



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 10:37 AM UTC

PDB ID : 8FIA / pdb_00008fia
Title : The structure of fly Teneurin self assembly
Authors : Bandekar, S.J.; Li, J.; Arac, D.
Deposited on : 2022-12-15
Resolution : 2.40 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

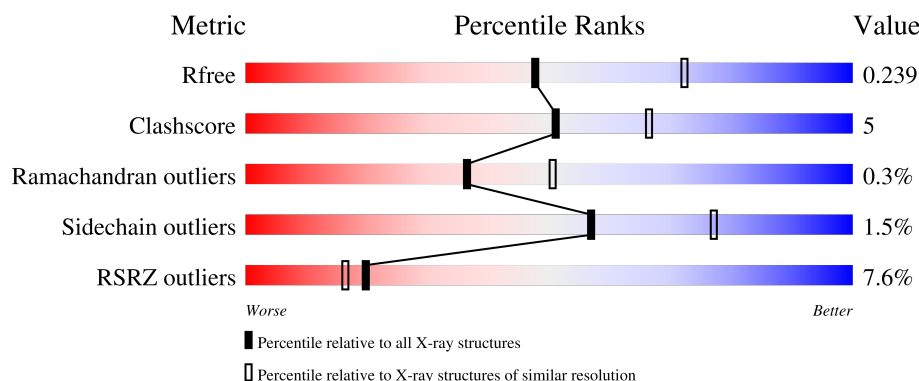
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	1962	7% 78% 12% 10%
2	B	6	67% 33%
3	C	3	33% 67%
4	D	6	50% 33% 17%
5	E	3	33% 67%

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Mol	Chain	Length	Quality of chain
6	F	2	 50%50%

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 14844 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.

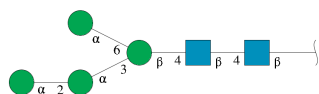
- Molecule 1 is a protein called Teneurin-m.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1772	Total	C	N	O	S	0	2	0
			14201	8978	2494	2676	53			

There are 9 discrepancies between the modelled and reference sequences:

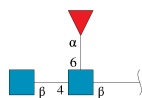
Chain	Residue	Modelled	Actual	Comment	Reference
A	776	ALA	-	expression tag	UNP O61307
A	777	ASP	-	expression tag	UNP O61307
A	778	PRO	-	expression tag	UNP O61307
A	2732	HIS	-	expression tag	UNP O61307
A	2733	HIS	-	expression tag	UNP O61307
A	2734	HIS	-	expression tag	UNP O61307
A	2735	HIS	-	expression tag	UNP O61307
A	2736	HIS	-	expression tag	UNP O61307
A	2737	HIS	-	expression tag	UNP O61307

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-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.



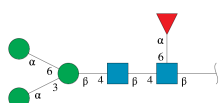
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 3 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.



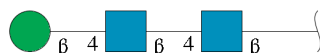
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	3	Total	C	N	O	0	0	0
			38	22	2	14			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	6	Total	C	N	O	0	0	0
			71	40	2	29			

- Molecule 5 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.



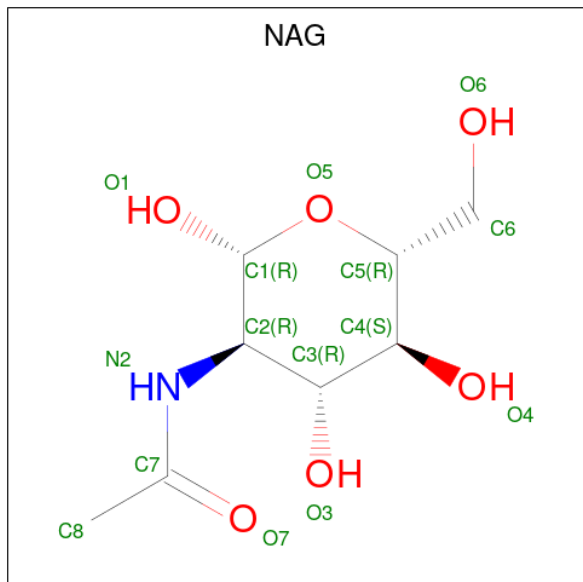
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



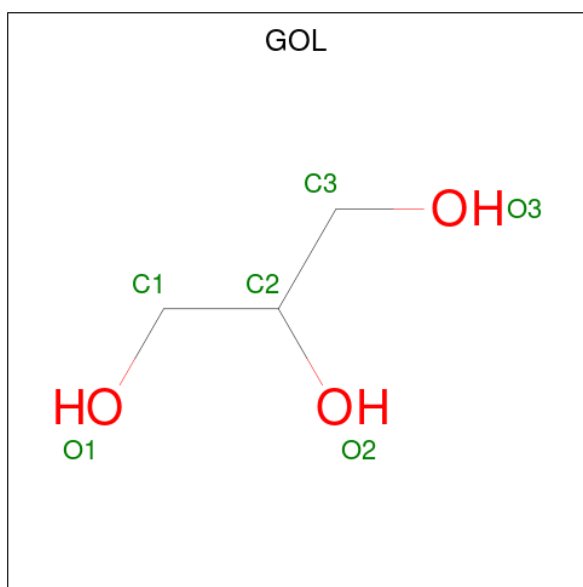
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



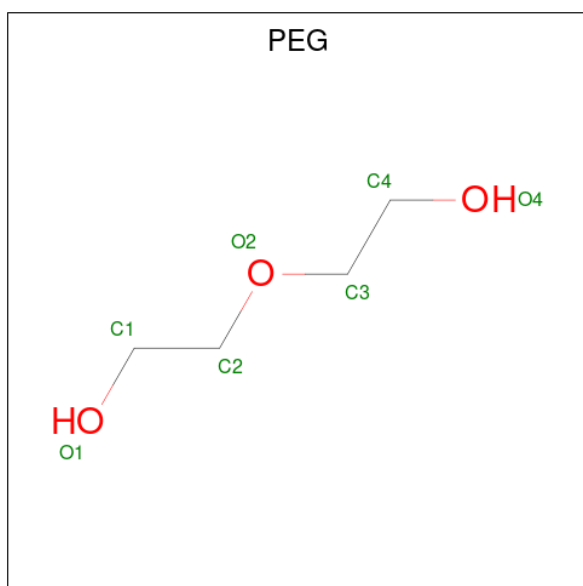
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			7	4	3		
9	A	1	Total	C	O	0	0
			7	4	3		

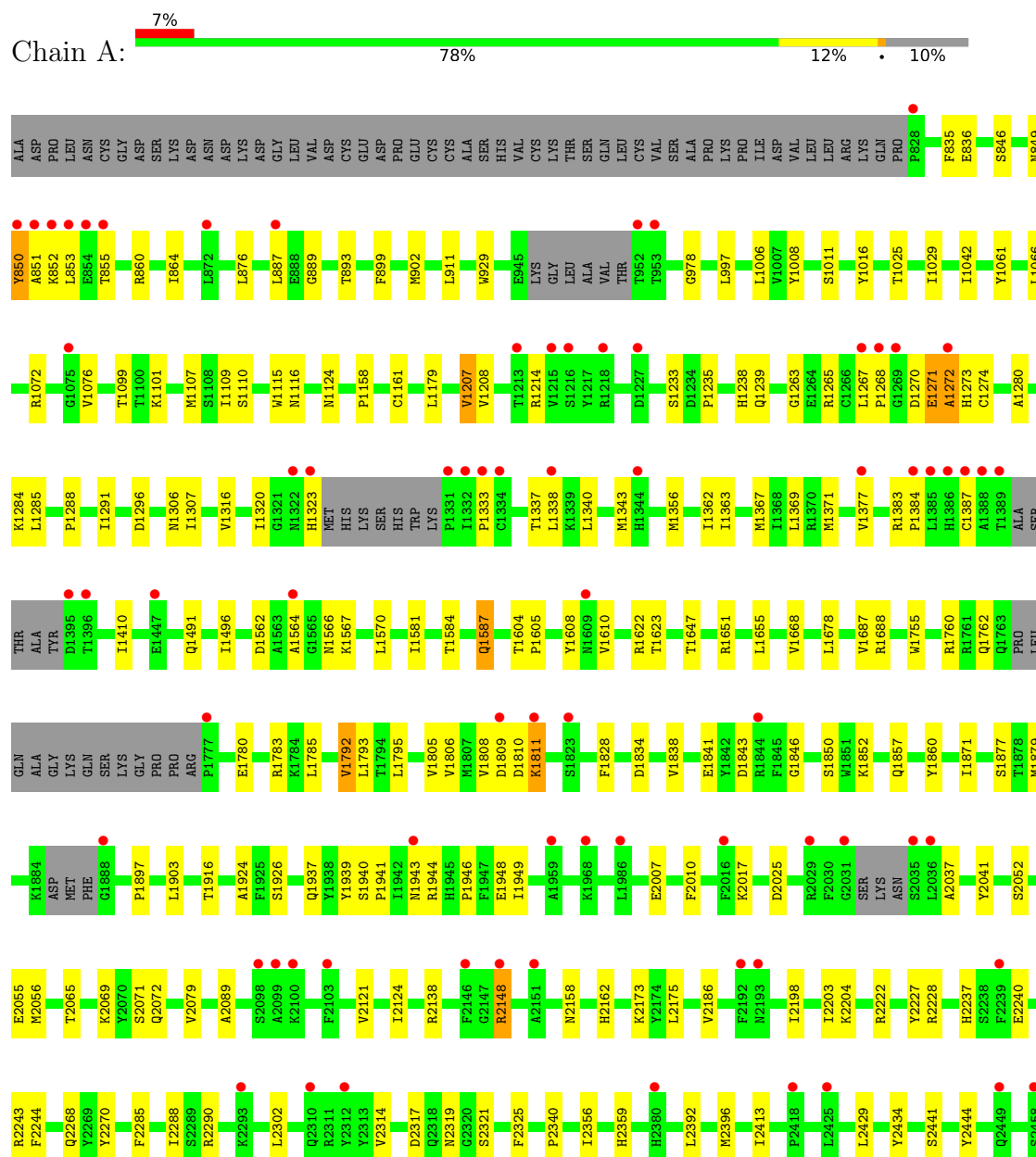
- Molecule 10 is water.

