wwPDB X-ray Structure Validation Summary Report (i)

Jan 7, 2024 – 02:26 pm GMT

PDB ID : 6FKN
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)

The following versions of software and data (see references (i)) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 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.
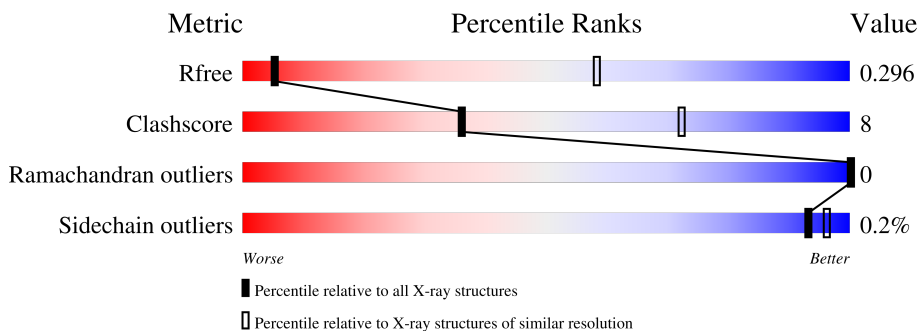
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1096 (5.80-3.80)
Clashscore	141614	1170 (5.80-3.80)
Ramachandran outliers	138981	1105 (5.80-3.80)
Sidechain outliers	138945	1085 (5.80-3.80)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	715	59% 13% 29%
1	C	715	59% 13% 28%
2	B	578	69% 14% 17%
2	D	578	68% 14% 18%
3	E	4	75% 25%
4	F	3	100%
5	G	5	20% 80%

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Mol	Chain	Length	Quality of chain
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
1	A	511	Total 3923	C 2466	N 654	O 777	S 26	0	0	0
1	C	512	Total 3931	C 2470	N 656	O 779	S 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
2	B	478	Total	C	N	O	S	0	0	0
			3743	2376	646	702	19			
2	D	473	Total	C	N	O	S	0	0	0
			3708	2355	639	695	19			

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-mannopyranos e-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluco pyranose.
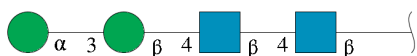
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	4	Total 50	C 28	N 2	O 20	0	0	0

- 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
4	F	3	Total 39	C 22	N 2	O 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.
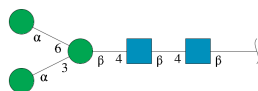
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	G	5	Total 61	C 34	N 2	O 25	0	0	0
5	H	5	Total 61	C 34	N 2	O 25	0	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

NAG

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

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. 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. 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: Plexin A, isoform A

Chain A:

- Molecule 1: Plexin A, isoform A

Chain C:

LEU ILE CYS ALA PHE THR THR GLU ASP LYS ALA LEU PHE THR ASN ALA THR LYS LYS ARG ASN GLY VAL ASN CYS THR THR PRO ARG THR ASP MET THR PRO GLN ILE GLU GLN LYS HIS HIS PHE THR ALA LYS LEU SER VAL ARG THR ARG ASN GLY PRO ASP LEU VAL SER THR

ASP PHE THR PHE ASP SER CYS SER THR HIS SER SER CYS THR ARG CYS VAL SER SER GLU PHE PRO CYS ASP TRP CYS VAL GLU ALA HIS ARG CYS THR HIS ASP THR ALA GLU ASN CYS ARG ASP ILE LEU VAL THR GLY VAL SER ARG ILE GLY PRO SER TYR ARG SER GLY PRO

GLY PHE CYS PRO THR GLY THR LYS HIS HIS HIS HIS HIS HIS

• Molecule 2: MIP07328p

Chain B:

GLU THR GLY ASP VAL LYS PRO ASP LEU GLN GLN THR LYS GLN ASP LYS VAL LEU ALA HIS F53 S57 T58 D59 K76 D77 V78 I79 Y80 L104 L107 K108 Y118 L119 R120 V121 E129 C133 G134 T135 N136 K139 H144 Y145 T146 P147 VAL GLU VAL SER SER GLU

GLU ALA GLY SER ALA GLY HIS ALA HIS ALA MET R165 R170 L177 Y180 L195 Y196 T199 V200 L209 I210 Y211 R212 E213 Q219 Y220 D221 L222 K223 G238 E250 V251 M252 R261 K267 Y274 V292 PRO G294 Y299 V310 E311 S312 V321

F322 T323 V326 N327 P330 E349 F350 K351 S352 GLN LYS ASP SER GLN SER HIS TRP LEU PRO VAL GLU ARG GLU GLN VAL PRO LYS PRO ARG PRO G374 V377 L383 I386 F390 H394 P395 L396 K412 V413 N414 R418 L419 I422 P426 D437

