



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:11 AM UTC

PDB ID : 7R3N / pdb_00007r3n
Title : mouse Interleukin-12 subunit beta - p80 homodimer in space group P21 crystal form 3
Authors : Bloch, Y.; Savvides, S.N.
Deposited on : 2022-02-07
Resolution : 3.16 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

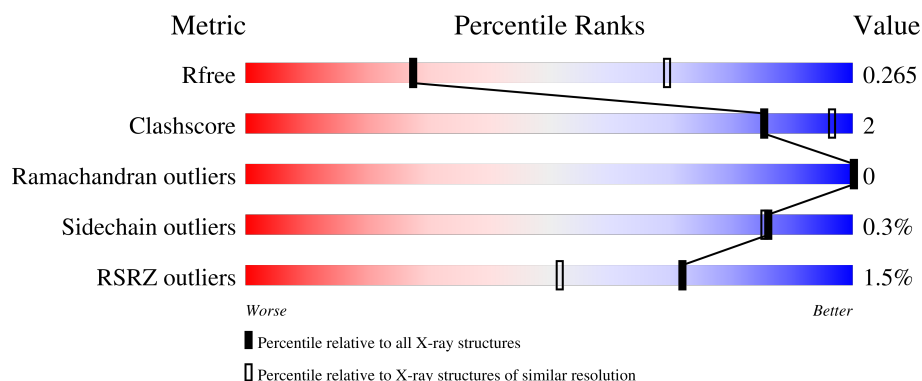
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.16 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.



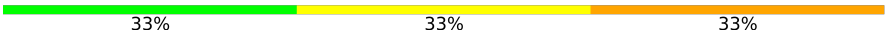
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)

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	335	82% 9% 9%
1	B	335	86% 5% 9%
1	C	335	3% 88% • 10%
1	D	335	86% 5% 9%
2	E	4	50% 25% 25%

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Mol	Chain	Length	Quality of chain
2	F	4	 25% 75%
2	H	4	 50% 25% 25%
3	G	3	 33% 33% 33%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9888 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 Interleukin-12 subunit beta.

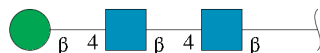
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	304	Total	C	N	O	S	0	1	0
			2414	1519	401	477	17			
1	B	304	Total	C	N	O	S	0	1	0
			2429	1527	409	476	17			
1	C	302	Total	C	N	O	S	0	0	0
			2401	1509	402	473	17			
1	D	305	Total	C	N	O	S	0	0	0
			2429	1525	411	476	17			

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



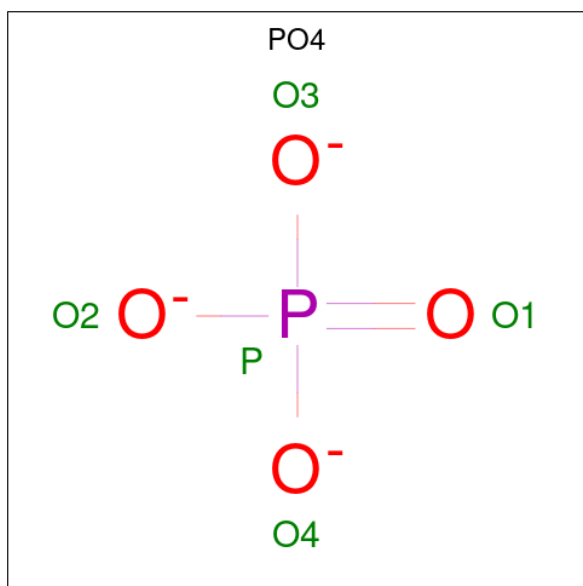
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	4	Total	C	N	O	0	0	0
			50	28	2	20			
2	F	4	Total	C	N	O	0	0	0
			50	28	2	20			
2	H	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 3 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
3	G	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		
4	D	1	Total	O	P	0	0
			5	4	1		
4	D	1	Total	O	P	0	0
			5	4	1		

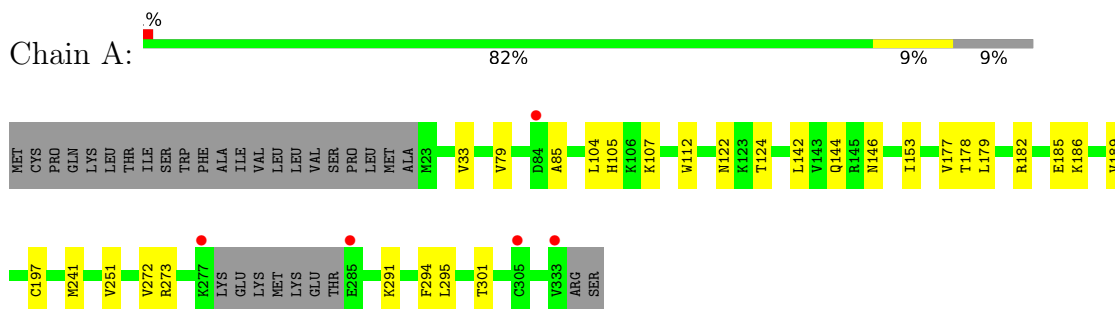
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O	0	0
			1	1		

