



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:36 AM UTC

PDB ID : 9PHS / pdb_00009phs
Title : Crystal structure of the A/Puerto Rico/8/1934 (H1N1) influenza virus hemagglutinin in complex with fusion inhibitor cyclic peptide CP141085 (CP1)
Authors : Kadam, R.U.; Wilson, I.A.
Deposited on : 2025-07-09
Resolution : 2.02 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

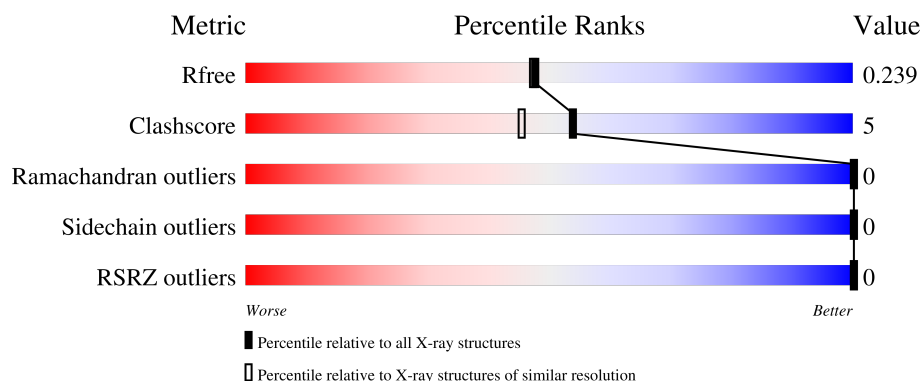
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.02 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	13299 (2.04-2.00)
Clashscore	190562	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)
RSRZ outliers	180081	13314 (2.04-2.00)

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	326	
1	C	326	
1	E	326	
2	B	176	
2	D	176	

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Mol	Chain	Length	Quality of chain
2	F	176	82% 15%
3	G	19	100%
3	H	19	95% 5%
3	K	19	79% 21%
4	I	3	33% 67%
4	J	3	67% 33%
4	L	3	100%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 12840 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 Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	321	Total	C	N	O	S	0	1	0
			2520	1587	440	480	13			
1	C	321	Total	C	N	O	S	0	0	0
			2532	1597	441	481	13			
1	E	321	Total	C	N	O	S	0	1	0
			2542	1603	443	483	13			

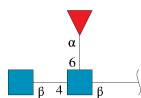
- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	171	Total	C	N	O	S	0	0	0
			1368	858	233	270	7			
2	D	171	Total	C	N	O	S	0	0	0
			1380	866	235	272	7			
2	F	171	Total	C	N	O	S	0	0	0
			1368	860	234	267	7			

- Molecule 3 is a protein called cyclic peptide CP141085.

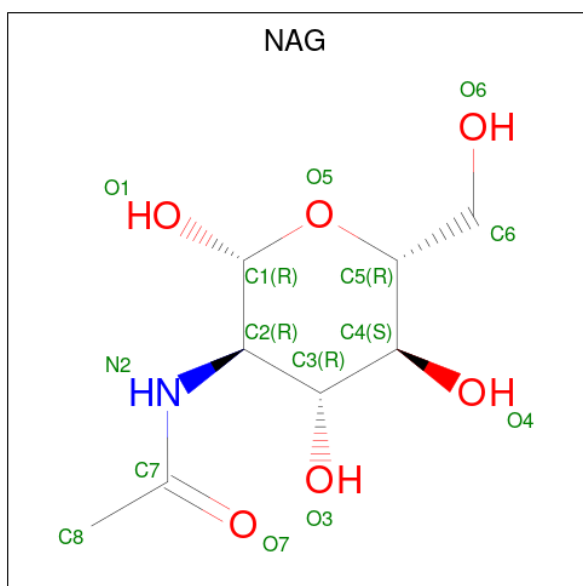
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	19	Total	C	N	O	S	0	0	0
			134	88	19	26	1			
3	H	19	Total	C	N	O	S	0	0	0
			134	88	19	26	1			
3	K	19	Total	C	N	O	S	0	0	0
			134	88	19	26	1			

- Molecule 4 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
4	L	3	Total	C	N	O	0	0	0
			38	22	2	14			
4	I	3	Total	C	N	O	0	0	0
			38	22	2	14			
4	J	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		

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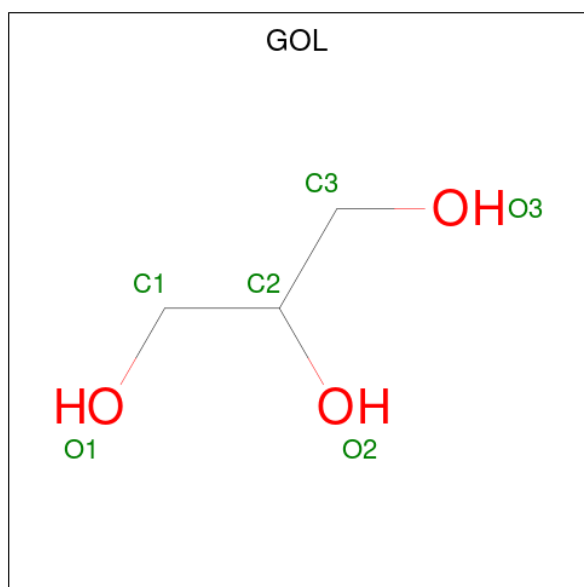
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	F	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Ca	0	0
			1	1		
6	C	1	Total	Ca	0	0
			1	1		
6	E	1	Total	Ca	0	0
			1	1		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		
7	F	1	Total	C	O	0	0
			6	3	3		

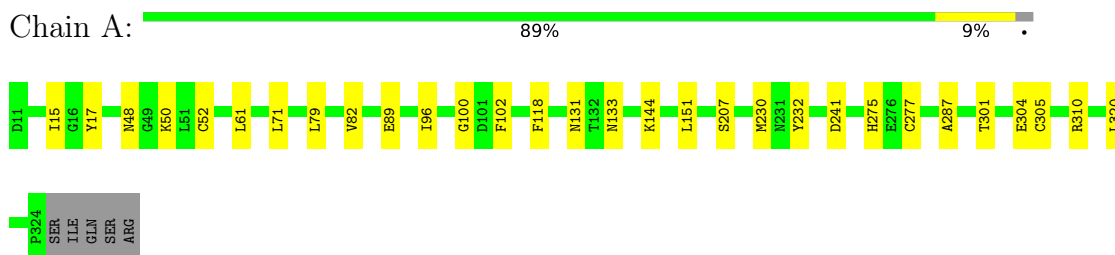
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	108	Total 108	O 108	0	0
8	B	57	Total 57	O 57	0	0
8	C	117	Total 117	O 117	0	0
8	D	48	Total 48	O 48	0	0
8	E	100	Total 100	O 100	0	0
8	F	45	Total 45	O 45	0	0
8	G	3	Total 3	O 3	0	0
8	H	2	Total 2	O 2	0	0
8	K	3	Total 3	O 3	0	0