N453 L466 V476 E485 L486 V497 S502 L503 L521 D531 L532 Q533 T534 H535 E536 L553 A563 L566 H569 ILE PRO ARG ASP ALA PRO GLY ALA GLU THR VAL SER PHE VAL THR MET ALA PRO PRO THR GLU GLU GLN LYS LEU LEU TYR SER ASN

VAL GLY SER GLY THR LYS HIS HIS HIS HIS HIS

• Molecule 2: MIP07328p

Chain D:

GLU THR GLY ASP VAL LYS PRO ASP LEU GLN GLN THR LYS GLN ASP LYS VAL LEU ALA HIS F53 S57 T58 D59 K76 D77 V78 I79 Y80 L104 L107 K108 Y118 L119 R120 V121 E129 C133 G134 T135 N136 K139 H144 Y145 T146 P147 VAL GLU VAL SER SER GLU

GLU ALA GLY SER ALA GLY HIS ALA HIS ALA MET R165 R170 L177 Y180 L195 T199 V200 L209 I210 Y211 R212 E213 Q219 Y220 D221 L222 K223 G238 E250 R261 K267 P293 GLY E295 F296 P297 V310 V321 F322 T323 V326 N327 A328 I329

P330 K351 K354 ASP SER GLN SER HIS TRP LEU PRO VAL GLU ARG GLU GLN VAL PRO LYS PRO ARG PRO G374 V377 L383 I386 F396 A400 L409 K412 V413 N414 R418 L419 I422 P426 N453 L466 V476 E485 L486 V497 S502 L503

I514 L521 D531 L532 Q533 T534 H535 E536 A541 THR SER GLN HIS LYS PHE GLY T549 K550 T551 Y552 L553 Q554 S555 S558 A563 L566 H569 ILE PRO ARG ASP ALA PRO GLY ALA GLU THR VAL SER PHE VAL THR MET ALA PRO PRO THR GLU GLU GLN LYS

LEU LEU TYR SER ASN VAL GLY SER GLY THR LYS HIS HIS HIS HIS HIS

• 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:

NAG1 NAG2 BMA3 MAN4

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

Chain F: 100%

NAG1 NAG2 BMA3

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

Chain G: 20%   80%

NAG1 NAG2 BMA3 MAN4 MAN5

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

Chain H: 60%   40%

NAG1 NAG2 BMA3 MAN4 MAN5

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.20 (at 4.88Å)	Xtriage
Refinement program	PHENIX (1.13rc2_2986: ???)	Depositor
R, R_{free}	0.285 , 0.297 0.285 , 0.296	Depositor DCC
R_{free} test set	819 reflections (5.35%)	wwPDB-VP
Wilson B-factor (Å^2)	185.7	Xtriage
Anisotropy	0.299	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 204.3	EDS
L-test for twinning[2]	$< |L| > = 0.46, < L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: BMA, MAN, NAG

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	0.32	0/4001	0.52	0/5436
1	C	0.32	0/4010	0.52	0/5450
2	B	0.31	0/3830	0.51	0/5200
2	D	0.31	0/3793	0.51	0/5150
All	All	0.32	0/15634	0.52	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 ⓘ

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	67	7
1	C	3931	0	3832	81	5
2	B	3743	0	3658	84	24
2	D	3708	0	3630	51	32
3	E	50	0	43	10	0
4	F	39	0	34	0	0
5	G	61	0	52	15	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	245	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 245 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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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%)	91	94
1	C	452/633 (71%)	450 (100%)	2 (0%)	91	94
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%)	93	96

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. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	278	GLN
2	B	394	HIS
1	C	278	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 ⓘ