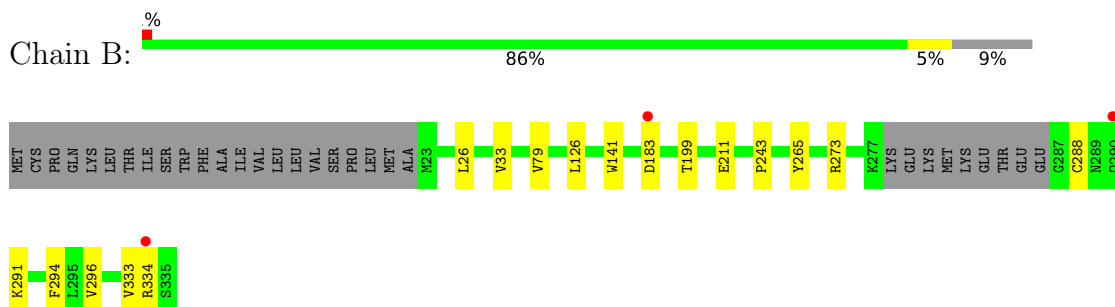
3 Residue-property plots [i](#)

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.

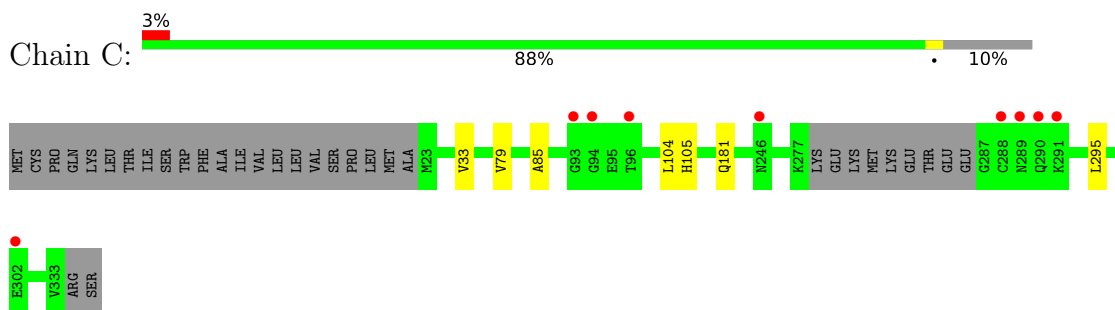
- Molecule 1: Interleukin-12 subunit beta



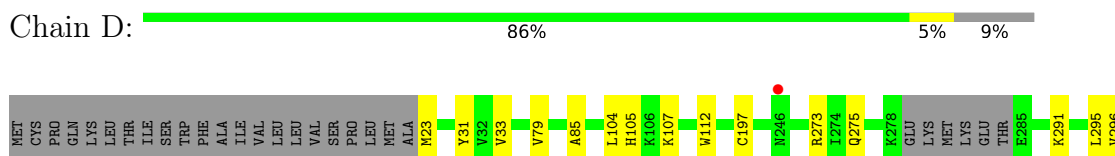
- Molecule 1: Interleukin-12 subunit beta



- Molecule 1: Interleukin-12 subunit beta



- Molecule 1: Interleukin-12 subunit beta





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

Chain E:



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

Chain F:



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

Chain H:



- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	112.81Å 65.17Å 134.31Å 90.00° 98.09° 90.00°	Depositor
Resolution (Å)	61.03 – 3.16 61.03 – 3.16	Depositor EDS
% Data completeness (in resolution range)	99.0 (61.03-3.16) 99.3 (61.03-3.16)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 3.13Å)	Xtriage
Refinement program	BUSTER, PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.220 , 0.258 0.234 , 0.265	Depositor DCC
R_{free} test set	2111 reflections (5.97%)	wwPDB-VP
Wilson B-factor (Å ²)	92.6	Xtriage
Anisotropy	0.327	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 78.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9888	wwPDB-VP
Average B, all atoms (Å ²)	117.0	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 45.29 % 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 1.3505e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, PO4, BMA, 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	0.54	0/2474	0.75	0/3356
1	B	0.44	0/2489	0.72	1/3373 (0.0%)
1	C	0.33	0/2457	0.63	0/3332
1	D	0.45	0/2485	0.68	0/3367
All	All	0.45	0/9905	0.70	1/13428 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	288	CYS	N-CA-C	7.28	119.90	111.02

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	197	CYS	Peptide
1	D	197	CYS	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2414	0	2285	17	0
1	B	2429	0	2327	10	0
1	C	2401	0	2288	4	0
1	D	2429	0	2328	11	0
2	E	50	0	43	1	0
2	F	50	0	43	0	0
2	H	50	0	43	1	0
3	G	39	0	34	1	0
4	A	5	0	0	0	0
4	B	10	0	0	1	0
4	D	10	0	0	0	0
5	A	1	0	0	0	0
All	All	9888	0	9391	42	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 2.

