



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 03:01 AM UTC

PDB ID : 6FKN / pdb_00006fkn
Title : Drosophila Plexin A in complex with Semaphorin 1b
Authors : Rozbesky, D.; Harlos, K.; Jones, E.Y.
Deposited on : 2018-01-24
Resolution : 4.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

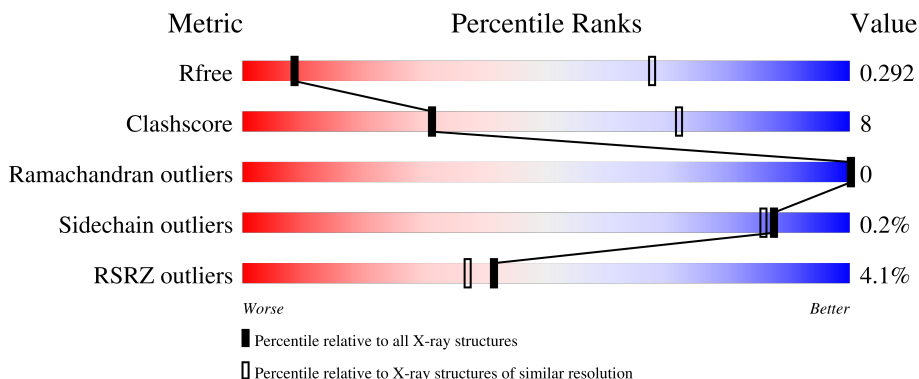
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.80 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	1018 (5.66-3.94)
Clashscore	190562	1001 (5.60-3.98)
Ramachandran outliers	187476	1104 (5.70-3.90)
Sidechain outliers	187428	1085 (5.70-3.90)
RSRZ outliers	180081	1013 (5.66-3.94)

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	715	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 58%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 14%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 26%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">2% 58% 14% 29%</p>
1	C	715	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 58%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 14%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 25%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">3% 58% 14% 28%</p>
2	B	578	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 69%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 14%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 13%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">4% 69% 14% 17%</p>
2	D	578	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 68%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 14%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 14%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">4% 68% 14% 18%</p>
3	E	4	<div style="width: 100%; height: 10px; background-color: yellow;"></div> <p style="text-align: center;">100%</p>

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Mol	Chain	Length	Quality of chain
4	F	3	 100%
5	G	5	 20% 80%
5	H	5	 60% 40%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	E	1	X	-	-	-
5	NAG	G	2	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15600 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 Plexin A, isoform A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	511	3923	2466	654	777	26	0	0	0
1	C	512	3931	2470	656	779	26	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	GLU	-	expression tag	UNP Q9V491
A	26	THR	-	expression tag	UNP Q9V491
A	27	GLY	-	expression tag	UNP Q9V491
A	731	GLY	-	expression tag	UNP Q9V491
A	732	THR	-	expression tag	UNP Q9V491
A	733	LYS	-	expression tag	UNP Q9V491
A	734	HIS	-	expression tag	UNP Q9V491
A	735	HIS	-	expression tag	UNP Q9V491
A	736	HIS	-	expression tag	UNP Q9V491
A	737	HIS	-	expression tag	UNP Q9V491
A	738	HIS	-	expression tag	UNP Q9V491
A	739	HIS	-	expression tag	UNP Q9V491
C	25	GLU	-	expression tag	UNP Q9V491
C	26	THR	-	expression tag	UNP Q9V491
C	27	GLY	-	expression tag	UNP Q9V491
C	731	GLY	-	expression tag	UNP Q9V491
C	732	THR	-	expression tag	UNP Q9V491
C	733	LYS	-	expression tag	UNP Q9V491
C	734	HIS	-	expression tag	UNP Q9V491
C	735	HIS	-	expression tag	UNP Q9V491
C	736	HIS	-	expression tag	UNP Q9V491
C	737	HIS	-	expression tag	UNP Q9V491
C	738	HIS	-	expression tag	UNP Q9V491
C	739	HIS	-	expression tag	UNP Q9V491

- Molecule 2 is a protein called MIP07328p.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	478	3743	2376	646	702	19	0	0	0
2	D	473	3708	2355	639	695	19	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	34	GLU	-	expression tag	UNP Q7KK54
B	35	THR	-	expression tag	UNP Q7KK54
B	36	GLY	-	expression tag	UNP Q7KK54
B	603	GLY	-	expression tag	UNP Q7KK54
B	604	THR	-	expression tag	UNP Q7KK54
B	605	LYS	-	expression tag	UNP Q7KK54
B	606	HIS	-	expression tag	UNP Q7KK54
B	607	HIS	-	expression tag	UNP Q7KK54
B	608	HIS	-	expression tag	UNP Q7KK54
B	609	HIS	-	expression tag	UNP Q7KK54
B	610	HIS	-	expression tag	UNP Q7KK54
B	611	HIS	-	expression tag	UNP Q7KK54
D	34	GLU	-	expression tag	UNP Q7KK54
D	35	THR	-	expression tag	UNP Q7KK54
D	36	GLY	-	expression tag	UNP Q7KK54
D	603	GLY	-	expression tag	UNP Q7KK54
D	604	THR	-	expression tag	UNP Q7KK54
D	605	LYS	-	expression tag	UNP Q7KK54
D	606	HIS	-	expression tag	UNP Q7KK54
D	607	HIS	-	expression tag	UNP Q7KK54
D	608	HIS	-	expression tag	UNP Q7KK54
D	609	HIS	-	expression tag	UNP Q7KK54
D	610	HIS	-	expression tag	UNP Q7KK54
D	611	HIS	-	expression tag	UNP Q7KK54

- Molecule 3 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.



