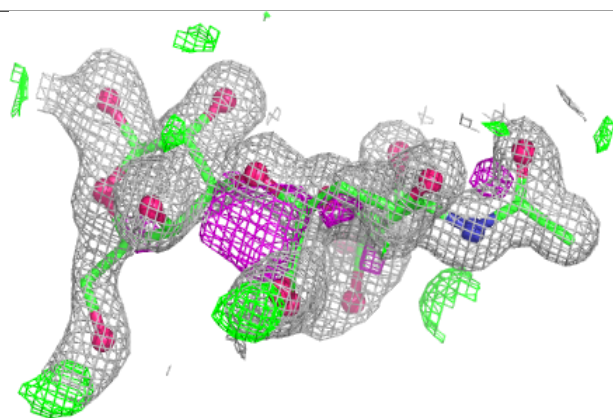
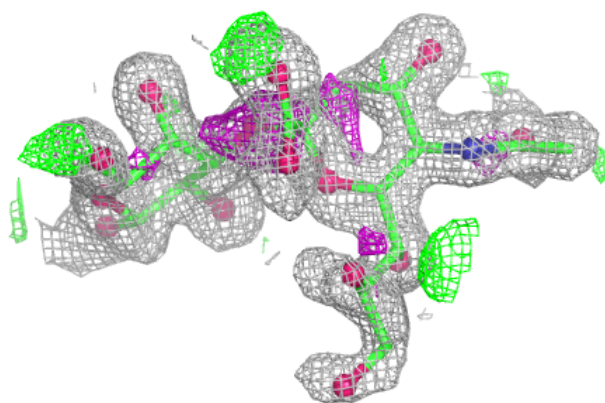
Electron density around Chain M:

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

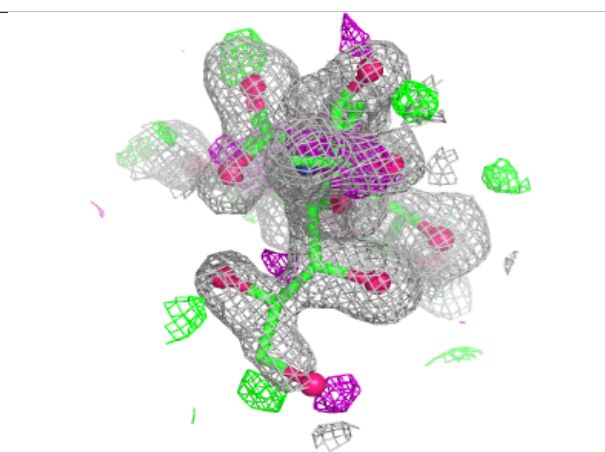
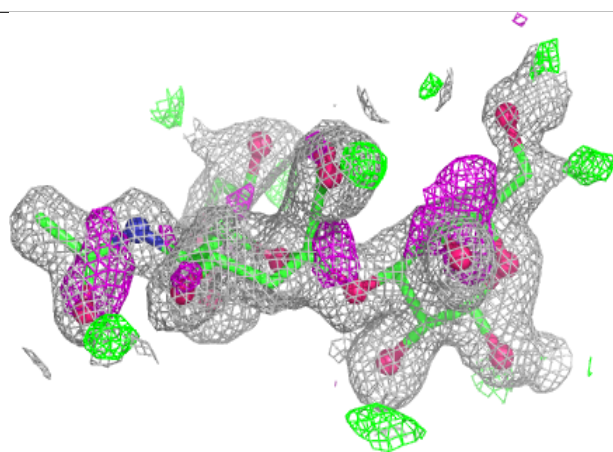
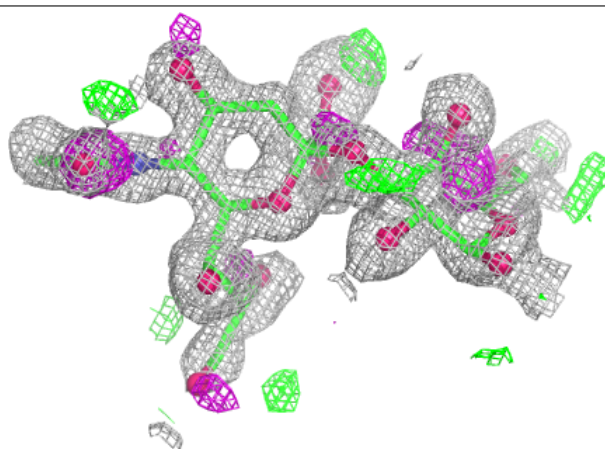