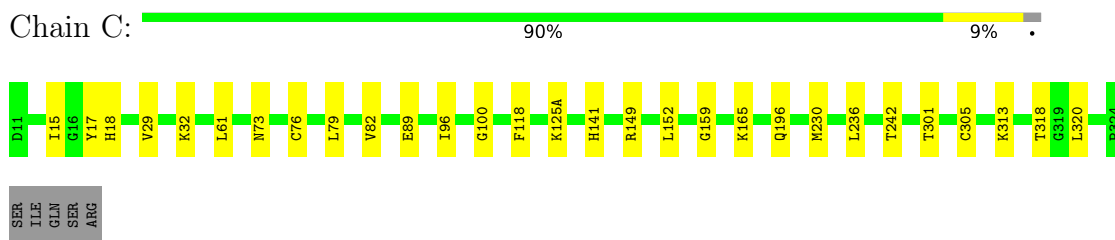
3 Residue-property plots

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.

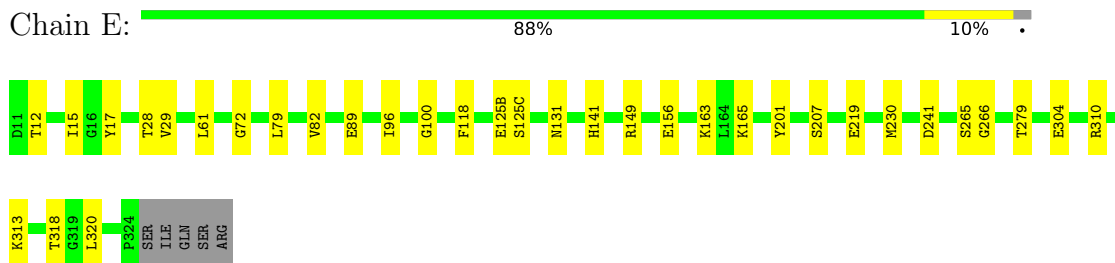
• Molecule 1: Hemagglutinin



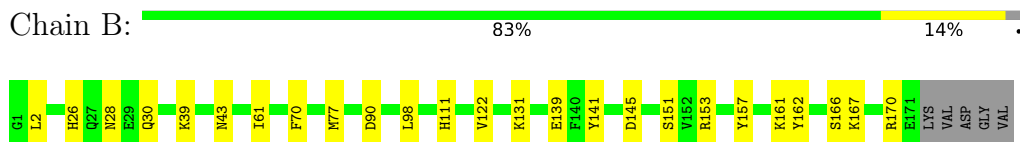
• Molecule 1: Hemagglutinin



• Molecule 1: Hemagglutinin



• Molecule 2: Hemagglutinin HA2 chain



• Molecule 2: Hemagglutinin HA2 chain

Chain D:  84% 13%

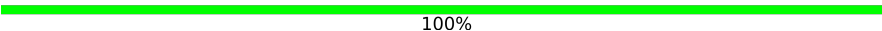


- Molecule 2: Hemagglutinin HA2 chain

Chain F:  82% 15%

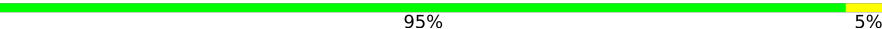


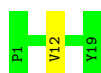
- Molecule 3: cyclic peptide CP141085

Chain G:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: cyclic peptide CP141085

Chain H:  95% 5%

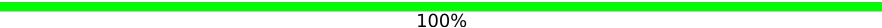


- Molecule 3: cyclic peptide CP141085

Chain K:  79% 21%



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

Chain L:  100%



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

Chain I:  33% 67%



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



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	189.80Å 108.83Å 118.24Å 90.00° 122.37° 90.00°	Depositor
Resolution (Å)	47.98 – 2.02 47.98 – 2.02	Depositor EDS
% Data completeness (in resolution range)	98.8 (47.98-2.02) 97.6 (47.98-2.02)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 2.03Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660, PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.215 , 0.248 (Not available) , 0.239	Depositor DCC
R_{free} test set	6603 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	38.5	Xtriage
Anisotropy	0.756	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 48.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.419 for $1/2^*h-3/2^*k,-1/2^*h-1/2^*k,-1/2^*h+1/2^*k-l$ 0.417 for $1/2^*h+3/2^*k,1/2^*h-1/2^*k,-1/2^*h-1/2^*k-l$	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	12840	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, DPR, FUC, CA, GOL

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	0.16	0/2583	0.39	0/3517
1	C	0.16	0/2596	0.39	0/3532
1	E	0.14	0/2606	0.38	0/3544
2	B	0.18	0/1395	0.39	0/1878
2	D	0.18	0/1407	0.38	0/1891
2	F	0.18	0/1395	0.37	0/1877
3	G	0.10	0/130	0.32	0/176
3	H	0.11	0/130	0.33	0/176
3	K	0.17	0/130	0.39	0/176
All	All	0.16	0/12372	0.38	0/16767

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	2520	0	2432	25	0
1	C	2532	0	2456	23	0
1	E	2542	0	2470	26	0
2	B	1368	0	1283	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1380	0	1308	18	0
2	F	1368	0	1289	23	0
3	G	134	0	129	0	0
3	H	134	0	129	1	0
3	K	134	0	129	4	0
4	I	38	0	34	1	0
4	J	38	0	34	0	0
4	L	38	0	34	0	0
5	A	14	0	13	0	0
5	B	14	0	13	0	0
5	C	14	0	13	0	0
5	D	14	0	13	0	0
5	E	28	0	26	1	0
5	F	14	0	13	0	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
6	E	1	0	0	0	0
7	A	6	0	8	1	0
7	B	6	0	8	0	0
7	C	6	0	8	1	0
7	D	6	0	8	2	0
7	F	6	0	8	0	0
8	A	108	0	0	0	0
8	B	57	0	0	0	0
8	C	117	0	0	4	0
8	D	48	0	0	0	0
8	E	100	0	0	2	0
8	F	45	0	0	1	0
8	G	3	0	0	0	0
8	H	2	0	0	0	0
8	K	3	0	0	0	0
All	All	12840	0	11858	119	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 5.