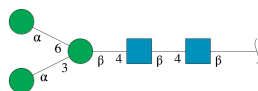
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	E	4	50	28	2	20	0	0	0

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



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

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

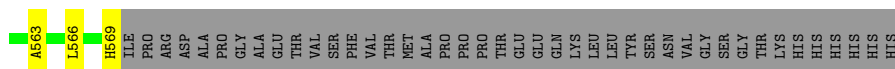


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	G	5	61	34	2	25	0	0	0
5	H	5	61	34	2	25	0	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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



- Molecule 3: 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: 100%



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

Chain F: 100%



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

Chain G: 20% 80%



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

Chain H: 60% 40%

4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	153.63Å 153.63Å 425.37Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	133.05 – 4.80 133.05 – 4.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (133.05-4.80) 89.0 (133.05-4.80)	Depositor EDS
R_{merge}	0.34	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 4.88Å)	Xtrriage
Refinement program	PHENIX (1.13rc2_2986: ???)	Depositor
R, R_{free}	0.285 , 0.297 0.283 , 0.292	Depositor DCC
R_{free} test set	819 reflections (5.35%)	wwPDB-VP
Wilson B-factor (Å ²)	185.7	Xtrriage
Anisotropy	0.299	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 224.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	15600	wwPDB-VP
Average B, all atoms (Å ²)	271.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.72% 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: MAN, NAG, BMA

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	0.24	0/4001	0.44	0/5436
1	C	0.24	0/4010	0.44	0/5450
2	B	0.22	0/3830	0.42	0/5200
2	D	0.23	0/3793	0.42	0/5150
All	All	0.24	0/15634	0.43	0/21236

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	3923	0	3825	72	7
1	C	3931	0	3832	84	5
2	B	3743	0	3658	83	24
2	D	3708	0	3630	52	32
3	E	50	0	43	9	0
4	F	39	0	34	0	0
5	G	61	0	52	16	0
5	H	61	0	52	0	0
6	A	42	0	39	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	42	0	39	2	0
All	All	15600	0	15204	253	37

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 8.

The worst 5 of 253 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:B:294:GLY:N	3:E:2:NAG:C7	1.96	1.28
2:B:386:ILE:HG23	2:B:390:PHE:CZ	1.69	1.25
2:D:293:PRO:CA	5:G:2:NAG:H82	1.67	1.24
2:B:386:ILE:HG22	2:B:390:PHE:CE2	1.81	1.16
2:B:349:GLU:OE2	1:C:486:PHE:CB	1.96	1.12

The worst 5 of 37 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:326:VAL:O	2:D:414:ASN:OD1[8_665]	1.13	1.07
2:D:549:THR:CG2	2:D:551:THR:CB[10_555]	1.13	1.07
2:B:414:ASN:CB	2:D:327:ASN:CB[8_665]	1.32	0.88
2:B:327:ASN:CB	2:D:414:ASN:CB[8_665]	1.36	0.84
1:A:391:ASN:ND2	2:D:514:ILE:CD1[8_665]	1.39	0.81

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	507/715 (71%)	485 (96%)	22 (4%)	0	100	100
1	C	510/715 (71%)	487 (96%)	23 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	470/578 (81%)	449 (96%)	21 (4%)	0	100	100
2	D	463/578 (80%)	443 (96%)	20 (4%)	0	100	100
All	All	1950/2586 (75%)	1864 (96%)	86 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	451/633 (71%)	449 (100%)	2 (0%)	84	83
1	C	452/633 (71%)	450 (100%)	2 (0%)	84	83
2	B	416/502 (83%)	416 (100%)	0	100	100
2	D	413/502 (82%)	413 (100%)	0	100	100
All	All	1732/2270 (76%)	1728 (100%)	4 (0%)	87	86

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

Mol	Chain	Res	Type
1	A	297	ILE
1	A	371	CYS
1	C	297	ILE
1	C	371	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	76	ASN
1	C	137	ASN
1	C	261	ASN
1	A	137	ASN
1	A	76	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

