



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 11:07 AM UTC

PDB ID : 6X1T / pdb_00006x1t
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 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

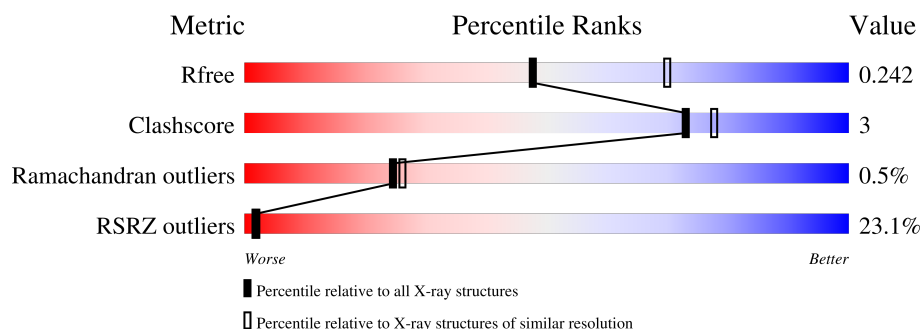
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (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	7% 86% 11% ••
1	C	228	11% 85% 11% •
1	E	228	23% 88% 9% •
1	G	228	34% 86% 9% 5%
1	H	228	7% 83% 14% •
1	J	228	33% 86% 10% •
2	B	214	3% 95% 5%

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Mol	Chain	Length	Quality of chain
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.

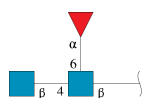
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	6	Total	C	N	O	P	0	0	0
			47	26	10	10	1			
3	N	6	Total	C	N	O	P	0	0	0
			44	25	9	9	1			
3	O	7	Total	C	N	O	P	0	0	0
			56	30	11	14	1			
3	P	5	Total	C	N	O	P	0	0	0
			39	22	8	8	1			
3	Q	7	Total	C	N	O	P	0	0	0
			56	30	11	14	1			
3	R	6	Total	C	N	O	P	0	0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



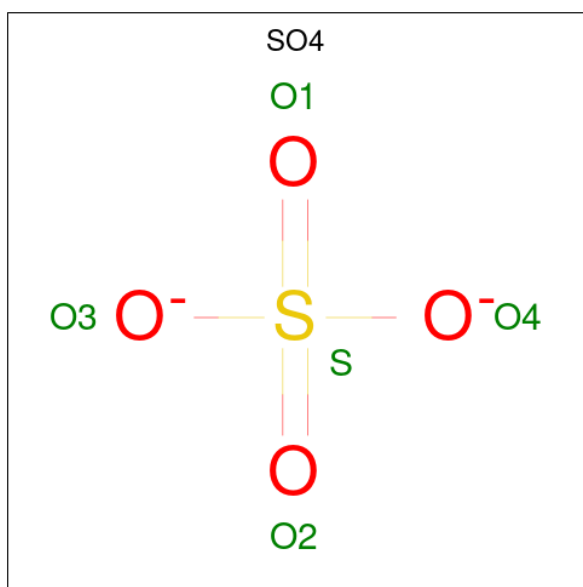
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	S	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	U	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	V	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	W	2	Total	C	N	O	0	0	0
			28	16	2	10			

- 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.



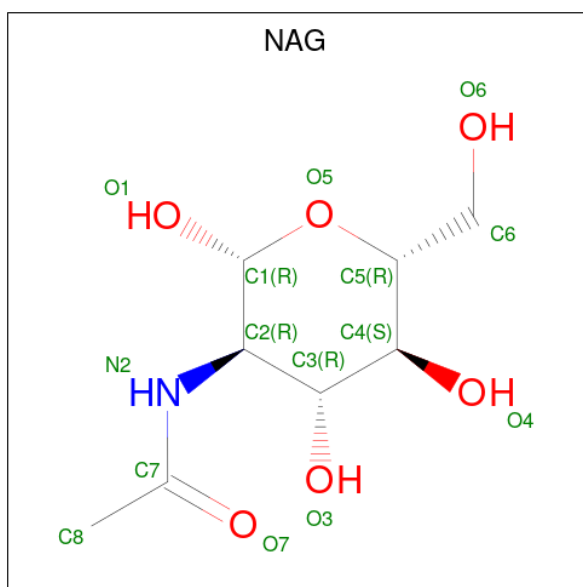
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	T	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 6 is SULFATE ION (CCD ID: 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 (CCD ID: 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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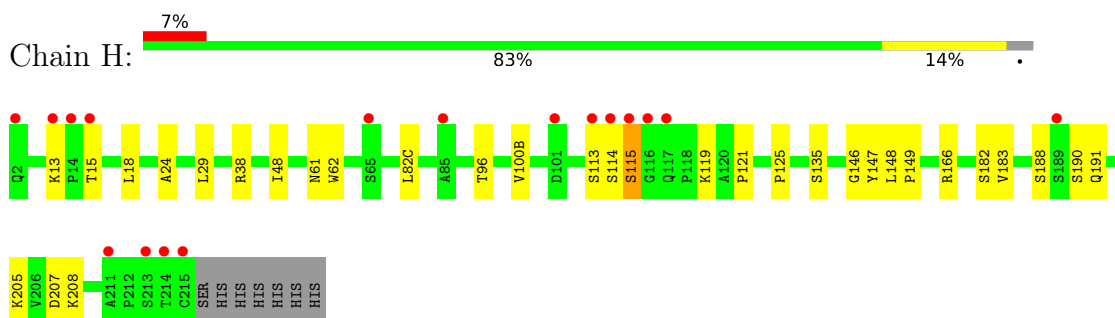
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	M	1	Total 1	O 1	0	0
8	N	1	Total 1	O 1	0	0
8	O	1	Total 1	O 1	0	0
8	P	1	Total 1	O 1	0	0
8	R	1	Total 1	O 1	0	0

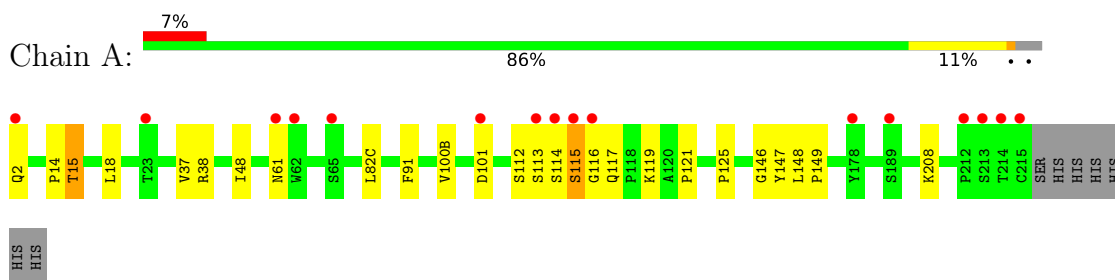
3 Residue-property plots [i](#)

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.

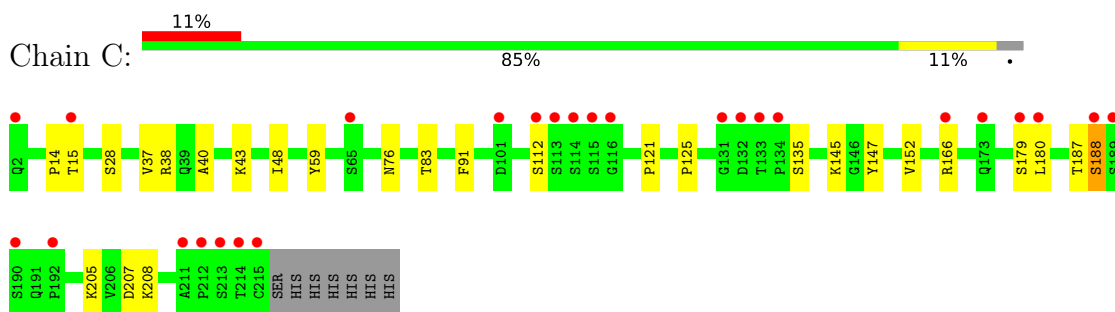
- Molecule 1: SC50-3 Heavy chain



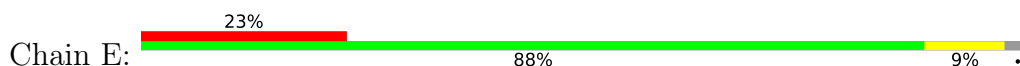
- Molecule 1: SC50-3 Heavy chain

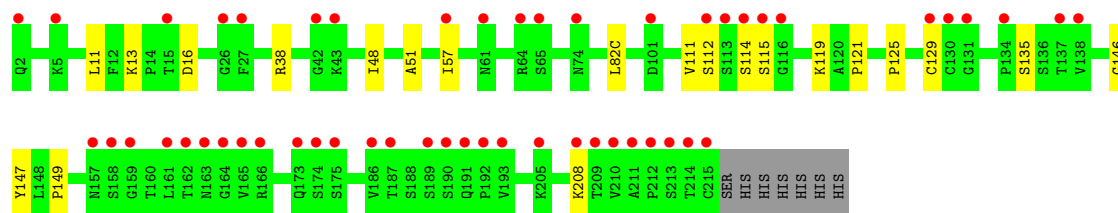


- Molecule 1: SC50-3 Heavy chain

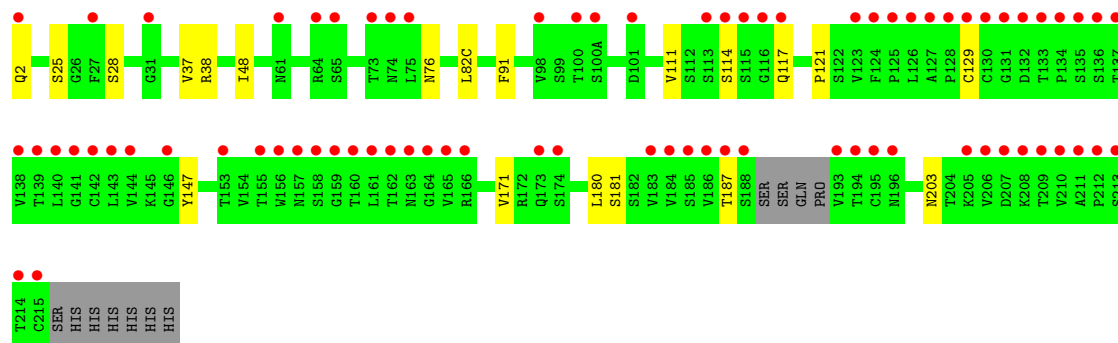
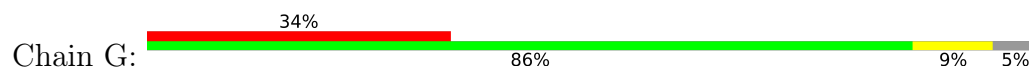


- Molecule 1: SC50-3 Heavy chain

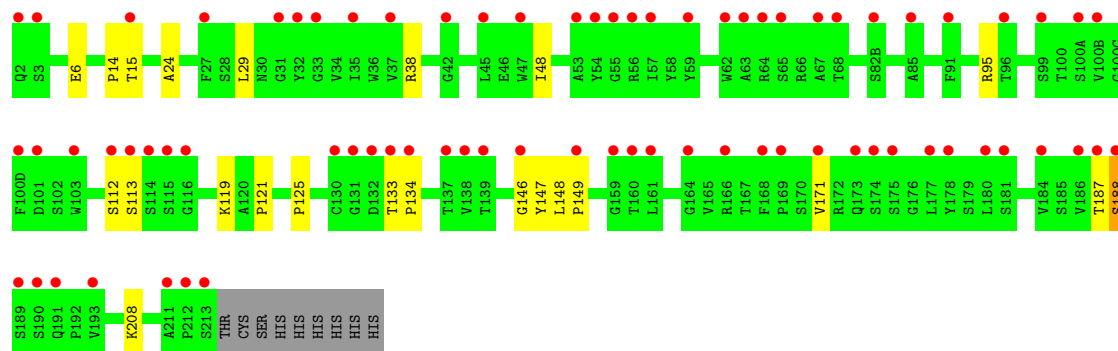
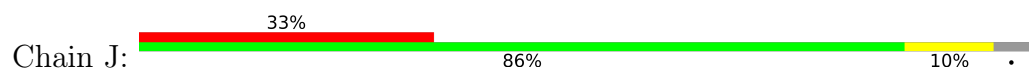