All (119) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:131:LYS:HG3	2:F:133:ILE:HD11	1.51	0.91
2:D:27:GLN:HG3	2:D:32:SER:HB2	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:98:LEU:HD21	2:F:99:LEU:HD13	1.74	0.70
2:D:14:TRP:HE1	7:D:202:GOL:H31	1.57	0.69
1:C:318:THR:HB	3:H:12:VAL:HG13	1.78	0.64
1:C:236:LEU:HB2	7:C:403:GOL:H12	1.82	0.61
2:D:164:GLU:CD	2:D:164:GLU:H	2.09	0.60
2:F:118:LEU:O	2:F:121:LYS:HG2	2.03	0.58
2:B:131:LYS:HG2	2:B:139:GLU:HB3	1.86	0.57
1:E:304:GLU:HB3	2:F:61:ILE:HG21	1.86	0.57
1:A:15:ILE:HD11	2:B:122:VAL:HG21	1.87	0.56
1:E:318:THR:HB	3:K:12:VAL:HG22	1.87	0.56
2:F:2:LEU:HD22	2:F:109:ASP:CG	2.31	0.56
2:F:164:GLU:O	2:F:168:LEU:HD23	2.05	0.56
2:B:161:LYS:HD3	2:B:162:TYR:CZ	2.41	0.55
1:C:15:ILE:HD11	2:D:122:VAL:HG21	1.87	0.55
1:C:141:HIS:CD2	1:C:149:ARG:HH22	2.24	0.55
1:E:79:LEU:O	1:E:82:VAL:HG22	2.05	0.55
1:A:79:LEU:O	1:A:82:VAL:HG22	2.06	0.55
3:K:8:ASP:OD1	3:K:12:VAL:HG12	2.07	0.55
1:A:96:ILE:HD11	1:A:102:PHE:HD2	1.73	0.53
2:B:167:LYS:NZ	2:B:170:ARG:HH22	2.07	0.53
1:E:163:LYS:HE2	1:E:201:TYR:OH	2.09	0.53
2:B:30:GLN:OE1	2:B:145:ASP:HB2	2.10	0.52
1:A:144:LYS:N	1:A:144:LYS:HD2	2.24	0.52
2:B:141:TYR:HB2	2:B:166:SER:HB3	1.92	0.52
1:A:310:ARG:NH1	2:B:90:ASP:OD1	2.40	0.52
2:B:167:LYS:HZ3	2:B:170:ARG:HH22	1.57	0.52
1:A:301:THR:HB	1:A:305:CYS:SG	2.50	0.51
1:C:61:LEU:HD12	1:C:89:GLU:HG2	1.92	0.51
1:C:32:LYS:NZ	8:C:507:HOH:O	2.43	0.51
1:C:100:GLY:HA3	1:C:230:MET:O	2.11	0.51
1:E:141:HIS:CD2	1:E:149:ARG:HH22	2.28	0.51
1:C:125(A):LYS:HG3	1:C:152:LEU:HD21	1.93	0.51
2:F:131:LYS:HG3	2:F:133:ILE:CD1	2.33	0.51
1:C:159:GLY:O	1:C:196:GLN:HG2	2.10	0.51
1:E:15:ILE:HD11	2:F:122:VAL:HG21	1.93	0.51
1:A:17:TYR:HB2	1:A:320:LEU:HD13	1.93	0.50
2:D:98:LEU:O	2:D:102:LEU:HG	2.11	0.50
1:A:96:ILE:HD12	1:A:232:TYR:CE1	2.46	0.50
2:B:151:SER:OG	2:B:157:TYR:HA	2.11	0.50
1:A:17:TYR:HB2	1:A:320:LEU:CD1	2.42	0.50
1:A:79:LEU:HG	7:A:403:GOL:H32	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:17:TYR:HB2	1:E:320:LEU:CD2	2.41	0.50
1:E:131:ASN:ND2	1:E:156:GLU:O	2.44	0.50
2:D:27:GLN:HG3	2:D:32:SER:CB	2.39	0.50
1:E:17:TYR:HB2	1:E:320:LEU:HD23	1.94	0.49
2:F:19:ASP:OD2	3:K:19:TYR:OH	2.30	0.49
1:C:18:HIS:CE1	4:I:3:FUC:H63	2.47	0.49
2:D:9:PHE:O	2:D:135:ASN:HA	2.13	0.49
2:D:14:TRP:NE1	7:D:202:GOL:H31	2.28	0.49
2:B:39:LYS:HE3	2:B:43:ASN:ND2	2.29	0.48
1:E:310:ARG:NH1	2:F:90:ASP:OD1	2.42	0.48
2:D:99:LEU:HD13	2:F:98:LEU:HD21	1.96	0.48
2:B:26:HIS:CE1	2:B:153:ARG:HH11	2.31	0.47
1:E:96:ILE:HG13	1:E:96:ILE:O	2.14	0.47
2:B:70:PHE:HE1	2:B:77:MET:HE2	1.80	0.47
1:E:125(B):GLU:OE2	1:E:125(C):SER:HB3	2.15	0.47
2:F:9:PHE:O	2:F:135:ASN:HA	2.15	0.47
2:D:141:TYR:HB2	2:D:166:SER:HB3	1.97	0.47
2:F:118:LEU:HA	2:F:121:LYS:HD2	1.97	0.47
1:E:100:GLY:HA3	1:E:230:MET:O	2.15	0.46
1:E:12:THR:OG1	2:F:27:GLN:HB3	2.14	0.46
1:A:207:SER:OG	1:A:241:ASP:OD1	2.29	0.46
1:A:100:GLY:HA3	1:A:230:MET:O	2.15	0.46
1:C:313:LYS:NZ	8:C:510:HOH:O	2.49	0.46
1:A:71:LEU:HD22	1:A:151:LEU:HD11	1.98	0.46
1:A:50:LYS:HD3	1:A:275:HIS:CG	2.51	0.46
1:C:79:LEU:O	1:C:82:VAL:HG22	2.16	0.45
2:F:11:GLU:OE1	2:F:135:ASN:ND2	2.50	0.45
2:D:39:LYS:HD2	2:D:40:SER:N	2.31	0.45
1:C:17:TYR:HB2	1:C:320:LEU:CD2	2.47	0.45
1:A:52:CYS:HB3	1:A:277:CYS:O	2.18	0.45
2:B:39:LYS:HD2	2:B:39:LYS:HA	1.69	0.44
1:C:165:LYS:NZ	1:E:219:GLU:HB3	2.32	0.44
2:B:161:LYS:HD3	2:B:162:TYR:CE2	2.53	0.44
2:F:161:LYS:HD2	2:F:162:TYR:CE2	2.52	0.44
1:A:131:ASN:HB3	1:A:133:ASN:ND2	2.33	0.43
2:F:26:HIS:NE2	2:F:153:ARG:HD3	2.33	0.43
1:A:304:GLU:HB3	2:B:61:ILE:HG21	2.00	0.43
1:A:320:LEU:CD2	2:B:111:HIS:HB3	2.48	0.43
1:C:29:VAL:HB	2:D:105:GLU:OE2	2.18	0.43
1:E:61:LEU:HD12	1:E:89:GLU:HG2	1.99	0.43
1:C:242:THR:HG21	8:C:611:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:73:ASN:HB3	1:C:76:CYS:SG	2.58	0.43
2:D:30:GLN:NE2	2:D:145:ASP:HB2	2.34	0.43
2:B:28:ASN:HD22	2:B:145:ASP:HA	1.83	0.43
1:A:118:PHE:C	1:A:118:PHE:CD1	2.97	0.43
1:E:29:VAL:HG11	2:F:102:LEU:HD23	2.01	0.43
1:E:125(B):GLU:H	1:E:125(B):GLU:HG3	1.60	0.43
2:F:26:HIS:CE1	2:F:153:ARG:HH11	2.37	0.43
1:C:242:THR:HG23	8:C:545:HOH:O	2.18	0.43
1:E:118:PHE:C	1:E:118:PHE:CD1	2.97	0.43
1:E:165:LYS:NZ	8:E:506:HOH:O	2.52	0.42
1:C:118:PHE:C	1:C:118:PHE:CD1	2.97	0.42
2:D:131:LYS:CG	2:D:139:GLU:HB3	2.49	0.42
2:F:163:SER:H	2:F:163:SER:HG	1.61	0.42
1:C:96:ILE:O	1:C:96:ILE:HG13	2.18	0.42
1:C:17:TYR:HB2	1:C:320:LEU:HD23	2.02	0.42
2:B:2:LEU:HB3	2:F:3:PHE:CZ	2.55	0.42
1:E:28:THR:HB	2:F:105:GLU:OE2	2.19	0.42
3:K:3:VAL:HG23	3:K:19:TYR:HB2	2.01	0.41
1:E:279:THR:HA	5:E:402:NAG:H81	2.01	0.41
1:A:133:ASN:ND2	1:A:133:ASN:H	2.18	0.41
1:A:320:LEU:HD23	2:B:111:HIS:CG	2.56	0.41
1:C:301:THR:HB	1:C:305:CYS:SG	2.59	0.41
2:D:18:ILE:H	2:D:18:ILE:HG13	1.59	0.41
1:E:313:LYS:NZ	8:E:510:HOH:O	2.54	0.41
2:D:55:VAL:HG22	2:D:99:LEU:HD21	2.02	0.41
2:D:51:LYS:NZ	2:D:103:GLU:OE1	2.51	0.41
1:A:48:ASN:ND2	1:A:287:ALA:HB3	2.36	0.41
1:C:29:VAL:HG21	2:D:102:LEU:HD23	2.02	0.41
1:E:265:SER:OG	1:E:266:GLY:N	2.54	0.41
1:A:131:ASN:HB3	1:A:133:ASN:HD21	1.86	0.41
1:A:61:LEU:HD12	1:A:89:GLU:HG2	2.03	0.40
1:E:72:GLY:O	1:E:149:ARG:HG2	2.20	0.40
2:F:72:LYS:NZ	8:F:302:HOH:O	2.40	0.40
1:A:52:CYS:HB3	1:A:277:CYS:C	2.45	0.40
1:E:207:SER:OG	1:E:241:ASP:OD1	2.35	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	320/326 (98%)	311 (97%)	9 (3%)	0	100	100
1	C	319/326 (98%)	310 (97%)	9 (3%)	0	100	100
1	E	320/326 (98%)	311 (97%)	9 (3%)	0	100	100
2	B	169/176 (96%)	166 (98%)	3 (2%)	0	100	100
2	D	169/176 (96%)	166 (98%)	3 (2%)	0	100	100
2	F	169/176 (96%)	167 (99%)	2 (1%)	0	100	100
3	G	17/19 (90%)	17 (100%)	0	0	100	100
3	H	17/19 (90%)	17 (100%)	0	0	100	100
3	K	17/19 (90%)	17 (100%)	0	0	100	100
All	All	1517/1563 (97%)	1482 (98%)	35 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	280/289 (97%)	280 (100%)	0	100	100
1	C	283/289 (98%)	283 (100%)	0	100	100
1	E	285/289 (99%)	285 (100%)	0	100	100
2	B	144/151 (95%)	144 (100%)	0	100	100
2	D	147/151 (97%)	147 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	143/151 (95%)	143 (100%)	0	100	100
3	G	13/13 (100%)	13 (100%)	0	100	100
3	H	13/13 (100%)	13 (100%)	0	100	100
3	K	13/13 (100%)	13 (100%)	0	100	100
All	All	1321/1359 (97%)	1321 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	133	ASN
2	B	28	ASN
2	B	60	ASN
2	B	146	ASN
1	C	92	ASN
1	C	95	ASN
1	C	141	HIS
1	C	196	GLN
1	E	141	HIS
2	F	135	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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.