17 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	$\# Z > 2$
3	NAG	E	1	3,2	14,14,15	0.37	0	17,19,21	0.51	0
3	NAG	E	2	3	14,14,15	0.28	0	17,19,21	0.51	0
3	BMA	E	3	3	11,11,12	0.37	0	15,15,17	1.12	2 (13%)
3	MAN	E	4	3	11,11,12	0.26	0	15,15,17	0.89	0
4	NAG	F	1	4,2	14,14,15	0.31	0	17,19,21	0.52	0
4	NAG	F	2	4	14,14,15	0.39	0	17,19,21	0.53	0
4	BMA	F	3	4	11,11,12	0.81	0	15,15,17	0.72	0
5	NAG	G	1	5,2	14,14,15	0.38	0	17,19,21	0.50	0
5	NAG	G	2	5	14,14,15	0.29	0	17,19,21	0.51	0
5	BMA	G	3	5	11,11,12	0.37	0	15,15,17	2.04	4 (26%)
5	MAN	G	4	5	11,11,12	1.02	1 (9%)	15,15,17	0.98	2 (13%)
5	MAN	G	5	5	11,11,12	0.26	0	15,15,17	0.63	0
5	NAG	H	1	5,2	14,14,15	0.30	0	17,19,21	0.53	0
5	NAG	H	2	5	14,14,15	0.38	0	17,19,21	0.51	0
5	BMA	H	3	5	11,11,12	0.82	0	15,15,17	0.75	0
5	MAN	H	4	5	11,11,12	0.95	1 (9%)	15,15,17	1.18	2 (13%)
5	MAN	H	5	5	11,11,12	0.80	0	15,15,17	1.07	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	1	3,2	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	BMA	E	3	3	-	0/2/19/22	0/1/1/1
3	MAN	E	4	3	-	1/2/19/22	0/1/1/1
4	NAG	F	1	4,2	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
4	BMA	F	3	4	-	2/2/19/22	0/1/1/1
5	NAG	G	1	5,2	-	2/6/23/26	0/1/1/1
5	NAG	G	2	5	-	2/6/23/26	0/1/1/1
5	BMA	G	3	5	-	1/2/19/22	0/1/1/1
5	MAN	G	4	5	-	0/2/19/22	0/1/1/1
5	MAN	G	5	5	-	1/2/19/22	0/1/1/1
5	NAG	H	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	H	2	5	-	0/6/23/26	0/1/1/1
5	BMA	H	3	5	-	2/2/19/22	0/1/1/1
5	MAN	H	4	5	-	0/2/19/22	0/1/1/1
5	MAN	H	5	5	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	4	MAN	C1-C2	2.42	1.58	1.52
5	G	4	MAN	O5-C5	2.09	1.47	1.43

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	3	BMA	C1-C2-C3	-5.81	101.19	109.64
5	H	4	MAN	C1-O5-C5	3.48	116.85	112.19
5	H	5	MAN	C1-O5-C5	3.11	116.35	112.19
5	G	3	BMA	O3-C3-C4	2.92	117.26	110.38
5	G	3	BMA	O3-C3-C2	2.62	115.40	110.05

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	E	1	NAG	C1

5 of 15 torsion outliers are listed below:

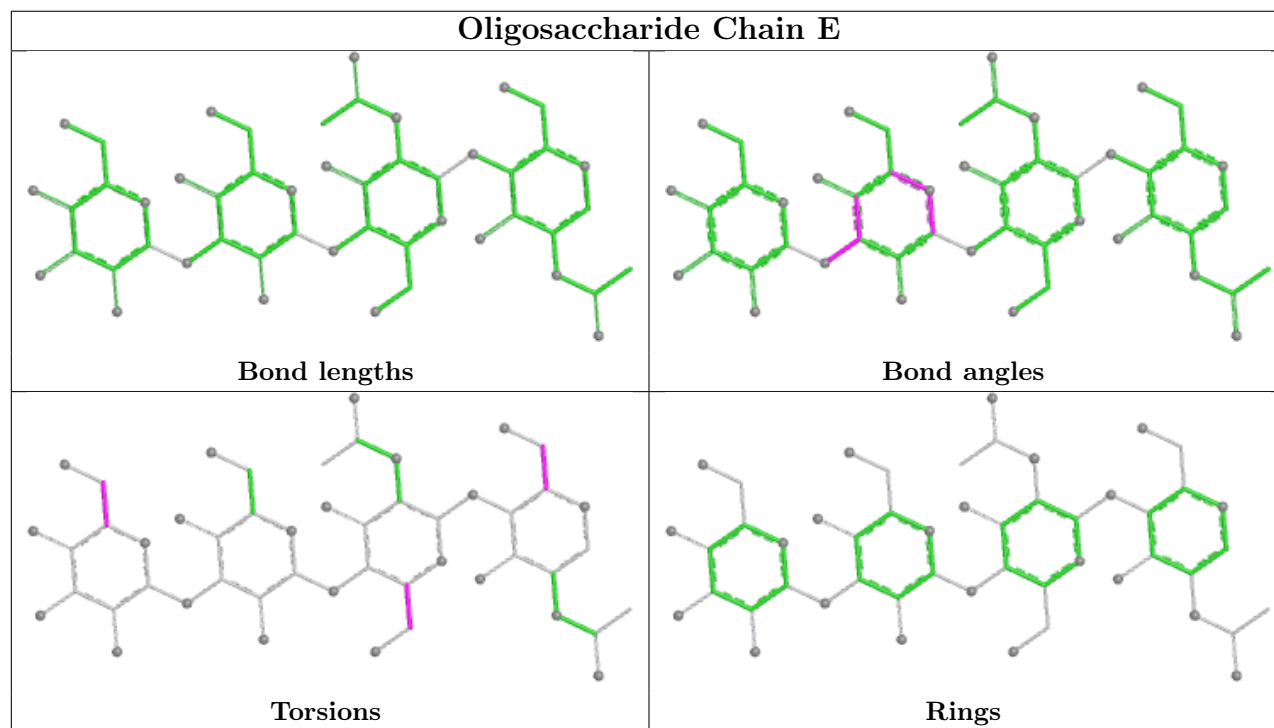
Mol	Chain	Res	Type	Atoms
3	E	2	NAG	O5-C5-C6-O6
5	G	2	NAG	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
5	G	2	NAG	C4-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6

