



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:31 AM UTC

PDB ID : 8GB5 / pdb_00008gb5
Title : Crystal structure of SARS-CoV-2 receptor binding domain in complex with neutralizing antibody 25F9
Authors : Yuan, M.; Zhu, X.; Wilson, I.A.
Deposited on : 2023-02-24
Resolution : 3.35 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:

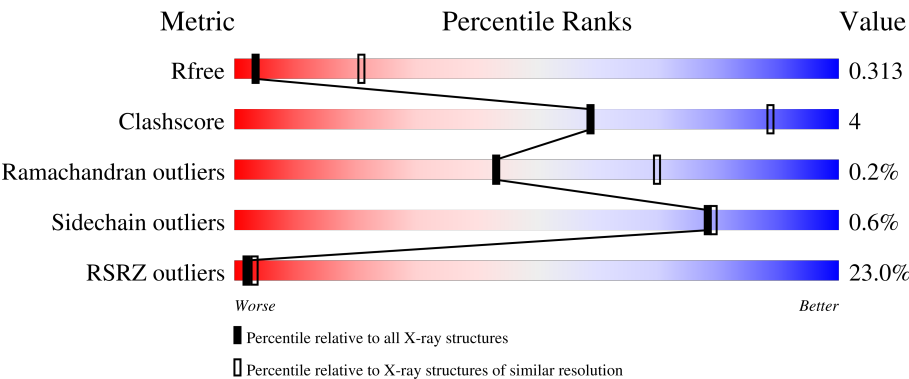
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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.



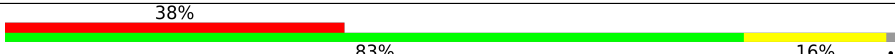
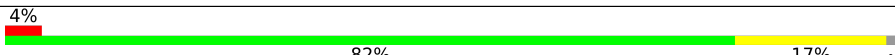
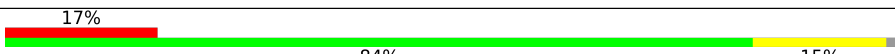
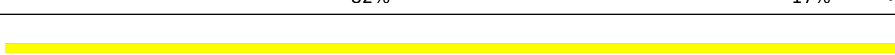
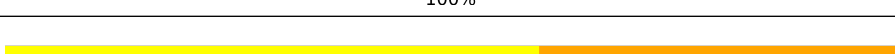
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1099 (3.40-3.32)
Clashscore	190562	1116 (3.40-3.32)
Ramachandran outliers	187476	1101 (3.40-3.32)
Sidechain outliers	187428	1101 (3.40-3.32)
RSRZ outliers	180081	1099 (3.40-3.32)

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	205	
1	D	205	
1	G	205	
1	J	205	
2	B	231	

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Mol	Chain	Length	Quality of chain
2	F	231	
2	I	231	
2	L	231	
3	C	216	
3	E	216	
3	H	216	
3	K	216	
4	M	3	
5	N	5	
6	O	4	
6	P	4	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 19740 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 Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	195	Total	C	N	O	S	0	0	0
			1543	989	257	289	8			
1	D	195	Total	C	N	O	S	0	0	0
			1543	989	257	289	8			
1	G	195	Total	C	N	O	S	0	0	0
			1543	989	257	289	8			
1	J	195	Total	C	N	O	S	0	0	0
			1543	989	257	289	8			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	531	GLY	-	expression tag	UNP P0DTC2
A	532	HIS	-	expression tag	UNP P0DTC2
A	533	HIS	-	expression tag	UNP P0DTC2
A	534	HIS	-	expression tag	UNP P0DTC2
A	535	HIS	-	expression tag	UNP P0DTC2
A	536	HIS	-	expression tag	UNP P0DTC2
A	537	HIS	-	expression tag	UNP P0DTC2
D	531	GLY	-	expression tag	UNP P0DTC2
D	532	HIS	-	expression tag	UNP P0DTC2
D	533	HIS	-	expression tag	UNP P0DTC2
D	534	HIS	-	expression tag	UNP P0DTC2
D	535	HIS	-	expression tag	UNP P0DTC2
D	536	HIS	-	expression tag	UNP P0DTC2
D	537	HIS	-	expression tag	UNP P0DTC2
G	531	GLY	-	expression tag	UNP P0DTC2
G	532	HIS	-	expression tag	UNP P0DTC2
G	533	HIS	-	expression tag	UNP P0DTC2
G	534	HIS	-	expression tag	UNP P0DTC2
G	535	HIS	-	expression tag	UNP P0DTC2
G	536	HIS	-	expression tag	UNP P0DTC2
G	537	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
J	531	GLY	-	expression tag	UNP P0DTC2
J	532	HIS	-	expression tag	UNP P0DTC2
J	533	HIS	-	expression tag	UNP P0DTC2
J	534	HIS	-	expression tag	UNP P0DTC2
J	535	HIS	-	expression tag	UNP P0DTC2
J	536	HIS	-	expression tag	UNP P0DTC2
J	537	HIS	-	expression tag	UNP P0DTC2

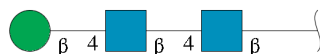
- Molecule 2 is a protein called 25F9 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	227	Total	C	N	O	S	0	0	0
			1725	1100	288	331	6			
2	F	227	Total	C	N	O	S	0	0	0
			1723	1099	288	331	5			
2	I	227	Total	C	N	O	S	0	0	0
			1725	1100	288	331	6			
2	L	228	Total	C	N	O	S	0	0	0
			1729	1102	289	332	6			

- Molecule 3 is a protein called 25F9 Light chain.

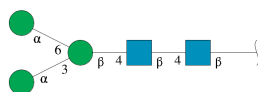
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	214	Total	C	N	O	S	0	0	0
			1585	984	273	323	5			
3	E	213	Total	C	N	O	S	0	0	0
			1579	981	273	321	4			
3	H	214	Total	C	N	O	S	0	0	0
			1585	984	273	323	5			
3	K	213	Total	C	N	O	S	0	0	0
			1579	981	272	322	4			

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



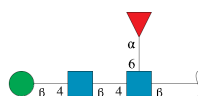
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	M	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



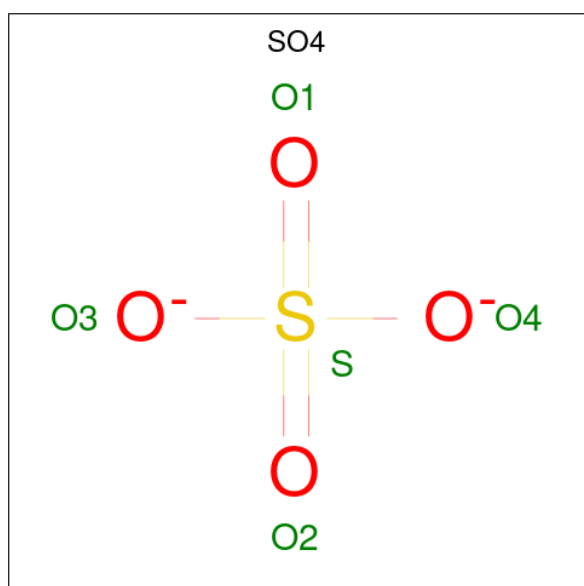
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	N	5	Total	C	N	O	0	0	0
			61	34	2	25			

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



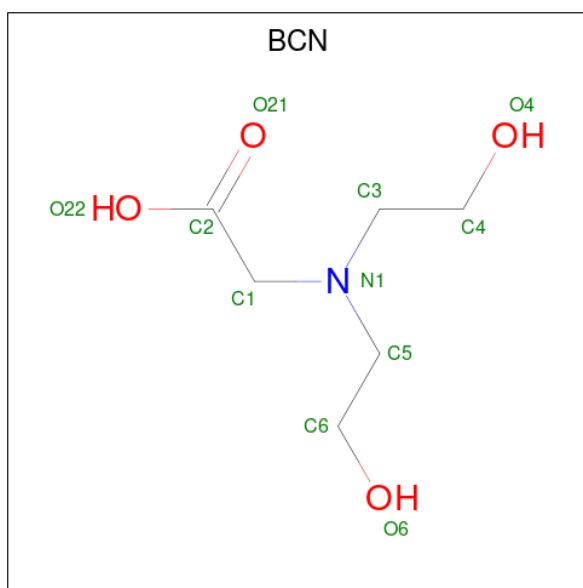
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	O	4	Total	C	N	O	0	0	0
			49	28	2	19			
6	P	4	Total	C	N	O	0	0	0
			49	28	2	19			

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



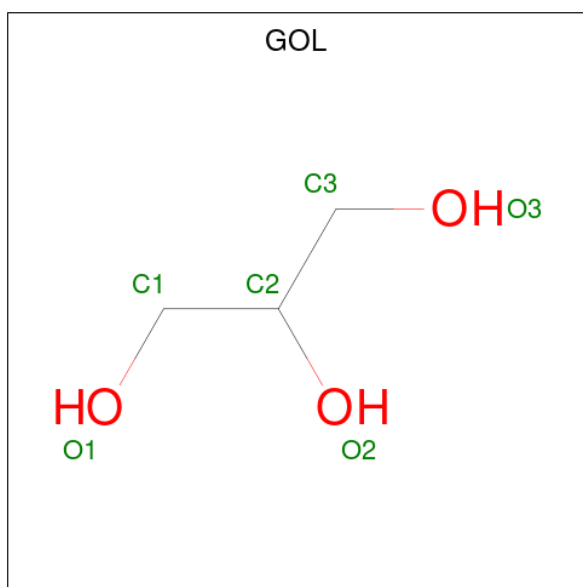
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total O S 5 4 1	0	0
7	D	1	Total O S 5 4 1	0	0
7	E	1	Total O S 5 4 1	0	0
7	E	1	Total O S 5 4 1	0	0
7	I	1	Total O S 5 4 1	0	0
7	J	1	Total O S 5 4 1	0	0
7	K	1	Total O S 5 4 1	0	0
7	K	1	Total O S 5 4 1	0	0

- Molecule 8 is BICINE (CCD ID: BCN) (formula: $C_6H_{13}NO_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total C N O 11 6 1 4	0	0
8	E	1	Total C N O 11 6 1 4	0	0
8	H	1	Total C N O 11 6 1 4	0	0

- Molecule 9 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	K	1	Total	C	O	0	0
			6	3	3		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	3	Total	O	0	0
			3	3		
10	B	3	Total	O	0	0
			3	3		
10	C	6	Total	O	0	0
			6	6		
10	D	2	Total	O	0	0
			2	2		
10	E	5	Total	O	0	0
			5	5		
10	F	4	Total	O	0	0
			4	4		
10	G	3	Total	O	0	0
			3	3		
10	H	6	Total	O	0	0
			6	6		
10	I	7	Total	O	0	0
			7	7		
10	J	2	Total	O	0	0
			2	2		
10	K	14	Total	O	0	0
			14	14		

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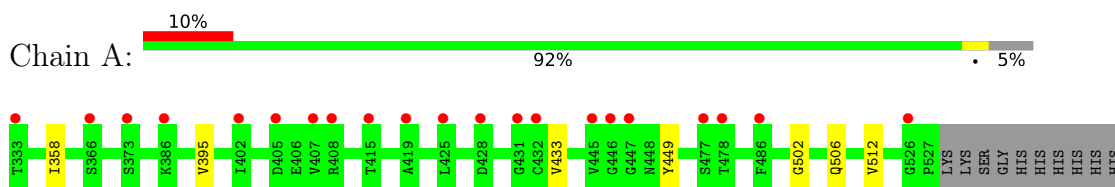
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	L	6	Total	O	0	0
			6	6		

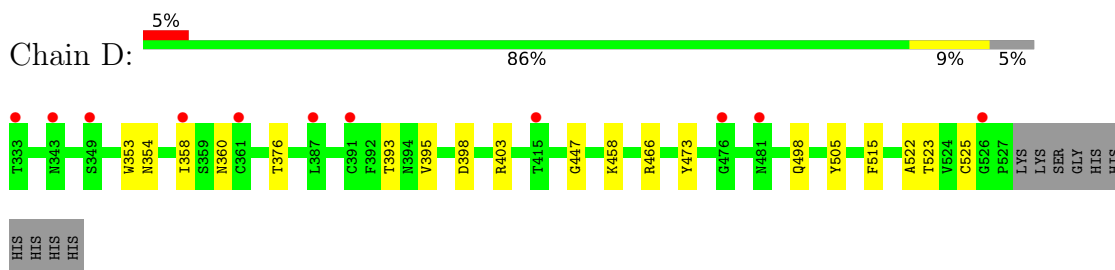
3 Residue-property plots [i](#)

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.