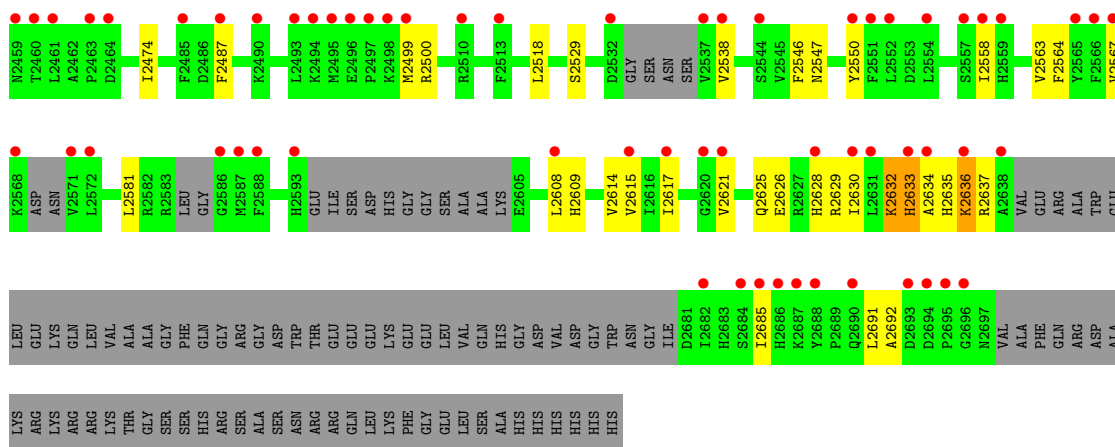
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	309	Total	O	0	0
			309	309		

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: Teneurin-m





- Molecule 2: alpha-D-mannopyranose-(1-2)-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 B: 67% 33%



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

Chain C: 33% 67%



- Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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 D: 50% 33% 17%



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 33% 67%



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	95.20Å 129.86Å 188.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.57 – 2.40 48.57 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.57-2.40) 87.6 (48.57-2.40)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.27 (at 2.27Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.216 , 0.243 0.216 , 0.239	Depositor DCC
R_{free} test set	2000 reflections (1.85%)	wwPDB-VP
Wilson B-factor (Å ²)	40.4	Xtriage
Anisotropy	0.337	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 44.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14844	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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: PEG, NAG, GOL, BMA, FUC, 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	0.67	0/14525	0.91	9/19683 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	978	GLY	CA-C-O	-7.19	117.28	122.45
1	A	2285	PHE	CB-CA-C	6.16	115.99	110.44
1	A	2072[A]	GLN	CA-C-O	6.13	127.02	119.79
1	A	2072[B]	GLN	CA-C-O	6.13	127.02	119.79
1	A	850	TYR	N-CA-C	6.01	117.70	111.03
1	A	836[A]	GLU	CA-C-O	5.47	126.11	119.38
1	A	836[B]	GLU	CA-C-O	5.47	126.11	119.38
1	A	1263	GLY	N-CA-C	-5.26	107.74	114.37
1	A	2052	SER	N-CA-C	-5.04	107.80	114.31