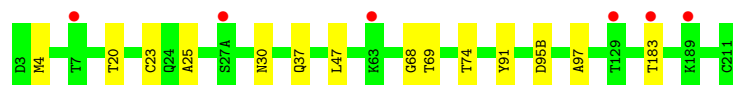
• Molecule 1: SC50-3 Heavy chain



• Molecule 1: SC50-3 Heavy chain

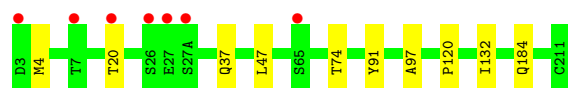


• Molecule 2: SC50-3 Light chain

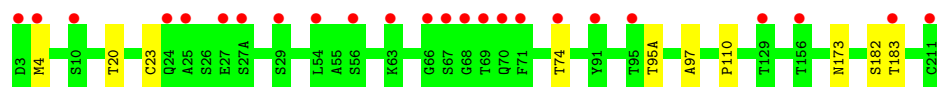


• Molecule 2: SC50-3 Light chain

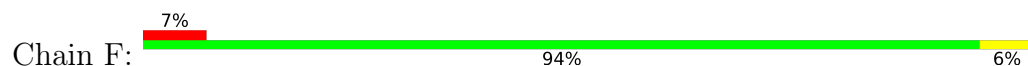




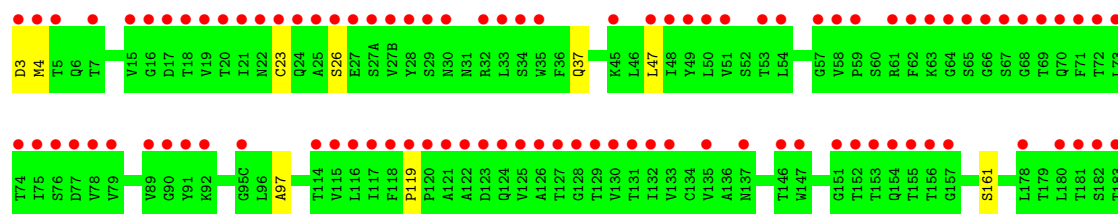
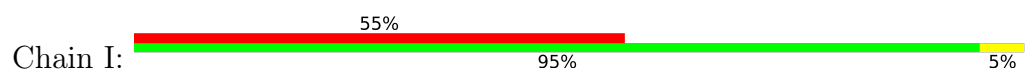
- Molecule 2: SC50-3 Light chain



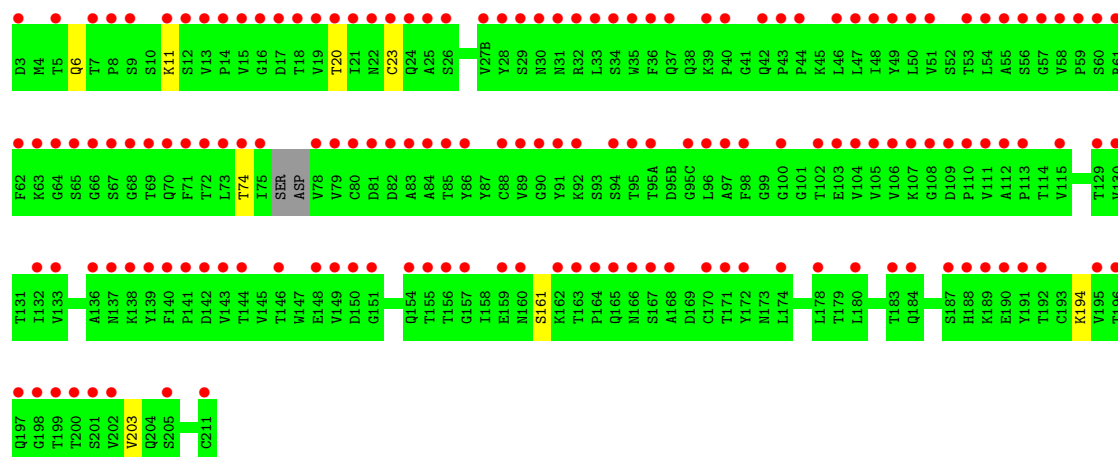
- Molecule 2: SC50-3 Light chain



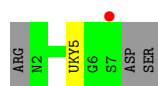
- Molecule 2: SC50-3 Light chain



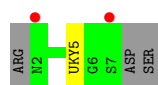
- Molecule 2: SC50-3 Light chain



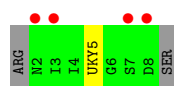
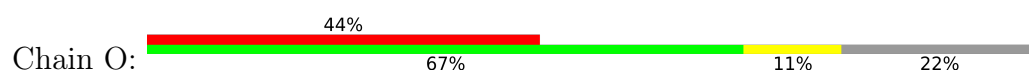
- Molecule 3: NM23-1-pTza peptide



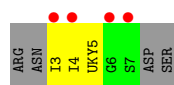
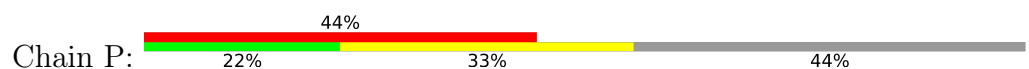
- Molecule 3: NM23-1-pTza peptide



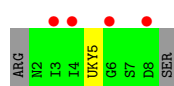
- Molecule 3: NM23-1-pTza peptide



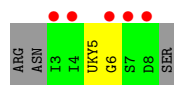
- Molecule 3: NM23-1-pTza peptide



- Molecule 3: NM23-1-pTza peptide



- Molecule 3: NM23-1-pTza peptide



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





- 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) 99.4 (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 (Not available) , 0.242	Depositor DCC
R_{free} test set	7567 reflections (4.85%)	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 , 32.8	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

5.1 Standard geometry

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

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	0.12	0/1690	0.40	0/2315
1	C	0.18	0/1690	0.40	0/2315
1	E	0.16	0/1690	0.44	0/2315
1	G	0.27	2/1660 (0.1%)	0.38	0/2272
1	H	0.32	2/1690 (0.1%)	0.44	0/2315
1	J	0.26	0/1677	0.46	0/2297
2	B	0.11	0/1628	0.34	0/2230
2	D	0.11	0/1628	0.34	0/2230
2	F	0.11	0/1628	0.34	0/2230
2	I	0.13	0/1628	0.35	0/2230
2	K	0.13	0/1613	0.36	0/2208
2	L	0.13	0/1628	0.35	0/2230
3	M	0.10	0/31	0.34	0/39
3	N	0.15	0/28	0.39	0/35
3	O	0.15	0/40	0.49	0/51
3	P	0.26	0/23	0.44	0/28
3	Q	0.10	0/40	0.34	0/51
3	R	0.15	0/29	0.39	0/36
All	All	0.18	4/20041 (0.0%)	0.39	0/27427

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	183	VAL	C-O	-5.63	1.17	1.23
1	G	181	SER	C-O	-5.25	1.17	1.23
1	H	182	SER	C-O	-5.17	1.18	1.23
1	G	180	LEU	C-O	-5.05	1.17	1.23