All (42) 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:D:273:ARG:HH11	1:D:291:LYS:HG3	1.57	0.70
1:A:144:GLN:O	1:A:182:ARG:NH2	2.28	0.65
1:B:126:LEU:HD23	1:B:141:TRP:HB3	1.82	0.62
1:A:178:THR:O	1:A:179:LEU:HD12	2.05	0.56
1:A:295:LEU:C	1:A:295:LEU:HD23	2.31	0.55
1:B:296:VAL:HG23	4:B:401:PO4:O4	2.08	0.53
1:B:33:VAL:HG11	1:B:79:VAL:HG21	1.90	0.53
1:A:272:VAL:HB	1:A:294[B]:PHE:CE1	2.44	0.53
1:B:199:THR:HG23	1:B:265:TYR:CE2	2.44	0.52
1:D:23:MET:HE3	1:D:31:TYR:CD2	2.44	0.52
1:D:105:HIS:CE1	2:H:1:NAG:H62	2.46	0.51
1:B:243:PRO:HG3	1:B:334:ARG:HG3	1.91	0.51
1:D:296:VAL:HG21	1:D:301:THR:HG23	1.93	0.51
1:A:107:LYS:HB2	1:A:112:TRP:CZ3	2.47	0.50
1:C:105:HIS:CE1	3:G:1:NAG:HO6	2.29	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:ASN:CB	1:A:185:GLU:OE1	2.61	0.48
1:D:33:VAL:HG11	1:D:79:VAL:HG21	1.95	0.48
1:A:85:ALA:HB2	1:A:104:LEU:HD13	1.96	0.48
1:C:33:VAL:HG11	1:C:79:VAL:HG21	1.94	0.48
1:A:33:VAL:HG11	1:A:79:VAL:HG21	1.95	0.47
1:D:296:VAL:HG21	1:D:301:THR:CG2	2.45	0.47
1:C:85:ALA:HB2	1:C:104:LEU:HD13	1.97	0.47
1:A:153:ILE:HG21	1:A:189:VAL:HG11	1.97	0.46
1:B:26:LEU:HD11	1:B:211:GLU:OE2	2.16	0.46
1:A:241:MET:SD	1:A:251:VAL:HG12	2.56	0.45
1:D:275:GLN:NE2	1:D:311:CYS:SG	2.89	0.45
1:A:122:ASN:OD1	1:A:124:THR:HG23	2.16	0.45
1:A:146:ASN:HB3	1:A:185:GLU:OE1	2.17	0.45
1:D:107:LYS:HB2	1:D:112:TRP:CZ3	2.52	0.44
1:A:142:LEU:HD23	1:A:186:LYS:HB2	1.98	0.44
1:A:177:VAL:HG12	1:A:179:LEU:HD13	2.00	0.44
1:B:199:THR:HG23	1:B:265:TYR:CZ	2.53	0.43
1:B:273:ARG:HH11	1:B:291:LYS:HG3	1.81	0.43
1:D:85:ALA:HB2	1:D:104:LEU:HD13	2.00	0.43
1:D:295:LEU:C	1:D:295:LEU:HD23	2.43	0.42
1:A:105:HIS:CE1	2:E:1:NAG:H62	2.55	0.42
1:A:251:VAL:HG22	1:A:301:THR:O	2.20	0.42
1:A:273:ARG:HD3	1:A:291:LYS:HB3	2.02	0.42
1:B:273:ARG:NH1	1:B:291:LYS:HG3	2.35	0.41
1:D:273:ARG:NH1	1:D:291:LYS:HG3	2.29	0.41
1:C:295:LEU:C	1:C:295:LEU:HD23	2.46	0.41
1:B:183:ASP:OD1	1:B:183:ASP:O	2.39	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	301/335 (90%)	292 (97%)	9 (3%)	0	100	100
1	B	301/335 (90%)	292 (97%)	9 (3%)	0	100	100
1	C	298/335 (89%)	293 (98%)	5 (2%)	0	100	100
1	D	301/335 (90%)	295 (98%)	6 (2%)	0	100	100
All	All	1201/1340 (90%)	1172 (98%)	29 (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	272/307 (89%)	272 (100%)	0	100	100
1	B	277/307 (90%)	274 (99%)	3 (1%)	65	75
1	C	272/307 (89%)	271 (100%)	1 (0%)	84	84
1	D	276/307 (90%)	276 (100%)	0	100	100
All	All	1097/1228 (89%)	1093 (100%)	4 (0%)	86	84

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	294[A]	PHE
1	B	294[B]	PHE
1	B	333	VAL
1	C	181	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	ASN
1	A	152	ASN
1	A	304	GLN

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Mol	Chain	Res	Type
1	B	47	ASN
1	B	87	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 ⓘ