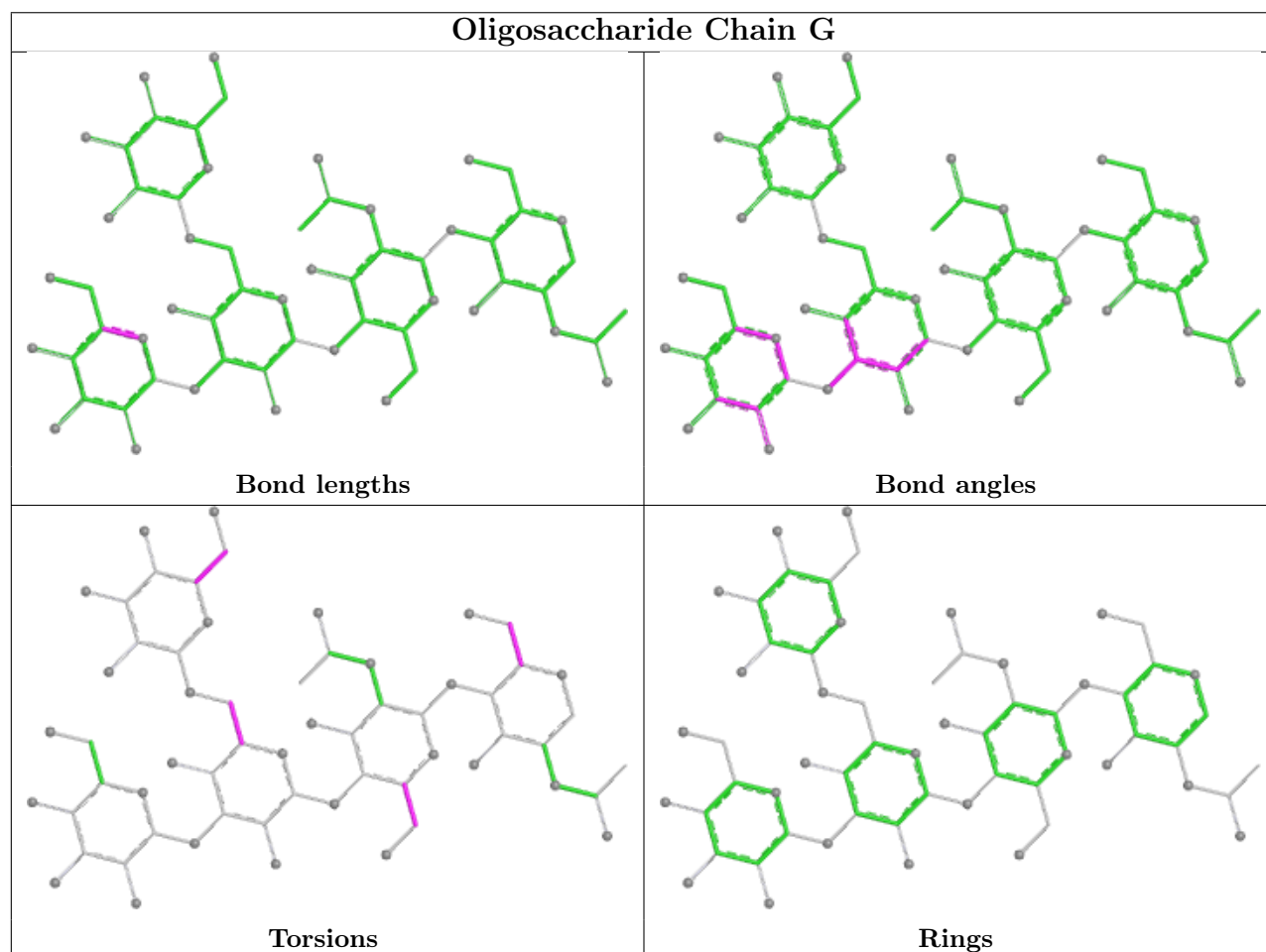
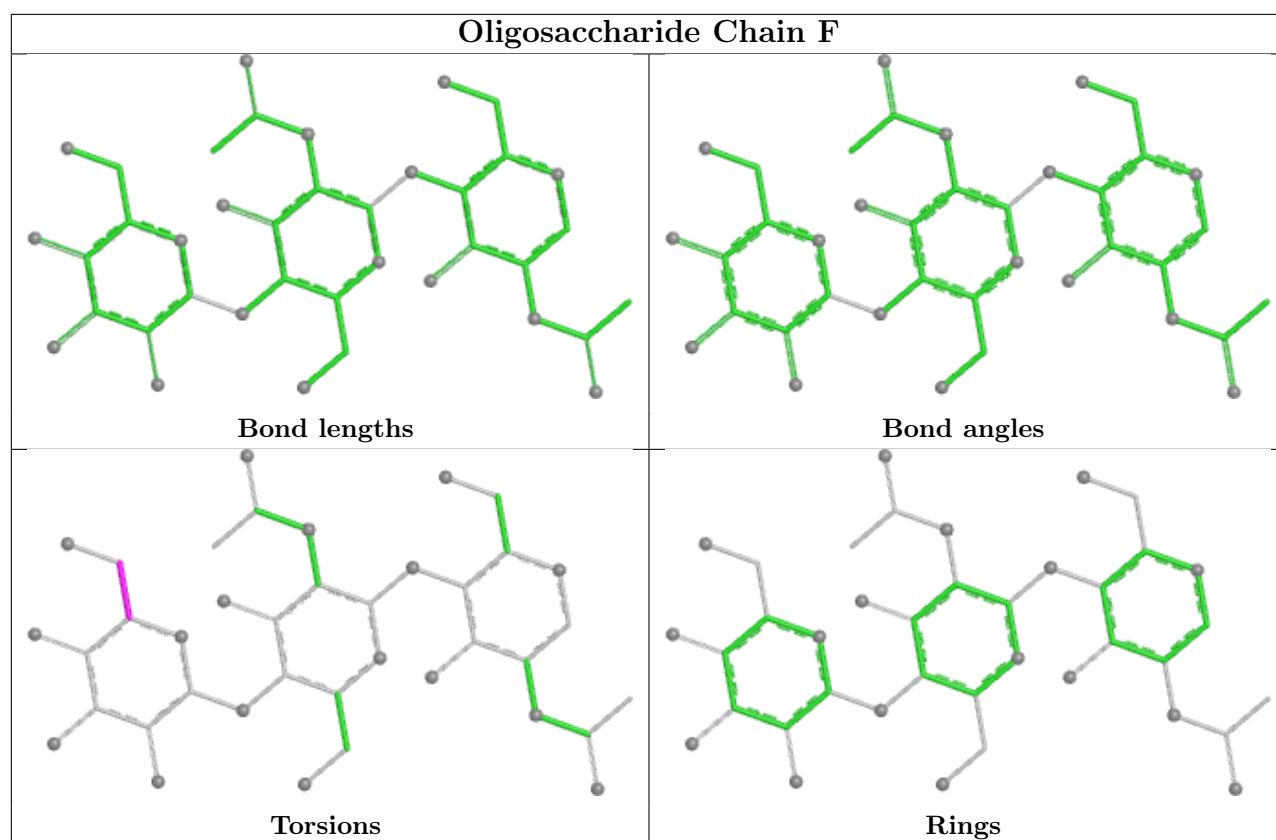
There are no ring outliers.