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	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	8	0
2	F	1593	0	1540	8	0
2	I	1593	0	1540	7	0
2	K	1579	0	1530	5	0
2	L	1593	0	1540	10	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	124	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 (124) 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
1:C:152:VAL:HG23	1:C:180:LEU:HD21	1.68	0.76
1:C:28:SER:HA	1:C:76:ASN:HD21	1.53	0.73
1:C:135:SER:HB3	2:F:110:PRO:HD2	1.70	0.73
2:K:11:LYS:HE3	2:K:11:LYS:HA	1.72	0.70
1:A:14:PRO:HD3	1:A:112:SER:O	1.94	0.68
2:B:20:THR:HG22	2:B:74:THR:HG23	1.77	0.66
1:H:61:ASN:ND2	2:L:95(B):ASP:OD2	2.29	0.66
1:J:125:PRO:HD3	1:J:208:LYS:HE2	1.78	0.64
2:L:20:THR:HG22	2:L:74:THR:HG23	1.79	0.64
1:G:28:SER:HA	1:G:76:ASN:HD21	1.61	0.64
1:H:190:SER:OG	1:G:203:ASN:ND2	2.29	0.63
2:F:49:TYR:HH	4:V:2:NAG:HO6	1.46	0.62
2:I:4:MET:HG2	2:I:97:ALA:HB3	1.80	0.62
2:F:6:GLN:HG3	2:F:23:CYS:SG	2.40	0.62
2:K:6:GLN:HG3	2:K:23:CYS:SG	2.38	0.62
1:J:95:ARG:HH11	1:J:95:ARG:HG2	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:PRO:HD3	1:C:208:LYS:HE2	1.85	0.59
2:D:20:THR:HG22	2:D:74:THR:HG23	1.85	0.59
1:E:13:LYS:NZ	1:E:16:ASP:OD1	2.31	0.58
1:G:2:GLN:N	1:G:25:SER:O	2.37	0.57
1:C:187:THR:OG1	1:C:188:SER:N	2.37	0.57
2:L:183:THR:HG21	1:A:61:ASN:CB	2.35	0.57
2:D:110:PRO:HD2	1:E:135:SER:HB3	1.87	0.56
5:T:1:NAG:H61	5:T:2:NAG:HN2	1.71	0.56
1:J:187:THR:OG1	1:J:188:SER:N	2.38	0.55
1:C:40:ALA:HB3	1:C:43:LYS:HD3	1.89	0.55
1:J:38:ARG:HB3	1:J:48:ILE:HD11	1.88	0.55
2:I:4:MET:HE3	2:I:23:CYS:SG	2.47	0.54
1:H:205:LYS:HB2	1:C:207:ASP:HB2	1.90	0.54
1:C:152:VAL:CG2	1:C:180:LEU:HD23	2.38	0.54
1:H:119:LYS:HD2	1:H:146:GLY:O	2.08	0.53
1:H:62:TRP:HB3	2:B:184:GLN:NE2	2.23	0.53
2:F:4:MET:HG2	2:F:97:ALA:HB3	1.90	0.53
1:A:115:SER:O	1:A:117:GLN:N	2.41	0.52
1:C:38:ARG:HB3	1:C:48:ILE:HD11	1.90	0.52
1:H:115:SER:HB3	1:A:14:PRO:HG2	1.90	0.52
1:A:119:LYS:HD2	1:A:146:GLY:O	2.10	0.52
1:H:114:SER:O	1:H:115:SER:OG	2.25	0.52
2:L:183:THR:HG21	1:A:61:ASN:HB3	1.91	0.51
2:L:4:MET:HG2	2:L:97:ALA:HB3	1.92	0.51
3:P:3:ILE:HG12	3:P:4:ILE:H	1.75	0.51
1:G:121:PRO:HB3	1:G:147:TYR:HB3	1.93	0.51
1:G:38:ARG:HB3	1:G:48:ILE:HD11	1.92	0.51
2:D:4:MET:HE3	2:D:23:CYS:SG	2.50	0.51
1:E:38:ARG:HB3	1:E:48:ILE:HD11	1.93	0.51
1:G:129:CYS:SG	2:I:119:PRO:HG3	2.52	0.50
1:H:121:PRO:HB3	1:H:147:TYR:HB3	1.93	0.50
1:E:82(C):LEU:HB3	1:E:111:VAL:HG11	1.93	0.50
1:H:125:PRO:HD3	1:H:208:LYS:HE2	1.94	0.50
1:H:115:SER:H	1:A:113:SER:HA	1.76	0.50
1:J:121:PRO:HB3	1:J:147:TYR:HB3	1.93	0.50
1:A:125:PRO:HD3	1:A:208:LYS:HE2	1.94	0.50
1:A:38:ARG:HB3	1:A:48:ILE:HD11	1.92	0.49
2:I:189:LYS:HD3	2:I:207:ASN:OD1	2.11	0.49
1:H:96:THR:HB	4:S:1:NAG:H82	1.95	0.49
2:F:11:LYS:HD2	6:F:304:SO4:O1	2.13	0.49
1:C:121:PRO:HB3	1:C:147:TYR:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:152:VAL:HG22	1:C:180:LEU:HD23	1.95	0.48
1:A:115:SER:HG	1:A:148:LEU:HD21	1.72	0.48
1:E:51:ALA:HA	1:E:57:ILE:HD13	1.95	0.48
1:A:121:PRO:HB3	1:A:147:TYR:HB3	1.95	0.48
1:A:14:PRO:O	1:A:15:THR:HG22	2.14	0.48
1:C:152:VAL:HG22	1:C:180:LEU:CD2	2.43	0.48
2:L:30:ASN:OD1	2:L:68:GLY:N	2.23	0.48
1:C:14:PRO:HD3	1:C:112:SER:O	2.14	0.48
1:H:191:GLN:O	1:G:203:ASN:ND2	2.47	0.47
2:B:4:MET:HG2	2:B:97:ALA:HB3	1.95	0.47
1:E:112:SER:HB2	1:E:114:SER:O	2.14	0.47
1:H:38:ARG:HB3	1:H:48:ILE:HD11	1.95	0.47
1:H:13:LYS:HD3	1:A:114:SER:HB2	1.97	0.47
1:H:113:SER:O	1:A:113:SER:N	2.45	0.47
1:A:15:THR:O	2:D:183:THR:OG1	2.32	0.47
2:I:3:ASP:HB3	2:I:26:SER:HB3	1.97	0.47
2:I:37:GLN:HB2	2:I:47:LEU:HD11	1.97	0.47
1:A:37:VAL:HG22	1:A:91:PHE:HB2	1.96	0.46
1:E:119:LYS:HD2	1:E:146:GLY:O	2.16	0.46
1:E:129:CYS:SG	2:F:119:PRO:HG3	2.56	0.46
1:A:100(B):VAL:HG13	2:B:91:TYR:HB2	1.98	0.46
2:D:4:MET:HG2	2:D:97:ALA:HB3	1.97	0.46
1:J:171:VAL:HG13	2:K:161:SER:HB2	1.98	0.45
2:B:37:GLN:HB2	2:B:47:LEU:HD11	1.99	0.45
1:E:121:PRO:HB3	1:E:147:TYR:HB3	1.97	0.45
1:H:166[A]:ARG:NH1	8:H:403:HOH:O	2.50	0.45
1:G:82(C):LEU:HB3	1:G:111:VAL:HG11	1.99	0.45
1:G:117:GLN:NE2	6:G:304:SO4:O2	2.45	0.45
1:J:119:LYS:HD2	1:J:146:GLY:O	2.17	0.45
4:W:1:NAG:H62	4:W:2:NAG:N2	2.32	0.45
1:C:37:VAL:HG22	1:C:91:PHE:HB2	1.99	0.45
2:F:37:GLN:HB2	2:F:47:LEU:HD11	1.99	0.45
2:L:37:GLN:HB2	2:L:47:LEU:HD11	1.99	0.44
1:H:148:LEU:HD12	1:H:149:PRO:HA	1.98	0.44
1:A:148:LEU:HD12	1:A:149:PRO:HA	2.00	0.44
1:A:2:GLN:HE21	1:A:2:GLN:N	2.16	0.43
1:G:171:VAL:HG13	2:I:161:SER:HB2	2.00	0.43
1:E:11:LEU:HB2	1:E:149:PRO:HG3	2.01	0.43
1:H:24:ALA:HB2	1:H:29:LEU:HG	2.00	0.43
1:H:135:SER:O	1:H:188:SER:OG	2.28	0.43
1:E:125:PRO:HD3	1:E:208:LYS:HE2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:THR:OG1	2:D:182:SER:HB2	2.19	0.43
1:H:100(B):VAL:HG13	2:L:91:TYR:HB2	2.01	0.42
1:C:59:TYR:O	2:D:95(A):THR:HA	2.19	0.42
1:J:24:ALA:HB2	1:J:29:LEU:HG	2.01	0.42
2:L:4:MET:HE3	2:L:23:CYS:SG	2.60	0.42
2:K:194:LYS:HG3	2:K:203:VAL:HG22	2.01	0.42
1:J:133:THR:HA	1:J:134:PRO:HD3	1.93	0.41
1:C:166[A]:ARG:NH1	2:D:173:ASN:OD1	2.52	0.41
1:A:101:ASP:HB3	8:A:403:HOH:O	2.20	0.41
2:L:25:ALA:O	2:L:69:THR:HB	2.20	0.41
1:J:6:GLU:OE2	8:J:401:HOH:O	2.21	0.41
1:J:148:LEU:HD12	1:J:149:PRO:HA	2.03	0.41
2:F:20:THR:HG22	2:F:74:THR:HG23	2.03	0.41
1:J:14:PRO:HD3	1:J:112:SER:O	2.20	0.41
1:H:166[A]:ARG:NH2	8:H:406:HOH:O	2.54	0.41
1:A:18:LEU:HB2	1:A:82(C):LEU:HD21	2.02	0.41
2:B:120:PRO:HD3	2:B:132:ILE:HG12	2.03	0.41
1:H:207:ASP:HB2	1:C:205:LYS:HB3	2.03	0.40
1:C:145:LYS:HA	1:C:179:SER:OG	2.21	0.40
1:H:18:LEU:HB2	1:H:82(C):LEU:HD21	2.04	0.40
1:G:37:VAL:HG22	1:G:91:PHE:HB2	2.04	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	223/228 (98%)	218 (98%)	2 (1%)	3 (1%)	9	7
1	C	223/228 (98%)	218 (98%)	3 (1%)	2 (1%)	14	13
1	E	223/228 (98%)	219 (98%)	3 (1%)	1 (0%)	30	32
1	G	217/228 (95%)	213 (98%)	2 (1%)	2 (1%)	14	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	223/228 (98%)	219 (98%)	2 (1%)	2 (1%)	14	13
1	J	221/228 (97%)	216 (98%)	3 (1%)	2 (1%)	14	13
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%)	24	26

All (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
1	C	15	THR
1	J	15	THR
1	H	115	SER
1	A	115	SER
1	G	114	SER
3	R	6	GLY
1	A	15	THR
1	G	187	THR

5.3.2 Protein sidechains ⓘ

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

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	M	5	3	12,14,15	1.96	3 (25%)	8,20,22	2.24	2 (25%)
3	UKY	Q	5	3	12,14,15	1.85	3 (25%)	8,20,22	2.17	2 (25%)
3	UKY	P	5	3	12,14,15	1.83	3 (25%)	8,20,22	2.17	2 (25%)
3	UKY	N	5	3	12,14,15	1.93	3 (25%)	8,20,22	2.27	2 (25%)
3	UKY	R	5	3	12,14,15	1.94	3 (25%)	8,20,22	2.29	2 (25%)
3	UKY	O	5	3	12,14,15	1.94	3 (25%)	8,20,22	2.09	2 (25%)

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	M	5	3	-	0/4/12/14	0/1/1/1
3	UKY	Q	5	3	-	0/4/12/14	0/1/1/1
3	UKY	P	5	3	-	0/4/12/14	0/1/1/1
3	UKY	N	5	3	-	0/4/12/14	0/1/1/1
3	UKY	R	5	3	-	0/4/12/14	0/1/1/1
3	UKY	O	5	3	-	0/4/12/14	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	5	UKY	CD1-NG	-4.50	1.34	1.37
3	R	5	UKY	CD1-NG	-4.38	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	5	UKY	CD1-NG	-4.27	1.34	1.37
3	N	5	UKY	CD1-NG	-4.21	1.34	1.37
3	P	5	UKY	CE1-CD1	3.98	1.44	1.37
3	O	5	UKY	CE1-CD1	3.96	1.44	1.37
3	N	5	UKY	CE1-CD1	3.96	1.44	1.37
3	R	5	UKY	CE1-CD1	3.92	1.44	1.37
3	M	5	UKY	CE1-CD1	3.91	1.44	1.37
3	Q	5	UKY	CD1-NG	-3.87	1.34	1.37
3	Q	5	UKY	CE1-CD1	3.86	1.44	1.37
3	P	5	UKY	CD1-NG	-3.73	1.34	1.37
3	O	5	UKY	NG-ND2	-2.47	1.32	1.35
3	Q	5	UKY	NG-ND2	-2.45	1.32	1.35
3	N	5	UKY	NG-ND2	-2.42	1.32	1.35
3	M	5	UKY	NG-ND2	-2.38	1.32	1.35
3	P	5	UKY	NG-ND2	-2.36	1.32	1.35
3	R	5	UKY	NG-ND2	-2.34	1.32	1.35

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	5	UKY	NG-ND2-NE2	4.47	110.76	107.13
3	N	5	UKY	NG-ND2-NE2	4.42	110.73	107.13
3	Q	5	UKY	NG-ND2-NE2	4.34	110.66	107.13
3	R	5	UKY	CB-NG-ND2	4.26	125.36	119.53
3	R	5	UKY	NG-ND2-NE2	4.20	110.55	107.13
3	O	5	UKY	NG-ND2-NE2	4.18	110.53	107.13
3	M	5	UKY	NG-ND2-NE2	4.17	110.52	107.13
3	M	5	UKY	CB-NG-ND2	4.09	125.12	119.53
3	N	5	UKY	CB-NG-ND2	3.85	124.80	119.53
3	Q	5	UKY	CB-NG-ND2	3.53	124.36	119.53
3	P	5	UKY	CB-NG-ND2	3.47	124.28	119.53
3	O	5	UKY	CB-NG-ND2	3.45	124.25	119.53

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 ⓘ

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	0.57	0
4	NAG	S	2	4	14,14,15	0.21	0	17,19,21	0.46	0
5	NAG	T	1	5,1	14,14,15	0.20	0	17,19,21	0.54	0
5	NAG	T	2	5	14,14,15	0.39	0	17,19,21	0.42	0
5	FUC	T	3	5	10,10,11	0.70	0	14,14,16	0.77	0
4	NAG	U	1	1,4	14,14,15	0.21	0	17,19,21	0.53	0
4	NAG	U	2	4	14,14,15	0.23	0	17,19,21	0.47	0
4	NAG	V	1	1,4	14,14,15	0.22	0	17,19,21	0.56	0
4	NAG	V	2	4	14,14,15	0.20	0	17,19,21	0.46	0
4	NAG	W	1	1,4	14,14,15	0.21	0	17,19,21	0.53	0
4	NAG	W	2	4	14,14,15	0.23	0	17,19,21	0.48	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	5,1	-	0/6/23/26	0/1/1/1
5	NAG	T	2	5	-	1/6/23/26	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
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 (4) torsion outliers are listed below:

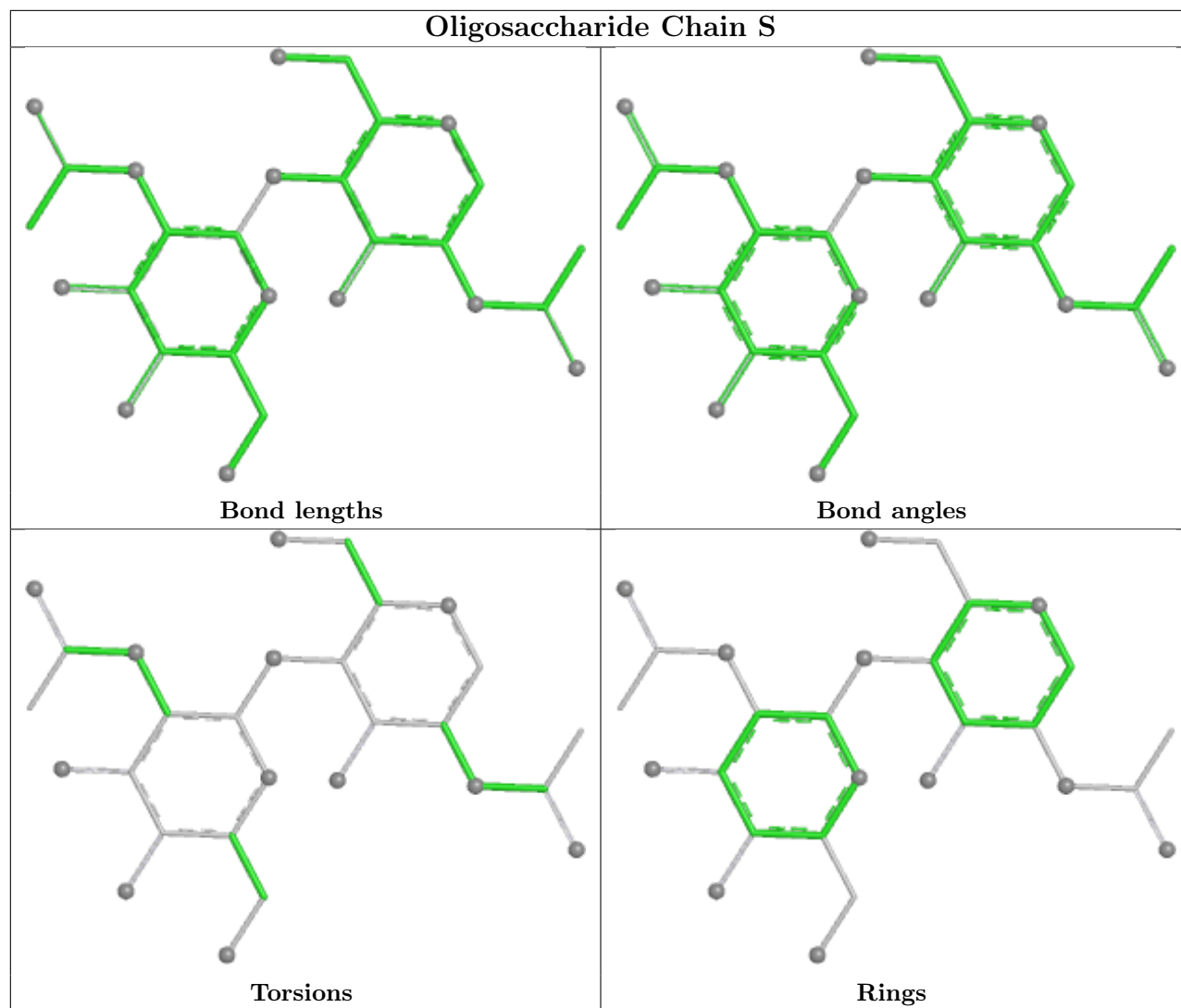
Mol	Chain	Res	Type	Atoms
4	W	2	NAG	C8-C7-N2-C2
4	W	2	NAG	O7-C7-N2-C2
4	W	2	NAG	O5-C5-C6-O6
5	T	2	NAG	C3-C2-N2-C7

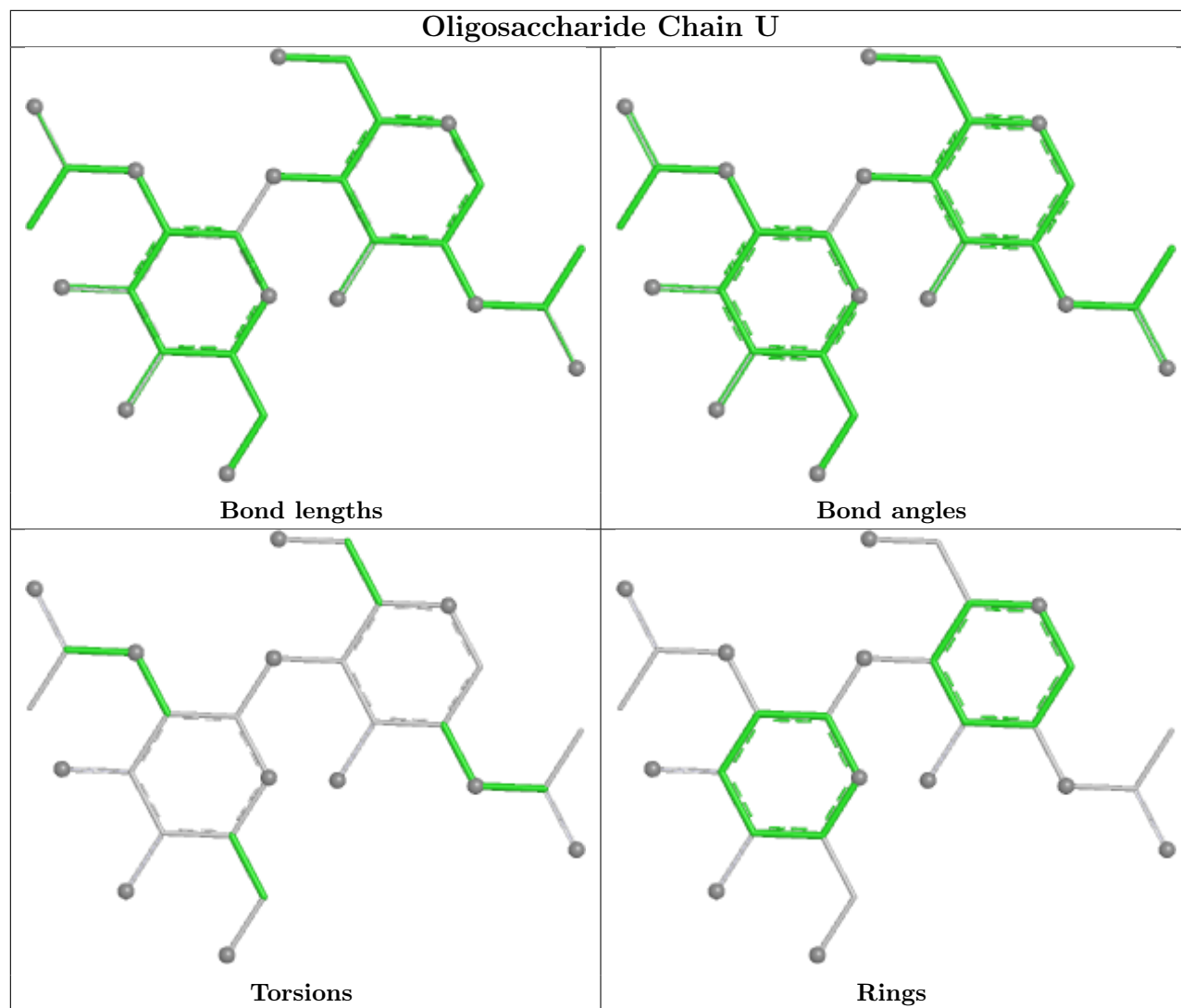
There are no ring outliers.

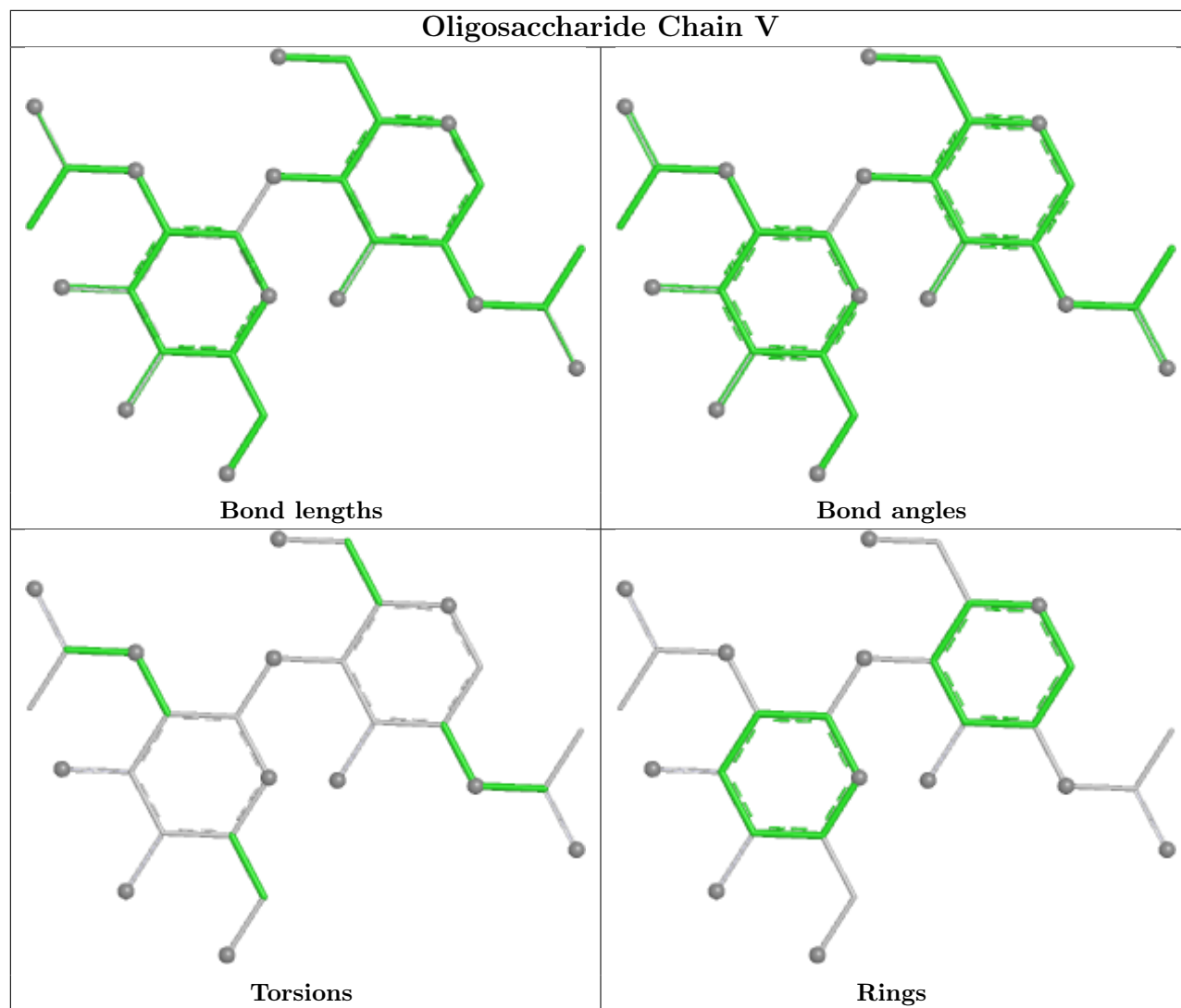
6 monomers are involved in 4 short contacts:

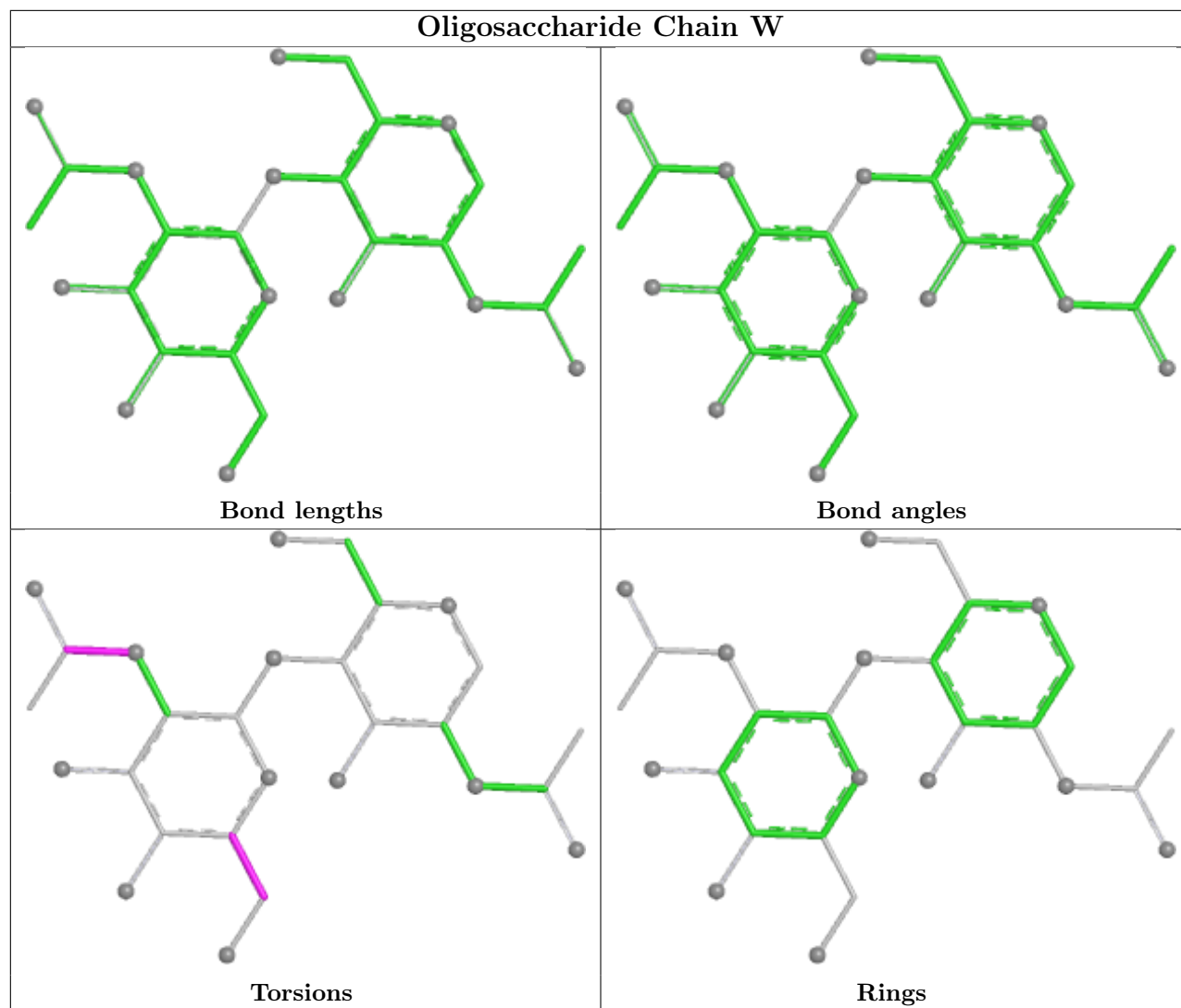
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	W	1	NAG	1	0
4	W	2	NAG	1	0
5	T	2	NAG	1	0
4	V	2	NAG	1	0
5	T	1	NAG	1	0
4	S	1	NAG	1	0

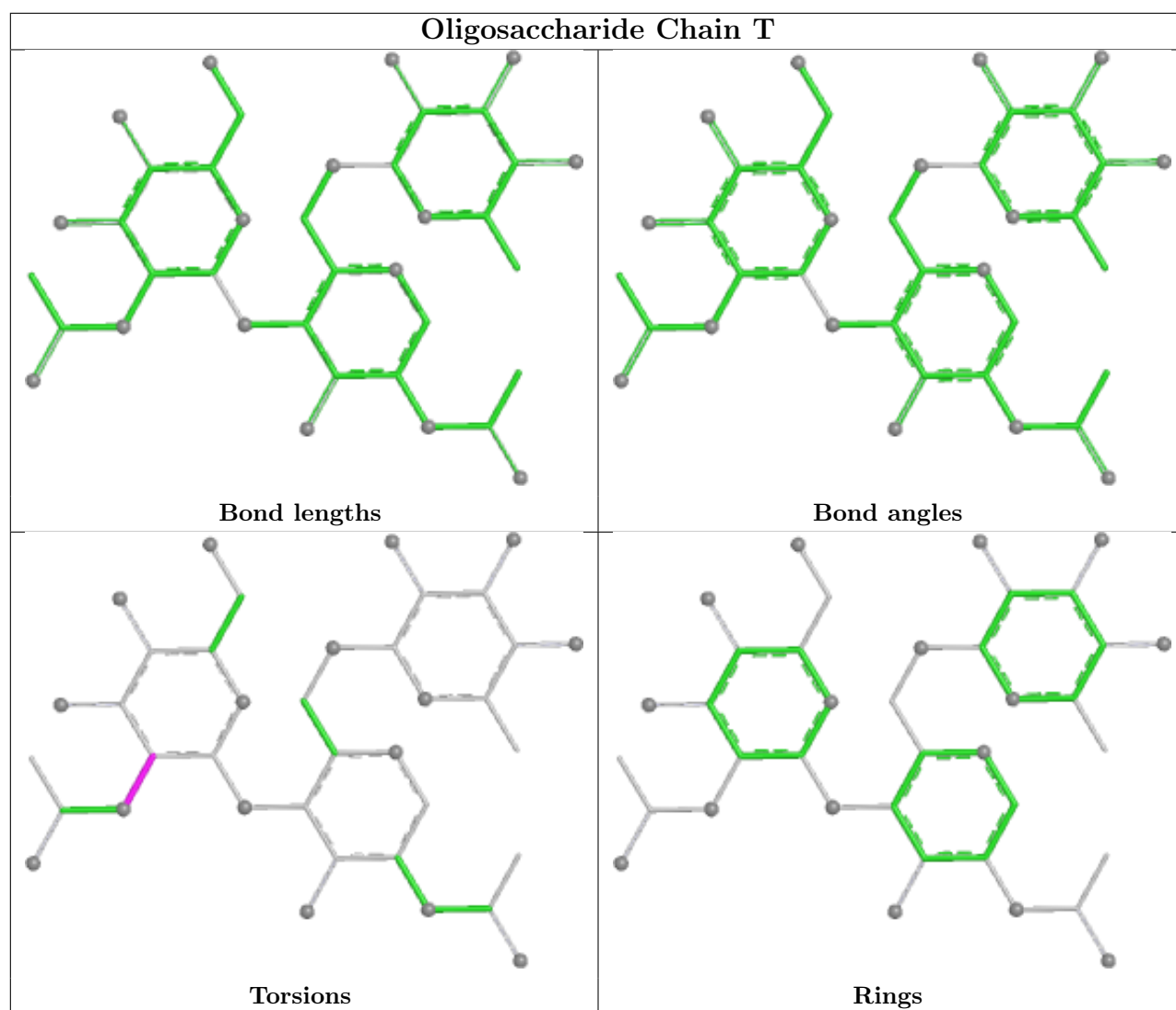
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











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	304	-	4,4,4	0.21	0	6,6,6	0.11	0
6	SO4	C	304	-	4,4,4	0.23	0	6,6,6	0.08	0
6	SO4	F	303	-	4,4,4	0.24	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	SO4	F	301	-	4,4,4	0.23	0	6,6,6	0.07	0
6	SO4	C	303	-	4,4,4	0.24	0	6,6,6	0.07	0
6	SO4	L	301	-	4,4,4	0.24	0	6,6,6	0.10	0
6	SO4	G	303	-	4,4,4	0.24	0	6,6,6	0.10	0
6	SO4	A	304	-	4,4,4	0.24	0	6,6,6	0.12	0
6	SO4	G	304	-	4,4,4	0.24	0	6,6,6	0.08	0
6	SO4	H	303	-	4,4,4	0.23	0	6,6,6	0.09	0
7	NAG	J	301	1	14,14,15	0.21	0	17,19,21	0.51	0
6	SO4	F	302	-	4,4,4	0.23	0	6,6,6	0.09	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%)	0.68	16 (7%) 21 25	18, 40, 62, 92	4 (1%)
1	C	221/228 (96%)	0.73	26 (11%) 9 10	20, 39, 70, 119	4 (1%)
1	E	221/228 (96%)	1.30	52 (23%) 2 2	29, 50, 82, 111	4 (1%)
1	G	217/228 (95%)	1.68	77 (35%) 1 0	24, 47, 98, 126	4 (1%)
1	H	221/228 (96%)	0.44	17 (7%) 19 23	15, 35, 59, 72	4 (1%)
1	J	219/228 (96%)	1.66	75 (34%) 1 0	27, 54, 80, 92	4 (1%)
2	B	214/214 (100%)	0.35	7 (3%) 49 55	19, 38, 49, 64	1 (0%)
2	D	214/214 (100%)	0.78	24 (11%) 10 11	22, 44, 67, 88	1 (0%)
2	F	214/214 (100%)	0.88	14 (6%) 25 29	23, 47, 64, 77	1 (0%)
2	I	214/214 (100%)	2.16	118 (55%) 0 0	34, 61, 83, 97	1 (0%)
2	K	212/214 (99%)	2.88	156 (73%) 0 0	37, 74, 90, 100	1 (0%)
2	L	214/214 (100%)	0.21	6 (2%) 55 61	21, 34, 53, 62	1 (0%)
3	M	5/9 (55%)	1.31	1 (20%) 3 3	38, 45, 49, 57	0
3	N	5/9 (55%)	2.08	2 (40%) 1 0	52, 53, 60, 67	0
3	O	6/9 (66%)	2.39	4 (66%) 0 0	56, 62, 78, 82	0
3	P	4/9 (44%)	4.05	4 (100%) 0 0	68, 72, 74, 78	0
3	Q	6/9 (66%)	2.32	4 (66%) 0 0	57, 64, 68, 70	0
3	R	5/9 (55%)	3.60	5 (100%) 0 0	57, 60, 72, 77	0
All	All	2633/2706 (97%)	1.16	608 (23%) 2 2	15, 46, 82, 126	30 (1%)

All (608) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	186	VAL	7.2
1	C	214	THR	6.8
2	I	126	ALA	6.7

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Mol	Chain	Res	Type	RSRZ
2	K	75	ILE	6.4
2	K	110	PRO	6.3
1	G	115	SER	6.2
1	C	215	CYS	6.2
1	G	210	VAL	6.1
1	A	213	SER	6.0
1	G	140	LEU	5.9
3	R	6	GLY	5.9
1	G	161	LEU	5.9
1	C	189	SER	5.9
1	G	160	THR	5.7
1	H	213	SER	5.6
2	K	13	VAL	5.6
2	K	106	VAL	5.6
2	K	108	GLY	5.6
1	G	166[A]	ARG	5.5
2	I	122	ALA	5.4
2	K	66	GLY	5.4
2	K	59	PRO	5.4
1	A	115	SER	5.4
2	K	21	ILE	5.3
1	E	115	SER	5.2
3	P	3	ILE	5.2
1	G	193	VAL	5.2
2	I	23	CYS	5.2
2	K	63	LYS	5.2
1	G	138	VAL	5.2
2	K	140	PHE	5.1
2	K	48	ILE	5.1
1	J	113	SER	5.1
1	H	2	GLN	5.1
2	K	189	LYS	5.0
1	A	116	GLY	5.0
1	E	214	THR	5.0
2	K	51	VAL	4.9
2	K	19	VAL	4.9
1	J	101	ASP	4.9
1	G	164	GLY	4.9
2	K	172	TYR	4.9
2	I	27(A)	SER	4.8
1	G	211	ALA	4.8
1	G	184	VAL	4.8