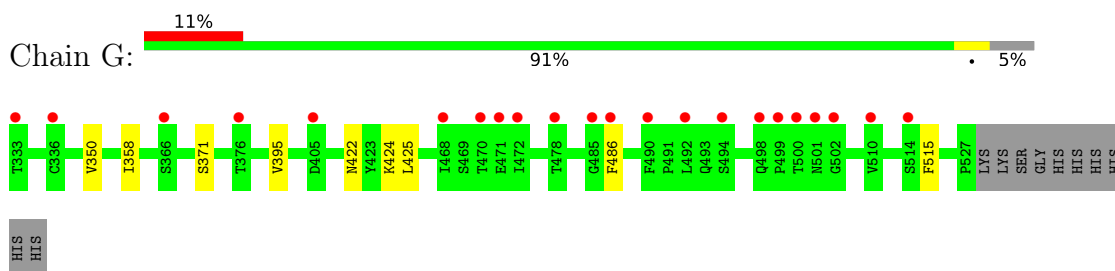
- Molecule 1: Spike protein S1



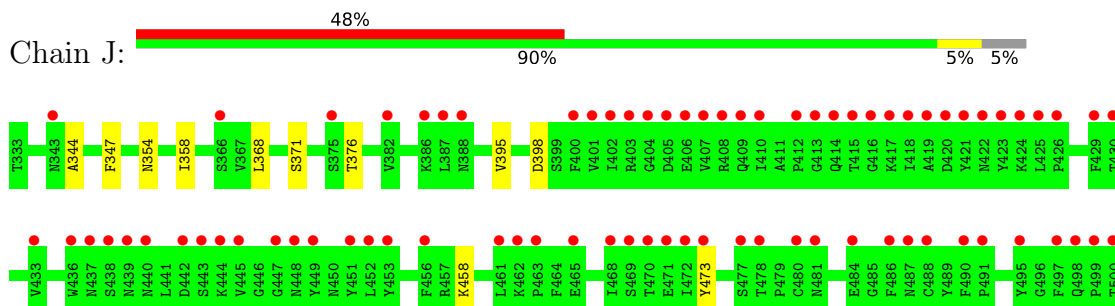
- Molecule 1: Spike protein S1

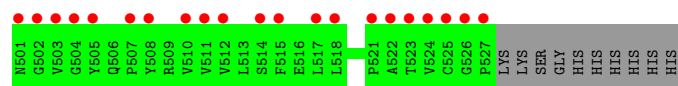


- Molecule 1: Spike protein S1

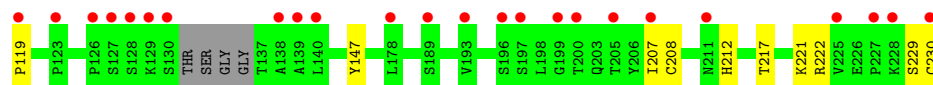
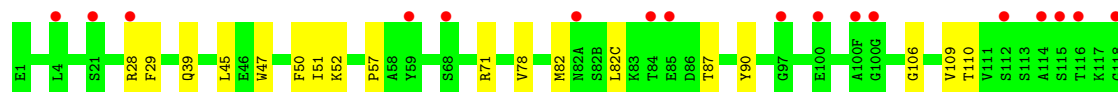
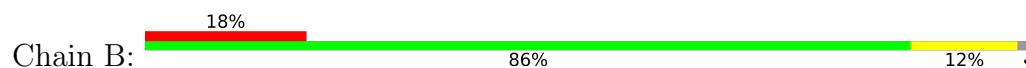


- Molecule 1: Spike protein S1

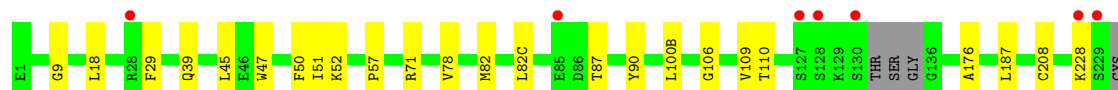
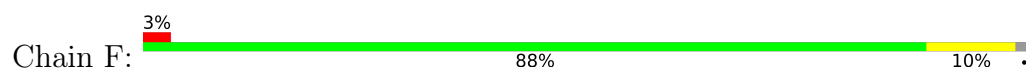




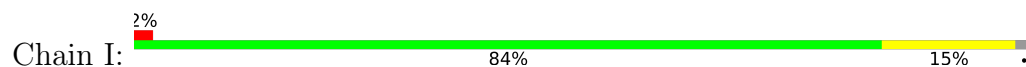
• Molecule 2: 25F9 Heavy chain



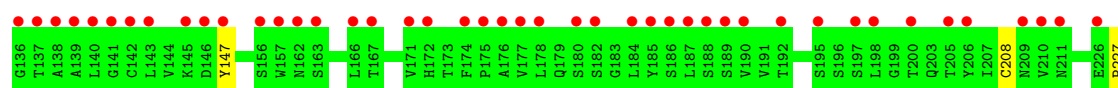
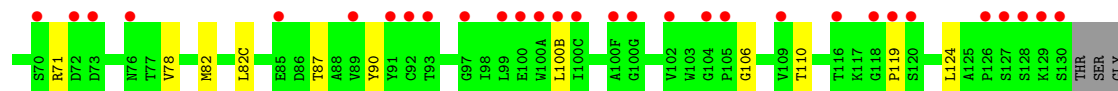
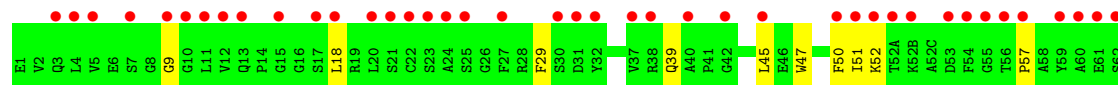
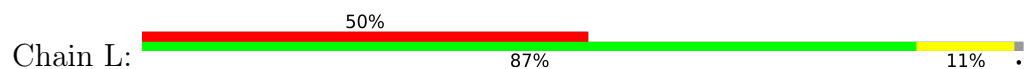
• Molecule 2: 25F9 Heavy chain



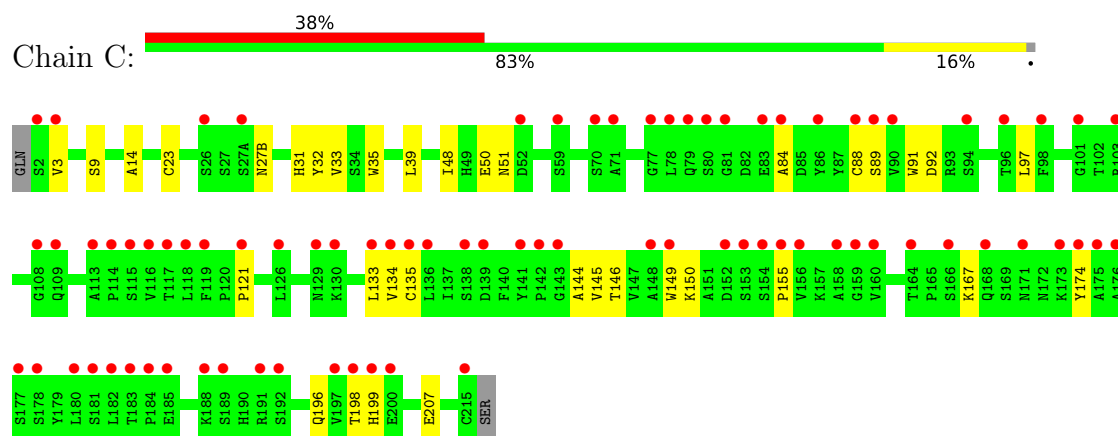
• Molecule 2: 25F9 Heavy chain



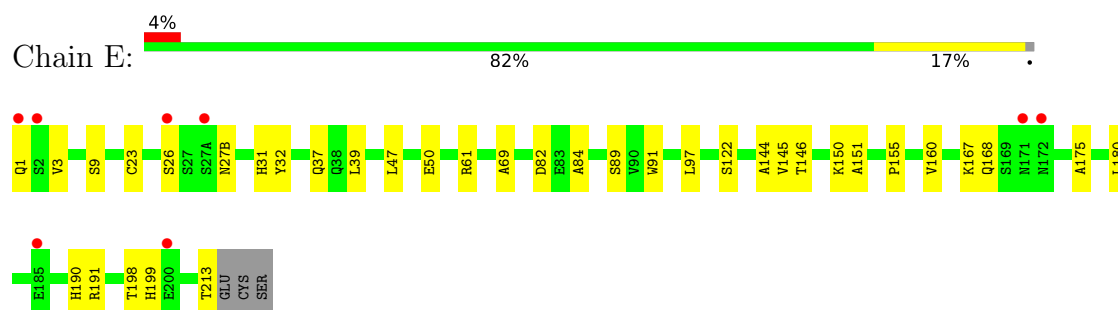
• Molecule 2: 25F9 Heavy chain



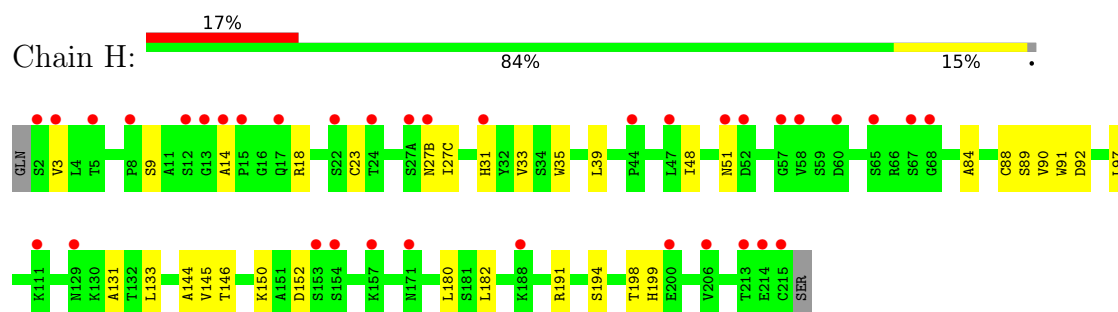
- Molecule 3: 25F9 Light chain



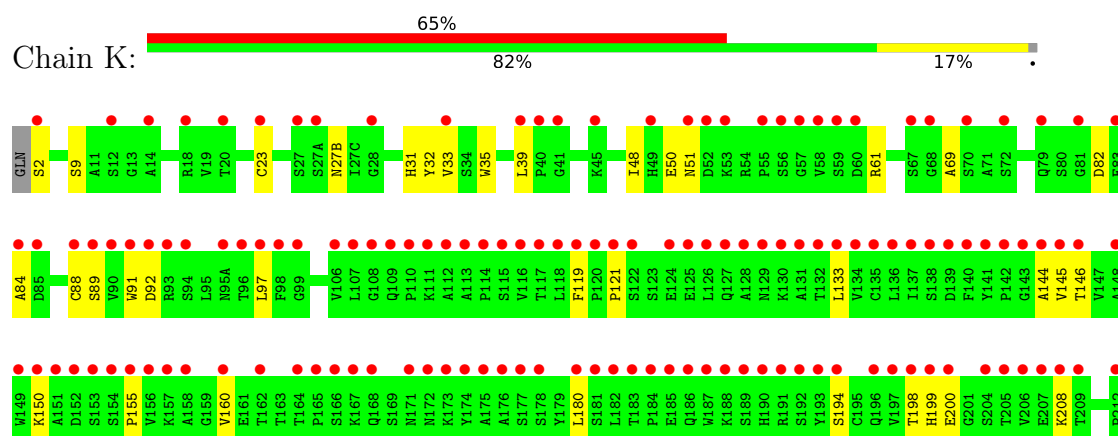
- Molecule 3: 25F9 Light chain



- Molecule 3: 25F9 Light chain



- Molecule 3: 25F9 Light chain





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

Chain M: 100%



- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N: 60% 40%



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

Chain O: 50% 25% 25%



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

Chain P: 25% 75%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	92.48Å 105.82Å 118.18Å 83.08° 67.47° 64.04°	Depositor
Resolution (Å)	47.49 – 3.35 47.49 – 3.35	Depositor EDS
% Data completeness (in resolution range)	98.5 (47.49-3.35) 98.4 (47.49-3.35)	Depositor EDS
R_{merge}	0.87	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.19.2	Depositor
R, R_{free}	0.275 , 0.320 0.274 , 0.313	Depositor DCC
R_{free} test set	3294 reflections (4.58%)	wwPDB-VP
Wilson B-factor (Å ²)	39.3	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 89.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	0.000 for h,h-k,h-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	19740	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 85.08 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3953e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.09	0/1587	0.26	0/2161
1	D	0.10	0/1587	0.28	0/2161
1	G	0.09	0/1587	0.25	0/2161
1	J	0.09	0/1587	0.29	0/2161
2	B	0.10	0/1769	0.31	0/2409
2	F	0.10	0/1767	0.33	0/2406
2	I	0.10	0/1769	0.33	0/2409
2	L	0.10	0/1773	0.32	0/2414
3	C	0.11	0/1623	0.34	0/2216
3	E	0.12	0/1617	0.34	0/2208
3	H	0.12	0/1623	0.34	0/2216
3	K	0.10	0/1617	0.30	0/2208
All	All	0.10	0/19906	0.31	0/27130