No monomer is involved in short contacts.

5.5 Carbohydrates

9 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	I	1	4,1	14,14,15	0.44	0	17,19,21	0.54	0
4	NAG	I	2	4	14,14,15	0.63	1 (7%)	17,19,21	0.41	0
4	FUC	I	3	4	10,10,11	0.82	0	14,14,16	0.79	0
4	NAG	J	1	4,1	14,14,15	0.45	0	17,19,21	0.55	0
4	NAG	J	2	4	14,14,15	0.34	0	17,19,21	0.37	0
4	FUC	J	3	4	10,10,11	0.78	1 (10%)	14,14,16	0.89	1 (7%)
4	NAG	L	1	4,1	14,14,15	0.41	0	17,19,21	0.44	0
4	NAG	L	2	4	14,14,15	0.37	0	17,19,21	0.38	0
4	FUC	L	3	4	10,10,11	0.65	0	14,14,16	0.73	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	I	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	I	2	4	-	1/6/23/26	0/1/1/1
4	FUC	I	3	4	-	-	0/1/1/1
4	NAG	J	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1
4	FUC	J	3	4	-	-	0/1/1/1
4	NAG	L	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	L	2	4	-	2/6/23/26	0/1/1/1
4	FUC	L	3	4	-	-	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	3	FUC	C1-C2	2.20	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	2	NAG	C1-C2	2.16	1.55	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	3	FUC	C1-C2-C3	2.04	112.62	109.64

There are no chirality outliers.