15 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	E	1	1,2	14,14,15	0.43	0	17,19,21	1.01	1 (5%)
2	NAG	E	2	2	14,14,15	0.33	0	17,19,21	1.27	1 (5%)
2	BMA	E	3	2	11,11,12	0.33	0	15,15,17	0.71	0
2	MAN	E	4	2	11,11,12	0.20	0	15,15,17	0.61	0
2	NAG	F	1	1,2	14,14,15	0.46	0	17,19,21	0.76	1 (5%)
2	NAG	F	2	2	14,14,15	0.34	0	17,19,21	1.11	1 (5%)
2	BMA	F	3	2	11,11,12	0.29	0	15,15,17	0.89	1 (6%)
2	MAN	F	4	2	11,11,12	0.24	0	15,15,17	0.53	0
3	NAG	G	1	1,3	14,14,15	0.55	0	17,19,21	0.98	1 (5%)
3	NAG	G	2	3	14,14,15	0.30	0	17,19,21	1.17	1 (5%)
3	BMA	G	3	3	11,11,12	0.27	0	15,15,17	0.53	0
2	NAG	H	1	1,2	14,14,15	0.27	0	17,19,21	0.87	1 (5%)
2	NAG	H	2	2	14,14,15	0.34	0	17,19,21	0.97	1 (5%)
2	BMA	H	3	2	11,11,12	0.30	0	15,15,17	0.57	0
2	MAN	H	4	2	11,11,12	0.21	0	15,15,17	0.47	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	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	BMA	E	3	2	-	0/2/19/22	0/1/1/1
2	MAN	E	4	2	-	0/2/19/22	0/1/1/1
2	NAG	F	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	BMA	F	3	2	-	1/2/19/22	0/1/1/1
2	MAN	F	4	2	-	0/2/19/22	0/1/1/1
3	NAG	G	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	BMA	G	3	3	-	0/2/19/22	0/1/1/1
2	NAG	H	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
2	BMA	H	3	2	-	0/2/19/22	0/1/1/1
2	MAN	H	4	2	-	0/2/19/22	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	G	2	NAG	O5-C1-C2	-4.43	104.44	111.29
2	E	2	NAG	O5-C1-C2	-4.32	104.60	111.29
2	F	2	NAG	O5-C1-C2	-3.93	105.22	111.29
3	G	1	NAG	C1-O5-C5	3.55	116.94	112.19
2	H	2	NAG	O5-C1-C2	-3.38	106.07	111.29
2	H	1	NAG	C1-O5-C5	3.22	116.50	112.19
2	E	1	NAG	C1-O5-C5	3.18	116.45	112.19
2	F	1	NAG	C1-O5-C5	2.57	115.63	112.19
2	F	3	BMA	C1-O5-C5	-2.43	108.93	112.19

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	2	NAG	C8-C7-N2-C2
2	F	2	NAG	O7-C7-N2-C2

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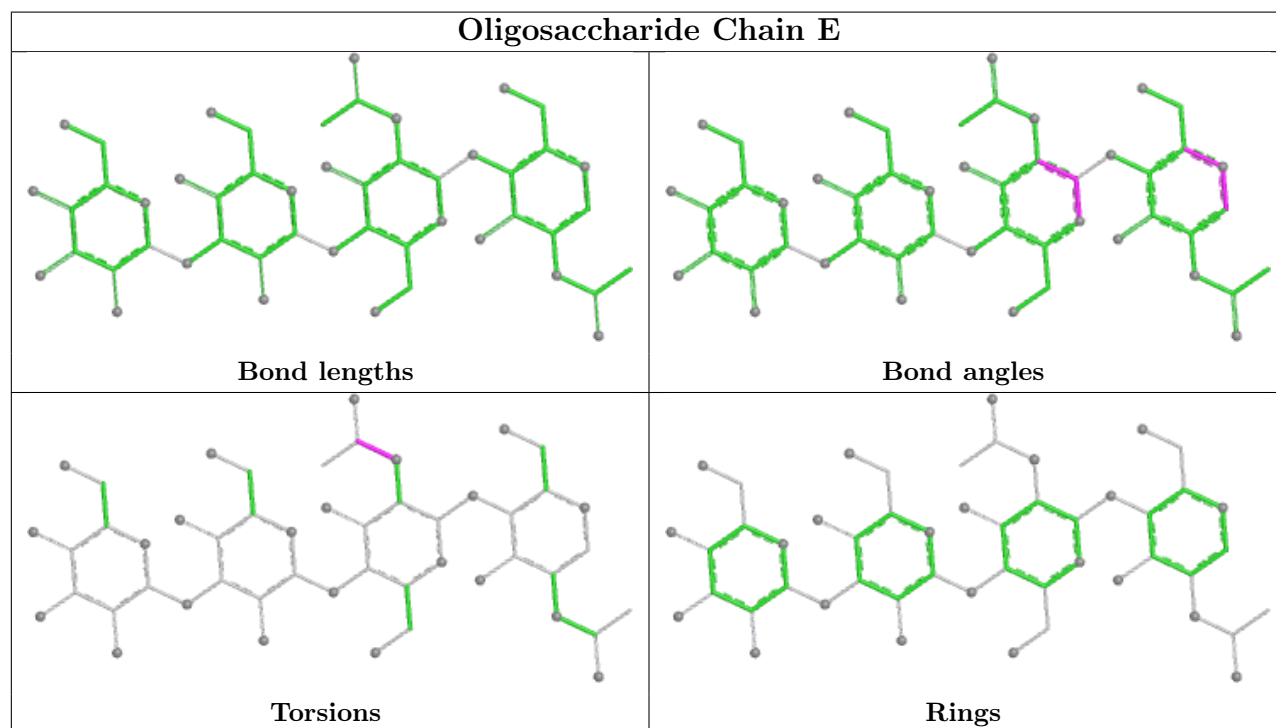
Mol	Chain	Res	Type	Atoms
3	G	2	NAG	C8-C7-N2-C2
3	G	2	NAG	O7-C7-N2-C2
3	G	1	NAG	C8-C7-N2-C2
3	G	1	NAG	O7-C7-N2-C2
2	H	2	NAG	C8-C7-N2-C2
2	F	3	BMA	O5-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
2	E	2	NAG	C8-C7-N2-C2
2	H	2	NAG	O7-C7-N2-C2
3	G	1	NAG	C4-C5-C6-O6
2	E	2	NAG	O7-C7-N2-C2