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1543	0	1459	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1543	0	1459	10	0
1	G	1543	0	1459	6	0
1	J	1543	0	1459	9	0
2	B	1725	0	1697	17	0
2	F	1723	0	1696	13	0
2	I	1725	0	1698	19	0
2	L	1729	0	1701	14	0
3	C	1585	0	1532	19	0
3	E	1579	0	1532	21	0
3	H	1585	0	1533	18	0
3	K	1579	0	1528	23	0
4	M	39	0	34	1	0
5	N	61	0	52	1	0
6	O	49	0	43	1	0
6	P	49	0	43	4	0
7	A	5	0	0	1	0
7	D	5	0	0	0	0
7	E	10	0	0	0	0
7	I	5	0	0	0	0
7	J	5	0	0	0	0
7	K	10	0	0	0	0
8	C	11	0	12	1	0
8	E	11	0	11	2	0
8	H	11	0	12	0	0
9	K	6	0	8	1	0
10	A	3	0	0	0	0
10	B	3	0	0	0	0
10	C	6	0	0	1	0
10	D	2	0	0	0	0
10	E	5	0	0	0	0
10	F	4	0	0	0	0
10	G	3	0	0	0	0
10	H	6	0	0	0	0
10	I	7	0	0	0	0
10	J	2	0	0	0	0
10	K	14	0	0	0	0
10	L	6	0	0	0	0
All	All	19740	0	18968	169	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (169) 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)
3:H:131:ALA:HB3	3:H:182:LEU:O	1.73	0.89
3:K:92:ASP:HB2	3:K:97:LEU:HD11	1.63	0.79
3:H:92:ASP:HB2	3:H:97:LEU:HD11	1.66	0.77
1:J:371:SER:HB2	6:P:1:NAG:H3	1.67	0.76
1:G:358:ILE:HB	1:G:395:VAL:HG23	1.69	0.73
6:P:2:NAG:H62	6:P:4:FUC:H5	1.70	0.73
1:D:358:ILE:HB	1:D:395:VAL:HG23	1.72	0.71
1:A:358:ILE:HB	1:A:395:VAL:HG23	1.74	0.70
2:I:150:GLU:HG3	2:I:151:PRO:HA	1.73	0.69
2:L:29:PHE:HZ	2:L:78:VAL:HG23	1.58	0.69
3:C:92:ASP:HB2	3:C:97:LEU:HD11	1.76	0.67
1:J:358:ILE:HB	1:J:395:VAL:HG23	1.75	0.66
2:B:119:PRO:HB3	2:B:147:TYR:HB3	1.78	0.66
2:I:140:LEU:HD22	2:I:225:VAL:HG11	1.77	0.65
2:L:228:LYS:HG2	2:L:229:SER:H	1.62	0.65
2:L:52:LYS:O	2:L:71:ARG:NH1	2.31	0.64
3:C:32:TYR:HB3	3:C:50:GLU:HA	1.79	0.63
2:F:29:PHE:HZ	2:F:78:VAL:HG23	1.63	0.62
3:C:33:VAL:N	3:C:51:ASN:OD1	2.27	0.62
3:C:27(B):ASN:O	3:C:31:HIS:HB2	2.00	0.61
2:B:29:PHE:HZ	2:B:78:VAL:HG23	1.65	0.60
3:E:167:LYS:HB2	8:E:303:BCN:H32	1.82	0.60
2:B:207:ILE:HG12	2:B:222:ARG:HG2	1.83	0.60
2:B:39:GLN:HB2	2:B:45:LEU:HD23	1.82	0.60
2:B:229:SER:OG	2:B:230:CYS:N	2.34	0.59
3:K:145:VAL:HG12	3:K:199:HIS:HB2	1.83	0.59
2:L:119:PRO:HB3	2:L:147:TYR:HB3	1.84	0.58
2:F:87:THR:HG23	2:F:110:THR:HA	1.85	0.58
3:H:145:VAL:HG12	3:H:199:HIS:HB2	1.87	0.57
2:L:82:MET:HB3	2:L:82(C):LEU:HD21	1.86	0.57
2:B:212:HIS:HB3	2:B:217:THR:HB	1.85	0.56
1:G:371:SER:HA	6:O:2:NAG:H83	1.88	0.56
3:K:9:SER:HB3	3:K:144:ALA:HB3	1.88	0.56
2:B:52:LYS:O	2:B:71:ARG:NH1	2.39	0.55
1:D:353:TRP:O	1:D:466:ARG:NH1	2.40	0.55
3:C:167:LYS:NZ	10:C:401:HOH:O	2.40	0.54
2:I:87:THR:HG23	2:I:110:THR:HA	1.89	0.54
2:I:29:PHE:HZ	2:I:78:VAL:HG23	1.73	0.54
2:I:176:ALA:HB2	2:I:187:LEU:HD23	1.89	0.54
3:H:133:LEU:HD22	3:H:180:LEU:HD23	1.90	0.54
2:I:153:THR:HG23	2:I:211:ASN:HB3	1.90	0.54
2:L:87:THR:HG23	2:L:110:THR:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:51:ILE:HG13	2:L:57:PRO:HG3	1.91	0.53
3:E:9:SER:HB3	3:E:144:ALA:HB3	1.90	0.53
1:J:344:ALA:HB3	1:J:347:PHE:HE1	1.74	0.53
2:F:52:LYS:O	2:F:71:ARG:NH1	2.42	0.52
2:I:207:ILE:HG12	2:I:222:ARG:HG2	1.90	0.52
2:B:87:THR:HG23	2:B:110:THR:HA	1.91	0.52
2:I:52:LYS:O	2:I:71:ARG:NH1	2.42	0.52
1:A:449:TYR:HE1	3:E:213:THR:HG22	1.75	0.52
3:H:35:TRP:HB2	3:H:48:ILE:HB	1.92	0.52
1:G:486:PHE:HB2	2:L:227:PRO:HG2	1.92	0.52
2:F:39:GLN:HB2	2:F:45:LEU:HD23	1.90	0.52
3:E:1:GLN:N	3:E:26:SER:OG	2.41	0.51
3:K:150:LYS:HD3	3:K:155:PRO:HA	1.92	0.51
2:B:51:ILE:HG13	2:B:57:PRO:HG3	1.92	0.51
2:I:82:MET:HB3	2:I:82(C):LEU:HD21	1.92	0.51
3:K:39:LEU:HD23	3:K:84:ALA:HB2	1.93	0.50
3:C:39:LEU:HD23	3:C:84:ALA:HB2	1.91	0.50
3:E:89:SER:HA	3:E:97:LEU:O	2.12	0.50
2:I:51:ILE:HG13	2:I:57:PRO:HG3	1.92	0.50
2:F:51:ILE:HG13	2:F:57:PRO:HG3	1.93	0.50
3:H:9:SER:HB3	3:H:144:ALA:HB3	1.93	0.50
2:I:154:VAL:HG22	2:I:210:VAL:HG22	1.94	0.50
3:K:133:LEU:HD22	3:K:180:LEU:HD23	1.93	0.50
3:K:35:TRP:HB2	3:K:48:ILE:HB	1.93	0.49
2:F:9:GLY:HA2	2:F:18:LEU:HD21	1.94	0.49
2:L:90:TYR:O	2:L:106:GLY:HA2	2.12	0.49
2:B:47:TRP:HZ2	2:B:50:PHE:HD2	1.60	0.49
3:E:145:VAL:HG12	3:E:199:HIS:HB2	1.94	0.49
3:K:31:HIS:CD2	3:K:91:TRP:HD1	2.31	0.49
4:M:1:NAG:H61	4:M:2:NAG:HN2	1.77	0.49
3:E:146:THR:OG1	3:E:198:THR:HB	2.12	0.49
2:L:39:GLN:HB2	2:L:45:LEU:HD23	1.93	0.49
3:H:27(B):ASN:O	3:H:31:HIS:HB2	2.13	0.49
3:H:39:LEU:HD23	3:H:84:ALA:HB2	1.95	0.48
7:A:601:SO4:O3	3:E:191:ARG:NH1	2.44	0.48
3:H:33:VAL:N	3:H:51:ASN:OD1	2.27	0.48
5:N:2:NAG:H4	5:N:3:BMA:H2	1.71	0.48
3:E:150:LYS:HD3	3:E:155:PRO:HA	1.96	0.47
3:C:35:TRP:HB2	3:C:48:ILE:HB	1.96	0.47
3:E:31:HIS:CD2	3:E:91:TRP:HD1	2.32	0.47
2:F:82:MET:HB3	2:F:82(C):LEU:HD21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:403:ARG:HG3	1:D:505:TYR:HA	1.96	0.47
2:F:90:TYR:O	2:F:106:GLY:HA2	2.14	0.47
2:I:39:GLN:HB2	2:I:45:LEU:HD23	1.97	0.47
3:K:9:SER:OG	3:K:200:GLU:OE2	2.31	0.47
3:C:196:GLN:HG2	3:C:207:GLU:HB2	1.96	0.46
3:E:37:GLN:HB2	3:E:47:LEU:HD11	1.97	0.46
3:E:151:ALA:HB1	3:E:190:HIS:CD2	2.50	0.46
3:K:31:HIS:HD2	3:K:91:TRP:HD1	1.62	0.46
3:H:31:HIS:CD2	3:H:91:TRP:HD1	2.32	0.46
1:J:354:ASN:O	1:J:398:ASP:HA	2.14	0.46
2:L:47:TRP:HZ2	2:L:50:PHE:HD2	1.64	0.46
3:E:31:HIS:HD2	3:E:91:TRP:HD1	1.64	0.46
3:C:9:SER:HB3	3:C:144:ALA:HB3	1.97	0.46
8:E:303:BCN:H41	8:E:303:BCN:H52	1.44	0.46
3:E:27(B):ASN:O	3:E:31:HIS:HB2	2.16	0.45
2:L:9:GLY:HA2	2:L:18:LEU:HD21	1.99	0.45
1:G:395:VAL:HG12	1:G:515:PHE:HD1	1.81	0.45
3:K:2:SER:O	3:K:2:SER:OG	2.32	0.45
3:E:122:SER:HB2	2:F:228:LYS:NZ	2.31	0.45
1:G:350:VAL:HG22	1:G:422:ASN:HB3	1.98	0.45
3:C:146:THR:OG1	3:C:198:THR:HB	2.17	0.45
2:F:176:ALA:HB2	2:F:187:LEU:HD23	1.98	0.45
3:H:14:ALA:HB3	3:K:69:ALA:HB2	1.99	0.45
1:D:458:LYS:HE3	1:D:473:TYR:CE1	2.51	0.44
3:E:61:ARG:NH2	3:E:82:ASP:OD2	2.49	0.44
3:E:160:VAL:HG22	3:E:180:LEU:HD13	1.99	0.44
2:I:47:TRP:HZ2	2:I:50:PHE:HD2	1.66	0.44
3:K:27(B):ASN:O	3:K:31:HIS:HB2	2.17	0.44
3:C:145:VAL:HG12	3:C:199:HIS:HB2	1.99	0.44
3:E:32:TYR:HB3	3:E:50:GLU:HA	1.98	0.44
3:H:152:ASP:OD1	3:H:191:ARG:HB3	2.16	0.44
3:C:150:LYS:HD3	3:C:155:PRO:HA	1.99	0.44
3:H:150:LYS:HB2	3:H:194:SER:HB2	1.99	0.44
1:J:344:ALA:HB3	1:J:347:PHE:CE1	2.53	0.44
3:C:133:LEU:HD23	3:C:149:TRP:CZ3	2.52	0.44
1:G:424:LYS:HD2	1:G:425:LEU:H	1.82	0.44
1:J:458:LYS:HE3	1:J:473:TYR:CE1	2.53	0.43
2:B:82:MET:HB3	2:B:82(C):LEU:HD21	1.99	0.43
1:D:447:GLY:HA2	1:D:498:GLN:HG2	2.00	0.43
2:I:87:THR:HA	2:I:109:VAL:O	2.18	0.43
1:D:376:THR:OG1	2:F:100(B):LEU:O	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:33:VAL:N	3:K:51:ASN:OD1	2.28	0.43
3:C:135:CYS:HB2	3:C:149:TRP:CH2	2.54	0.43
3:H:27(C):ILE:HG12	3:H:90:VAL:HG21	2.00	0.43
2:I:153:THR:CG2	2:I:211:ASN:HB3	2.48	0.43
3:K:89:SER:HA	3:K:97:LEU:O	2.18	0.43
2:B:90:TYR:O	2:B:106:GLY:HA2	2.18	0.42
1:D:354:ASN:O	1:D:398:ASP:HA	2.18	0.42
3:E:39:LEU:HD23	3:E:84:ALA:HB2	2.00	0.42
3:K:121:PRO:HD3	3:K:133:LEU:HD12	1.99	0.42
3:K:61:ARG:NH2	3:K:82:ASP:OD2	2.52	0.42
1:A:433:VAL:HG22	1:A:512:VAL:HG13	2.01	0.42
2:I:123:PRO:O	2:I:124:LEU:HD23	2.20	0.42
3:K:119:PHE:CG	2:L:124:LEU:HD13	2.54	0.42
3:C:89:SER:HA	3:C:97:LEU:O	2.19	0.42
1:J:371:SER:HA	6:P:2:NAG:H83	2.02	0.42
3:H:146:THR:OG1	3:H:198:THR:HB	2.20	0.42
2:B:28:ARG:H	2:B:28:ARG:HG2	1.67	0.42
1:D:360:ASN:H	1:D:523:THR:HB	1.85	0.42
2:B:119:PRO:HD2	2:B:217:THR:HG21	2.02	0.41
3:K:208:LYS:HD3	3:K:208:LYS:HA	1.90	0.41
2:B:87:THR:HA	2:B:109:VAL:O	2.20	0.41
3:H:133:LEU:HD13	3:H:182:LEU:HD21	2.02	0.41
3:H:89:SER:HA	3:H:97:LEU:O	2.20	0.41
3:C:174:TYR:OH	8:C:301:BCN:H12	2.20	0.41
2:I:117:LYS:HD3	2:I:118:GLY:O	2.19	0.41
2:F:47:TRP:HZ2	2:F:50:PHE:HD2	1.67	0.41
1:J:368:LEU:HD12	6:P:1:NAG:H83	2.02	0.41
3:K:160:VAL:HG22	3:K:180:LEU:HD13	2.02	0.41
2:B:29:PHE:CZ	2:B:78:VAL:HG23	2.52	0.41
3:C:14:ALA:HB3	3:E:69:ALA:HB2	2.01	0.41
3:K:32:TYR:HB3	3:K:50:GLU:HA	2.02	0.41
2:B:221:LYS:HD2	2:B:221:LYS:HA	1.85	0.41
3:H:18:ARG:HB3	9:K:301:GOL:H32	2.02	0.41
3:K:146:THR:OG1	3:K:198:THR:HB	2.21	0.41
3:C:121:PRO:HG3	3:C:133:LEU:HD12	2.03	0.41
3:C:31:HIS:CD2	3:C:91:TRP:HD1	2.39	0.40
1:J:376:THR:OG1	2:L:100(B):LEU:O	2.27	0.40
1:A:502:GLY:O	1:A:506:GLN:HG3	2.22	0.40
1:D:395:VAL:HG12	1:D:515:PHE:HD1	1.87	0.40
1:D:393:THR:HA	1:D:522:ALA:HA	2.03	0.40
3:E:168:GLN:OE1	3:E:175:ALA:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:87:THR:HA	2:F:109:VAL:O	2.22	0.40
2:I:126:PRO:HD3	2:I:140:LEU:HD23	2.03	0.40
2:I:228:LYS:HD2	2:I:228:LYS:HA	1.71	0.40
3:K:150:LYS:HB2	3:K:194:SER:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	193/205 (94%)	189 (98%)	4 (2%)	0	100	100
1	D	193/205 (94%)	185 (96%)	8 (4%)	0	100	100
1	G	193/205 (94%)	187 (97%)	6 (3%)	0	100	100
1	J	193/205 (94%)	187 (97%)	6 (3%)	0	100	100
2	B	223/231 (96%)	216 (97%)	7 (3%)	0	100	100
2	F	223/231 (96%)	216 (97%)	7 (3%)	0	100	100
2	I	223/231 (96%)	216 (97%)	7 (3%)	0	100	100
2	L	224/231 (97%)	218 (97%)	6 (3%)	0	100	100
3	C	212/216 (98%)	201 (95%)	9 (4%)	2 (1%)	14	41
3	E	211/216 (98%)	202 (96%)	8 (4%)	1 (0%)	24	52
3	H	212/216 (98%)	204 (96%)	7 (3%)	1 (0%)	24	52
3	K	211/216 (98%)	202 (96%)	9 (4%)	0	100	100
All	All	2511/2608 (96%)	2423 (96%)	84 (3%)	4 (0%)	43	70