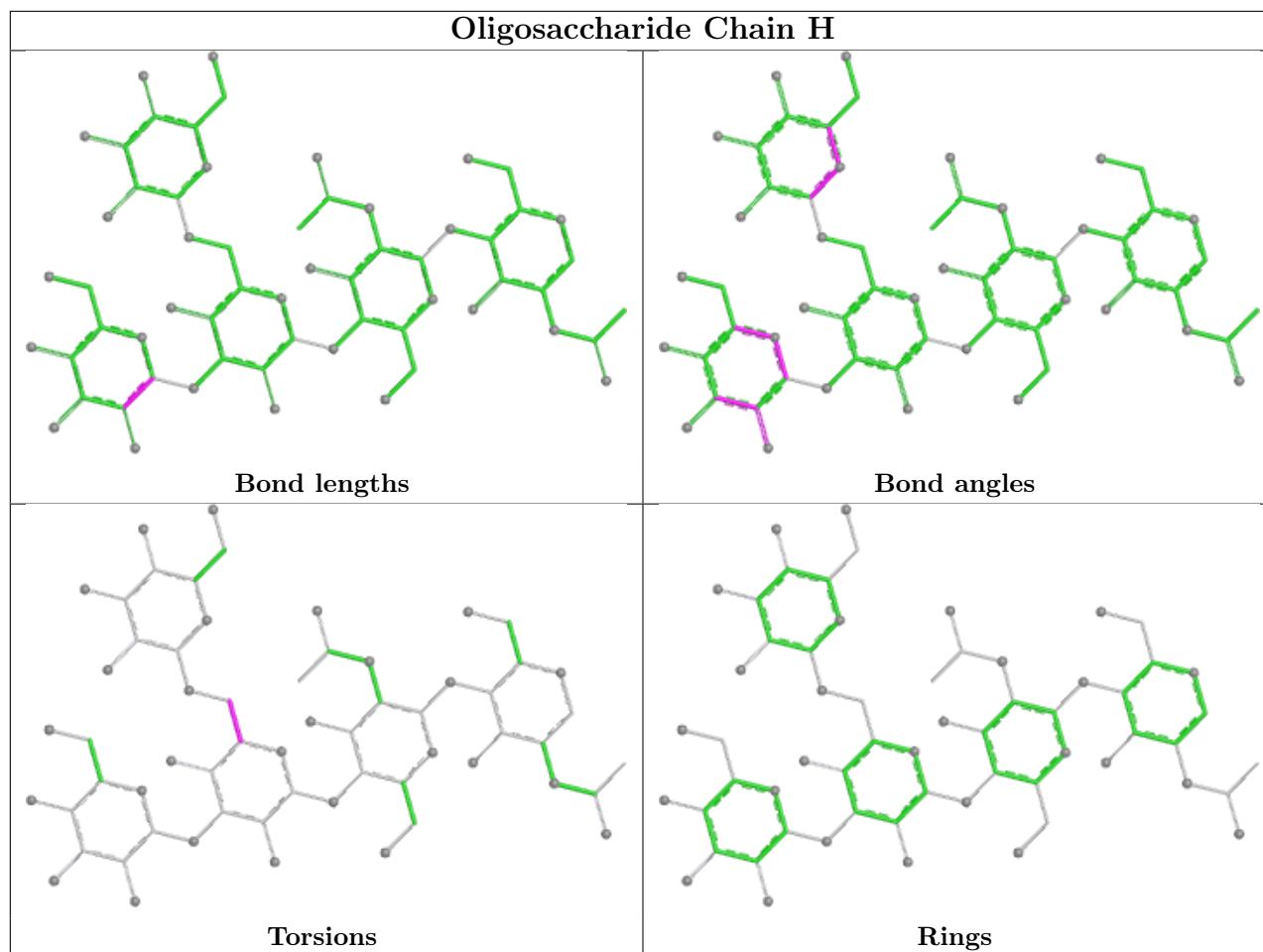
5 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	2	NAG	10	0
3	E	1	NAG	3	0
3	E	4	MAN	1	0
3	E	2	NAG	5	0
5	G	1	NAG	6	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](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	NAG	C	803	1	14,14,15	0.66	1 (7%)	17,19,21	0.45	0
6	NAG	C	802	1	14,14,15	0.22	0	17,19,21	0.61	0
6	NAG	A	802	1	14,14,15	0.24	0	17,19,21	0.60	0
6	NAG	A	801	1	14,14,15	0.22	0	17,19,21	0.82	0
6	NAG	A	803	1	14,14,15	0.68	1 (7%)	17,19,21	0.46	0
6	NAG	C	801	1	14,14,15	0.22	0	17,19,21	0.81	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
6	NAG	C	803	1	-	3/6/23/26	0/1/1/1
6	NAG	C	802	1	-	2/6/23/26	0/1/1/1
6	NAG	A	802	1	-	2/6/23/26	0/1/1/1
6	NAG	A	801	1	-	1/6/23/26	0/1/1/1
6	NAG	A	803	1	-	3/6/23/26	0/1/1/1
6	NAG	C	801	1	-	1/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	803	NAG	C1-C2	2.36	1.55	1.52
6	C	803	NAG	C1-C2	2.26	1.55	1.52