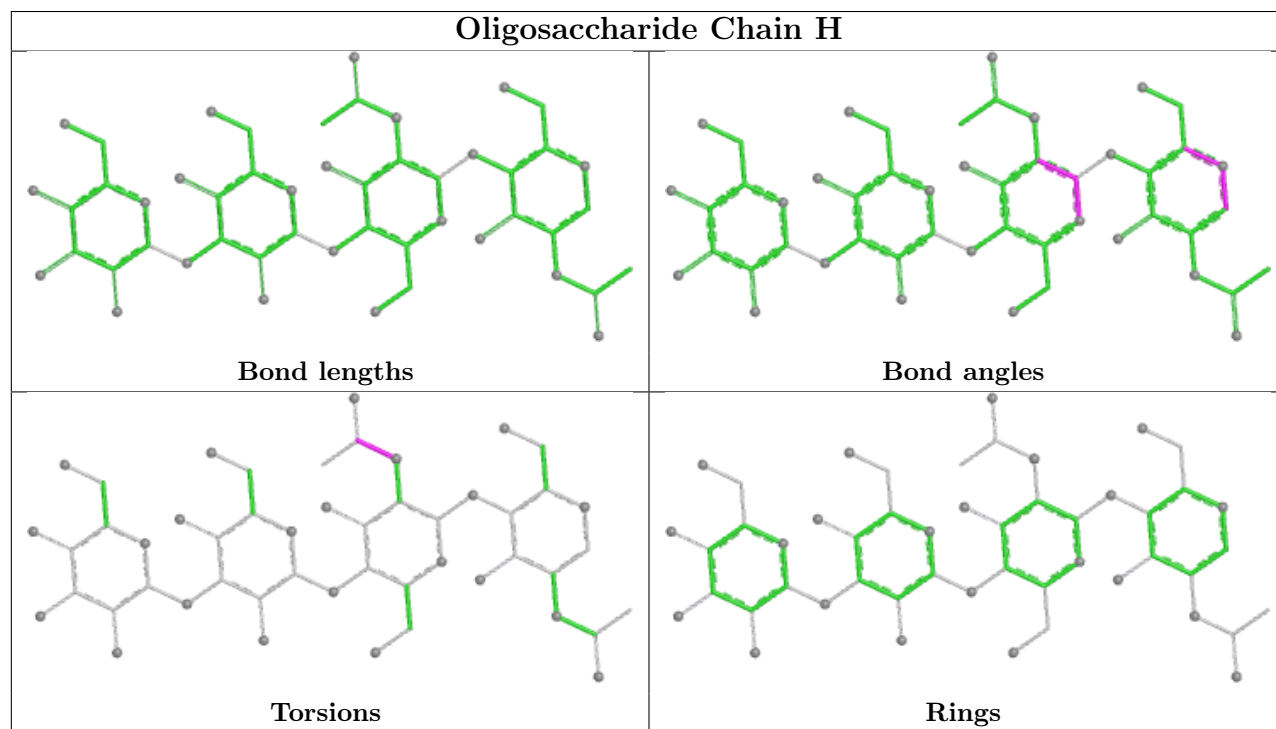
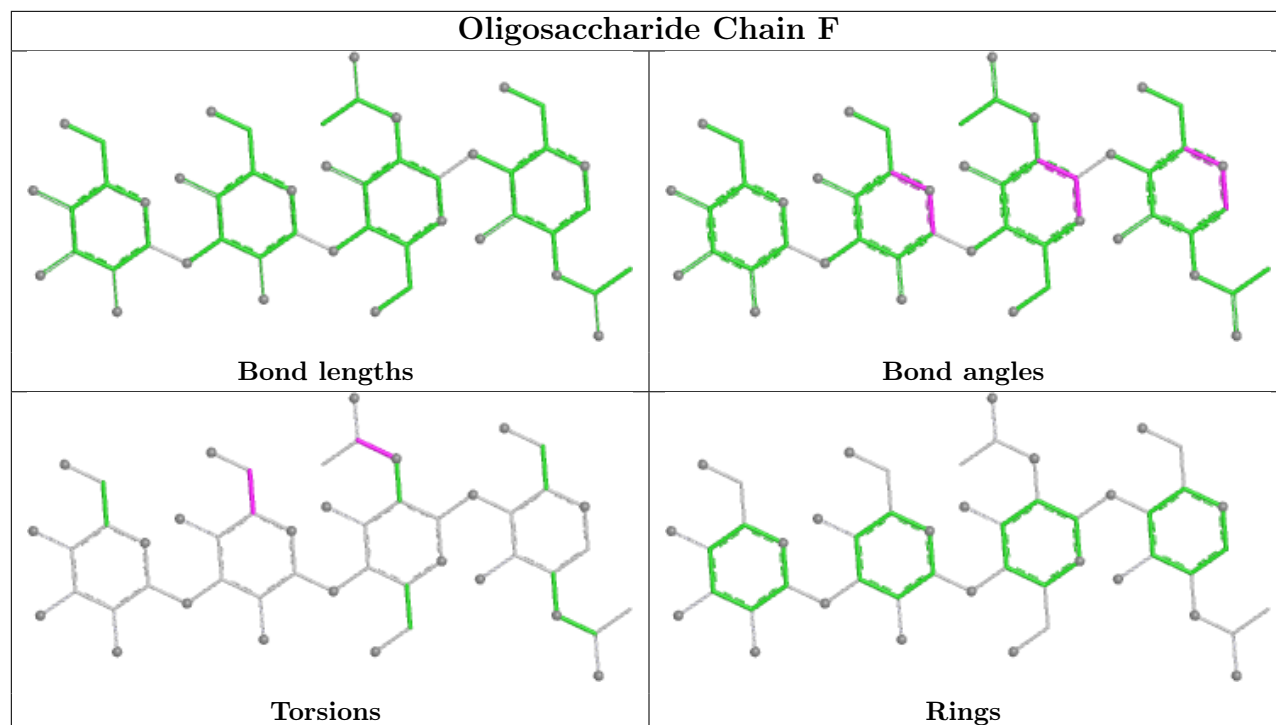
There are no ring outliers.