Electron density around Chain N:

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

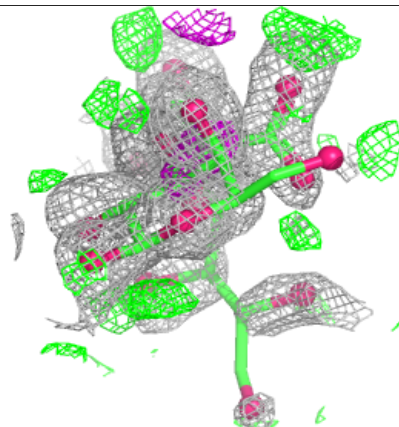
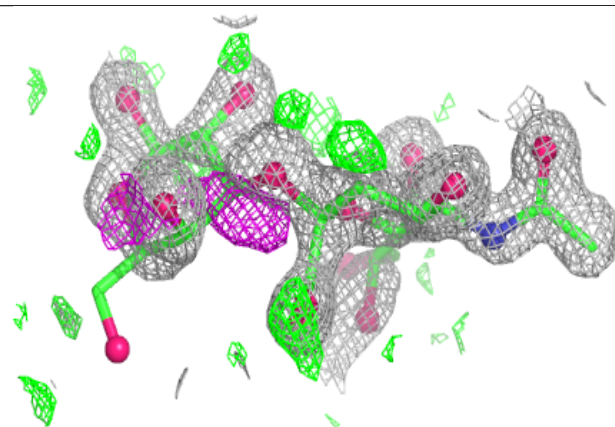
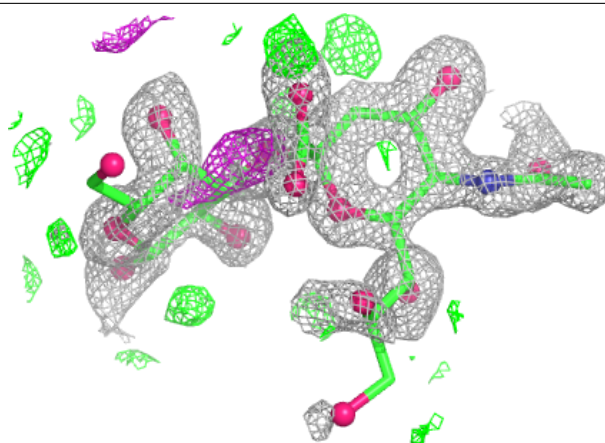
**Electron density around Chain O:**