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	14201	0	13874	149	0
2	B	72	0	61	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	38	0	34	1	0
4	D	71	0	61	2	0
5	E	39	0	34	1	0
6	F	28	0	25	1	0
7	A	42	0	39	1	0
8	A	30	0	40	0	0
9	A	14	0	20	1	0
10	A	309	0	0	2	0
All	All	14844	0	14188	150	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 (150) 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:1267:LEU:HB3	1:A:1270:ASP:HB3	1.59	0.83
1:A:1940:SER:HB3	1:A:1943:ASN:HD22	1.49	0.76
1:A:1805:VAL:HG21	5:E:1:NAG:H82	1.70	0.74
1:A:1271:GLU:HB3	1:A:1274:CYS:SG	2.30	0.72
1:A:1604:THR:CG2	1:A:1608:TYR:HB3	2.21	0.71
1:A:1233:SER:HB3	1:A:1291:ILE:HD11	1.74	0.70
1:A:2240:GLU:HB3	1:A:2243:ARG:HB2	1.74	0.70
1:A:1604:THR:HG22	1:A:1608:TYR:HB3	1.73	0.69
1:A:1025:THR:HB	1:A:1029:ILE:HD11	1.73	0.68
1:A:1271:GLU:HG3	1:A:1284:LYS:HD2	1.74	0.68
1:A:1828:PHE:HB2	1:A:1838:VAL:HB	1.75	0.68
1:A:1384:PRO:HG2	1:A:1387:CYS:SG	2.34	0.67
1:A:2609:HIS:HA	1:A:2614:VAL:HG12	1.78	0.65
1:A:1852:LYS:HG2	1:A:1857:GLN:HG2	1.80	0.64
1:A:1834:ASP:HB3	4:D:1:NAG:H82	1.79	0.63
1:A:1239:GLN:HA	1:A:1285:LEU:HD12	1.81	0.61
1:A:1107:MET:SD	1:A:1124:ASN:HB2	2.41	0.60
1:A:2635:HIS:O	1:A:2636:LYS:C	2.43	0.60
1:A:1806:VAL:HG11	1:A:2429:LEU:HD21	1.84	0.60
1:A:1271:GLU:O	1:A:1272:ALA:C	2.43	0.60
1:A:1320:ILE:HG12	1:A:1340:LEU:HD12	1.82	0.60
1:A:2222:ARG:HB2	1:A:2227:TYR:HE2	1.66	0.60
1:A:2288:ILE:HD12	1:A:2290:ARG:HD2	1.85	0.59
1:A:1795:LEU:HB3	1:A:2487:PHE:HE1	1.68	0.59
1:A:997:LEU:HD11	1:A:1610:VAL:HG11	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1333:PRO:HG2	1:A:1338:LEU:HD22	1.85	0.58
1:A:2581:LEU:HD13	1:A:2608:LEU:HD21	1.85	0.57
1:A:2069:LYS:HB3	1:A:2079:VAL:HB	1.87	0.57
1:A:1363:ILE:HD11	1:A:1410:ILE:HG23	1.87	0.57
1:A:1792:VAL:HG13	1:A:2434:TYR:HE2	1.69	0.57
1:A:1647:THR:HG21	1:A:1651:ARG:HH21	1.70	0.57
1:A:1760:ARG:HB3	1:A:1780:GLU:HB2	1.86	0.56
1:A:849:ASN:HA	1:A:853:LEU:HD13	1.87	0.56
1:A:1564:ALA:HB3	1:A:1566:ASN:HD22	1.70	0.56
1:A:1841:GLU:HB2	1:A:1850:SER:HB3	1.88	0.56
1:A:1320:ILE:HD11	1:A:1371:MET:SD	2.46	0.55
1:A:1903:LEU:HB2	1:A:1916:THR:HB	1.88	0.55
1:A:846:SER:O	1:A:849:ASN:ND2	2.40	0.55
1:A:2392:LEU:HB3	1:A:2396:MET:HE2	1.89	0.55
1:A:1570:LEU:HD13	1:A:1581:ILE:HG12	1.88	0.55
1:A:1235:PRO:HA	1:A:1288:PRO:HG2	1.88	0.54
1:A:1622:ARG:HG2	1:A:1623:THR:HG23	1.88	0.54
1:A:2625:GLN:HA	1:A:2628:HIS:CD2	2.43	0.54
1:A:1158:PRO:HG2	1:A:1161:CYS:HB3	1.89	0.54
1:A:2203:ILE:HG13	1:A:2204:LYS:HG2	1.90	0.53
1:A:1877:SER:HB3	1:A:1897:PRO:HB3	1.89	0.53
1:A:1943:ASN:O	1:A:1944:ARG:HB2	2.08	0.53
1:A:1809:ASP:O	1:A:1810:ASP:C	2.52	0.52
1:A:1647:THR:HG21	1:A:1651:ARG:HE	1.72	0.52
1:A:2629:ARG:HA	1:A:2632:LYS:HE3	1.91	0.52
1:A:1367:MET:SD	1:A:1384:PRO:HD3	2.49	0.52
1:A:1076:VAL:HG13	1:A:1101:LYS:HB3	1.91	0.52
1:A:893:THR:HG22	1:A:899:PHE:HB3	1.92	0.52
1:A:2228:ARG:HB2	1:A:2237:HIS:HB3	1.91	0.52
1:A:1808:VAL:HG12	1:A:1809:ASP:N	2.24	0.52
1:A:1678:LEU:CD1	1:A:1687:VAL:HG22	2.40	0.52
1:A:2564:PHE:HB2	1:A:2615:VAL:HG22	1.92	0.51
1:A:1099:THR:HG23	1:A:1356:MET:HE2	1.93	0.51
1:A:2685:ILE:HB	1:A:2692:ALA:HB2	1.92	0.51
1:A:2158:ASN:HD21	1:A:2162:HIS:HB2	1.76	0.51
1:A:1238:HIS:NE2	1:A:1265:ARG:HD2	2.25	0.51
1:A:1937:GLN:HG2	1:A:1948:GLU:HG2	1.93	0.51
1:A:2626:GLU:O	1:A:2630:ILE:HG13	2.11	0.50
1:A:852:LYS:HD3	1:A:887:LEU:HA	1.92	0.50
1:A:2017:LYS:HB2	1:A:2025:ASP:HB3	1.94	0.50
1:A:1587:GLN:HB2	1:A:1605:PRO:HG2	1.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2173:LYS:HB2	1:A:2186:VAL:HB	1.94	0.50
1:A:1214:ARG:CZ	3:C:3:FUC:H5	2.42	0.50
1:A:1604:THR:HG21	1:A:1608:TYR:HB3	1.94	0.49
1:A:1941:PRO:HB2	1:A:2198:ILE:HG22	1.94	0.49
1:A:1110:SER:HB2	1:A:1116:ASN:HA	1.94	0.49
1:A:864:ILE:HG21	1:A:911:LEU:HD11	1.95	0.48
1:A:1562:ASP:CG	1:A:1566:ASN:HB2	2.38	0.48
1:A:2121:VAL:O	1:A:2124:ILE:HG12	2.14	0.48
1:A:2629:ARG:HG2	1:A:2632:LYS:NZ	2.28	0.48
1:A:1562:ASP:C	1:A:1564:ALA:H	2.22	0.48
1:A:2055:GLU:HG2	1:A:2065:THR:HG22	1.96	0.48
1:A:2007:GLU:HB2	1:A:2010:PHE:HB3	1.96	0.47
1:A:1808:VAL:O	1:A:1809:ASP:C	2.57	0.47
1:A:1066:LEU:HD23	1:A:1072:ARG:HA	1.96	0.47
1:A:2518:LEU:HB2	1:A:2529:SER:HB2	1.95	0.47
1:A:2547:ASN:CG	7:A:2810:NAG:HN2	2.22	0.47
1:A:1871:ILE:HD13	1:A:2500:ARG:HD3	1.97	0.47
1:A:2317:ASP:OD2	1:A:2321:SER:HB2	2.15	0.47
1:A:853:LEU:C	1:A:855:THR:H	2.23	0.47
1:A:1688:ARG:HH11	1:A:1688:ARG:HB3	1.80	0.46
1:A:1337:THR:C	1:A:1338:LEU:HD23	2.40	0.46
1:A:1011:SER:HA	1:A:1016:TYR:CG	2.51	0.46
1:A:1280:ALA:HA	1:A:1316:VAL:CG2	2.46	0.46
1:A:860:ARG:HG2	1:A:929:TRP:CZ2	2.51	0.46
1:A:1008:TYR:HB2	1:A:1115:TRP:CE2	2.51	0.46
1:A:1296:ASP:OD1	1:A:1296:ASP:N	2.44	0.46
1:A:2632:LYS:O	1:A:2633:HIS:C	2.59	0.46
1:A:1207:VAL:HG22	1:A:1208:VAL:HG23	1.97	0.45
1:A:1939:TYR:CE2	1:A:1946:PRO:HB3	2.51	0.45
1:A:2474:ILE:HG22	9:A:2806:PEG:H42	1.97	0.45
1:A:1006:LEU:HD12	1:A:1006:LEU:HA	1.89	0.45
1:A:2138:ARG:HE	1:A:2138:ARG:HB2	1.67	0.45
1:A:1307:ILE:HG13	1:A:1362:ILE:HD13	1.99	0.44
1:A:1655:LEU:HG	1:A:1668:VAL:HG22	1.99	0.44
1:A:835:PHE:CE1	1:A:902:MET:HE1	2.52	0.44
1:A:2041:TYR:HE1	1:A:2056:MET:HE3	1.82	0.44
1:A:1491:GLN:HG2	10:A:2935:HOH:O	2.18	0.44
1:A:1099:THR:CG2	1:A:1356:MET:HE2	2.48	0.43
1:A:1179:LEU:HD21	1:A:1496:ILE:HD12	2.00	0.43
1:A:1343:MET:HE2	1:A:1369:LEU:CD2	2.48	0.43
1:A:2625:GLN:HA	1:A:2628:HIS:HD2	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2340:PRO:HB3	1:A:2413:ILE:HD11	2.00	0.43
1:A:1793:LEU:HD23	1:A:1795:LEU:HD11	2.02	0.42
1:A:2629:ARG:O	1:A:2632:LYS:HB2	2.18	0.42
1:A:1843:ASP:OD1	1:A:1846:GLY:N	2.52	0.42
1:A:2302:LEU:HD22	1:A:2314:VAL:HG21	2.00	0.42
1:A:2633:HIS:O	1:A:2636:LYS:HG3	2.19	0.42
1:A:1267:LEU:HD13	1:A:1268:PRO:HD2	2.01	0.42
1:A:1271:GLU:O	1:A:1273:HIS:N	2.53	0.42
1:A:1320:ILE:HG12	1:A:1340:LEU:CD1	2.47	0.42
1:A:2089:ALA:HA	4:D:6:FUC:H3	2.01	0.42
1:A:849:ASN:ND2	1:A:850:TYR:N	2.68	0.42
1:A:1755:TRP:CZ3	1:A:1785:LEU:HB2	2.55	0.42
1:A:1042:ILE:HD11	1:A:1061:TYR:HE2	1.85	0.42
1:A:1306:ASN:HD21	1:A:1323:HIS:HB3	1.85	0.42
1:A:1783:ARG:HG2	1:A:2487:PHE:CZ	2.55	0.42
1:A:2268:GLN:NE2	1:A:2270:TYR:OH	2.52	0.42
1:A:2037:ALA:HB3	1:A:2268:GLN:HE22	1.84	0.42
1:A:1860:TYR:OH	1:A:2499:MET:HE2	2.20	0.42
1:A:852:LYS:HB2	1:A:887:LEU:O	2.20	0.41
1:A:1852:LYS:HD3	1:A:1857:GLN:NE2	2.35	0.41
1:A:1924:ALA:HB3	1:A:1939:TYR:HB2	2.01	0.41
1:A:2148:ARG:HA	1:A:2148:ARG:HD2	1.90	0.41
1:A:2632:LYS:O	1:A:2635:HIS:HB2	2.20	0.41
1:A:2441:SER:HA	1:A:2444:TYR:CZ	2.55	0.41
6:F:1:NAG:H62	6:F:2:NAG:H82	2.02	0.41
1:A:1367:MET:HE3	1:A:1367:MET:HB2	1.92	0.41
1:A:876:LEU:HD12	1:A:876:LEU:HA	1.86	0.41
1:A:1566:ASN:OD1	1:A:1584:THR:HG21	2.21	0.41
1:A:2319:ASN:O	1:A:2359:HIS:HA	2.21	0.41
1:A:2558:ILE:HG12	1:A:2563:VAL:HG21	2.03	0.41
1:A:2302:LEU:HD12	1:A:2356:ILE:HG13	2.03	0.41
1:A:1340:LEU:HD13	1:A:1377:VAL:CG2	2.51	0.41
1:A:1567:LYS:H	1:A:1584:THR:HB	1.86	0.41
1:A:2071:SER:HB2	10:A:3092:HOH:O	2.21	0.40
1:A:2240:GLU:HB2	1:A:2244:PHE:CE2	2.57	0.40
1:A:2314:VAL:HG22	1:A:2325:PHE:CD2	2.57	0.40
1:A:2628:HIS:O	1:A:2632:LYS:HG3	2.21	0.40
1:A:851:ALA:HB3	1:A:889:GLY:HA2	2.04	0.40
1:A:1267:LEU:HA	1:A:1267:LEU:HD22	1.77	0.40
1:A:1810:ASP:O	1:A:1811:LYS:HB2	2.21	0.40
1:A:2550:TYR:HD1	1:A:2567:VAL:O	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2546:PHE:O	1:A:2547:ASN:C	2.63	0.40
1:A:2634:ALA:O	1:A:2635:HIS:C	2.64	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	1750/1962 (89%)	1663 (95%)	82 (5%)	5 (0%)	36 50

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1272	ALA
1	A	2636	LYS
1	A	1811	LYS
1	A	1271	GLU
1	A	1109	ILE

5.3.2 Protein sidechains [i](#)

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	1167/1708 (68%)	1150 (98%)	17 (2%)	57 77