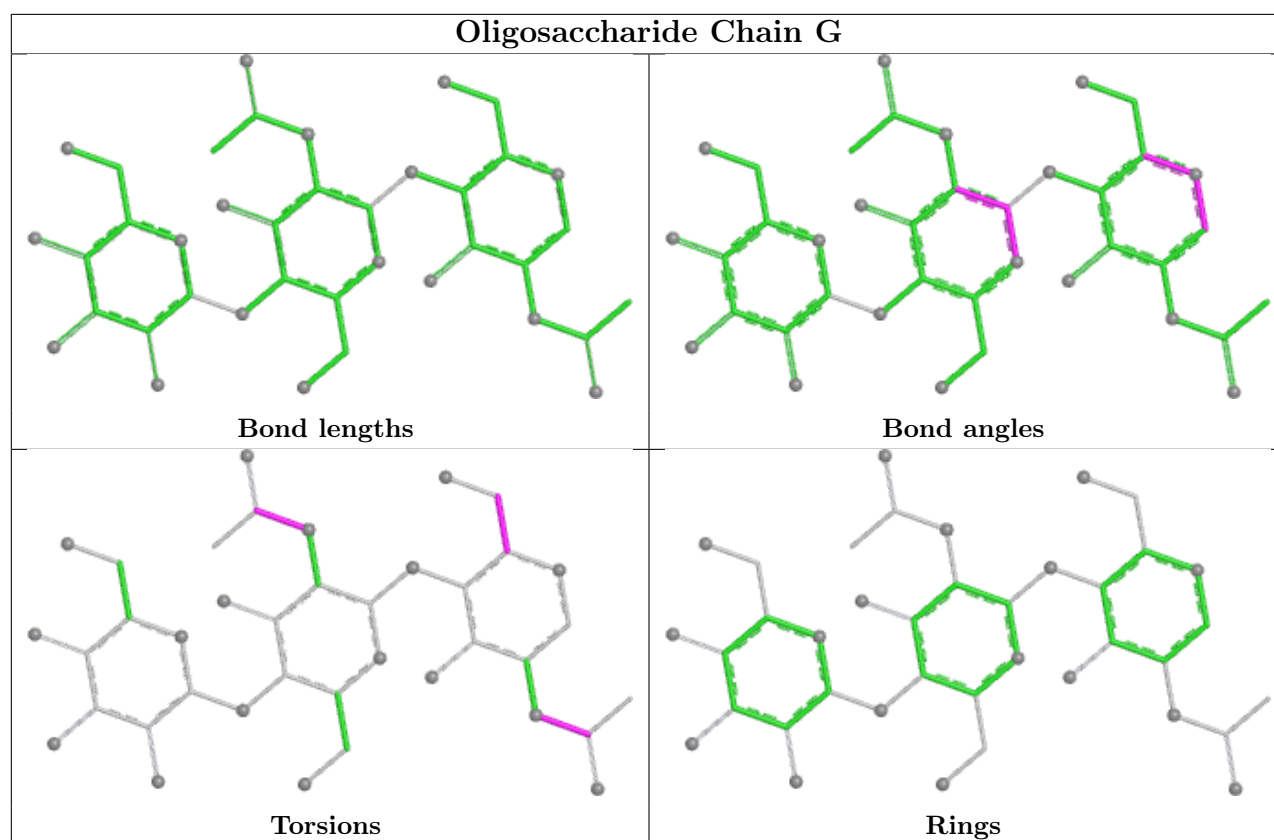
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	1	NAG	1	0
2	H	1	NAG	1	0
2	E	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](#)

5 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	$\# Z > 2$
4	PO4	D	402	-	4,4,4	2.48	3 (75%)	6,6,6	0.43	0
4	PO4	B	402	-	4,4,4	2.52	3 (75%)	6,6,6	0.47	0
4	PO4	B	401	-	4,4,4	2.53	3 (75%)	6,6,6	0.48	0
4	PO4	A	401	-	4,4,4	2.52	3 (75%)	6,6,6	0.45	0
4	PO4	D	401	-	4,4,4	2.38	3 (75%)	6,6,6	0.41	0