There are no bond angle outliers.

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	801	NAG	C3-C2-N2-C7
6	C	801	NAG	C3-C2-N2-C7
6	A	803	NAG	C4-C5-C6-O6
6	C	803	NAG	C4-C5-C6-O6
6	A	802	NAG	C4-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	803	NAG	1	0
6	A	801	NAG	1	0
6	A	803	NAG	6	0
6	C	801	NAG	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	511/715 (71%)	0.18	13 (2%) 58 46	220, 261, 332, 388	0
1	C	512/715 (71%)	0.31	21 (4%) 41 37	203, 246, 315, 370	0
2	B	478/578 (82%)	0.33	22 (4%) 37 34	207, 259, 319, 370	0
2	D	473/578 (81%)	0.34	25 (5%) 32 31	256, 296, 362, 422	0
All	All	1974/2586 (76%)	0.29	81 (4%) 41 37	203, 265, 336, 422	0

The worst 5 of 81 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	503	LEU	6.5
1	C	520	VAL	5.7
1	C	461	PHE	5.1
2	D	342	ILE	4.7
2	D	63	ILE	4.5

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.

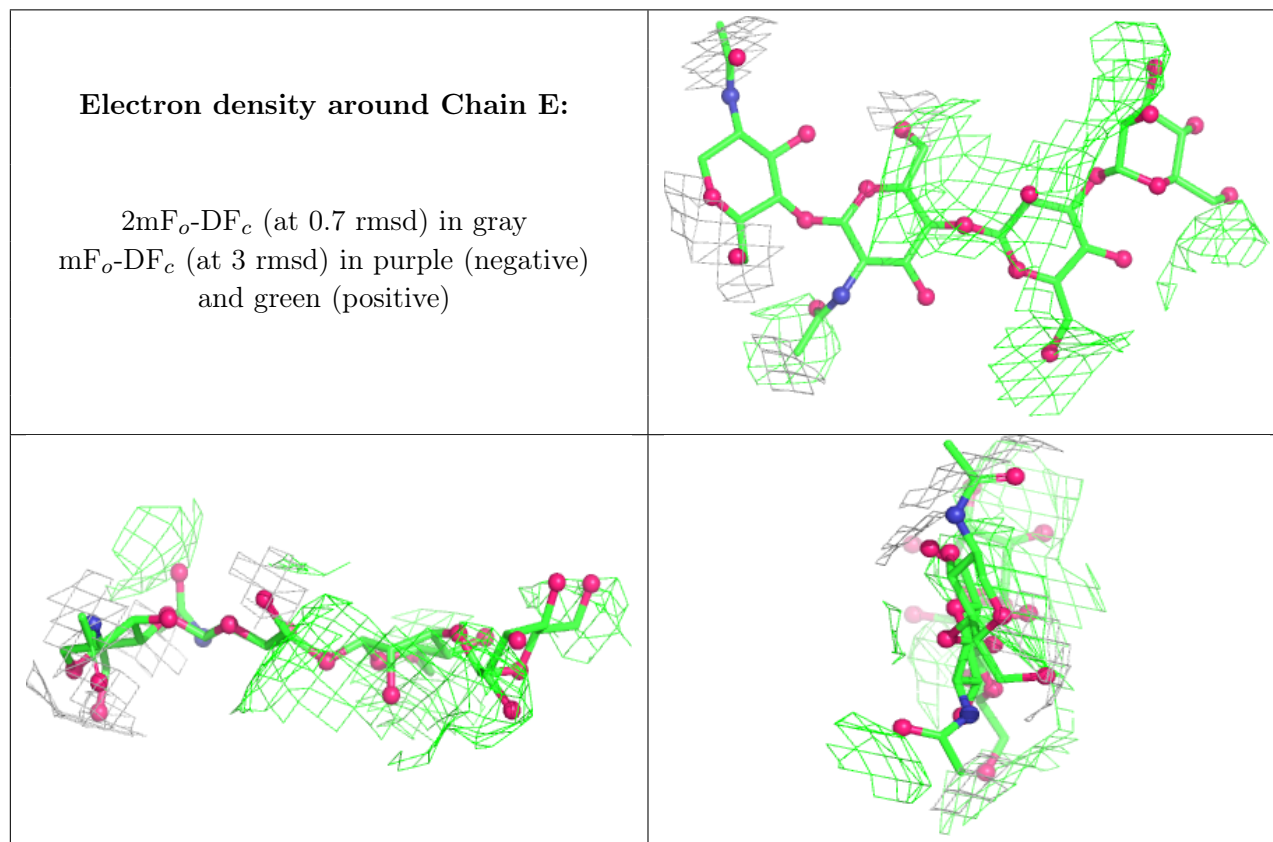
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	BMA	F	3	11/12	0.17	0.17	329,330,331,331	0
5	BMA	G	3	11/12	0.21	0.15	344,345,347,347	0