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1207	VAL
1	A	1383	ARG
1	A	1587	GLN
1	A	1762	GLN
1	A	1792	VAL
1	A	1879	MET
1	A	1926	SER
1	A	1949	ILE
1	A	2148	ARG
1	A	2175	LEU
1	A	2538	VAL
1	A	2617	ILE
1	A	2621	VAL
1	A	2632	LYS
1	A	2633	HIS
1	A	2637	ARG
1	A	2691	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1741	GLN
1	A	1812	GLN
1	A	1943	ASN
1	A	2170	ASN
1	A	2268	GLN
1	A	2282	HIS
1	A	2307	HIS
1	A	2366	HIS
1	A	2374	GLN
1	A	2453	GLN
1	A	2459	ASN
1	A	2628	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

20 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	B	1	1,2	14,14,15	0.41	0	17,19,21	0.88	1 (5%)
2	NAG	B	2	2	14,14,15	0.43	0	17,19,21	0.72	0
2	BMA	B	3	2	11,11,12	0.37	0	15,15,17	0.92	1 (6%)
2	MAN	B	4	2	11,11,12	0.21	0	15,15,17	0.66	0
2	MAN	B	5	2	11,11,12	0.19	0	15,15,17	0.60	0
2	MAN	B	6	2	11,11,12	0.28	0	15,15,17	0.65	0
3	NAG	C	1	3,1	14,14,15	0.39	0	17,19,21	1.42	3 (17%)
3	NAG	C	2	3	14,14,15	0.33	0	17,19,21	0.71	0
3	FUC	C	3	3	10,10,11	0.26	0	14,14,16	0.63	0
4	NAG	D	1	1,4	14,14,15	0.41	0	17,19,21	1.10	1 (5%)
4	NAG	D	2	4	14,14,15	0.42	0	17,19,21	0.86	1 (5%)
4	BMA	D	3	4	11,11,12	0.36	0	15,15,17	0.65	0
4	MAN	D	4	4	11,11,12	0.25	0	15,15,17	0.58	0
4	MAN	D	5	4	11,11,12	0.25	0	15,15,17	0.60	0
4	FUC	D	6	4	10,10,11	0.29	0	14,14,16	0.55	0
5	NAG	E	1	1,5	14,14,15	0.46	0	17,19,21	0.66	0
5	NAG	E	2	5	14,14,15	0.37	0	17,19,21	0.86	1 (5%)
5	BMA	E	3	5	11,11,12	0.29	0	15,15,17	0.67	0
6	NAG	F	1	1,6	14,14,15	0.38	0	17,19,21	0.89	1 (5%)
6	NAG	F	2	6	14,14,15	0.38	0	17,19,21	0.76	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
2	NAG	B	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1
2	BMA	B	3	2	-	1/2/19/22	0/1/1/1
2	MAN	B	4	2	-	0/2/19/22	0/1/1/1
2	MAN	B	5	2	-	0/2/19/22	0/1/1/1
2	MAN	B	6	2	-	0/2/19/22	0/1/1/1
3	NAG	C	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	FUC	C	3	3	-	-	0/1/1/1
4	NAG	D	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	1/6/23/26	0/1/1/1
4	BMA	D	3	4	-	0/2/19/22	0/1/1/1
4	MAN	D	4	4	-	0/2/19/22	0/1/1/1
4	MAN	D	5	4	-	0/2/19/22	0/1/1/1
4	FUC	D	6	4	-	-	0/1/1/1
5	NAG	E	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	2	5	-	2/6/23/26	0/1/1/1
5	BMA	E	3	5	-	0/2/19/22	0/1/1/1
6	NAG	F	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	F	2	6	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	NAG	C2-N2-C7	-3.46	118.27	122.90
3	C	1	NAG	O5-C1-C2	-3.17	106.39	111.29
4	D	1	NAG	O5-C1-C2	-2.82	106.93	111.29
2	B	3	BMA	C1-O5-C5	2.50	115.53	112.19
2	B	1	NAG	O5-C1-C2	-2.27	107.78	111.29
3	C	1	NAG	C4-C3-C2	-2.12	107.92	111.02
6	F	1	NAG	C2-N2-C7	-2.12	120.06	122.90
5	E	2	NAG	O5-C1-C2	-2.05	108.11	111.29
4	D	2	NAG	C2-N2-C7	-2.04	120.17	122.90

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1	NAG	C8-C7-N2-C2
3	C	1	NAG	O7-C7-N2-C2

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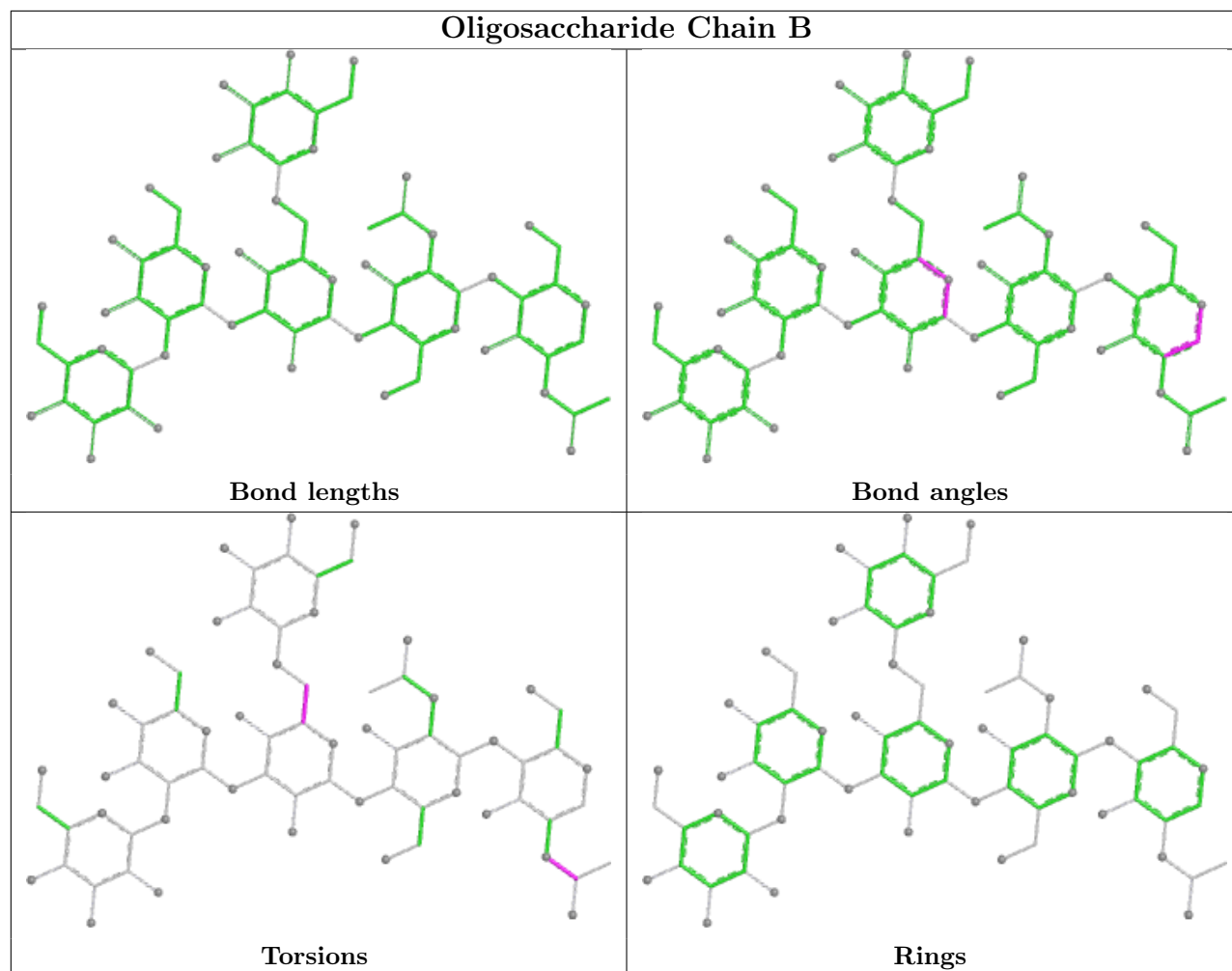
Mol	Chain	Res	Type	Atoms
4	D	1	NAG	C8-C7-N2-C2
4	D	1	NAG	O7-C7-N2-C2
2	B	1	NAG	C8-C7-N2-C2
2	B	1	NAG	O7-C7-N2-C2
5	E	2	NAG	C8-C7-N2-C2
6	F	1	NAG	C8-C7-N2-C2
6	F	1	NAG	O7-C7-N2-C2
5	E	2	NAG	O7-C7-N2-C2
2	B	3	BMA	O5-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
6	F	2	NAG	O5-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6