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	402	PO4	P-O2	-2.88	1.46	1.54
4	A	401	PO4	P-O2	-2.85	1.46	1.54
4	A	401	PO4	P-O3	-2.82	1.46	1.54
4	B	401	PO4	P-O4	-2.76	1.46	1.54
4	B	401	PO4	P-O2	-2.76	1.46	1.54
4	D	402	PO4	P-O4	-2.75	1.46	1.54
4	D	402	PO4	P-O3	-2.74	1.46	1.54
4	B	401	PO4	P-O3	-2.73	1.46	1.54
4	B	402	PO4	P-O4	-2.68	1.46	1.54
4	B	402	PO4	P-O3	-2.67	1.46	1.54
4	D	401	PO4	P-O2	-2.65	1.46	1.54
4	D	402	PO4	P-O2	-2.65	1.46	1.54
4	A	401	PO4	P-O4	-2.64	1.46	1.54
4	D	401	PO4	P-O4	-2.57	1.47	1.54
4	D	401	PO4	P-O3	-2.52	1.47	1.54

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	401	PO4	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	304/335 (90%)	-0.17	5 (1%)	70 50	45, 78, 153, 174	1 (0%)
1	B	304/335 (90%)	-0.20	3 (0%)	79 62	32, 120, 203, 238	1 (0%)
1	C	302/335 (90%)	0.09	9 (2%)	52 32	106, 153, 203, 218	0
1	D	305/335 (91%)	-0.23	1 (0%)	90 81	51, 93, 177, 216	0
All	All	1215/1340 (90%)	-0.13	18 (1%)	72 52	32, 114, 199, 238	2 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	94	GLY	5.4
1	D	246	ASN	3.4
1	C	290	GLN	3.3
1	C	246	ASN	3.3
1	C	302	GLU	3.0
1	A	305	CYS	2.6
1	C	291	LYS	2.6
1	A	277	LYS	2.5
1	C	96	THR	2.4
1	C	289	ASN	2.4
1	A	285	GLU	2.3
1	A	333	VAL	2.3
1	B	334	ARG	2.3
1	B	290	GLN	2.3
1	A	84	ASP	2.1
1	C	288	CYS	2.1
1	C	93	GLY	2.1
1	B	183	ASP	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 ⓘ

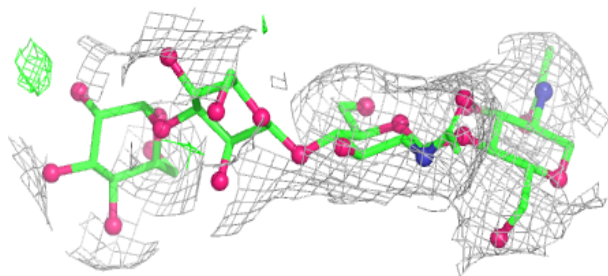
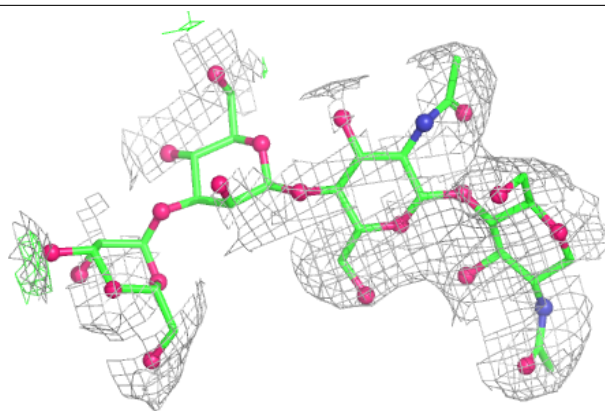
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MAN	H	4	11/12	0.32	0.12	222,229,243,247	0
2	BMA	H	3	11/12	0.38	0.15	205,212,223,235	0
3	BMA	G	3	11/12	0.49	0.11	149,163,166,169	0
2	NAG	F	2	14/15	0.64	0.11	157,174,180,181	0
2	MAN	F	4	11/12	0.65	0.08	167,180,187,188	0
2	MAN	E	4	11/12	0.68	0.08	118,141,148,151	0
3	NAG	G	1	14/15	0.71	0.10	142,151,158,160	0
2	BMA	F	3	11/12	0.75	0.06	174,183,192,193	0
3	NAG	G	2	14/15	0.77	0.09	146,162,166,168	0
2	NAG	F	1	14/15	0.78	0.11	150,163,174,182	0
2	NAG	H	2	14/15	0.79	0.17	145,188,196,197	0
2	BMA	E	3	11/12	0.84	0.09	79,103,130,139	0
2	NAG	E	2	14/15	0.91	0.08	69,83,88,89	0
2	NAG	H	1	14/15	0.92	0.13	100,108,131,138	0
2	NAG	E	1	14/15	0.95	0.07	54,64,69,76	0