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	3	VAL
3	E	3	VAL
3	H	3	VAL
3	C	134	VAL

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	168/177 (95%)	168 (100%)	0	100	100
1	D	168/177 (95%)	167 (99%)	1 (1%)	78	79
1	G	168/177 (95%)	168 (100%)	0	100	100
1	J	168/177 (95%)	168 (100%)	0	100	100
2	B	193/195 (99%)	192 (100%)	1 (0%)	81	80
2	F	192/195 (98%)	191 (100%)	1 (0%)	81	80
2	I	193/195 (99%)	192 (100%)	1 (0%)	81	80
2	L	193/195 (99%)	192 (100%)	1 (0%)	81	80
3	C	178/180 (99%)	176 (99%)	2 (1%)	65	73
3	E	177/180 (98%)	176 (99%)	1 (1%)	78	79
3	H	178/180 (99%)	176 (99%)	2 (1%)	65	73
3	K	177/180 (98%)	175 (99%)	2 (1%)	65	73
All	All	2153/2208 (98%)	2141 (99%)	12 (1%)	78	79

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	208	CYS
3	C	23	CYS
3	C	88	CYS
1	D	525	CYS
3	E	23	CYS
2	F	208	CYS
3	H	23	CYS

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Mol	Chain	Res	Type
3	H	88	CYS
2	I	208	CYS
3	K	23	CYS
3	K	88	CYS
2	L	208	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	370	ASN
1	A	388	ASN
2	B	39	GLN
2	B	179	GLN
3	C	38	GLN
1	D	360	ASN
1	D	370	ASN
1	D	388	ASN
1	D	474	GLN
1	D	493	GLN
1	D	498	GLN
2	F	81	GLN
1	G	388	ASN
3	H	38	GLN
3	H	186	GLN
2	I	39	GLN
2	I	179	GLN
1	J	370	ASN
3	K	38	GLN
3	K	196	GLN
2	L	39	GLN

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 ⓘ

16 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	M	1	4,1	14,14,15	0.23	0	17,19,21	0.49	0
4	NAG	M	2	4	14,14,15	0.33	0	17,19,21	0.40	0
4	BMA	M	3	4	11,11,12	0.52	0	15,15,17	0.92	1 (6%)
5	NAG	N	1	1,5	14,14,15	0.79	1 (7%)	17,19,21	0.69	0
5	NAG	N	2	5	14,14,15	0.54	0	17,19,21	1.36	2 (11%)
5	BMA	N	3	5	11,11,12	0.96	1 (9%)	15,15,17	1.59	5 (33%)
5	MAN	N	4	5	11,11,12	0.92	0	15,15,17	0.95	1 (6%)
5	MAN	N	5	5	11,11,12	0.68	0	15,15,17	1.00	2 (13%)
6	NAG	O	1	1,6	14,14,15	0.73	1 (7%)	17,19,21	0.69	0
6	NAG	O	2	6	14,14,15	0.39	0	17,19,21	0.99	2 (11%)
6	BMA	O	3	6	11,11,12	0.76	0	15,15,17	0.66	0
6	FUC	O	4	6	10,10,11	0.68	0	14,14,16	0.77	0
6	NAG	P	1	1,6	14,14,15	0.48	0	17,19,21	1.07	1 (5%)
6	NAG	P	2	6	14,14,15	0.87	1 (7%)	17,19,21	1.10	2 (11%)
6	BMA	P	3	6	11,11,12	0.67	0	15,15,17	0.66	0
6	FUC	P	4	6	10,10,11	0.79	0	14,14,16	0.98	1 (7%)

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	M	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	M	2	4	-	1/6/23/26	0/1/1/1
4	BMA	M	3	4	-	0/2/19/22	0/1/1/1
5	NAG	N	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	N	2	5	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BMA	N	3	5	-	2/2/19/22	0/1/1/1
5	MAN	N	4	5	-	1/2/19/22	0/1/1/1
5	MAN	N	5	5	-	1/2/19/22	0/1/1/1
6	NAG	O	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	O	2	6	-	2/6/23/26	0/1/1/1
6	BMA	O	3	6	-	0/2/19/22	0/1/1/1
6	FUC	O	4	6	-	-	0/1/1/1
6	NAG	P	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	P	2	6	-	2/6/23/26	0/1/1/1
6	BMA	P	3	6	-	1/2/19/22	0/1/1/1
6	FUC	P	4	6	-	-	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	P	2	NAG	C1-C2	3.00	1.56	1.52
5	N	1	NAG	C1-C2	2.72	1.56	1.52
6	O	1	NAG	O5-C1	-2.19	1.40	1.43
5	N	3	BMA	C2-C3	2.07	1.55	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	2	NAG	C2-N2-C7	3.85	128.05	122.90
6	P	1	NAG	C1-O5-C5	3.68	117.12	112.19
6	P	2	NAG	C2-N2-C7	3.52	127.62	122.90
5	N	3	BMA	C3-C4-C5	2.98	115.63	110.23
5	N	3	BMA	C2-C3-C4	2.91	115.98	110.86
6	O	2	NAG	C2-N2-C7	2.89	126.77	122.90
4	M	3	BMA	C1-O5-C5	2.64	115.73	112.19
5	N	2	NAG	C1-C2-N2	2.50	114.38	110.43
6	P	4	FUC	C1-O5-C5	2.36	118.53	112.97
5	N	3	BMA	O3-C3-C4	-2.25	105.08	110.38
5	N	5	MAN	C1-O5-C5	2.23	115.17	112.19
5	N	4	MAN	O2-C2-C3	-2.12	105.75	110.15
6	P	2	NAG	C1-C2-N2	2.10	113.74	110.43
5	N	5	MAN	O2-C2-C3	-2.10	105.81	110.15
5	N	3	BMA	O5-C5-C6	2.05	111.65	107.66
5	N	3	BMA	C1-C2-C3	2.03	112.60	109.64
6	O	2	NAG	C1-C2-N2	2.03	113.63	110.43

There are no chirality outliers.

All (19) torsion outliers are listed below:

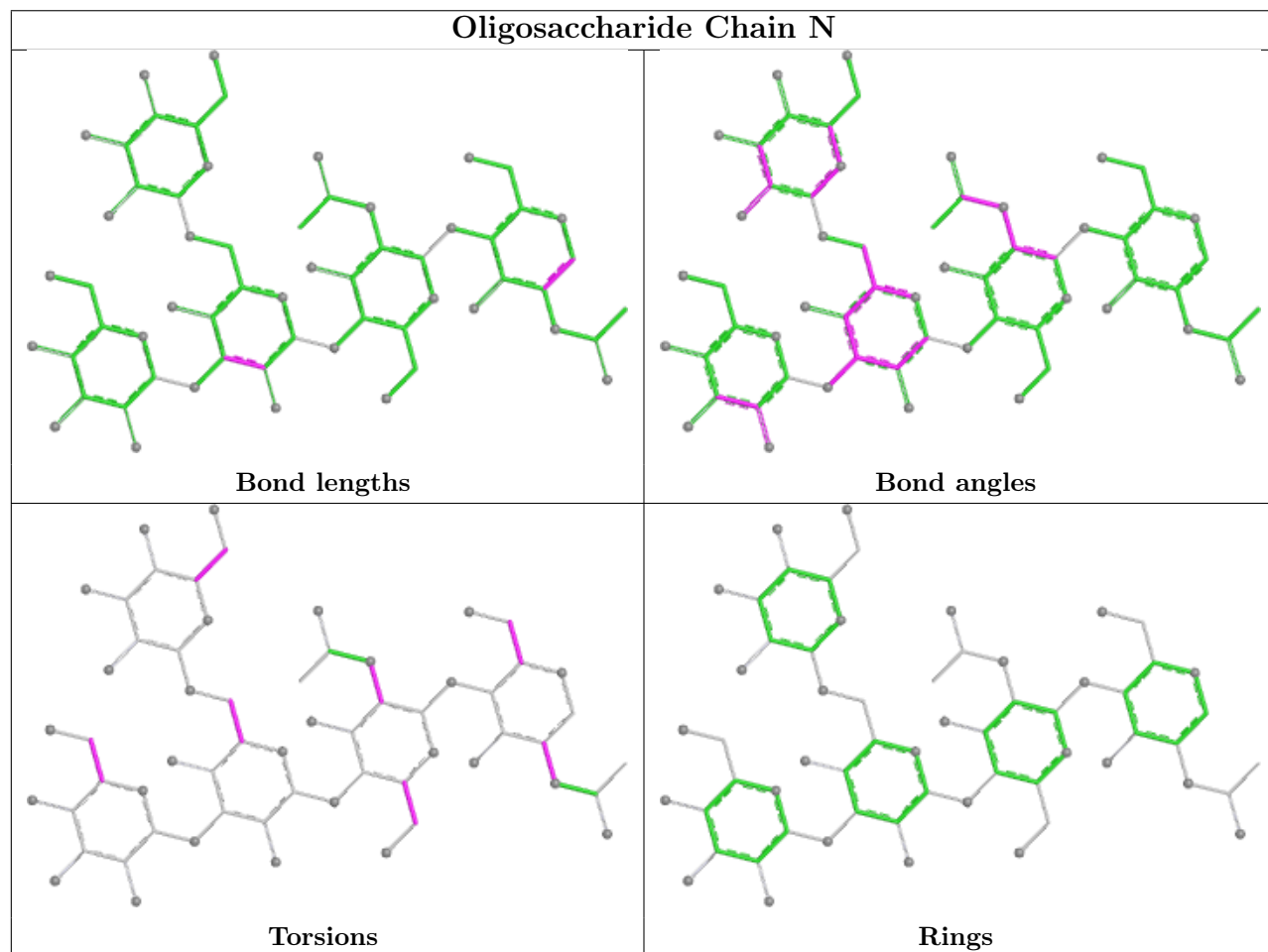
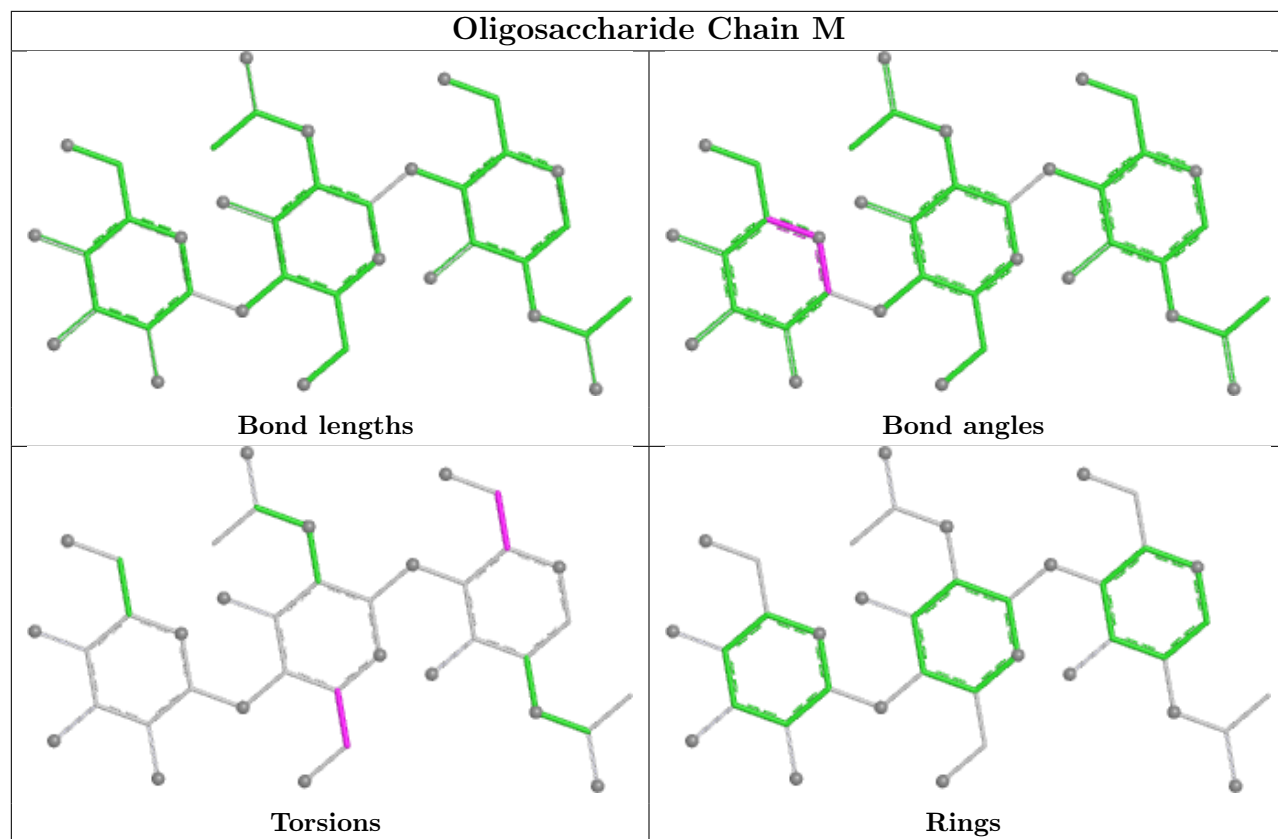
Mol	Chain	Res	Type	Atoms
5	N	2	NAG	C1-C2-N2-C7
6	O	2	NAG	C1-C2-N2-C7
6	P	2	NAG	C1-C2-N2-C7
5	N	2	NAG	C4-C5-C6-O6
5	N	2	NAG	O5-C5-C6-O6
4	M	1	NAG	O5-C5-C6-O6
5	N	3	BMA	O5-C5-C6-O6
4	M	1	NAG	C4-C5-C6-O6
5	N	4	MAN	O5-C5-C6-O6
6	P	2	NAG	O5-C5-C6-O6
4	M	2	NAG	O5-C5-C6-O6
5	N	3	BMA	C4-C5-C6-O6
6	O	2	NAG	O5-C5-C6-O6
6	P	3	BMA	O5-C5-C6-O6
5	N	5	MAN	O5-C5-C6-O6
5	N	1	NAG	C4-C5-C6-O6
5	N	1	NAG	C3-C2-N2-C7
5	N	1	NAG	O5-C5-C6-O6
6	O	1	NAG	C3-C2-N2-C7

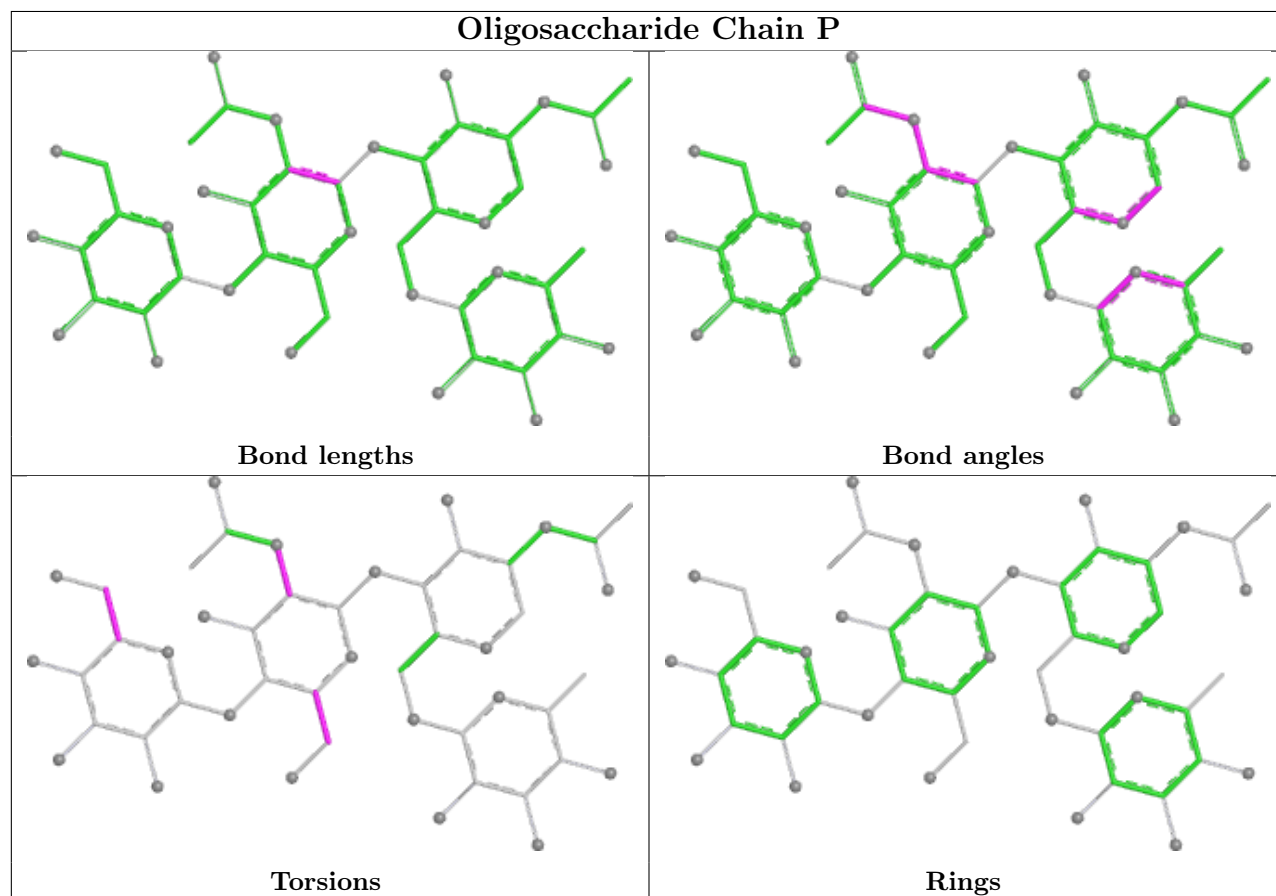
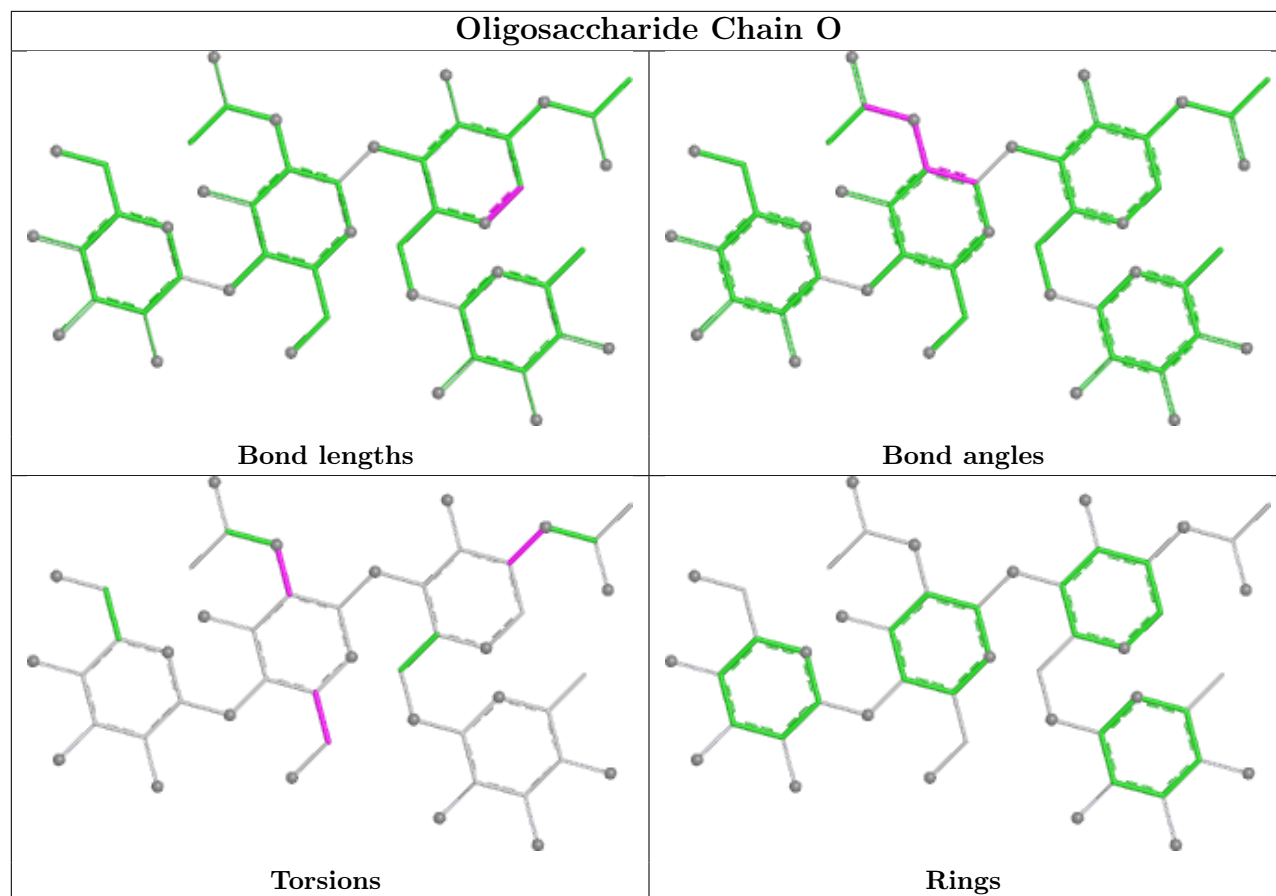
There are no ring outliers.