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Mol	Chain	Res	Type	RSRZ
2	K	73	LEU	4.8
2	K	105	VAL	4.8
1	H	101	ASP	4.7
2	K	139	TYR	4.7
1	C	213	SER	4.7
1	J	190	SER	4.7
2	K	79	VAL	4.7
2	K	54	LEU	4.7
1	C	115	SER	4.7
2	K	12	SER	4.7
2	K	78	VAL	4.7
3	N	2	ASN	4.6
2	I	51	VAL	4.6
2	I	25	ALA	4.6
3	P	7	SER	4.6
2	I	120	PRO	4.6
1	J	114	SER	4.6
2	I	69	THR	4.6
1	G	187	THR	4.5
1	G	134	PRO	4.5
1	A	215	CYS	4.5
1	G	156	TRP	4.5
1	G	162	THR	4.5
1	A	189	SER	4.4
1	E	192	PRO	4.4
2	I	66	GLY	4.4
1	J	211	ALA	4.4
2	K	72	THR	4.4
2	K	35	TRP	4.4
1	E	114	SER	4.4
2	I	71	PHE	4.4
2	I	203	VAL	4.3
2	I	184	GLN	4.3
2	K	23	CYS	4.3
1	J	189	SER	4.3
1	H	65	SER	4.3
1	E	213	SER	4.3
2	K	33	LEU	4.3
3	R	3	ILE	4.3
2	K	11	LYS	4.2
2	K	15	VAL	4.2
2	K	111	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
2	K	141	PRO	4.2
2	K	109	ASP	4.2
2	K	7	THR	4.2
2	I	22	ASN	4.2
2	I	121	ALA	4.2
2	I	127	THR	4.2
1	E	129	CYS	4.1
2	I	125	VAL	4.1
1	G	124	PHE	4.1
1	G	137	THR	4.1
2	K	20	THR	4.1
1	G	188	SER	4.1
1	G	212	PRO	4.1
2	K	8	PRO	4.1
2	K	74	THR	4.1
1	G	141	GLY	4.1
2	K	62	PHE	4.1
2	K	64	GLY	4.1
2	I	21	ILE	4.1
2	B	27(A)	SER	4.1
2	K	14	PRO	4.1
2	K	112	ALA	4.0
1	G	215	CYS	4.0
1	E	101	ASP	4.0
1	E	215	CYS	4.0
1	G	195[A]	CYS	4.0
1	G	214	THR	4.0
2	I	29	SER	4.0
1	G	128	PRO	4.0
1	G	185[A]	SER	4.0
2	K	27(B)	VAL	3.9
2	K	151	GLY	3.9
1	G	213	SER	3.9
1	G	165	VAL	3.9
2	K	143	VAL	3.9
1	G	133	THR	3.9
1	C	113	SER	3.9
1	E	2	GLN	3.9
2	K	107	LYS	3.9
1	A	214	THR	3.9
1	C	15	THR	3.9
1	G	194	THR	3.9

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Mol	Chain	Res	Type	RSRZ
1	G	123	VAL	3.8
1	G	206	VAL	3.8
1	J	166[A]	ARG	3.8
2	I	27(B)	VAL	3.8
1	C	190	SER	3.8
1	G	113	SER	3.8
2	I	63	LYS	3.8
2	K	68	GLY	3.8
1	G	157	ASN	3.8
2	I	48	ILE	3.8
2	K	86	TYR	3.7
1	A	101	ASP	3.7
1	G	132	ASP	3.7
2	K	165	GLN	3.7
1	J	188	SER	3.7
2	K	16	GLY	3.7
1	G	155	THR	3.7
2	K	211	CYS	3.7
1	G	131	GLY	3.7
1	A	61	ASN	3.7
2	K	69	THR	3.7
1	E	113	SER	3.7
1	G	135	SER	3.7
2	I	26	SER	3.7
2	D	68	GLY	3.7
2	K	47	LEU	3.7
2	K	46	LEU	3.6
2	K	22	ASN	3.6
2	K	137	ASN	3.6
2	I	185	TYR	3.6
1	G	126	LEU	3.6
2	I	211	CYS	3.6
2	I	147	TRP	3.6
2	I	92	LYS	3.6
2	K	28	TYR	3.6
2	K	201	SER	3.6
2	K	71	PHE	3.6
3	P	4	ILE	3.6
2	I	64	GLY	3.6
1	G	101	ASP	3.6
2	K	200	THR	3.6
2	K	202	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
2	K	65	SER	3.6
1	E	166[A]	ARG	3.6
2	K	92	LYS	3.6
1	E	211	ALA	3.6
3	O	7	SER	3.5
2	K	91	TYR	3.5
2	K	36	PHE	3.5
2	D	3	ASP	3.5
2	I	74	THR	3.5
1	A	113	SER	3.5
2	D	67	SER	3.5
2	K	57	GLY	3.5
2	F	22	ASN	3.5
1	G	209	THR	3.5
2	K	18	THR	3.5
2	K	156	THR	3.5
1	E	186	VAL	3.5
2	K	89	VAL	3.5
2	K	55	ALA	3.5
1	C	2	GLN	3.5
1	J	212	PRO	3.5
1	E	164	GLY	3.5
2	K	142	ASP	3.5
1	C	134	PRO	3.4
1	G	139	THR	3.4
1	J	115	SER	3.4
2	I	27	GLU	3.4
1	J	56	ARG	3.4
2	I	3	ASP	3.4
2	I	123	ASP	3.4
1	J	171	VAL	3.4
2	I	195	VAL	3.4
2	K	83	ALA	3.4
2	D	211	CYS	3.4
2	K	70	GLN	3.4
1	G	127	ALA	3.4
2	K	56	SER	3.4
2	I	128	GLY	3.4
1	J	3	SER	3.3
1	J	213	SER	3.3
2	I	130	VAL	3.3
2	K	167	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	J	42	GLY	3.3
1	J	169	PRO	3.3
2	I	68	GLY	3.3
2	K	30	ASN	3.3
2	K	61	ARG	3.3
1	E	174	SER	3.3
3	R	8	ASP	3.3
2	I	178	LEU	3.3
1	J	133	THR	3.3
2	K	168	ALA	3.2
2	I	4	MET	3.2
1	J	15	THR	3.2
2	I	18	THR	3.2
2	I	181	THR	3.2
2	I	35	TRP	3.2
1	J	112	SER	3.2
1	G	125	PRO	3.2
3	Q	3	ILE	3.2
2	K	60	SER	3.2
1	G	116	GLY	3.2
2	K	81	ASP	3.2
3	O	2	ASN	3.2
2	I	180	LEU	3.2
2	K	199	THR	3.2
2	I	208	ARG	3.1
2	I	189	LYS	3.1
1	J	168	PHE	3.1
1	E	163	ASN	3.1
2	I	30	ASN	3.1
2	K	25	ALA	3.1
2	K	82	ASP	3.1
1	E	161	LEU	3.1
1	C	188	SER	3.1
1	G	174	SER	3.1
1	J	100(D)	PHE	3.1
1	G	196	ASN	3.1
2	K	95(C)	GLY	3.1
3	Q	8	ASP	3.1
2	K	113	PRO	3.1
2	I	75	ILE	3.1
2	I	117	ILE	3.1
1	E	137	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	J	131	GLY	3.1
2	K	198	GLY	3.1
2	K	84	ALA	3.1
1	G	98	VAL	3.1
1	J	100(B)	VAL	3.1
2	I	54	LEU	3.1
1	G	208	LYS	3.1
2	I	28	TYR	3.1
1	J	175	SER	3.1
2	F	12	SER	3.1
1	G	142[A]	CYS	3.1
2	I	157	GLY	3.1
2	K	80	CYS	3.1
2	K	97	ALA	3.1
2	I	50	LEU	3.1
2	K	171	THR	3.0
1	G	65	SER	3.0
2	F	24	GLN	3.0
1	G	74	ASN	3.0
2	K	98	PHE	3.0
2	K	180	LEU	3.0
2	I	155	THR	3.0
2	K	85	THR	3.0
2	K	37	GLN	3.0
1	J	130	CYS	3.0
1	E	210	VAL	3.0
2	K	103	GLU	3.0
2	K	104	VAL	3.0
2	I	91	TYR	3.0
2	K	196	THR	3.0
2	K	187	SER	3.0
1	J	134	PRO	3.0
2	B	27	GLU	3.0
2	I	202	VAL	3.0
2	K	197	GLN	3.0
1	E	65	SER	3.0
2	K	34	SER	3.0
2	K	17	ASP	3.0
2	I	62	PHE	2.9
1	J	63	ALA	2.9
1	E	130	CYS	2.9
1	G	129	CYS	2.9

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Mol	Chain	Res	Type	RSRZ
2	I	19	VAL	2.9
2	K	58	VAL	2.9
1	E	191	GLN	2.9
1	A	114	SER	2.9
1	J	99	SER	2.9
2	B	26	SER	2.9
1	H	116	GLY	2.9
1	C	101	ASP	2.9
1	E	42	GLY	2.9
1	E	74	ASN	2.9
1	G	159	GLY	2.9
1	E	134	PRO	2.9
2	K	178	LEU	2.9
2	K	32	ARG	2.9
1	C	173	GLN	2.9
2	L	7	THR	2.9
2	I	129	THR	2.9
1	E	112	SER	2.9
2	K	67	SER	2.9
2	K	191	TYR	2.9
1	J	62	TRP	2.9
2	I	73	LEU	2.9
2	D	70	GLN	2.9
1	G	130	CYS	2.9
2	K	88	CYS	2.9
1	J	100(A)	SER	2.9
1	E	26	GLY	2.9
1	J	164	GLY	2.9
2	I	207	ASN	2.9
1	J	2	GLN	2.9
1	J	27	PHE	2.9
2	K	195	VAL	2.9
2	K	170	CYS	2.9
2	L	183	THR	2.9
2	K	157	GLY	2.8
1	E	64	ARG	2.8
2	K	164	PRO	2.8
1	E	173	GLN	2.8
2	I	118	PHE	2.8
2	F	159	GLU	2.8
1	G	207	ASP	2.8
2	I	32	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
2	I	187	SER	2.8
2	I	209	GLY	2.8
1	A	2	GLN	2.8
2	K	96	LEU	2.8
1	J	67	ALA	2.8
2	I	206	PHE	2.8
1	E	165	VAL	2.8
1	E	193	VAL	2.8
1	H	15	THR	2.8
1	J	137	THR	2.8
2	D	69	THR	2.8
2	K	129	THR	2.8
1	H	113	SER	2.8
2	K	9	SER	2.8
2	K	188	HIS	2.8
2	I	204	GLN	2.8
2	I	132	ILE	2.8
1	C	131	GLY	2.8
2	K	24	GLN	2.8
3	P	6	GLY	2.8
2	K	49	TYR	2.8
2	D	25	ALA	2.8
2	I	58	VAL	2.8
1	E	209	THR	2.7
2	F	20	THR	2.7
2	I	20	THR	2.7
2	I	131	THR	2.7
1	C	180	LEU	2.7
2	I	191	TYR	2.7
1	E	138	VAL	2.7
2	I	5	THR	2.7
2	I	200	THR	2.7
1	J	146	GLY	2.7
1	J	174	SER	2.7
2	F	122	ALA	2.7
1	G	173	GLN	2.7
1	J	31	GLY	2.7
1	J	82(B)	SER	2.7
3	M	7	SER	2.7
1	G	143	LEU	2.7
1	H	214	THR	2.7
2	I	72	THR	2.7