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



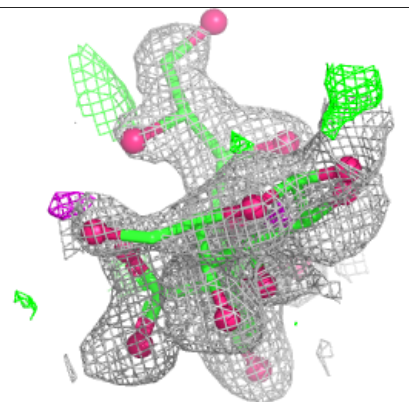
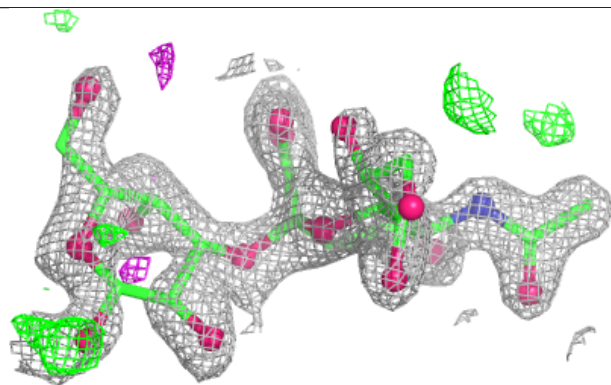
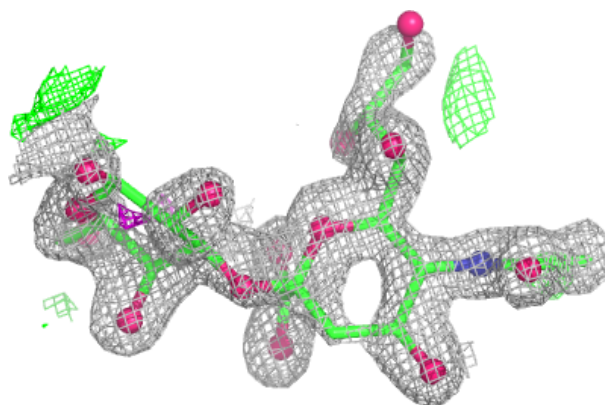
Electron density around Chain P:

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

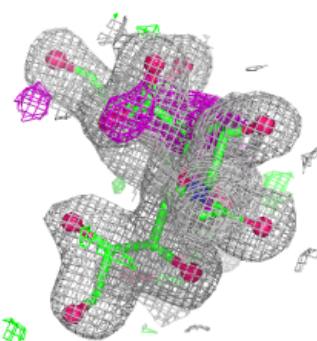
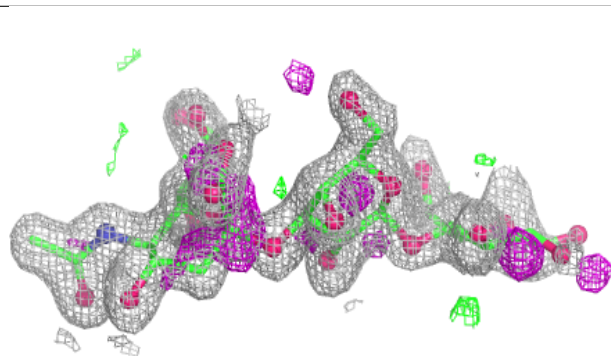
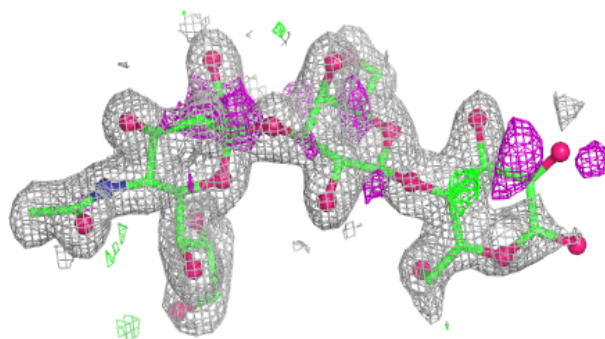