8 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	M	2	NAG	1	0
6	P	2	NAG	2	0
6	P	1	NAG	2	0
4	M	1	NAG	1	0
5	N	2	NAG	1	0
6	O	2	NAG	1	0
5	N	3	BMA	1	0
6	P	4	FUC	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

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	$\# Z > 2$
7	SO4	J	601	-	4,4,4	0.24	0	6,6,6	0.09	0
7	SO4	E	301	-	4,4,4	0.22	0	6,6,6	0.09	0
7	SO4	A	601	-	4,4,4	0.23	0	6,6,6	0.12	0
8	BCN	E	303	-	10,10,10	1.02	0	11,11,11	1.07	0
7	SO4	D	601	-	4,4,4	0.23	0	6,6,6	0.10	0
8	BCN	H	301	-	10,10,10	0.98	0	11,11,11	1.08	0
7	SO4	I	301	-	4,4,4	0.23	0	6,6,6	0.12	0
7	SO4	K	303	-	4,4,4	0.23	0	6,6,6	0.06	0
9	GOL	K	301	-	5,5,5	0.94	0	5,5,5	1.06	0
8	BCN	C	301	-	10,10,10	1.00	0	11,11,11	1.00	0
7	SO4	E	302	-	4,4,4	0.24	0	6,6,6	0.04	0
7	SO4	K	302	-	4,4,4	0.25	0	6,6,6	0.05	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BCN	C	301	-	-	4/10/10/10	-
8	BCN	E	303	-	-	3/10/10/10	-
8	BCN	H	301	-	-	5/10/10/10	-
9	GOL	K	301	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	H	301	BCN	N1-C1-C2-O22
8	C	301	BCN	N1-C1-C2-O21
8	C	301	BCN	N1-C1-C2-O22
8	H	301	BCN	N1-C1-C2-O21
8	E	303	BCN	N1-C5-C6-O6
8	E	303	BCN	N1-C3-C4-O4
8	E	303	BCN	C4-C3-N1-C5
8	H	301	BCN	C2-C1-N1-C3
8	C	301	BCN	C4-C3-N1-C1
8	C	301	BCN	C4-C3-N1-C5
8	H	301	BCN	C6-C5-N1-C1
8	H	301	BCN	C2-C1-N1-C5

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	601	SO4	1	0
8	E	303	BCN	2	0
9	K	301	GOL	1	0
8	C	301	BCN	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	195/205 (95%)	0.90	21 (10%) 11 10	42, 73, 90, 105	0
1	D	195/205 (95%)	0.67	11 (5%) 30 22	40, 61, 85, 103	0
1	G	195/205 (95%)	1.11	22 (11%) 10 10	44, 79, 112, 117	0
1	J	195/205 (95%)	2.09	98 (50%) 0 0	59, 99, 125, 138	0
2	B	227/231 (98%)	1.35	41 (18%) 3 4	66, 85, 108, 124	0
2	F	227/231 (98%)	0.34	7 (3%) 51 38	31, 54, 88, 112	0
2	I	227/231 (98%)	0.52	5 (2%) 62 46	36, 66, 89, 106	0
2	L	228/231 (98%)	2.05	116 (50%) 0 0	70, 99, 118, 140	0
3	C	214/216 (99%)	1.57	81 (37%) 1 1	35, 84, 105, 124	0
3	E	213/216 (98%)	0.42	8 (3%) 44 31	25, 51, 76, 105	0
3	H	214/216 (99%)	1.05	36 (16%) 4 5	33, 63, 91, 106	0
3	K	213/216 (98%)	2.65	140 (65%) 0 0	56, 93, 118, 142	0
All	All	2543/2608 (97%)	1.22	586 (23%) 2 3	25, 75, 112, 142	0

All (586) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	K	214	GLU	6.0
3	K	189	SER	5.7
3	K	171	ASN	5.6
3	K	28	GLY	5.5
3	K	57	GLY	5.3
3	K	153	SER	5.2
2	B	227	PRO	5.1
2	L	139	ALA	5.0
3	K	173	LYS	5.0
3	K	129	ASN	5.0
1	J	501	ASN	4.9

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Mol	Chain	Res	Type	RSRZ
3	K	95(A)	ASN	4.7
3	K	213	THR	4.7
1	J	444	LYS	4.7
3	C	171	ASN	4.7
3	H	213	THR	4.6
3	K	115	SER	4.6
3	K	51	ASN	4.6
2	L	141	GLY	4.5
3	K	152	ASP	4.4
1	J	445	VAL	4.4
2	L	100(F)	ALA	4.4
3	H	52	ASP	4.4
3	K	174	TYR	4.4
3	K	184	PRO	4.4
1	J	502	GLY	4.4
3	K	188	LYS	4.4
1	J	481	ASN	4.4
3	K	121	PRO	4.4
3	K	156	VAL	4.3
2	B	230	CYS	4.3
2	L	21	SER	4.3
3	C	130	LYS	4.2
3	K	130	LYS	4.2
3	K	126	LEU	4.2
2	L	137	THR	4.2
3	K	27(A)	SER	4.2
3	C	153	SER	4.2
2	L	56	THR	4.2
3	K	168	GLN	4.1
1	J	443	SER	4.1
3	K	155	PRO	4.1
2	L	118	GLY	4.1
3	K	96	THR	4.1
3	C	184	PRO	4.1
3	K	2	SER	4.1
3	K	58	VAL	4.1
1	J	500	THR	4.1
3	C	173	LYS	4.1
1	J	425	LEU	4.0
2	L	99	LEU	4.0
1	G	500	THR	4.0
3	K	185	GLU	4.0

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Mol	Chain	Res	Type	RSRZ
3	C	191	ARG	4.0
2	L	197	SER	4.0
3	C	84	ALA	4.0
3	H	214	GLU	4.0
3	K	200	GLU	4.0
1	J	416	GLY	3.9
3	C	108	GLY	3.9
3	K	176	ALA	3.9
1	J	417	LYS	3.9
2	L	140	LEU	3.9
3	C	115	SER	3.9
3	K	134	VAL	3.9
3	K	70	SER	3.9
3	K	111	LYS	3.9
1	J	517	LEU	3.9
3	K	160	VAL	3.9
2	L	31	ASP	3.9
2	L	189	SER	3.9
3	K	113	ALA	3.9
3	K	149	TRP	3.9
1	J	403	ARG	3.8
3	H	215	CYS	3.8
2	L	13	GLN	3.8
3	K	199	HIS	3.8
1	J	518	LEU	3.8
3	K	56	SER	3.8
2	L	92	CYS	3.8
2	B	197	SER	3.8
3	K	181	SER	3.8
3	K	166	SER	3.8
3	K	207	GLU	3.8
1	J	437	ASN	3.7
1	J	461	LEU	3.7
2	L	100(B)	LEU	3.7
2	L	62	SER	3.7
1	G	494	SER	3.7
1	J	527	PRO	3.6
3	K	148	ALA	3.6
3	K	151	ALA	3.6
2	L	25	SER	3.6
3	K	196	GLN	3.6
3	K	128	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	J	498	GLN	3.6
2	L	12	VAL	3.6
3	K	197	VAL	3.6
1	J	452	LEU	3.6
1	J	472	ILE	3.6
2	F	130	SER	3.6
1	A	415	THR	3.6
3	C	96	THR	3.6
2	L	136	GLY	3.6
1	J	499	PRO	3.6
1	J	507	PRO	3.6
1	J	406	GLU	3.6
1	G	366	SER	3.6
3	C	70	SER	3.6
1	J	526	GLY	3.5
3	K	133	LEU	3.5
1	J	418	ILE	3.5
3	K	109	GLN	3.5
1	J	413	GLY	3.5
3	K	91	TRP	3.5
3	K	164	THR	3.5
2	L	126	PRO	3.5
2	L	210	VAL	3.5
3	K	122	SER	3.5
2	B	100(F)	ALA	3.5
2	L	11	LEU	3.5
2	L	23	SER	3.5
3	K	182	LEU	3.5
1	J	419	ALA	3.4
3	E	1	GLN	3.4
1	J	521	PRO	3.4
3	H	27(A)	SER	3.4
3	K	138	SER	3.4
1	J	405	ASP	3.4
3	K	97	LEU	3.4
1	J	438	SER	3.4
1	J	477	SER	3.4
3	K	157	LYS	3.4
2	L	198	LEU	3.4
3	K	180	LEU	3.4
2	L	97	GLY	3.4
3	K	144	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
2	B	85	GLU	3.4
1	J	421	TYR	3.4
2	L	4	LEU	3.4
3	C	156	VAL	3.4
1	J	522	ALA	3.4
2	I	126	PRO	3.4
3	K	150	LYS	3.4
3	K	204	SER	3.3
1	D	361	CYS	3.3
3	K	60	ASP	3.3
1	J	439	ASN	3.3
3	K	90	VAL	3.3
2	L	85	GLU	3.3
3	K	124	GLU	3.3
2	L	9	GLY	3.3
3	C	158	ALA	3.3
3	K	108	GLY	3.3
1	J	420	ASP	3.3
3	K	92	ASP	3.3
3	C	121	PRO	3.3
2	B	200	THR	3.3
3	K	136	LEU	3.3
1	D	343	ASN	3.3
3	K	187	TRP	3.3
2	L	100	GLU	3.3
3	K	59	SER	3.3
3	K	114	PRO	3.3
3	K	107	LEU	3.3
3	K	186	GLN	3.3
3	C	81	GLY	3.3
3	H	68	GLY	3.3
1	J	408	ARG	3.2
3	K	154	SER	3.2
3	H	58	VAL	3.2
3	K	146	THR	3.2
1	J	448	ASN	3.2
2	L	24	ALA	3.2
1	J	471	GLU	3.2
1	J	495	TYR	3.2
2	L	27	PHE	3.2
1	J	382	VAL	3.2
2	L	147	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
2	L	130	SER	3.2
3	K	52	ASP	3.2
2	B	138	ALA	3.2
1	J	449	TYR	3.2
2	L	175	PRO	3.2
1	J	514	SER	3.2
3	H	5	THR	3.2
3	K	198	THR	3.2
2	L	53	ASP	3.2
1	J	488	CYS	3.2
3	K	208	LYS	3.2
3	K	212	PRO	3.2
3	C	79	GLN	3.2
1	J	470	THR	3.2
3	C	117	THR	3.2
3	K	183	THR	3.2
3	K	167	LYS	3.1
1	J	480	CYS	3.1
3	K	41	GLY	3.1
3	K	141	TYR	3.1
2	B	115	SER	3.1
3	C	166	SER	3.1
1	J	447	GLY	3.1
3	C	83	GLU	3.1
3	K	110	PRO	3.1
2	B	128	SER	3.1
2	B	199	GLY	3.1
3	H	27(B)	ASN	3.1
2	B	127	SER	3.1
3	H	12	SER	3.1
3	H	3	VAL	3.1
2	L	52(B)	LYS	3.1
2	L	162	ASN	3.1
3	H	13	GLY	3.1
3	C	152	ASP	3.1
2	L	3	GLN	3.0
3	C	3	VAL	3.0
3	K	131	ALA	3.0
3	K	175	ALA	3.0
2	B	68	SER	3.0
2	B	119	PRO	3.0
2	B	114	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	476	GLY	3.0
3	K	127	GLN	3.0
3	K	132	THR	3.0
3	K	158	ALA	3.0
3	H	171	ASN	3.0
1	J	497	PHE	3.0
1	J	402	ILE	3.0
1	G	471	GLU	3.0
3	K	72	SER	3.0
2	L	177	VAL	3.0
1	J	414	GLN	2.9
1	D	387	LEU	2.9
3	K	135	CYS	2.9
3	H	67	SER	2.9
3	K	94	SER	2.9
3	K	40	PRO	2.9
2	L	138	ALA	2.9
1	J	490	PHE	2.9
3	C	136	LEU	2.9
3	C	168	GLN	2.9
2	L	10	GLY	2.9
3	H	154	SER	2.9
3	H	188	LYS	2.9
3	K	118	LEU	2.9
2	B	82(A)	ASN	2.9
3	E	172	ASN	2.9
1	J	525	CYS	2.9
2	L	171	VAL	2.9
1	J	508	TYR	2.9
2	L	174	PHE	2.9
3	C	174	TYR	2.9
3	K	49	HIS	2.8
2	L	73	ASP	2.8
1	J	503	VAL	2.8
3	C	90	VAL	2.8
1	A	366	SER	2.8
1	J	409	GLN	2.8
2	L	17	SER	2.8
2	L	180	SER	2.8
3	C	89	SER	2.8
2	L	105	PRO	2.8
2	L	5	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
3	K	106	VAL	2.8
1	J	422	ASN	2.8
1	G	336	CYS	2.8
2	F	128	SER	2.8
2	L	127	SER	2.8
3	K	194	SER	2.8
2	L	102	VAL	2.8
3	H	200	GLU	2.8
1	J	407	VAL	2.8
1	J	511	VAL	2.8
3	K	67	SER	2.8
2	L	100(C)	ILE	2.8
1	J	440	ASN	2.8
2	B	126	PRO	2.8
3	C	80	SER	2.8
3	C	94	SER	2.8
3	K	165	PRO	2.7
3	C	180	LEU	2.7
1	G	486	PHE	2.7
1	J	410	ILE	2.7
2	L	7	SER	2.7
3	C	181	SER	2.7
3	H	2	SER	2.7
2	B	84	THR	2.7
1	G	405	ASP	2.7
2	L	211	ASN	2.7
3	H	51	ASN	2.7
3	K	112	ALA	2.7
1	J	504	GLY	2.7
2	B	112	SER	2.7
2	L	93	THR	2.7
2	L	72	ASP	2.7
3	K	145	VAL	2.7
3	K	55	PRO	2.7
3	K	143	GLY	2.7
1	G	333	THR	2.7
1	J	469	SER	2.7
2	L	89	VAL	2.7
2	L	119	PRO	2.7
3	K	137	ILE	2.7
1	G	502	GLY	2.7
2	F	228	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
3	C	177	SER	2.7
3	K	178	SER	2.7
3	C	126	LEU	2.7
3	K	172	ASN	2.7
2	B	118	GLY	2.6
3	C	159	GLY	2.6
3	K	81	GLY	2.6
1	G	470	THR	2.6
1	J	415	THR	2.6
3	K	162	THR	2.6
1	J	387	LEU	2.6
1	J	510	VAL	2.6
2	L	163	SER	2.6
2	L	166	LEU	2.6
2	L	182	SER	2.6
3	K	206	VAL	2.6
3	H	111	LYS	2.6
1	J	524	VAL	2.6
1	J	451	TYR	2.6
3	H	15	PRO	2.6
1	G	376	THR	2.6
3	H	24	THR	2.6
3	K	39	LEU	2.6
1	J	424	LYS	2.6
2	F	229	SER	2.6
2	L	195	SER	2.6
3	K	27	SER	2.6
2	L	54	PHE	2.6
3	K	79	GLN	2.6
1	J	484	GLU	2.6
3	C	148	ALA	2.6
2	B	228	LYS	2.6
1	D	391	CYS	2.6
3	E	26	SER	2.6
3	K	98	PHE	2.6
3	C	109	GLN	2.6
2	B	211	ASN	2.6
2	B	100	GLU	2.6
3	E	185	GLU	2.6
3	C	71	ALA	2.6
3	K	84	ALA	2.6
1	D	349	SER	2.5