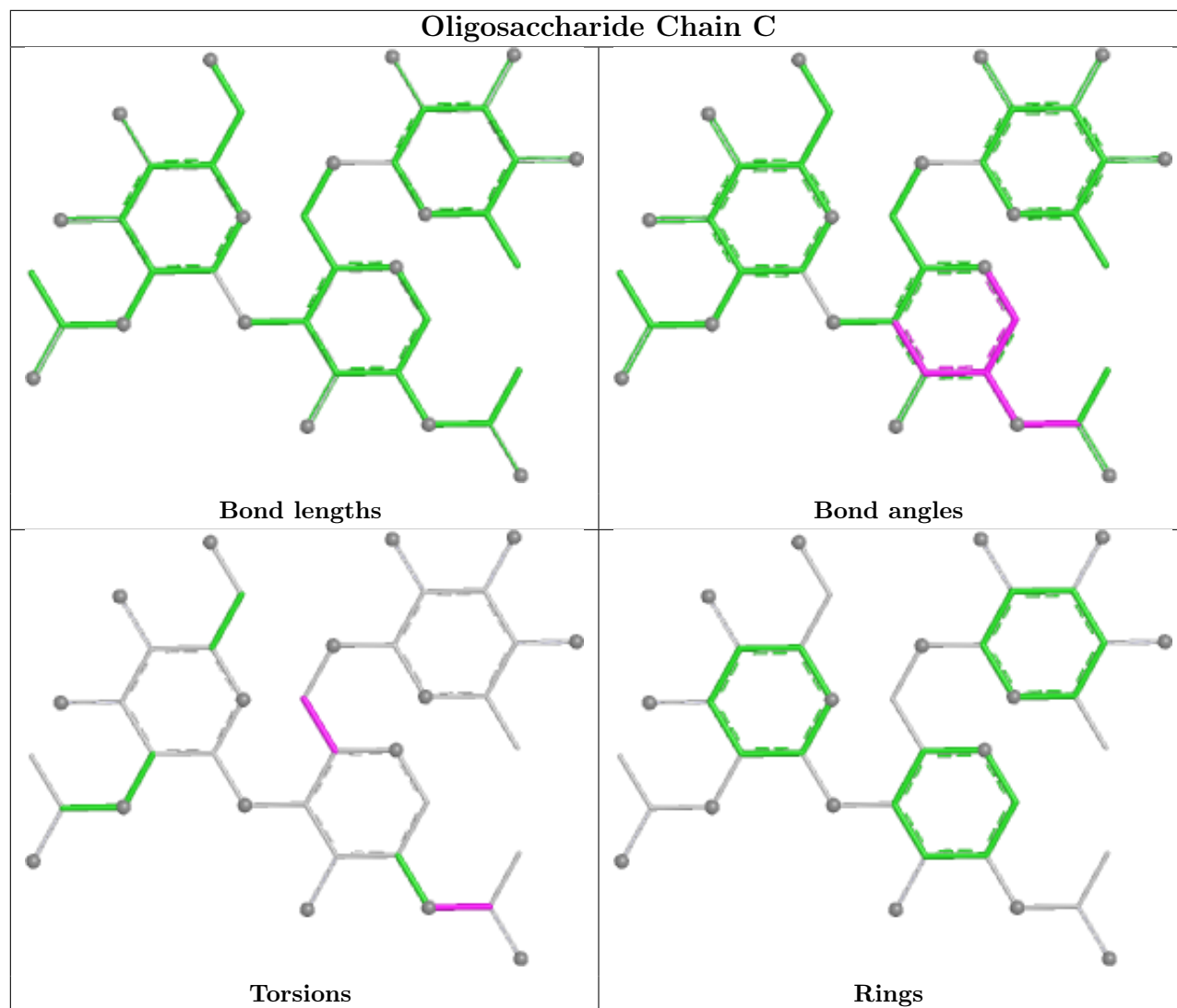
There are no ring outliers.

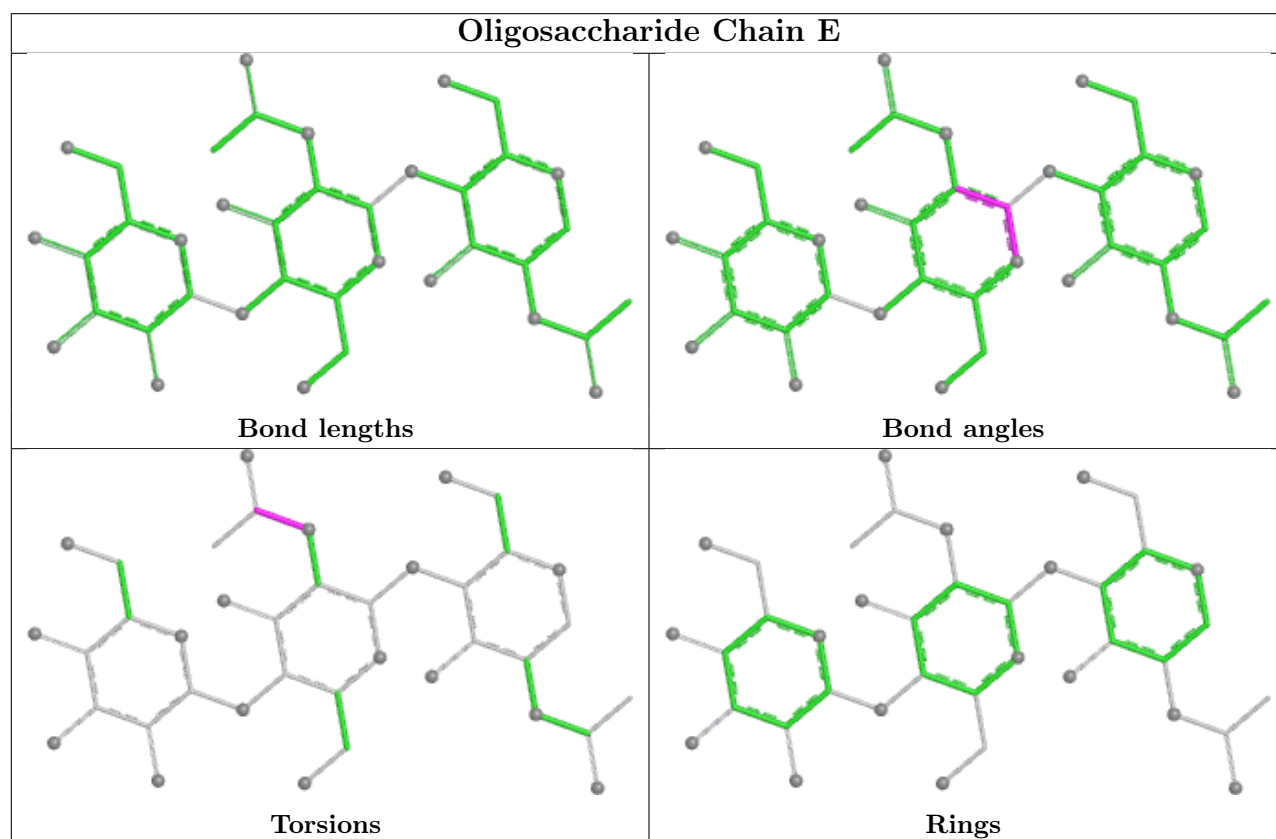
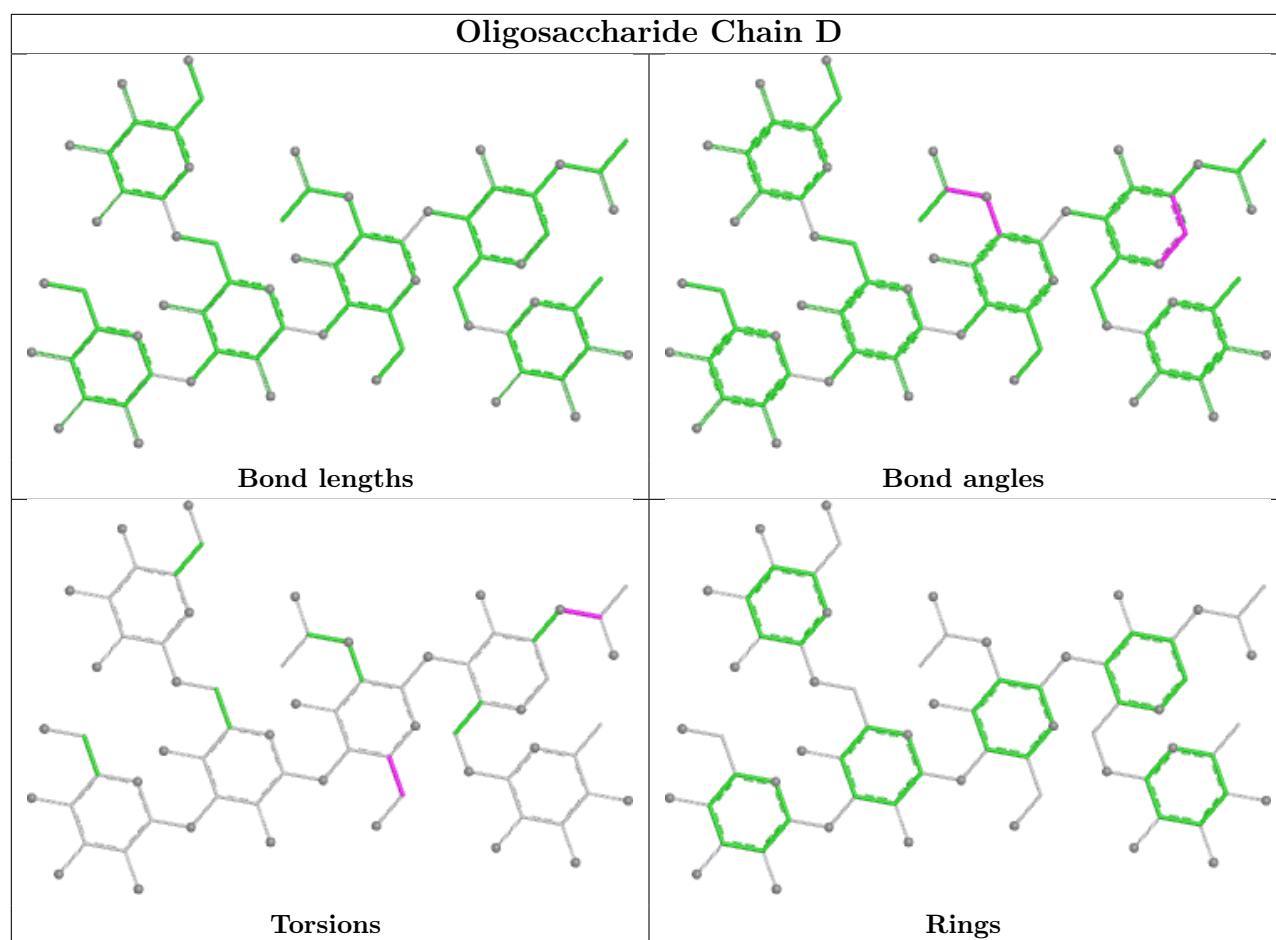
6 monomers are involved in 5 short contacts:

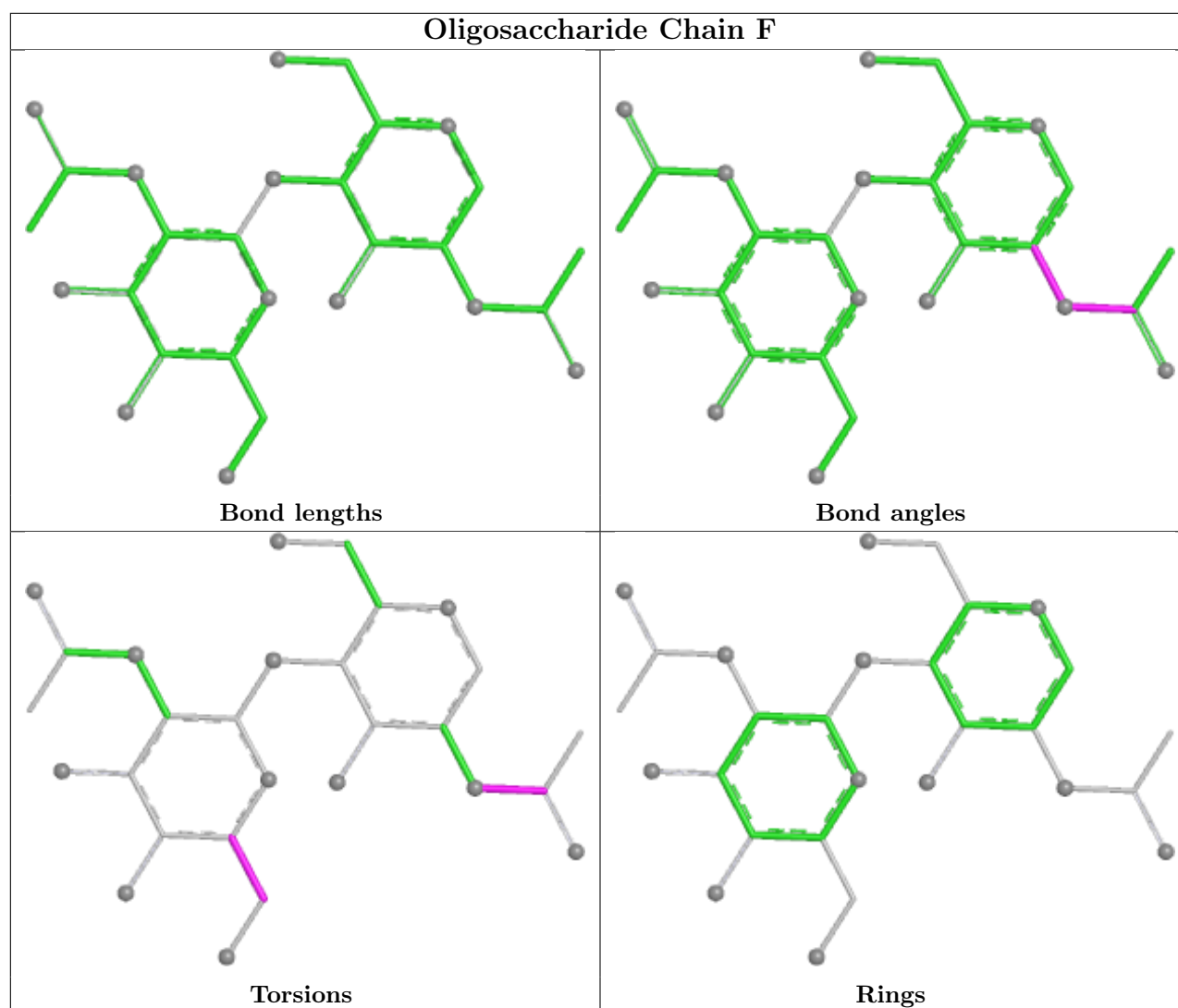
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	6	FUC	1	0
3	C	3	FUC	1	0
5	E	1	NAG	1	0
6	F	1	NAG	1	0
6	F	2	NAG	1	0
4	D	1	NAG	1	0

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](#)

10 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	NAG	A	2810	1	14,14,15	0.30	0	17,19,21	0.89	0
9	PEG	A	2806	-	6,6,6	0.11	0	5,5,5	0.07	0
7	NAG	A	2801	1	14,14,15	0.37	0	17,19,21	1.01	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	PEG	A	2805	-	6,6,6	0.10	0	5,5,5	0.11	0
8	GOL	A	2808	-	5,5,5	0.08	0	5,5,5	0.34	0
8	GOL	A	2807	-	5,5,5	0.08	0	5,5,5	0.31	0
8	GOL	A	2804	-	5,5,5	0.08	0	5,5,5	0.29	0
7	NAG	A	2802	1	14,14,15	0.30	0	17,19,21	0.84	0
8	GOL	A	2803	-	5,5,5	0.08	0	5,5,5	0.30	0
8	GOL	A	2809	-	5,5,5	0.08	0	5,5,5	0.32	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	A	2810	1	-	5/6/23/26	0/1/1/1
9	PEG	A	2806	-	-	1/4/4/4	-
7	NAG	A	2801	1	-	3/6/23/26	0/1/1/1
9	PEG	A	2805	-	-	0/4/4/4	-
8	GOL	A	2808	-	-	0/4/4/4	-
8	GOL	A	2807	-	-	0/4/4/4	-
8	GOL	A	2804	-	-	0/4/4/4	-
7	NAG	A	2802	1	-	4/6/23/26	0/1/1/1
8	GOL	A	2803	-	-	0/4/4/4	-
8	GOL	A	2809	-	-	0/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	2801	NAG	C2-N2-C7	-2.60	119.42	122.90
7	A	2801	NAG	O5-C1-C2	2.10	114.54	111.29

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	2801	NAG	C8-C7-N2-C2
7	A	2801	NAG	O7-C7-N2-C2
7	A	2802	NAG	C3-C2-N2-C7
7	A	2802	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
7	A	2802	NAG	O7-C7-N2-C2
7	A	2810	NAG	C8-C7-N2-C2
7	A	2810	NAG	O7-C7-N2-C2
7	A	2801	NAG	O5-C5-C6-O6
7	A	2810	NAG	O5-C5-C6-O6
7	A	2802	NAG	O5-C5-C6-O6
7	A	2810	NAG	C1-C2-N2-C7
7	A	2810	NAG	C3-C2-N2-C7
9	A	2806	PEG	C4-C3-O2-C2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	2810	NAG	1	0
9	A	2806	PEG	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	1772/1962 (90%)	0.56	135 (7%)	20 16	36, 63, 114, 166	2 (0%)