All (11) torsion outliers are listed below:

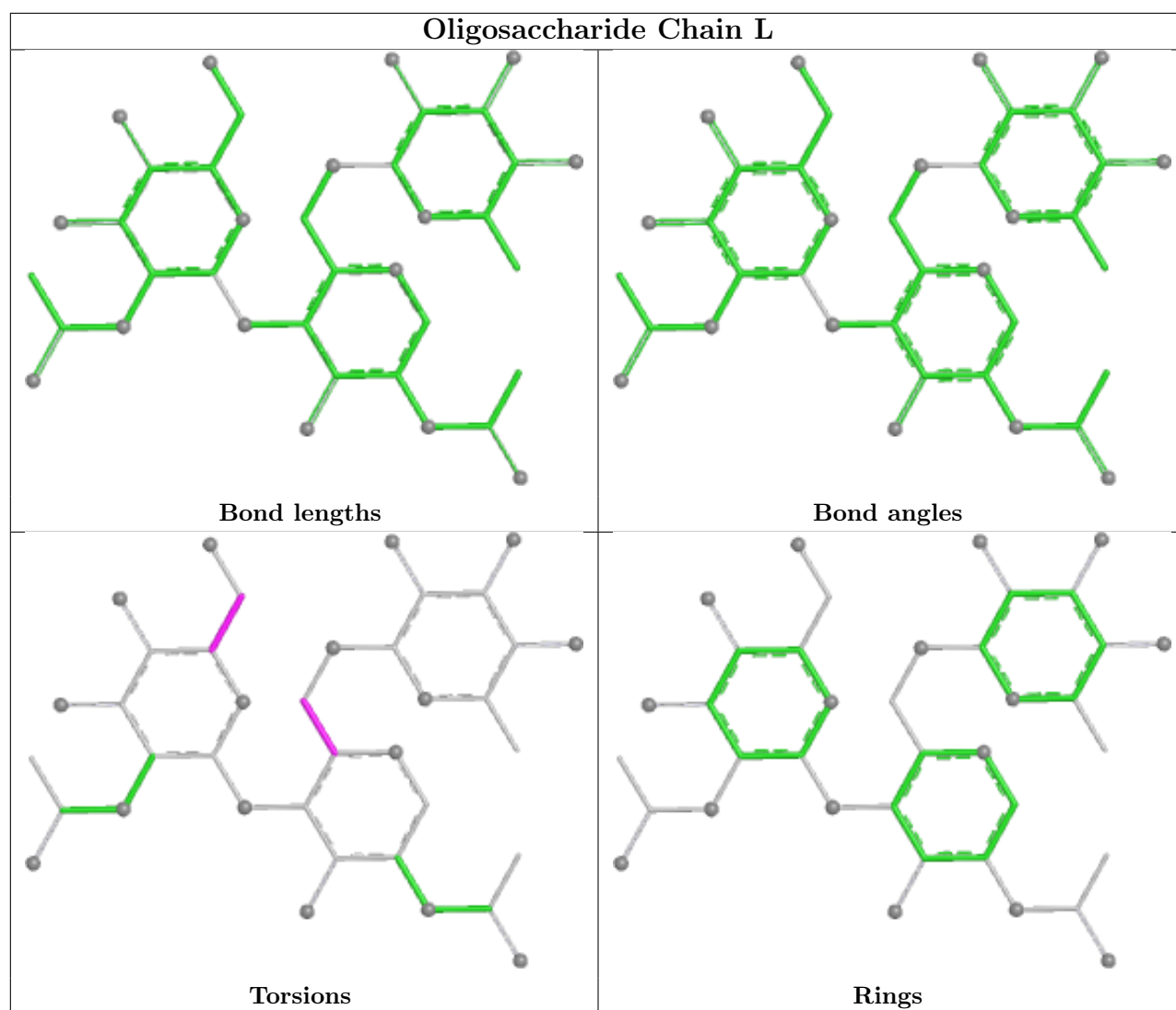
Mol	Chain	Res	Type	Atoms
4	J	2	NAG	O5-C5-C6-O6
4	L	2	NAG	O5-C5-C6-O6
4	L	1	NAG	C4-C5-C6-O6
4	I	1	NAG	C4-C5-C6-O6
4	J	1	NAG	C4-C5-C6-O6
4	L	1	NAG	O5-C5-C6-O6
4	I	1	NAG	O5-C5-C6-O6
4	J	2	NAG	C4-C5-C6-O6
4	J	1	NAG	O5-C5-C6-O6
4	L	2	NAG	C4-C5-C6-O6
4	I	2	NAG	O5-C5-C6-O6

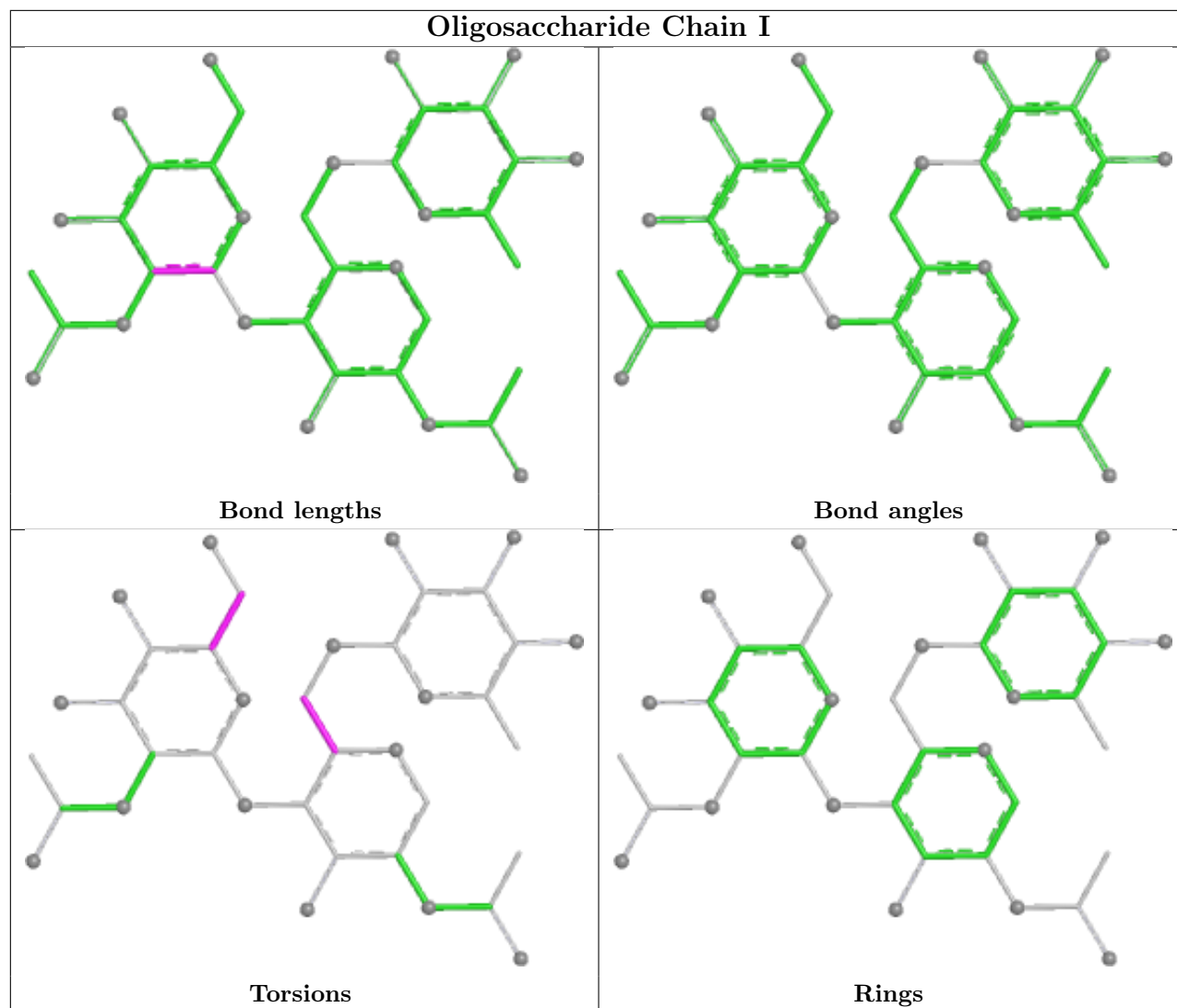
There are no ring outliers.