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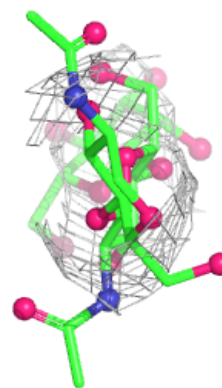
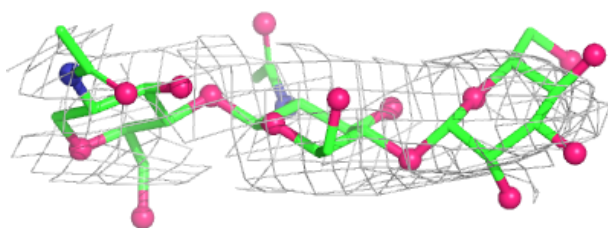
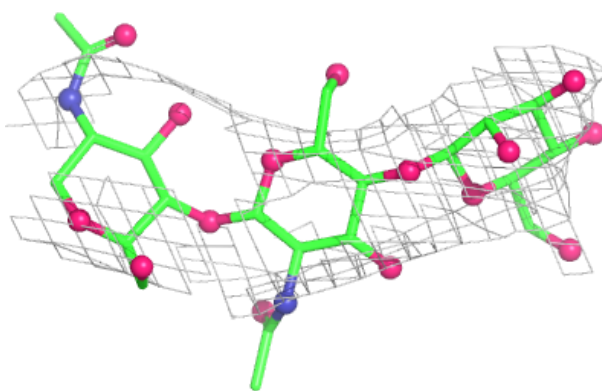
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	MAN	H	4	11/12	0.37	0.14	417,421,424,425	0
5	MAN	H	5	11/12	0.38	0.18	414,416,418,418	0
3	BMA	E	3	11/12	0.43	0.12	286,288,292,293	0
5	MAN	G	5	11/12	0.49	0.09	327,330,331,332	0
5	BMA	H	3	11/12	0.64	0.12	408,411,412,413	0
5	NAG	G	2	14/15	0.66	0.15	324,326,327,327	0
5	MAN	G	4	11/12	0.67	0.10	335,336,339,339	0
3	MAN	E	4	11/12	0.71	0.11	275,276,280,281	0
5	NAG	H	2	14/15	0.75	0.12	370,372,373,375	0
5	NAG	H	1	14/15	0.77	0.16	328,329,331,331	0
3	NAG	E	2	14/15	0.80	0.12	272,273,276,277	0
4	NAG	F	1	14/15	0.82	0.12	284,290,295,295	0
4	NAG	F	2	14/15	0.83	0.10	312,315,317,317	0
5	NAG	G	1	14/15	0.87	0.10	300,303,305,307	0
3	NAG	E	1	14/15	0.88	0.17	247,251,253,255	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.

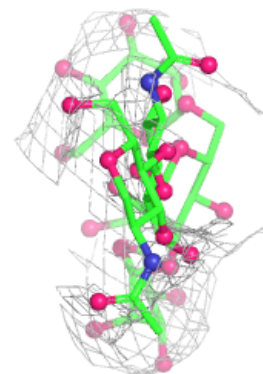
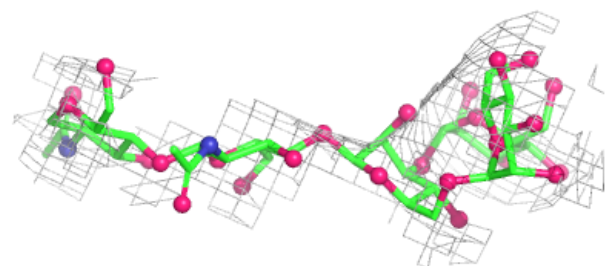
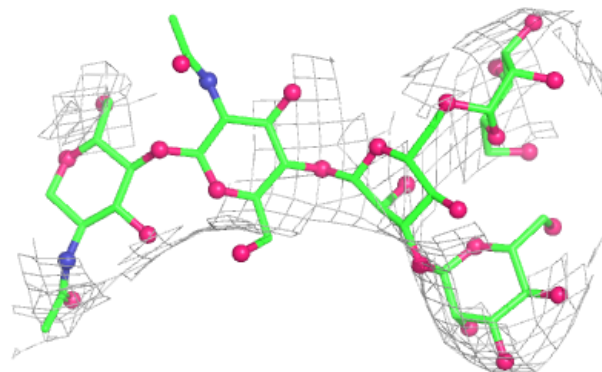