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Mol	Chain	Res	Type	RSRZ
2	K	53	THR	2.7
1	C	192	PRO	2.7
1	E	212	PRO	2.7
1	J	173	GLN	2.6
2	I	17	ASP	2.6
1	J	139	THR	2.6
2	D	183	THR	2.6
1	C	65	SER	2.6
2	F	211	CYS	2.6
2	I	77	ASP	2.6
2	I	135	VAL	2.6
1	E	131	GLY	2.6
1	J	159	GLY	2.6
2	I	183	THR	2.6
2	K	102	THR	2.6
1	G	136	SER	2.6
2	D	4	MET	2.6
2	F	60	SER	2.6
3	N	7	SER	2.6
2	F	92	LYS	2.6
1	C	211	ALA	2.6
1	G	64	ARG	2.6
2	K	31	ASN	2.6
1	G	73	THR	2.6
1	G	144	VAL	2.6
2	K	163	THR	2.6
2	F	27(A)	SER	2.6
2	K	205	SER	2.6
2	L	189	LYS	2.6
2	K	42	GLN	2.6
1	G	183	VAL	2.6
2	I	119	PRO	2.6
2	K	5	THR	2.6
2	K	44	PRO	2.6
1	G	158	SER	2.6
1	G	163	ASN	2.5
2	K	3	ASP	2.5
1	J	116	GLY	2.5
2	L	129	THR	2.5
1	E	189	SER	2.5
2	K	162	LYS	2.5
1	J	57	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
3	R	4	ILE	2.5
2	D	24	GLN	2.5
2	I	49	TYR	2.5
1	H	14	PRO	2.5
2	K	39	LYS	2.5
1	E	187	THR	2.5
2	D	74	THR	2.5
2	K	144	THR	2.5
2	I	70	GLN	2.5
2	K	174	LEU	2.5
3	O	8	ASP	2.5
2	D	66	GLY	2.5
2	F	23	CYS	2.5
2	D	95	THR	2.5
1	A	65	SER	2.5
1	C	166[A]	ARG	2.5
1	J	177	LEU	2.5
2	I	45	LYS	2.5
1	E	157	ASN	2.5
1	C	116	GLY	2.5
3	Q	6	GLY	2.5
2	I	152	THR	2.4
2	K	95(A)	THR	2.4
2	K	148	GLU	2.4
2	K	26	SER	2.4
1	G	205	LYS	2.4
1	H	117	GLN	2.4
1	H	85	ALA	2.4
2	K	155	THR	2.4
1	H	189	SER	2.4
2	D	10	SER	2.4
1	J	37	VAL	2.4
2	D	63	LYS	2.4
2	I	116	LEU	2.4
2	I	24	GLN	2.4
1	J	187	THR	2.4
1	E	27	PHE	2.4
2	K	138	LYS	2.4
2	K	149	VAL	2.4
1	J	191	GLN	2.4
2	K	40	PRO	2.4
1	E	116	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	J	68	THR	2.4
2	I	192	THR	2.4
2	D	27(A)	SER	2.4
2	I	15	VAL	2.4
2	K	133	VAL	2.4
2	D	54	LEU	2.4
2	I	188	HIS	2.4
1	G	117	GLN	2.4
2	I	124	GLN	2.4
2	I	154	GLN	2.4
2	I	186	ASN	2.3
2	I	210	ASP	2.3
2	K	160	ASN	2.3
2	I	198	GLY	2.3
1	C	179	SER	2.3
1	G	100(A)	SER	2.3
1	J	181	SER	2.3
2	B	65	SER	2.3
2	I	34	SER	2.3
1	H	215	CYS	2.3
2	D	71	PHE	2.3
2	K	130	VAL	2.3
1	G	75	LEU	2.3
1	C	132	ASP	2.3
1	J	47	TRP	2.3
2	I	114	THR	2.3
2	K	183	THR	2.3
1	J	184	VAL	2.3
2	I	79	VAL	2.3
2	I	133	VAL	2.3
1	G	31	GLY	2.3
1	E	15	THR	2.3
1	J	160	THR	2.3
1	H	115	SER	2.3
2	L	27(A)	SER	2.3
2	I	65	SER	2.3
1	G	27	PHE	2.3
2	I	115	VAL	2.3
1	E	208	LYS	2.3
2	F	123	ASP	2.3
2	I	151	GLY	2.3
1	A	62	TRP	2.3

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Mol	Chain	Res	Type	RSRZ
1	J	103	TRP	2.3
2	B	20	THR	2.3
1	E	158	SER	2.3
1	G	114	SER	2.3
3	Q	4	ILE	2.3
1	J	45	LEU	2.2
1	J	149	PRO	2.2
2	K	90	GLY	2.2
1	A	178	TYR	2.2
1	J	54	TYR	2.2
1	J	178	TYR	2.2
2	D	156	THR	2.2
1	J	65	SER	2.2
2	F	26	SER	2.2
2	I	76	SER	2.2
2	K	94	SER	2.2
1	E	205	LYS	2.2
1	E	61	ASN	2.2
1	J	64	ARG	2.2
2	I	61	ARG	2.2
1	G	146	GLY	2.2
1	G	100	THR	2.2
2	D	129	THR	2.2
2	I	153	THR	2.2
2	K	95	THR	2.2
1	E	190	SER	2.2
1	E	57	ILE	2.2
1	J	186	VAL	2.2
1	J	132	ASP	2.2
2	K	154	GLN	2.2
2	K	184	GLN	2.2
1	C	112	SER	2.2
1	J	96	THR	2.2
2	B	7	THR	2.2
2	D	29	SER	2.2
1	J	59	TYR	2.2
3	O	3	ILE	2.2
2	I	78	VAL	2.2
2	D	27	GLU	2.2
2	I	95(C)	GLY	2.2
2	I	53	THR	2.2
2	I	67	SER	2.2

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Mol	Chain	Res	Type	RSRZ
2	I	199	THR	2.2
2	I	47	LEU	2.1
2	I	137	ASN	2.1
2	K	166	ASN	2.1
2	I	90	GLY	2.1
1	H	13	LYS	2.1
1	E	43	LYS	2.1
1	J	138	VAL	2.1
2	I	89	VAL	2.1
1	G	2	GLN	2.1
2	I	16	GLY	2.1
2	I	57	GLY	2.1
1	E	162	THR	2.1
1	E	175	SER	2.1
2	I	156	THR	2.1
1	J	53	ALA	2.1
1	J	85	ALA	2.1
2	I	182	SER	2.1
2	K	146	THR	2.1
2	I	33	LEU	2.1
1	J	193	VAL	2.1
2	I	59	PRO	2.1
1	E	159	GLY	2.1
1	J	33	GLY	2.1
1	A	23	THR	2.1
2	I	146	THR	2.1
3	R	7	SER	2.1
1	J	161	LEU	2.1
1	J	180	LEU	2.1
2	F	3	ASP	2.1
1	A	212	PRO	2.1
1	C	212	PRO	2.1
2	K	115	VAL	2.1
1	J	91	PHE	2.1
1	E	5	LYS	2.0
1	H	114	SER	2.0
1	C	133	THR	2.0
1	G	153	THR	2.0
2	D	56	SER	2.0
2	I	7	THR	2.0
1	H	211	ALA	2.0
2	K	136	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
2	K	159	GLU	2.0
2	K	190	GLU	2.0
1	G	61	ASN	2.0
2	K	50	LEU	2.0
2	K	150	ASP	2.0
1	J	35	ILE	2.0
2	K	43	PRO	2.0
1	J	32	TYR	2.0
2	D	91	TYR	2.0
1	J	55	GLY	2.0
2	K	100	GLY	2.0
2	L	63	LYS	2.0
1	C	114	SER	2.0
2	K	29	SER	2.0
2	K	192	THR	2.0
2	B	3	ASP	2.0
2	K	132	ILE	2.0

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.

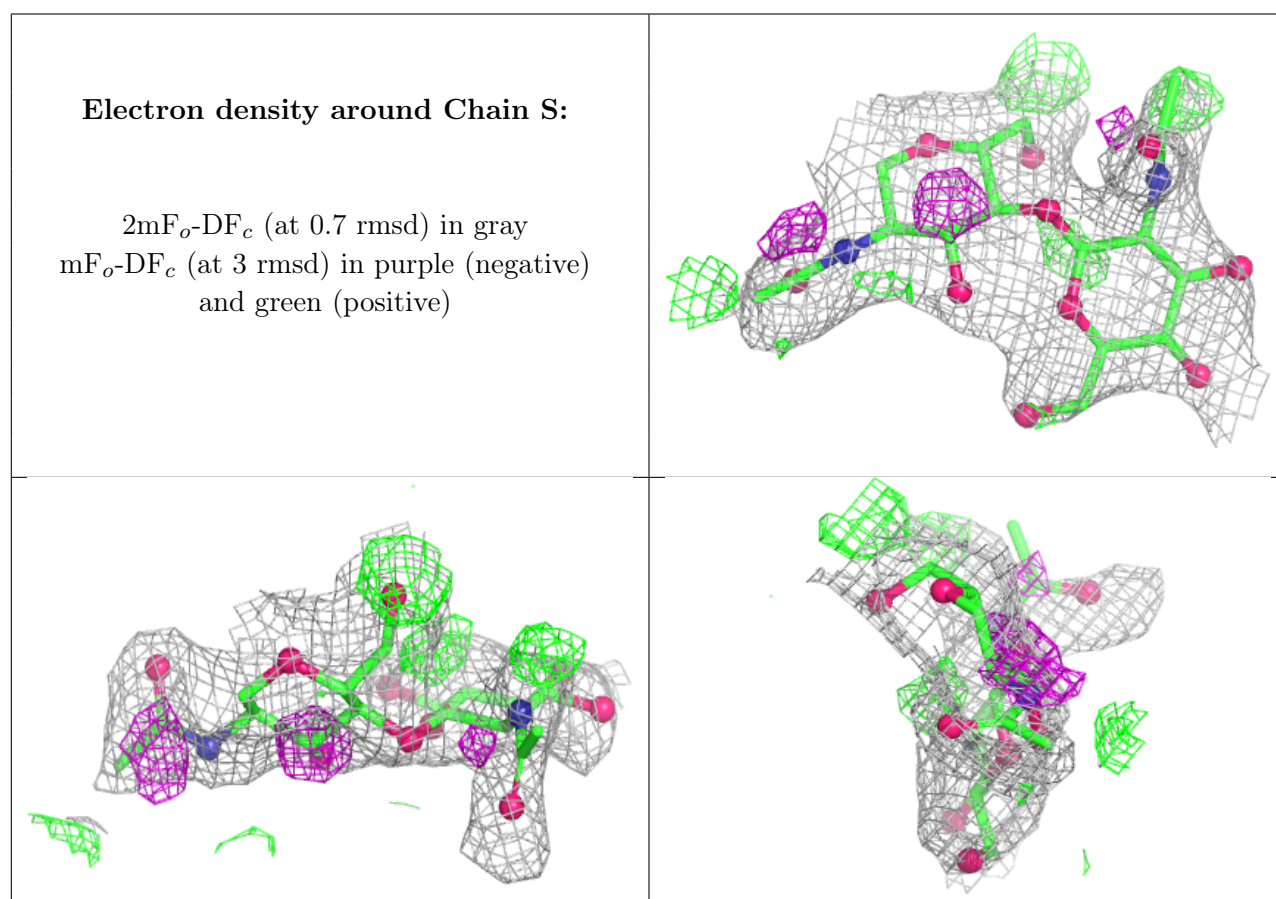
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	UKY	P	5	14/15	0.89	0.13	47,68,73,75	0
3	UKY	R	5	14/15	0.91	0.13	35,64,70,72	0
3	UKY	O	5	14/15	0.92	0.12	29,50,57,57	0
3	UKY	Q	5	14/15	0.93	0.10	34,53,62,64	0
3	UKY	N	5	14/15	0.95	0.08	41,48,54,60	0
3	UKY	M	5	14/15	0.97	0.07	27,35,44,49	0

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.