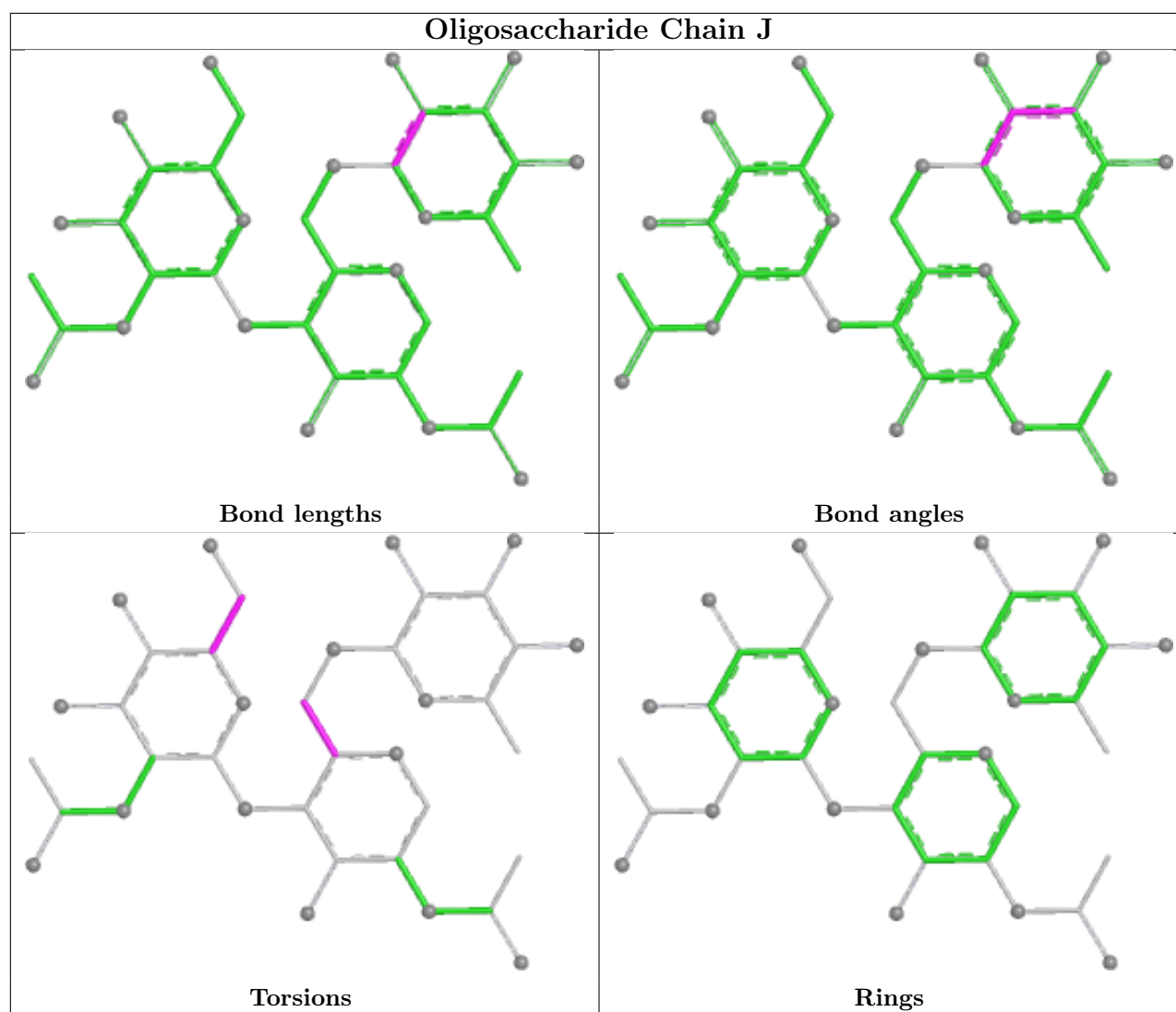
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	3	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 [i](#)

Of 15 ligands modelled in this entry, 3 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	C	401	1	14,14,15	0.34	0	17,19,21	0.44	0
5	NAG	D	201	2	14,14,15	0.48	0	17,19,21	1.15	1 (5%)
5	NAG	B	201	2	14,14,15	0.20	0	17,19,21	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	F	201	2	14,14,15	0.19	0	17,19,21	0.66	0
7	GOL	C	403	-	5,5,5	0.83	0	5,5,5	1.15	1 (20%)
5	NAG	E	402	1	14,14,15	0.29	0	17,19,21	0.44	0
7	GOL	F	202	-	5,5,5	1.00	0	5,5,5	1.03	0
7	GOL	D	202	-	5,5,5	0.96	0	5,5,5	1.05	0
5	NAG	E	401	1	14,14,15	0.33	0	17,19,21	0.41	0
5	NAG	A	401	1	14,14,15	0.34	0	17,19,21	0.46	0
7	GOL	B	202	-	5,5,5	0.98	0	5,5,5	1.04	0
7	GOL	A	403	-	5,5,5	0.95	0	5,5,5	1.07	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
5	NAG	C	401	1	-	2/6/23/26	0/1/1/1
5	NAG	D	201	2	-	2/6/23/26	0/1/1/1
5	NAG	B	201	2	-	4/6/23/26	0/1/1/1
5	NAG	F	201	2	-	4/6/23/26	0/1/1/1
7	GOL	C	403	-	-	2/4/4/4	-
5	NAG	E	402	1	-	0/6/23/26	0/1/1/1
7	GOL	F	202	-	-	4/4/4/4	-
7	GOL	D	202	-	-	2/4/4/4	-
5	NAG	E	401	1	-	2/6/23/26	0/1/1/1
5	NAG	A	401	1	-	2/6/23/26	0/1/1/1
7	GOL	B	202	-	-	2/4/4/4	-
7	GOL	A	403	-	-	1/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	201	NAG	C1-O5-C5	3.60	117.01	112.19
7	C	403	GOL	C3-C2-C1	-2.17	103.84	111.80