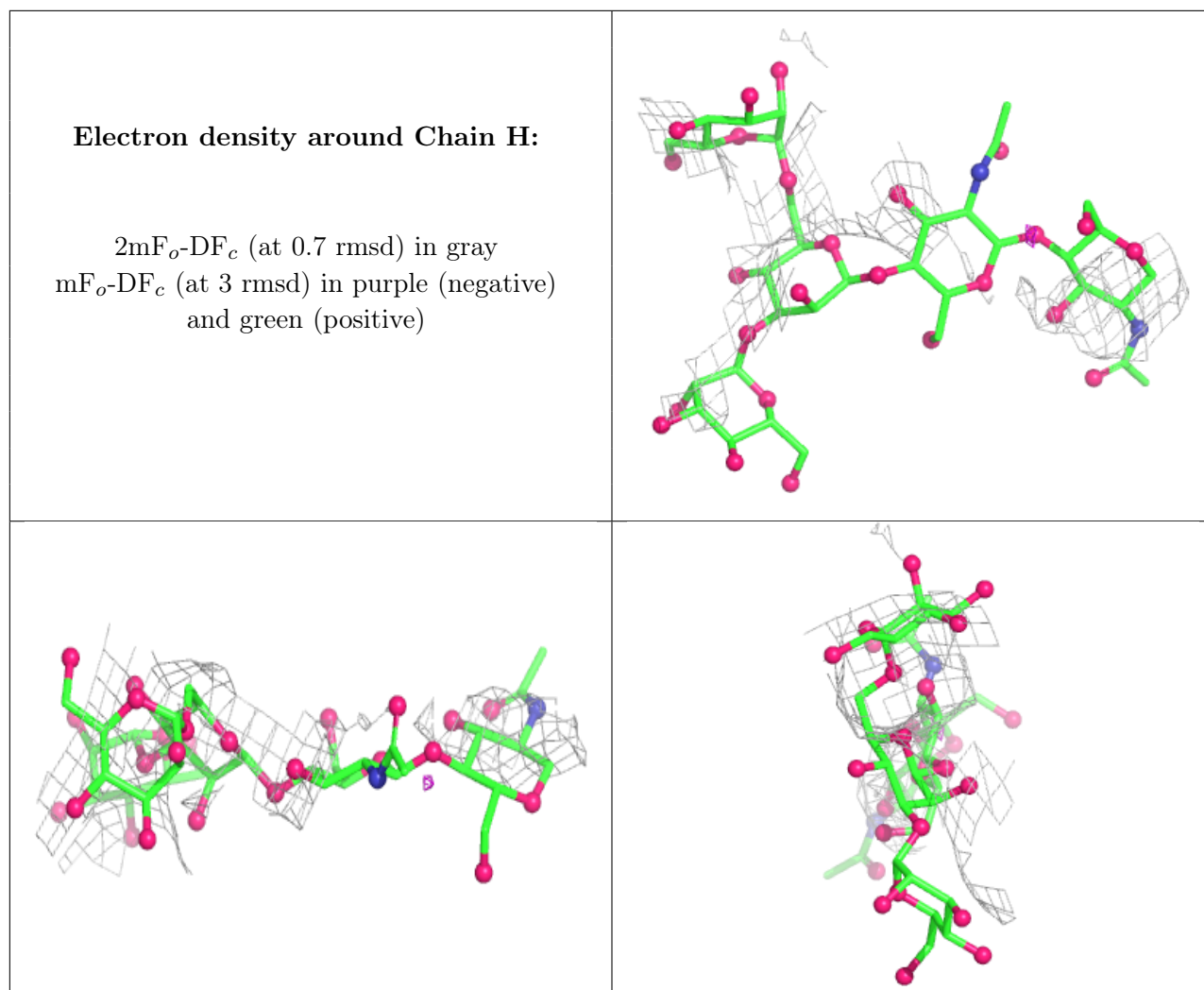
Electron density around Chain F:

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

**Electron density around Chain 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
6	NAG	C	803	14/15	0.47	0.14	282,283,284,285	0
6	NAG	A	803	14/15	0.51	0.14	286,289,290,290	0
6	NAG	C	802	14/15	0.75	0.20	272,280,285,287	0
6	NAG	A	802	14/15	0.76	0.15	272,278,282,283	0
6	NAG	C	801	14/15	0.80	0.10	250,254,256,256	0
6	NAG	A	801	14/15	0.83	0.08	259,261,262,263	0

6.5 Other polymers [i](#)

There are no such residues in this entry.