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Mol	Chain	Res	Type	RSRZ
2	L	186	SER	2.5
2	L	129	LYS	2.5
3	C	175	ALA	2.5
3	K	83	GLU	2.5
1	D	358	ILE	2.5
2	B	130	SER	2.5
2	L	55	GLY	2.5
3	H	153	SER	2.5
1	J	386	LYS	2.5
1	J	401	VAL	2.5
3	K	139	ASP	2.5
1	J	430	THR	2.5
2	L	157	TRP	2.5
2	L	32	TYR	2.5
2	B	4	LEU	2.5
3	C	77	GLY	2.5
2	B	21	SER	2.5
3	C	2	SER	2.5
3	C	154	SER	2.5
3	C	185	GLU	2.5
1	D	481	ASN	2.5
3	C	164	THR	2.5
1	D	526	GLY	2.5
3	H	17	GLN	2.5
2	I	128	SER	2.5
3	C	215	CYS	2.5
3	H	14	ALA	2.5
1	J	465	GLU	2.5
3	C	200	GLU	2.5
1	J	388	ASN	2.5
2	L	145	LYS	2.5
3	K	68	GLY	2.5
2	B	225	VAL	2.5
2	L	188	SER	2.4
2	L	229	SER	2.4
3	C	138	SER	2.4
1	J	436	TRP	2.4
2	L	167	THR	2.4
2	L	187	LEU	2.4
2	L	205	THR	2.4
1	J	453	TYR	2.4
1	J	473	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
3	K	193	TYR	2.4
3	K	89	SER	2.4
3	K	191	ARG	2.4
1	J	343	ASN	2.4
1	J	505	TYR	2.4
3	C	197	VAL	2.4
3	K	190	HIS	2.4
1	J	486	PHE	2.4
2	B	28	ARG	2.4
2	L	143	LEU	2.4
1	J	512	VAL	2.4
2	L	37	VAL	2.4
1	A	446	GLY	2.4
2	B	100(G)	GLY	2.4
2	L	51	ILE	2.4
3	C	113	ALA	2.4
3	C	133	LEU	2.4
3	C	149	TRP	2.4
2	L	15	GLY	2.4
3	H	57	GLY	2.4
3	K	85	ASP	2.4
3	C	78	LEU	2.4
3	C	182	LEU	2.4
2	L	70	SER	2.4
3	K	23	CYS	2.4
1	A	526	GLY	2.3
3	C	86	TYR	2.3
2	L	45	LEU	2.3
3	K	116	VAL	2.3
2	F	127	SER	2.3
2	L	156	SER	2.3
1	A	402	ILE	2.3
1	A	425	LEU	2.3
2	L	184	LEU	2.3
3	K	119	PHE	2.3
2	L	61	GLU	2.3
1	A	445	VAL	2.3
1	J	491	PRO	2.3
2	B	97	GLY	2.3
2	L	100(A)	TRP	2.3
2	L	60	ALA	2.3
3	K	88	CYS	2.3

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Mol	Chain	Res	Type	RSRZ
3	C	129	ASN	2.3
3	C	139	ASP	2.3
1	J	412	PRO	2.3
1	A	447	GLY	2.3
1	A	478	THR	2.3
1	J	366	SER	2.3
2	L	120	SER	2.3
2	L	128	SER	2.3
3	C	183	THR	2.3
3	C	198	THR	2.3
3	H	65	SER	2.3
3	K	209	THR	2.3
2	L	59	TYR	2.3
1	J	429	PHE	2.3
3	C	135	CYS	2.3
1	A	405	ASP	2.3
3	C	160	VAL	2.3
1	G	499	PRO	2.3
2	B	207	ILE	2.3
1	D	415	THR	2.3
1	J	523	THR	2.3
3	K	117	THR	2.3
1	J	400	PHE	2.3
1	J	423	TYR	2.3
2	B	193	VAL	2.3
3	C	134	VAL	2.3
2	L	42	GLY	2.2
2	L	57	PRO	2.2
3	C	142	PRO	2.2
3	C	143	GLY	2.2
3	H	8	PRO	2.2
3	H	44	PRO	2.2
3	K	142	PRO	2.2
2	L	172	HIS	2.2
2	L	192	THR	2.2
3	K	140	PHE	2.2
2	B	129	LYS	2.2
3	H	22	SER	2.2
2	F	28	ARG	2.2
1	G	498	GLN	2.2
2	B	123	PRO	2.2
2	L	20	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	J	456	PHE	2.2
2	B	116	THR	2.2
3	C	188	LYS	2.2
3	K	192	SER	2.2
2	B	139	ALA	2.2
2	L	104	GLY	2.2
3	C	155	PRO	2.2
3	H	47	LEU	2.2
1	A	386	LYS	2.2
1	J	515	PHE	2.2
1	A	333	THR	2.2
1	D	333	THR	2.2
3	H	31	HIS	2.2
3	C	141	TYR	2.2
3	C	26	SER	2.2
3	E	2	SER	2.2
3	K	12	SER	2.2
2	B	140	LEU	2.2
3	K	125	GLU	2.2
1	G	485	GLY	2.2
1	A	408	ARG	2.2
3	K	93	ARG	2.2
2	L	109	VAL	2.2
1	G	472	ILE	2.2
2	B	196	SER	2.2
2	B	178	LEU	2.2
2	L	40	ALA	2.2
2	L	52	LYS	2.2
3	H	157	LYS	2.2
3	K	45	LYS	2.2
3	K	53	LYS	2.2
3	C	52	ASP	2.2
1	G	478	THR	2.1
1	J	433	VAL	2.1
1	J	478	THR	2.1
2	B	205	THR	2.1
2	B	59	TYR	2.1
1	G	492	LEU	2.1
2	L	18	LEU	2.1
2	B	189	SER	2.1
3	K	14	ALA	2.1
3	E	171	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	490	PHE	2.1
1	J	442	ASP	2.1
2	L	142	CYS	2.1
2	L	52(A)	THR	2.1
1	J	468	ILE	2.1
2	L	91	TYR	2.1
2	L	176	ALA	2.1
1	J	375	SER	2.1
1	J	404	GLY	2.1
1	J	426	PRO	2.1
2	F	85	GLU	2.1
2	L	226	GLU	2.1
3	C	189	SER	2.1
3	E	27(A)	SER	2.1
3	K	177	SER	2.1
3	C	119	PHE	2.1
2	L	22	CYS	2.1
3	H	206	VAL	2.1
2	L	200	THR	2.1
3	K	20	THR	2.1
1	A	419	ALA	2.1
3	C	176	ALA	2.1
3	K	120	PRO	2.1
2	L	30	SER	2.1
2	L	50	PHE	2.1
3	C	88	CYS	2.1
3	C	118	LEU	2.1
3	H	60	ASP	2.1
1	A	431	GLY	2.1
2	L	100(G)	GLY	2.1
1	A	373	SER	2.1
1	A	477	SER	2.1
1	G	514	SER	2.1
3	C	178	SER	2.1
1	G	510	VAL	2.1
2	L	190	VAL	2.1
2	L	76	ASN	2.1
1	G	468	ILE	2.1
2	L	38	ARG	2.1
3	K	18	ARG	2.1
2	L	116	THR	2.1
2	L	185	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
2	L	206	TYR	2.1
3	E	200	GLU	2.1
3	C	116	VAL	2.0
3	C	59	SER	2.0
2	L	209	ASN	2.0
1	A	432	CYS	2.0
2	I	125	ALA	2.0
2	I	192	THR	2.0
2	L	146	ASP	2.0
1	J	463	PRO	2.0
3	C	103	ARG	2.0
3	C	27(A)	SER	2.0
3	C	192	SER	2.0
1	G	501	ASN	2.0
1	J	487	ASN	2.0
3	H	129	ASN	2.0
3	C	199	HIS	2.0
2	I	137	THR	2.0
3	K	205	THR	2.0
1	A	428	ASP	2.0
1	A	486	PHE	2.0
3	C	98	PHE	2.0
3	C	101	GLY	2.0
3	K	99	GLY	2.0
1	J	462	LYS	2.0
3	C	114	PRO	2.0
1	A	407	VAL	2.0
3	K	33	VAL	2.0
2	L	178	LEU	2.0