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2461	LEU	6.2
1	A	2638	ALA	5.3
1	A	850	TYR	5.2
1	A	851	ALA	5.1
1	A	1268	PRO	4.8
1	A	1272	ALA	4.8
1	A	1888	GLY	4.7
1	A	2460	THR	4.7
1	A	1395	ASP	4.6
1	A	2498	LYS	4.3
1	A	1385	LEU	4.3
1	A	2588	PHE	4.3
1	A	2690	GLN	4.1
1	A	2458	SER	4.0
1	A	2497	PRO	4.0
1	A	2565	TYR	4.0
1	A	2537	VAL	3.9
1	A	1389	THR	3.9
1	A	2532	ASP	3.8
1	A	828	PRO	3.8
1	A	1777	PRO	3.7
1	A	2695	PRO	3.6
1	A	1331	PRO	3.6
1	A	853	LEU	3.6
1	A	887	LEU	3.6
1	A	2587	MET	3.5
1	A	2566	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	2495	MET	3.3
1	A	2634	ALA	3.3
1	A	2696	GLY	3.3
1	A	852	LYS	3.3
1	A	2035	SER	3.3
1	A	1384	PRO	3.2
1	A	1215	VAL	3.2
1	A	2571	VAL	3.2
1	A	1609	ASN	3.2
1	A	2494	LYS	3.2
1	A	2487	PHE	3.1
1	A	2615	VAL	3.1
1	A	2572	LEU	3.1
1	A	1267	LEU	3.1
1	A	1218	ARG	3.0
1	A	2029	ARG	3.0
1	A	2586	GLY	2.9
1	A	2558	ILE	2.9
1	A	1332	ILE	2.9
1	A	1986	LEU	2.9
1	A	2513	PHE	2.8
1	A	1386	HIS	2.8
1	A	952	THR	2.8
1	A	1227	ASP	2.8
1	A	2031	GLY	2.8
1	A	2688	TYR	2.8
1	A	2551	PHE	2.8
1	A	2682	ILE	2.7
1	A	2293	LYS	2.7
1	A	2559	HIS	2.7
1	A	2550	TYR	2.7
1	A	1388	ALA	2.7
1	A	1396	THR	2.7
1	A	1447	GLU	2.7
1	A	2538	VAL	2.7
1	A	2567	VAL	2.7
1	A	855	THR	2.7
1	A	2687	LYS	2.6
1	A	1333	PRO	2.6
1	A	1943	ASN	2.6
1	A	1216	SER	2.6
1	A	872	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	2449	GLN	2.6
1	A	1811	LYS	2.6
1	A	2192	PHE	2.5
1	A	2100	LYS	2.5
1	A	2633	HIS	2.5
1	A	2620	GLY	2.5
1	A	2146	PHE	2.5
1	A	2552	LEU	2.5
1	A	1823	SER	2.5
1	A	2593	HIS	2.5
1	A	1269	GLY	2.4
1	A	1344	HIS	2.4
1	A	2099	ALA	2.4
1	A	2310	GLN	2.4
1	A	2686	HIS	2.4
1	A	2684	SER	2.4
1	A	1338	LEU	2.4
1	A	2098	SER	2.3
1	A	2554	LEU	2.3
1	A	2608	LEU	2.3
1	A	854	GLU	2.3
1	A	1323	HIS	2.3
1	A	2693	ASP	2.3
1	A	1387	CYS	2.3
1	A	2499	MET	2.3
1	A	2496	GLU	2.3
1	A	2036	LEU	2.3
1	A	2459	ASN	2.2
1	A	1075	GLY	2.2
1	A	2490	LYS	2.2
1	A	2493	LEU	2.2
1	A	2016	PHE	2.2
1	A	2148	ARG	2.2
1	A	2510	ARG	2.2
1	A	2694	ASP	2.2
1	A	2463	PRO	2.2
1	A	2425	LEU	2.2
1	A	2631	LEU	2.2
1	A	2193	ASN	2.2
1	A	1844	ARG	2.2
1	A	2418	PRO	2.2
1	A	2103	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	2621	VAL	2.1
1	A	1959	ALA	2.1
1	A	953	THR	2.1
1	A	2630	ILE	2.1
1	A	2685	ILE	2.1
1	A	1377	VAL	2.1
1	A	1564	ALA	2.1
1	A	1334	CYS	2.1
1	A	2557	SER	2.1
1	A	2239	PHE	2.1
1	A	1322	ASN	2.1
1	A	2617	ILE	2.1
1	A	2636	LYS	2.1
1	A	1809	ASP	2.1
1	A	2380	HIS	2.1
1	A	2628	HIS	2.1
1	A	2151	ALA	2.0
1	A	1213	THR	2.0
1	A	1968	LYS	2.0
1	A	2464	ASP	2.0
1	A	2485	PHE	2.0
1	A	2568	LYS	2.0
1	A	2312	TYR	2.0
1	A	2544	SER	2.0

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

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

6.3 Carbohydrates [i](#)

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

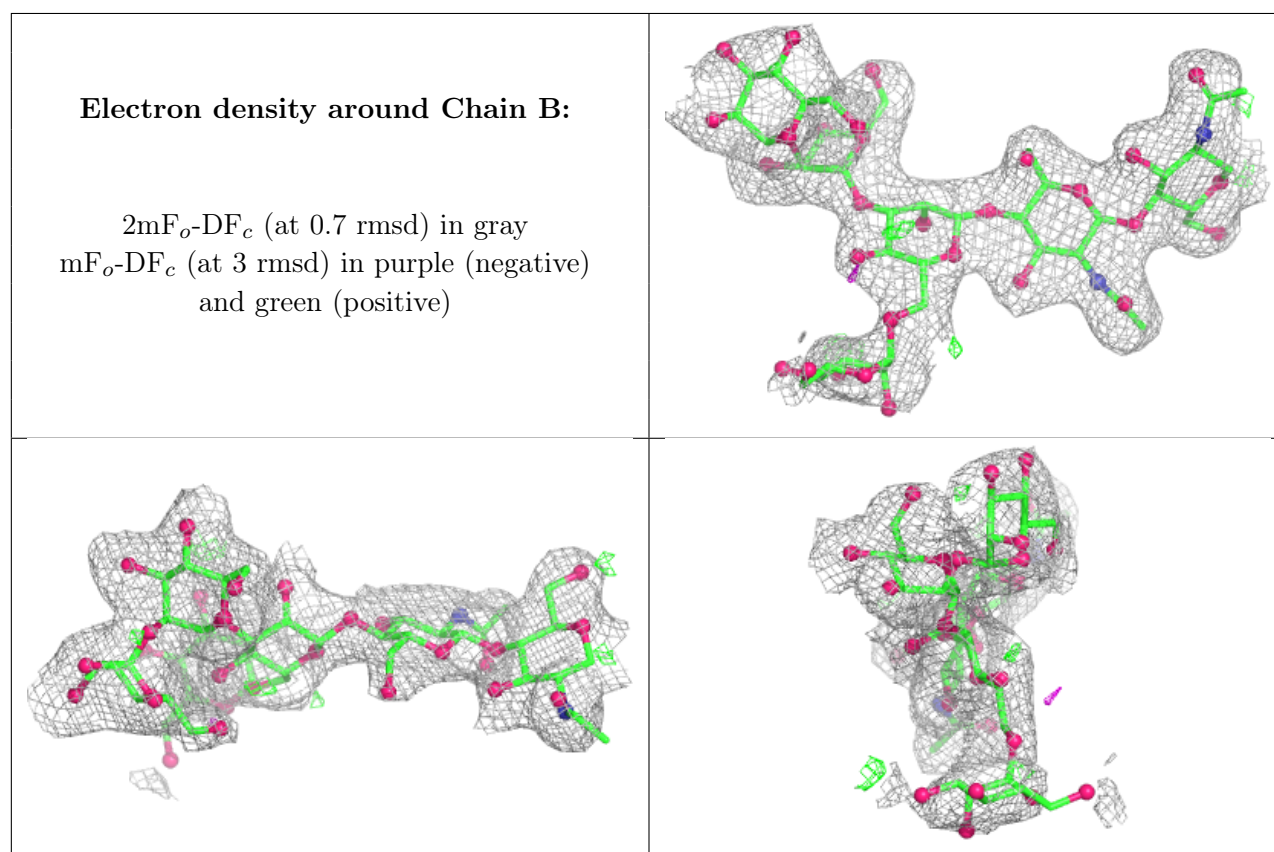
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	BMA	E	3	11/12	0.26	0.18	114,116,119,120	0
2	MAN	B	6	11/12	0.39	0.21	103,109,117,119	0
3	NAG	C	2	14/15	0.49	0.18	99,114,123,123	0
4	MAN	D	5	11/12	0.55	0.17	98,107,120,125	0

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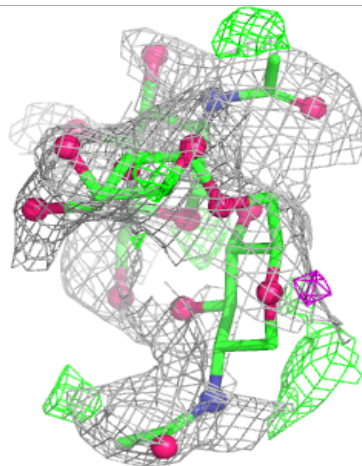
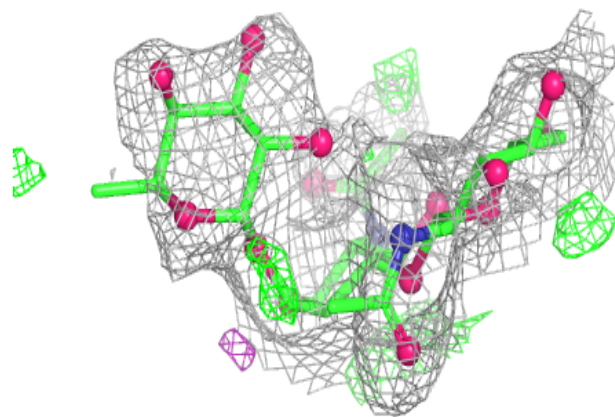
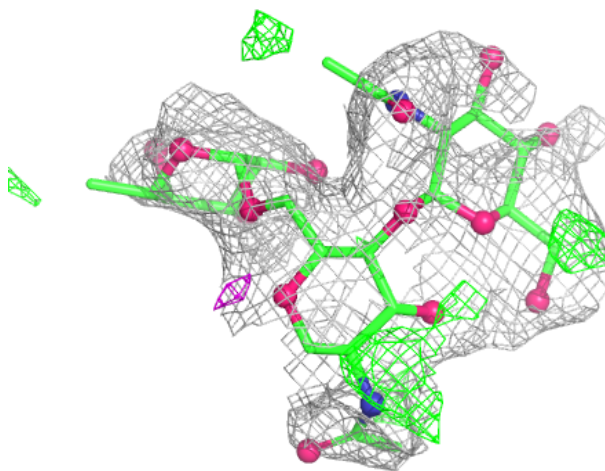
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	C	1	14/15	0.57	0.17	84,106,112,115	0
6	NAG	F	2	14/15	0.57	0.17	101,112,114,114	0
3	FUC	C	3	10/11	0.58	0.19	94,108,111,111	0
4	NAG	D	2	14/15	0.70	0.15	90,98,103,105	0
2	MAN	B	5	11/12	0.71	0.13	80,92,94,96	0
5	NAG	E	2	14/15	0.73	0.15	82,97,109,110	0
4	MAN	D	4	11/12	0.77	0.14	83,90,95,97	0
4	FUC	D	6	10/11	0.78	0.17	81,91,95,98	0
6	NAG	F	1	14/15	0.79	0.14	94,104,110,111	0
4	BMA	D	3	11/12	0.81	0.12	88,95,97,101	0
4	NAG	D	1	14/15	0.82	0.12	74,81,90,90	0
2	BMA	B	3	11/12	0.84	0.12	66,70,81,98	0
2	MAN	B	4	11/12	0.87	0.11	65,76,80,87	0
5	NAG	E	1	14/15	0.90	0.11	59,73,82,84	0
2	NAG	B	2	14/15	0.92	0.09	45,57,64,67	0
2	NAG	B	1	14/15	0.93	0.10	50,59,71,72	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.