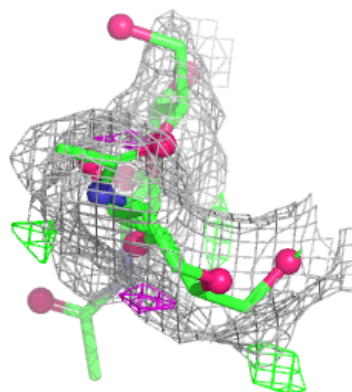
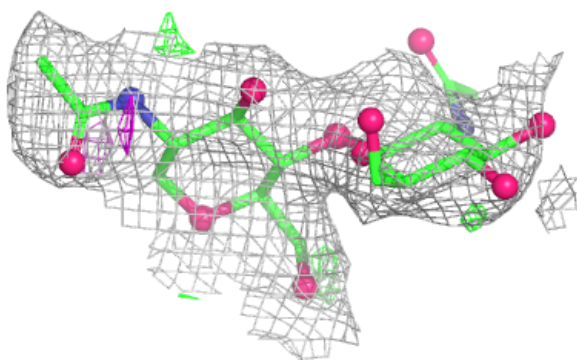
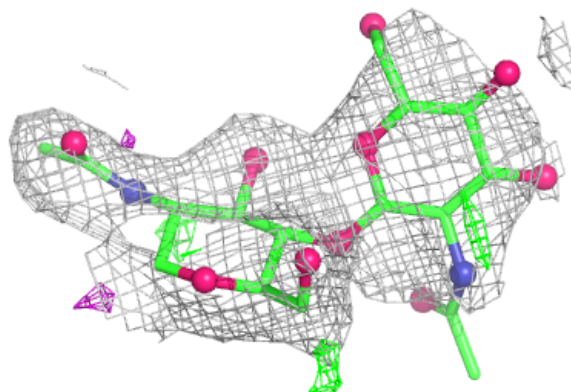
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	FUC	T	3	10/11	0.25	0.26	64,92,102,106	0
4	NAG	W	2	14/15	0.47	0.22	113,120,125,127	0
5	NAG	T	2	14/15	0.52	0.25	69,99,114,130	0
4	NAG	V	2	14/15	0.57	0.21	83,94,99,101	0
4	NAG	U	2	14/15	0.62	0.20	79,92,95,98	0
4	NAG	S	2	14/15	0.64	0.21	62,78,83,86	0
4	NAG	W	1	14/15	0.71	0.18	61,88,103,111	0
4	NAG	U	1	14/15	0.73	0.17	46,67,77,87	0
4	NAG	V	1	14/15	0.75	0.17	53,69,84,89	0
4	NAG	S	1	14/15	0.77	0.18	35,48,71,79	0
5	NAG	T	1	14/15	0.85	0.15	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.



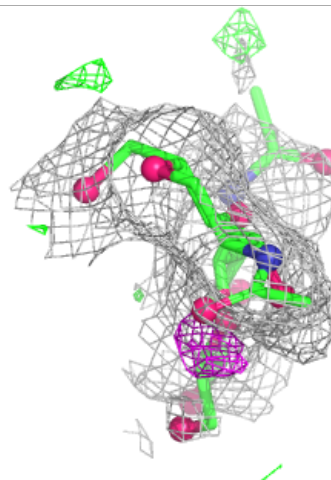
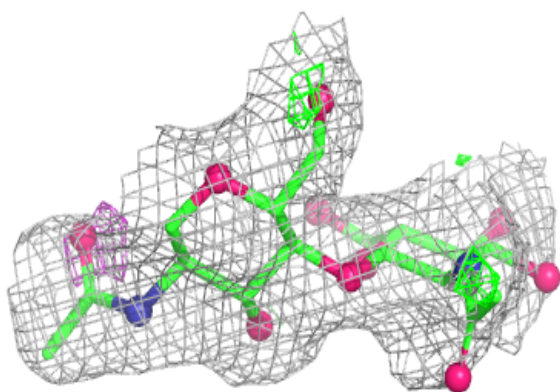
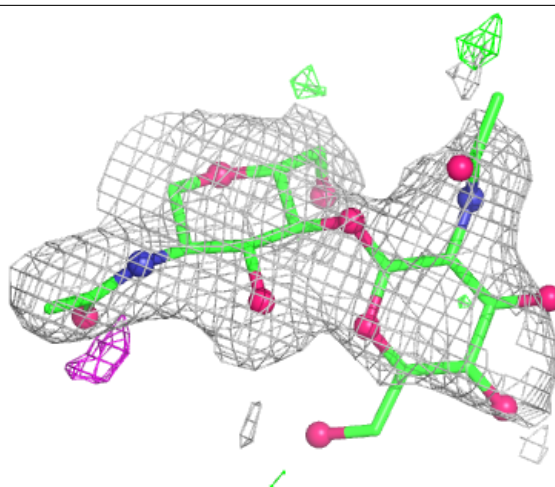
Electron density around Chain U:

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



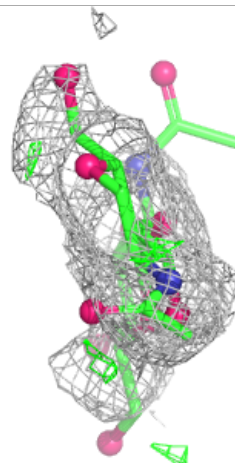
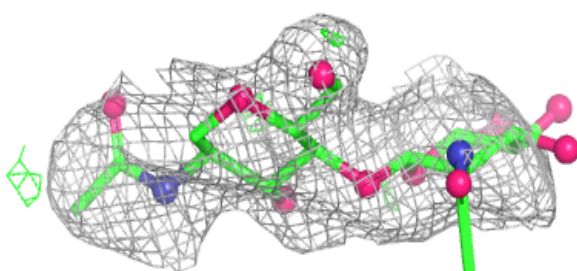
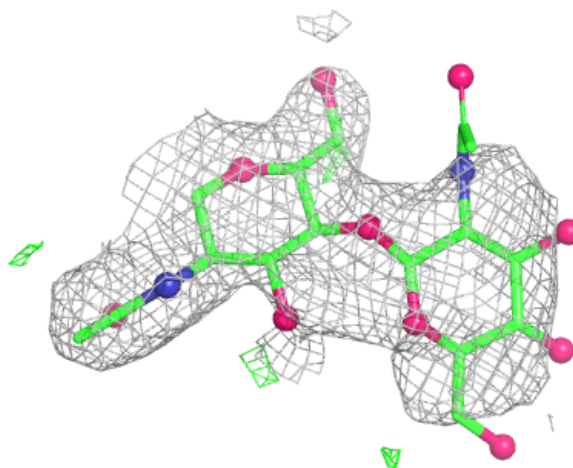
Electron density around Chain V:

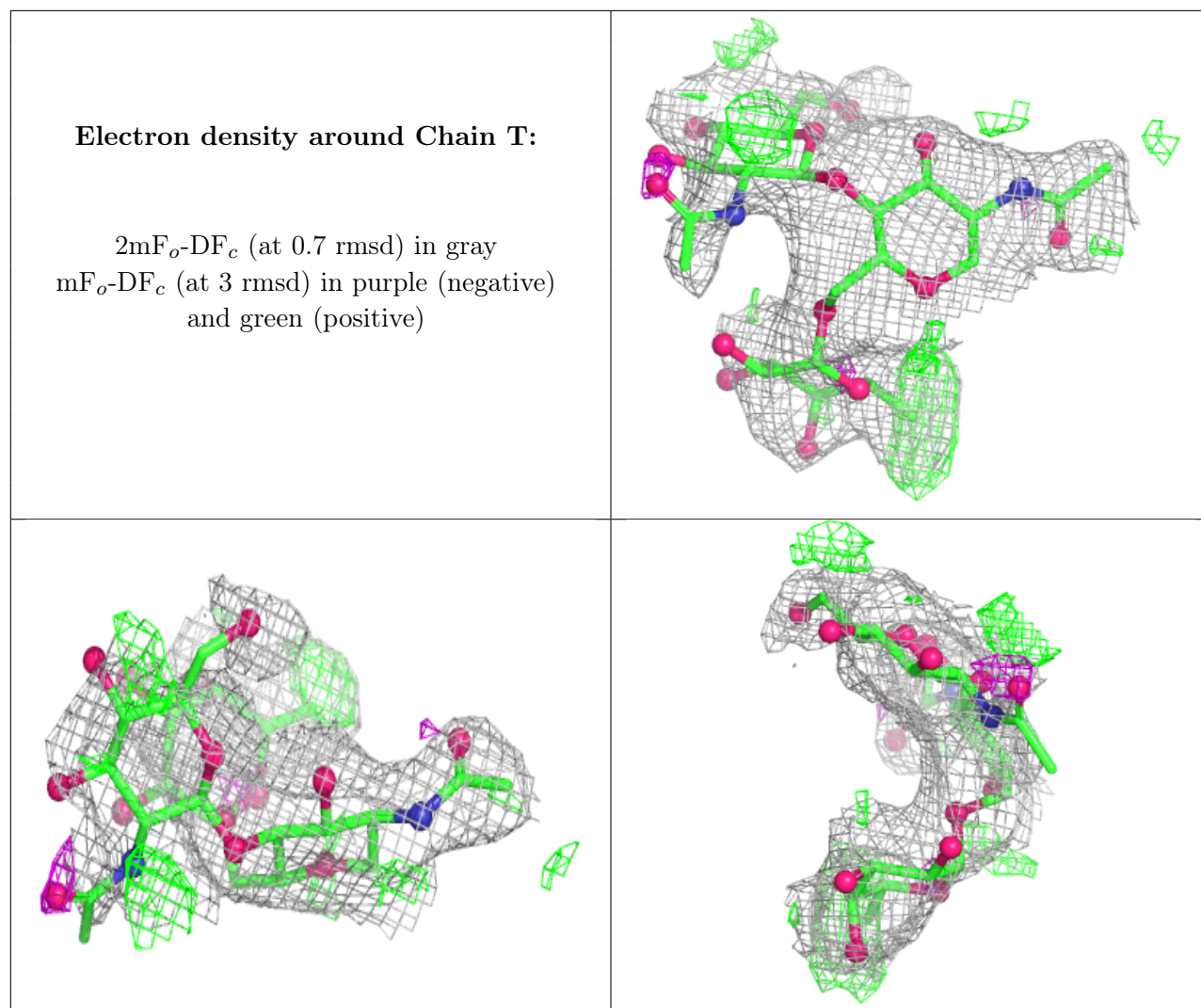
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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
6	SO4	H	303	5/5	0.64	0.17	60,67,82,94	0
6	SO4	F	303	5/5	0.72	0.13	59,68,87,88	0
7	NAG	J	301	14/15	0.72	0.19	69,82,88,94	0
6	SO4	F	304	5/5	0.73	0.11	75,88,91,103	0
6	SO4	F	302	5/5	0.73	0.12	76,83,91,96	0
6	SO4	G	304	5/5	0.75	0.14	60,82,83,94	0
6	SO4	C	303	5/5	0.78	0.13	59,76,81,84	0
6	SO4	C	304	5/5	0.80	0.12	64,75,88,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	SO4	F	301	5/5	0.82	0.11	78,87,98,104	0
6	SO4	A	304	5/5	0.87	0.30	39,42,63,68	0
6	SO4	G	303	5/5	0.87	0.36	26,44,65,70	0
6	SO4	L	301	5/5	0.89	0.15	42,60,69,73	0

6.5 Other polymers [i](#)

There are no such residues in this entry.