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	201	NAG	C1-C2-N2-C7
7	B	202	GOL	C1-C2-C3-O3
7	C	403	GOL	O1-C1-C2-C3
7	F	202	GOL	O1-C1-C2-C3
5	F	201	NAG	C4-C5-C6-O6
5	C	401	NAG	O5-C5-C6-O6
5	A	401	NAG	O5-C5-C6-O6
5	F	201	NAG	O5-C5-C6-O6
5	B	201	NAG	O5-C5-C6-O6
5	E	401	NAG	O5-C5-C6-O6
5	C	401	NAG	C4-C5-C6-O6
5	A	401	NAG	C4-C5-C6-O6
7	D	202	GOL	O1-C1-C2-C3
7	F	202	GOL	C1-C2-C3-O3
7	B	202	GOL	O2-C2-C3-O3
7	F	202	GOL	O1-C1-C2-O2
7	F	202	GOL	O2-C2-C3-O3
5	E	401	NAG	C4-C5-C6-O6
7	C	403	GOL	O1-C1-C2-O2
5	B	201	NAG	C4-C5-C6-O6
5	B	201	NAG	C1-C2-N2-C7
5	F	201	NAG	C1-C2-N2-C7
7	A	403	GOL	O2-C2-C3-O3
5	B	201	NAG	C3-C2-N2-C7
5	F	201	NAG	C3-C2-N2-C7
7	D	202	GOL	O1-C1-C2-O2
5	D	201	NAG	C3-C2-N2-C7

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	403	GOL	1	0
5	E	402	NAG	1	0
7	D	202	GOL	2	0
7	A	403	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	321/326 (98%)	-0.96	0 100 100	27, 45, 60, 79	1 (0%)
1	C	321/326 (98%)	-0.96	0 100 100	35, 45, 63, 79	0
1	E	321/326 (98%)	-0.96	0 100 100	25, 46, 62, 77	1 (0%)
2	B	171/176 (97%)	-0.96	0 100 100	37, 50, 81, 89	0
2	D	171/176 (97%)	-0.96	0 100 100	37, 50, 78, 87	0
2	F	171/176 (97%)	-0.97	0 100 100	36, 50, 78, 89	0
3	G	18/19 (94%)	-0.86	0 100 100	47, 57, 70, 71	0
3	H	18/19 (94%)	-0.73	0 100 100	50, 59, 66, 67	0
3	K	18/19 (94%)	-0.91	0 100 100	51, 57, 70, 71	0
All	All	1530/1563 (97%)	-0.96	0 100 100	25, 47, 73, 89	2 (0%)

There are no RSRZ outliers to report.

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	DPR	G	1	7/8	0.98	0.06	70,72,73,76	0
3	DPR	H	1	7/8	0.99	0.05	66,67,71,71	0
3	DPR	K	1	7/8	0.99	0.04	70,72,74,74	0

6.3 Carbohydrates

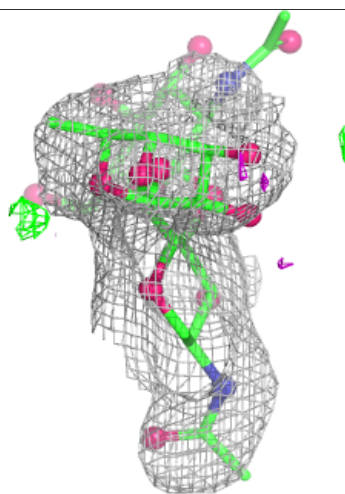
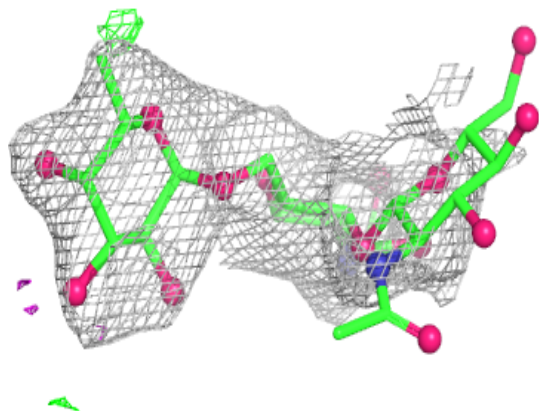
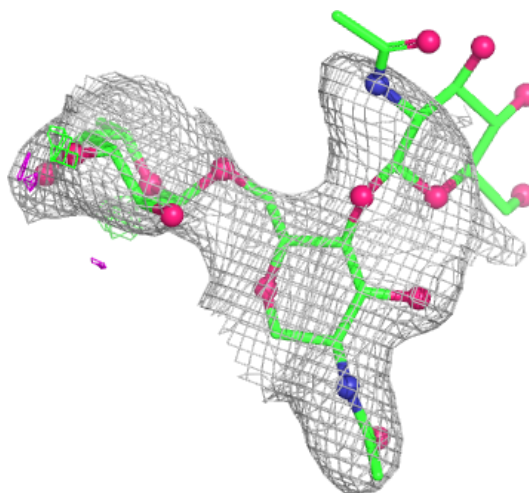
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	J	2	14/15	0.93	0.10	88,109,116,116	0
4	NAG	L	2	14/15	0.95	0.09	113,123,130,137	0
4	FUC	J	3	10/11	0.97	0.07	50,63,73,77	0
4	NAG	I	1	14/15	-	-	68,77,86,91	0
4	NAG	I	2	14/15	-	-	91,103,108,109	0
4	FUC	I	3	10/11	-	-	50,64,70,76	0
4	FUC	L	3	10/11	0.98	0.07	48,65,76,78	0
4	NAG	J	1	14/15	0.98	0.05	76,82,91,94	0
4	NAG	L	1	14/15	0.99	0.04	75,84,95,106	0