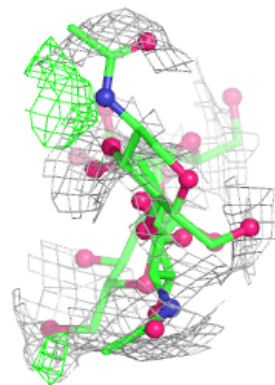
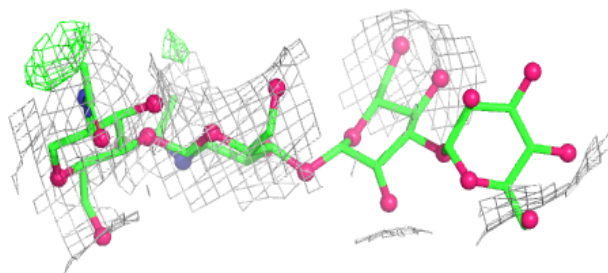
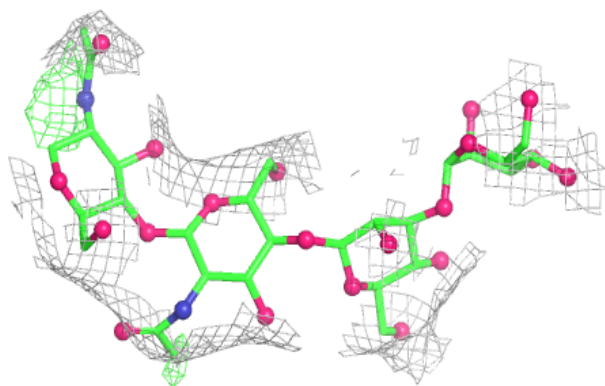
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

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

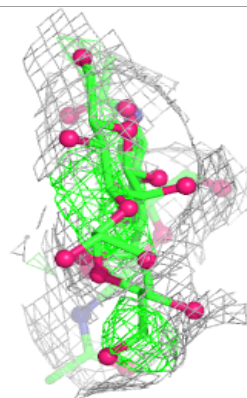
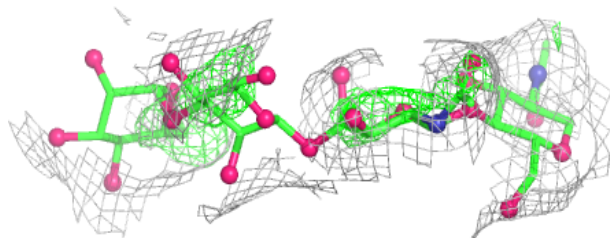
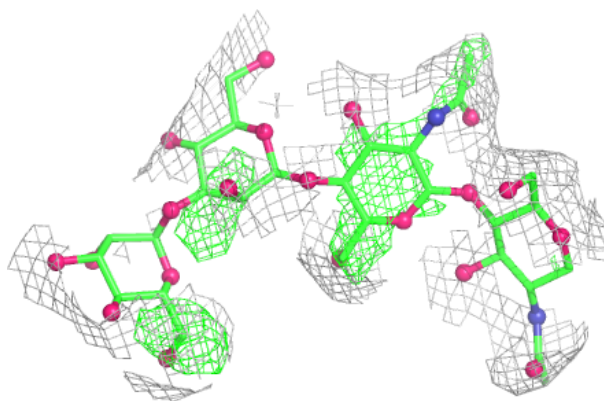
**Electron density around Chain F:**

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

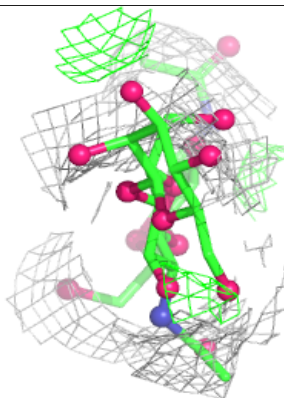
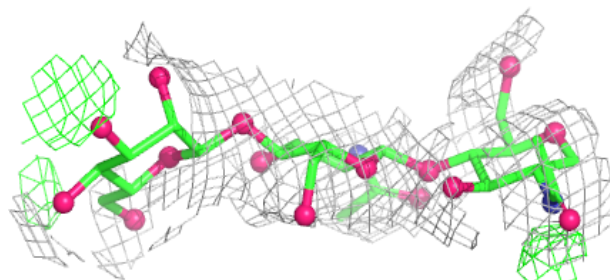
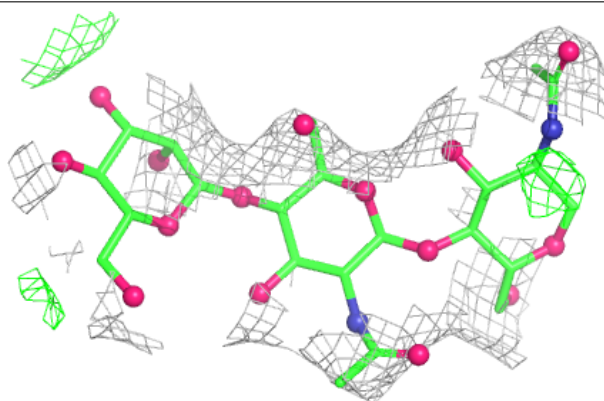


Electron density around Chain H:

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

**Electron density around Chain G:**

$2mF_o-DF_c$ (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
4	PO4	B	402	5/5	0.82	0.14	124,124,124,124	0
4	PO4	B	401	5/5	0.83	0.22	127,127,134,145	0
4	PO4	D	402	5/5	0.86	0.18	109,109,119,121	0
4	PO4	A	401	5/5	0.87	0.11	72,85,103,108	0
4	PO4	D	401	5/5	0.95	0.07	62,71,87,88	0

6.5 Other polymers [i](#)

There are no such residues in this entry.