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

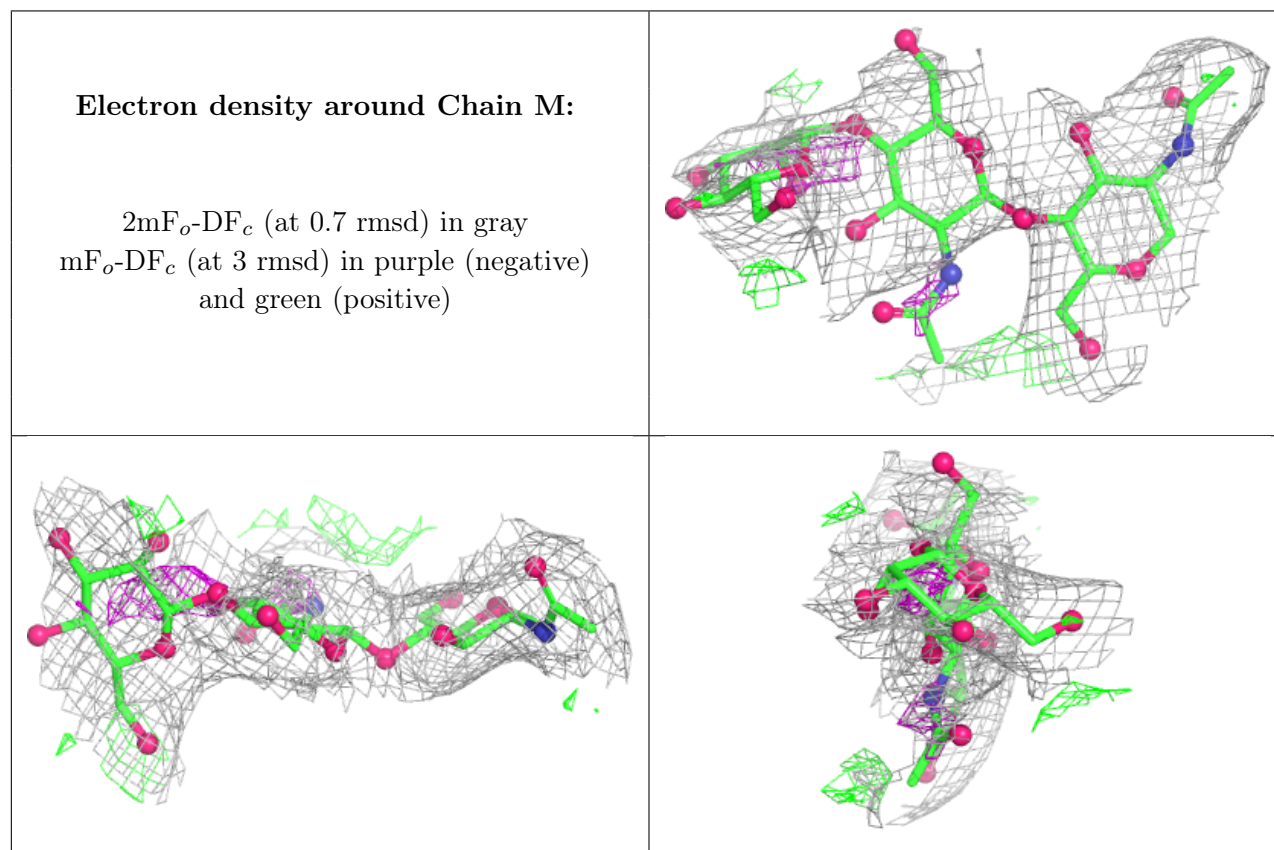
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

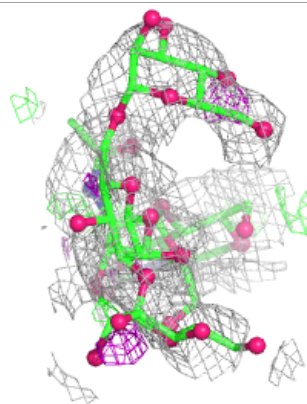
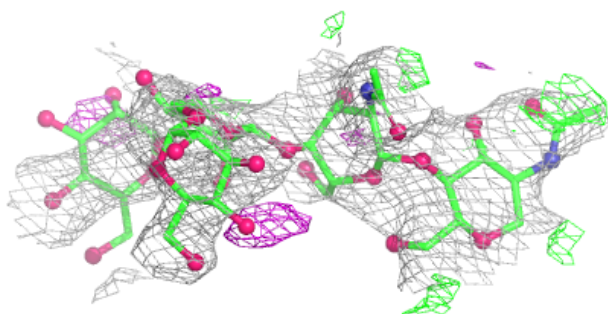
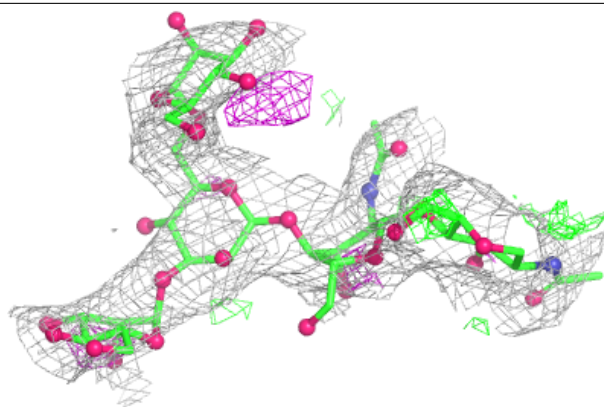
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	BMA	P	3	11/12	0.46	0.18	73,82,100,100	0
4	BMA	M	3	11/12	0.48	0.18	62,90,107,116	0
5	MAN	N	5	11/12	0.49	0.19	65,81,100,101	0
4	NAG	M	2	14/15	0.50	0.20	75,93,115,117	0
6	FUC	P	4	10/11	0.51	0.23	47,98,115,115	0
6	BMA	O	3	11/12	0.55	0.17	67,74,107,116	0
5	MAN	N	4	11/12	0.57	0.20	60,100,116,132	0
6	NAG	O	2	14/15	0.58	0.17	89,101,107,109	0
5	NAG	N	2	14/15	0.58	0.20	68,86,98,115	0
5	BMA	N	3	11/12	0.60	0.16	72,86,101,106	0
6	FUC	O	4	10/11	0.63	0.19	57,89,102,108	0
6	NAG	P	2	14/15	0.66	0.19	73,91,116,118	0
5	NAG	N	1	14/15	0.73	0.20	61,71,102,105	0
6	NAG	P	1	14/15	0.76	0.20	56,82,112,112	0
6	NAG	O	1	14/15	0.79	0.16	51,84,96,105	0
4	NAG	M	1	14/15	0.84	0.12	32,57,83,96	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.



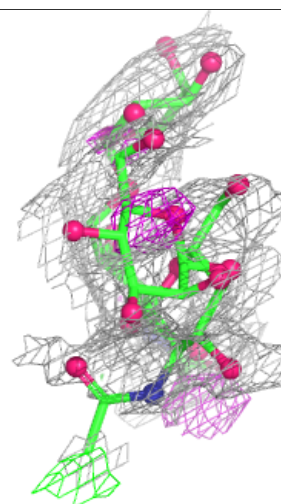
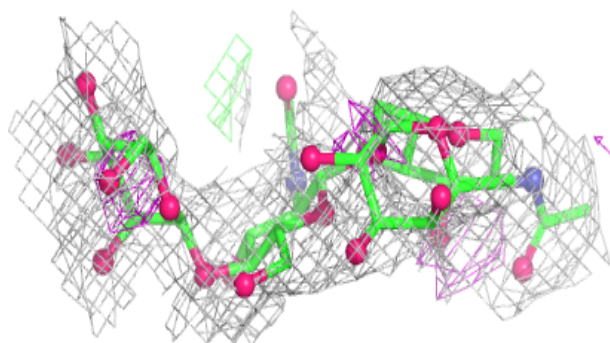
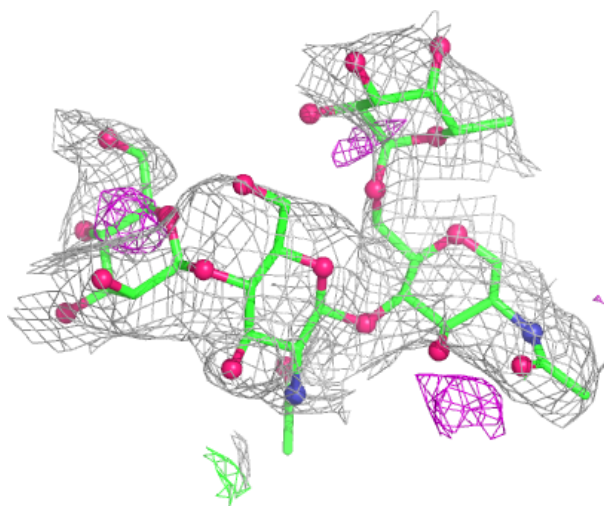
Electron density around Chain N:

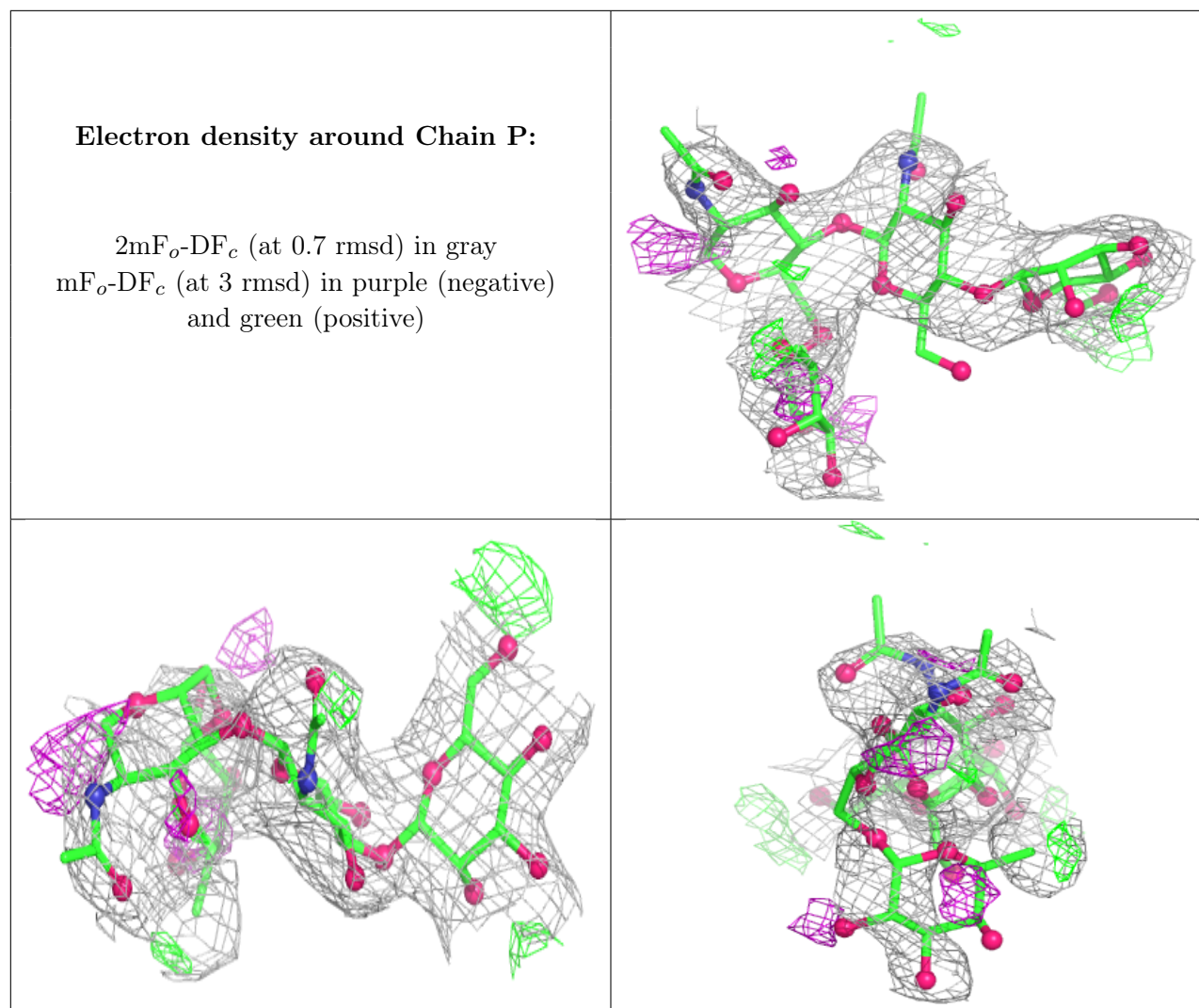
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





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($\text{\AA}^2$)	Q<0.9
7	SO4	I	301	5/5	0.79	0.29	70,90,120,123	0
8	BCN	E	303	11/11	0.84	0.16	47,68,75,79	0
7	SO4	E	301	5/5	0.86	0.32	81,84,104,125	0
7	SO4	K	303	5/5	0.86	0.11	68,71,93,99	0
7	SO4	E	302	5/5	0.86	0.12	48,52,87,114	0
8	BCN	H	301	11/11	0.86	0.12	39,51,67,68	0
9	GOL	K	301	6/6	0.88	0.13	29,40,56,56	0
8	BCN	C	301	11/11	0.89	0.11	38,49,66,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	SO4	K	302	5/5	0.90	0.13	57,65,85,104	0
7	SO4	J	601	5/5	0.90	0.13	57,76,99,99	0
7	SO4	D	601	5/5	0.96	0.09	57,72,93,102	0
7	SO4	A	601	5/5	0.98	0.07	53,57,75,80	0

6.5 Other polymers [i](#)

There are no such residues in this entry.