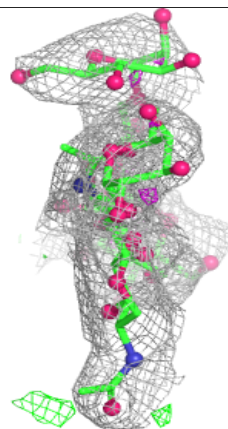
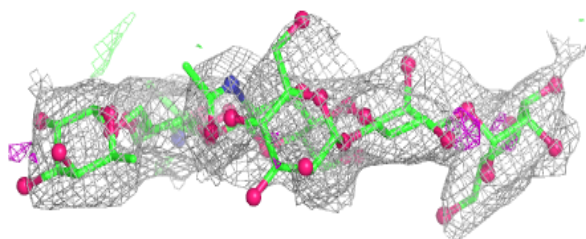
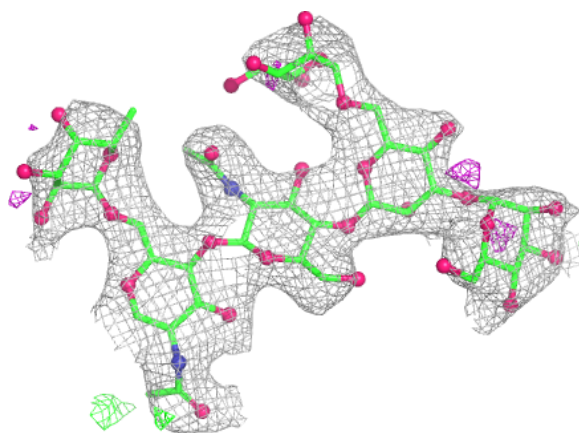
Electron density around Chain C:

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

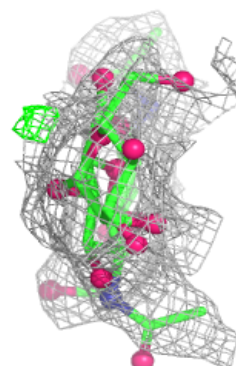
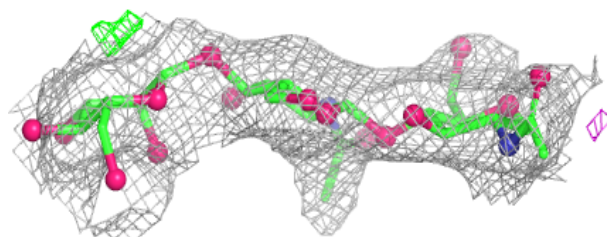
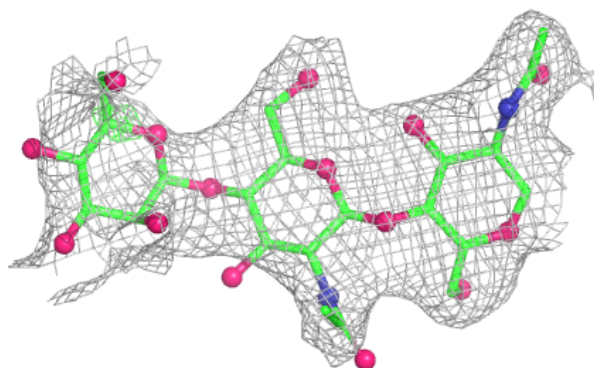


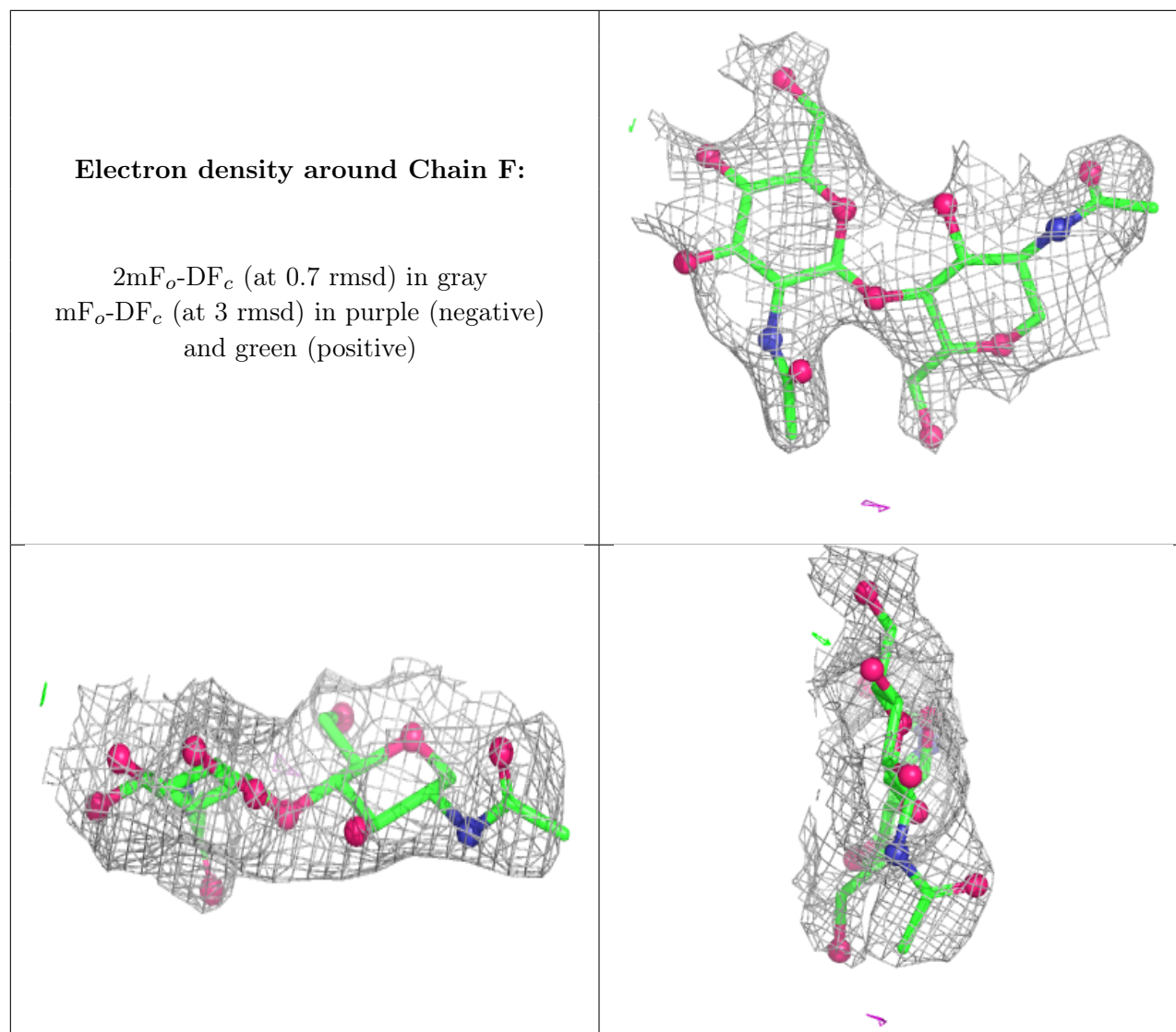
Electron density around Chain D:

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

**Electron density around Chain E:**

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	NAG	A	2810	14/15	0.45	0.19	96,116,120,121	0
7	NAG	A	2801	14/15	0.46	0.20	91,99,107,107	0
7	NAG	A	2802	14/15	0.50	0.17	111,117,123,124	0
8	GOL	A	2808	6/6	0.66	0.15	78,88,91,93	0
9	PEG	A	2806	7/7	0.77	0.20	61,63,70,81	0
9	PEG	A	2805	7/7	0.79	0.17	63,74,81,82	0
8	GOL	A	2809	6/6	0.83	0.18	53,67,70,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	GOL	A	2803	6/6	0.90	0.15	51,58,60,66	0
8	GOL	A	2804	6/6	0.90	0.18	51,55,60,64	0
8	GOL	A	2807	6/6	0.92	0.11	42,52,56,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.