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

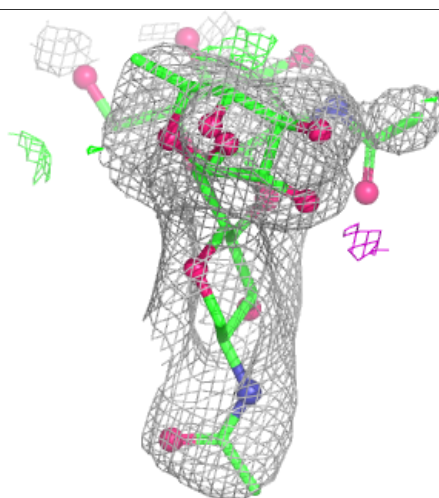
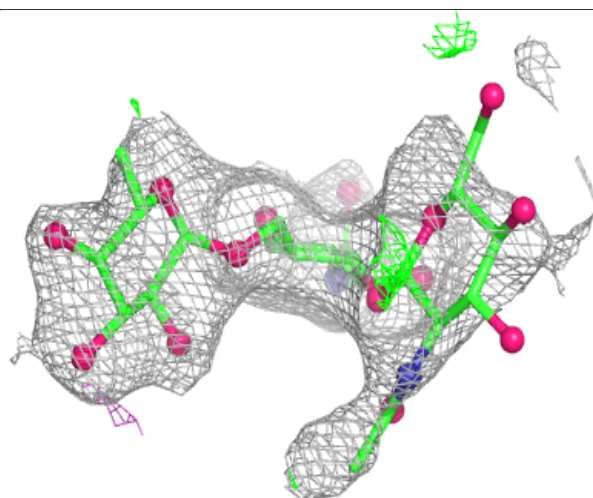
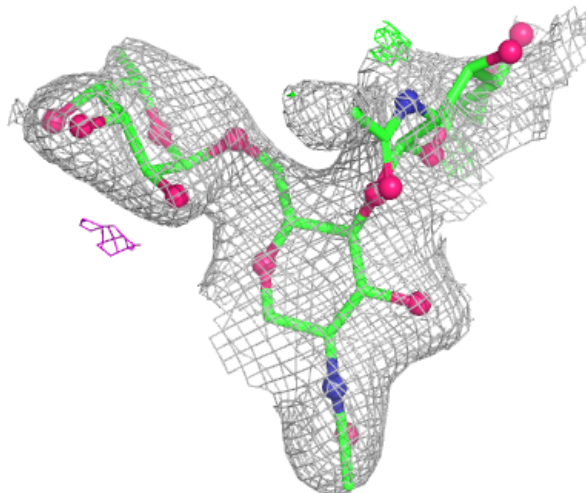
Electron density around Chain L:

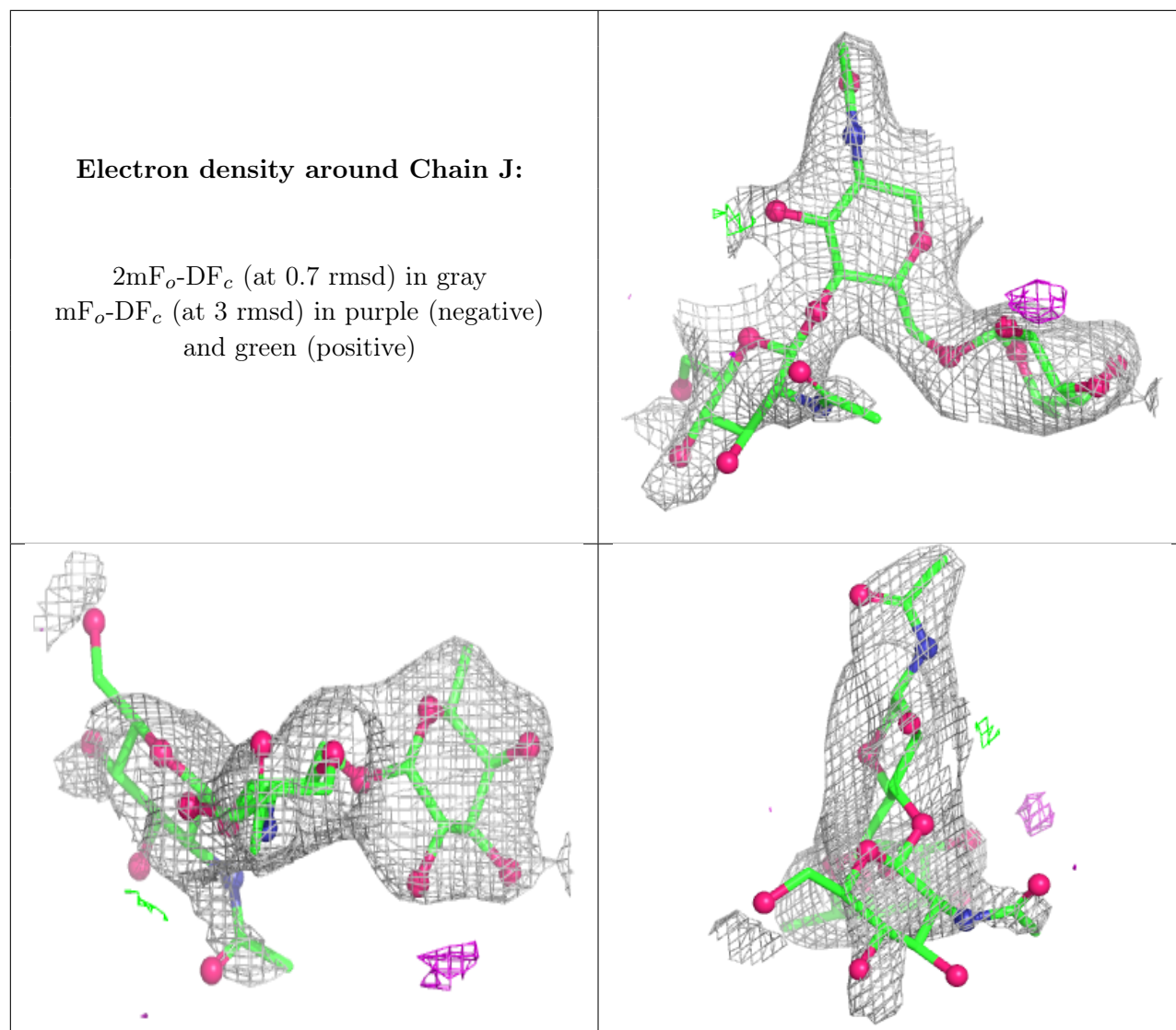
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain I:

$2mF_o-DF_c$ (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
5	NAG	A	401	14/15	0.90	0.07	88,99,102,102	0
5	NAG	E	401	14/15	0.91	0.08	90,101,105,107	0
5	NAG	C	401	14/15	0.92	0.08	88,100,106,109	0
5	NAG	E	402	14/15	0.95	0.05	74,99,108,108	0
5	NAG	F	201	14/15	0.95	0.06	89,94,100,102	0
7	GOL	A	403	6/6	0.95	0.10	53,58,64,66	0
5	NAG	D	201	14/15	0.96	0.06	86,97,102,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	B	201	14/15	0.97	0.04	84,97,104,109	0
7	GOL	B	202	6/6	0.97	0.05	57,60,63,66	0
7	GOL	D	202	6/6	0.97	0.06	58,64,66,70	0
7	GOL	C	403	6/6	0.98	0.07	50,53,54,57	0
7	GOL	F	202	6/6	0.98	0.05	60,65,67,71	0
6	CA	E	403	1/1	1.00	0.01	38,38,38,38	0
6	CA	A	402	1/1	1.00	0.01	39,39,39,39	0
6	CA	C	402	1/1	1.00	0.03	39,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.