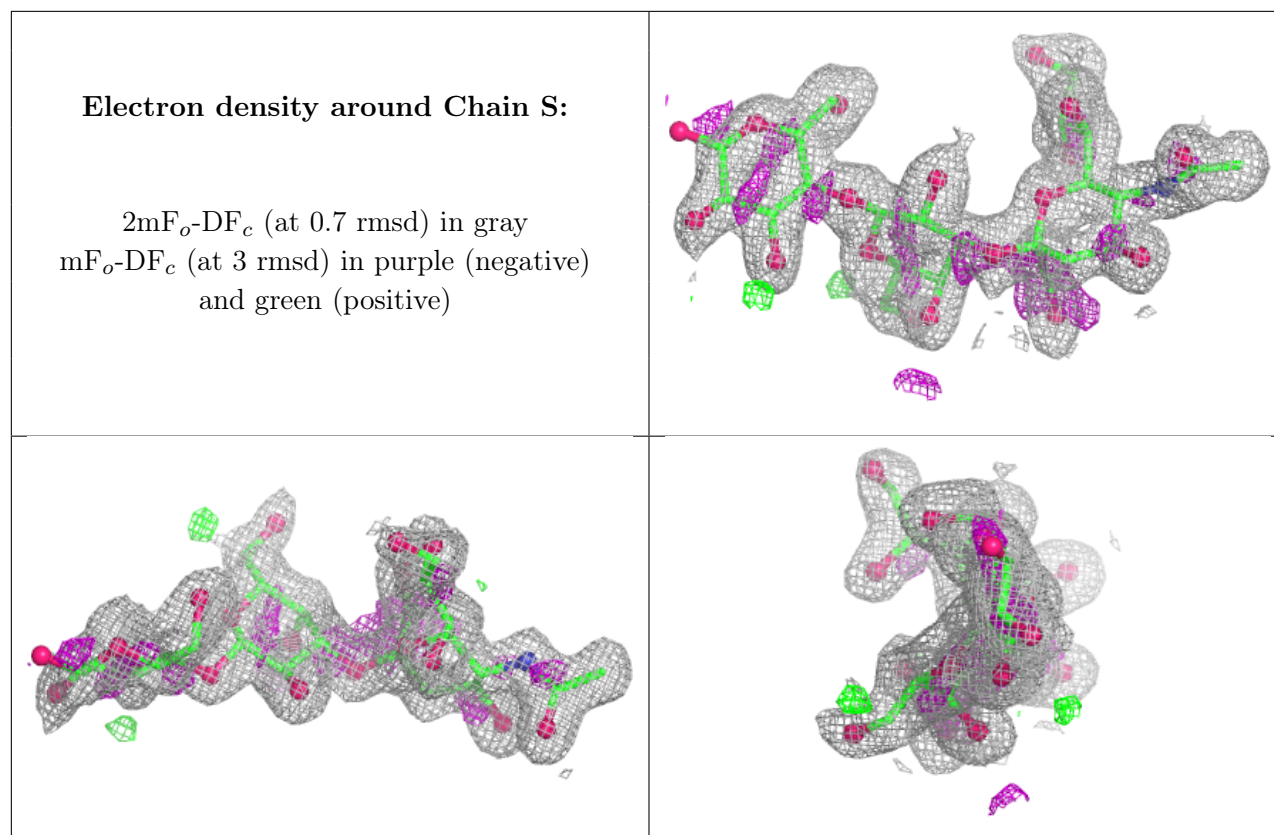
Electron density around Chain Q:

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

**Electron density around Chain R:**

$2mF_o-DF_c$ (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
6	EDO	E	404	4/4	0.73	0.18	26,35,37,42	0
6	EDO	A	404	4/4	0.79	0.19	27,27,36,42	0
6	EDO	G	404	4/4	0.79	0.18	38,41,42,51	0
6	EDO	B	405	4/4	0.80	0.17	28,31,33,42	0
6	EDO	F	403	4/4	0.80	0.15	30,32,36,47	0
6	EDO	B	406	4/4	0.80	0.14	33,35,41,43	0
7	IPA	J	407	4/4	0.80	0.22	34,39,41,46	0
6	EDO	H	404	4/4	0.81	0.14	47,47,50,50	0
6	EDO	E	406	4/4	0.81	0.17	30,34,37,38	0
7	IPA	D	405	4/4	0.83	0.20	34,36,38,44	0
6	EDO	H	405	4/4	0.83	0.16	35,39,47,53	0
7	IPA	I	405	4/4	0.84	0.19	34,35,39,44	0
7	IPA	H	406	4/4	0.85	0.14	29,30,32,35	0
6	EDO	A	406	4/4	0.85	0.17	46,47,48,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	EDO	A	405	4/4	0.85	0.14	24,31,31,43	0
7	IPA	B	409	4/4	0.86	0.20	27,29,34,41	0
6	EDO	A	407	4/4	0.86	0.15	41,41,46,47	0
7	IPA	G	405	4/4	0.86	0.15	30,31,32,38	0
6	EDO	C	403	4/4	0.88	0.28	22,25,27,28	0
6	EDO	B	408	4/4	0.89	0.14	25,28,39,50	0
6	EDO	I	403	4/4	0.89	0.13	31,34,45,47	0
7	IPA	A	408	4/4	0.89	0.17	30,32,35,43	0
6	EDO	A	403	4/4	0.90	0.25	22,22,24,36	0
7	IPA	C	406	4/4	0.90	0.14	28,29,30,30	0
6	EDO	D	403	4/4	0.90	0.11	31,36,42,43	0
7	IPA	E	407	4/4	0.90	0.14	29,29,30,31	0
6	EDO	E	403	4/4	0.91	0.12	24,25,25,36	0
6	EDO	B	407	4/4	0.91	0.12	22,30,38,40	0
6	EDO	J	406	4/4	0.91	0.12	25,32,37,38	0
6	EDO	J	405	4/4	0.92	0.12	30,36,37,37	0
7	IPA	F	404	4/4	0.92	0.13	29,35,38,40	0
6	EDO	G	403	4/4	0.92	0.12	24,30,32,36	0
6	EDO	D	404	4/4	0.93	0.10	22,27,33,36	0
6	EDO	B	403	4/4	0.93	0.10	23,27,28,32	0
6	EDO	J	403	4/4	0.93	0.09	25,30,31,34	0
6	EDO	J	404	4/4	0.93	0.10	29,37,40,41	0
6	EDO	H	403	4/4	0.94	0.10	23,31,33,35	0
6	EDO	E	405	4/4	0.94	0.11	19,31,32,34	0
6	EDO	B	404	4/4	0.95	0.09	26,30,30,31	0
6	EDO	C	404	4/4	0.95	0.09	27,30,31,33	0
6	EDO	C	405	4/4	0.95	0.11	23,32,39,40	0
6	EDO	I	404	4/4	0.96	0.08	24,32,35,35	0
5	CL	G	402	1/1	0.96	0.15	31,31,31,31	0
4	CA	D	401	1/1	0.96	0.06	24,24,24,24	1
4	CA	H	401	1/1	0.97	0.05	28,28,28,28	1
5	CL	C	402	1/1	0.97	0.12	26,26,26,26	0
4	CA	C	401	1/1	0.97	0.05	23,23,23,23	1
4	CA	A	401	1/1	0.97	0.06	22,22,22,22	1
4	CA	G	401	1/1	0.97	0.04	23,23,23,23	1
5	CL	H	402	1/1	0.98	0.17	31,31,31,31	0
5	CL	I	402	1/1	0.98	0.14	32,32,32,32	0
4	CA	E	401	1/1	0.98	0.05	21,21,21,21	1
4	CA	I	401	1/1	0.98	0.07	25,25,25,25	1
4	CA	J	401	1/1	0.98	0.05	26,26,26,26	1
5	CL	A	402	1/1	0.98	0.09	25,25,25,25	0
4	CA	F	401	1/1	0.98	0.05	25,25,25,25	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	CL	D	402	1/1	0.98	0.08	26,26,26,26	0
5	CL	E	402	1/1	0.98	0.09	24,24,24,24	0
5	CL	F	402	1/1	0.98	0.13	33,33,33,33	0
4	CA	B	401	1/1	0.98	0.04	21,21,21,21	1
5	CL	B	402	1/1	0.99	0.13	25,25,25,25	0
5	CL	J	402	1/1	0.99	0.12	29,29,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.