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	0.36	0	17,19,21	0.50	0
3	NAG	E	2	3	14,14,15	0.29	0	17,19,21	0.49	0
3	BMA	E	3	3	11,11,12	0.38	0	15,15,17	1.23	3 (20%)
3	MAN	E	4	3	11,11,12	0.27	0	15,15,17	1.13	1 (6%)
4	NAG	F	1	2,4	14,14,15	0.31	0	17,19,21	0.50	0
4	NAG	F	2	4	14,14,15	0.36	0	17,19,21	0.51	0
4	BMA	F	3	4	11,11,12	0.83	0	15,15,17	0.75	0
5	NAG	G	1	2,5	14,14,15	0.36	0	17,19,21	0.48	0
5	NAG	G	2	5	14,14,15	0.29	0	17,19,21	0.49	0
5	BMA	G	3	5	11,11,12	0.38	0	15,15,17	2.32	4 (26%)
5	MAN	G	4	5	11,11,12	1.01	1 (9%)	15,15,17	1.05	2 (13%)
5	MAN	G	5	5	11,11,12	0.26	0	15,15,17	0.73	0
5	NAG	H	1	2,5	14,14,15	0.30	0	17,19,21	0.51	0
5	NAG	H	2	5	14,14,15	0.36	0	17,19,21	0.49	0
5	BMA	H	3	5	11,11,12	0.83	0	15,15,17	0.77	0
5	MAN	H	4	5	11,11,12	0.97	1 (9%)	15,15,17	1.22	2 (13%)
5	MAN	H	5	5	11,11,12	0.82	0	15,15,17	1.08	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	2,4	-	1/6/23/26	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	2,5	-	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	2,5	-	1/6/23/26	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	2.54	1.58	1.52
5	G	4	MAN	O5-C5	2.00	1.47	1.43

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	G	3	BMA	C1-C2-C3	-6.90	101.19	109.67
5	H	4	MAN	C1-O5-C5	3.44	116.85	112.19
3	E	4	MAN	O5-C1-C2	-3.07	106.03	110.77
5	H	5	MAN	C1-O5-C5	3.07	116.35	112.19
5	G	3	BMA	O3-C3-C4	2.99	117.26	110.35

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	E	1	NAG	C1

5 of 17 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
3	E	2	NAG	5	0
3	E	1	NAG	4	0
5	G	2	NAG	9	0
3	E	4	MAN	1	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.

Oligosaccharide Chain E

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain F

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain G

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain H

Bond lengths

Bond angles

Torsions

Rings
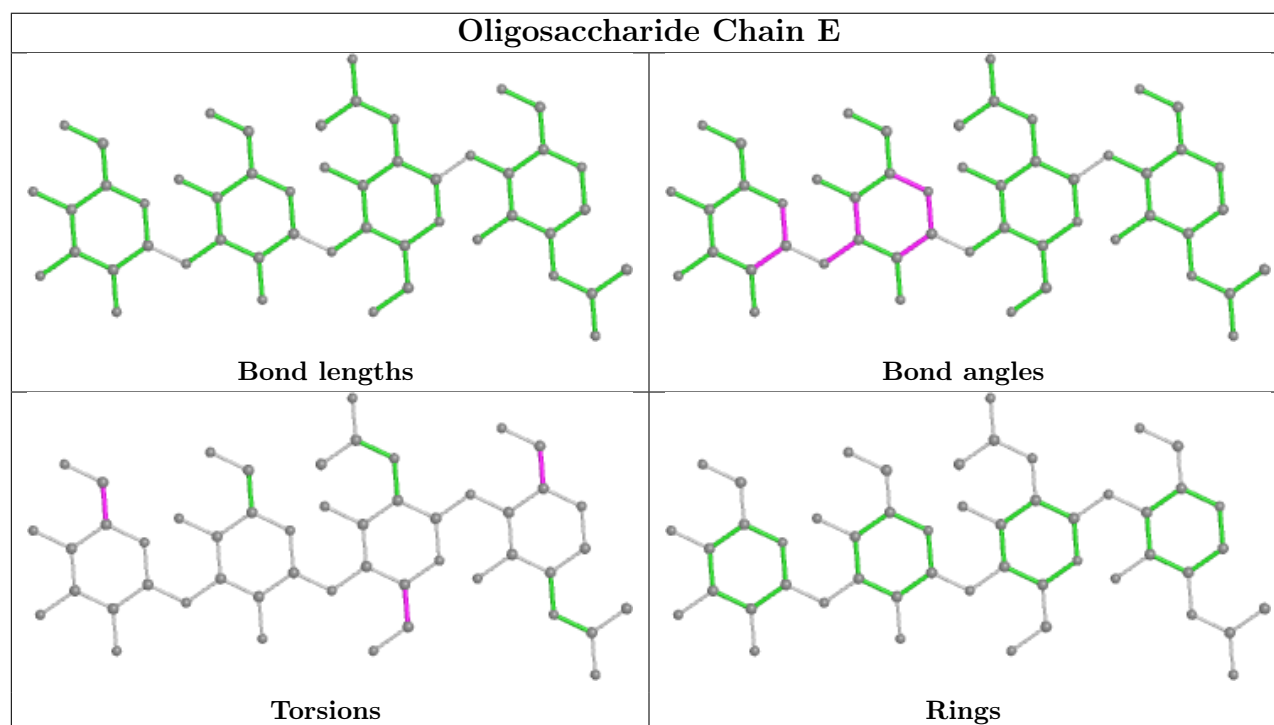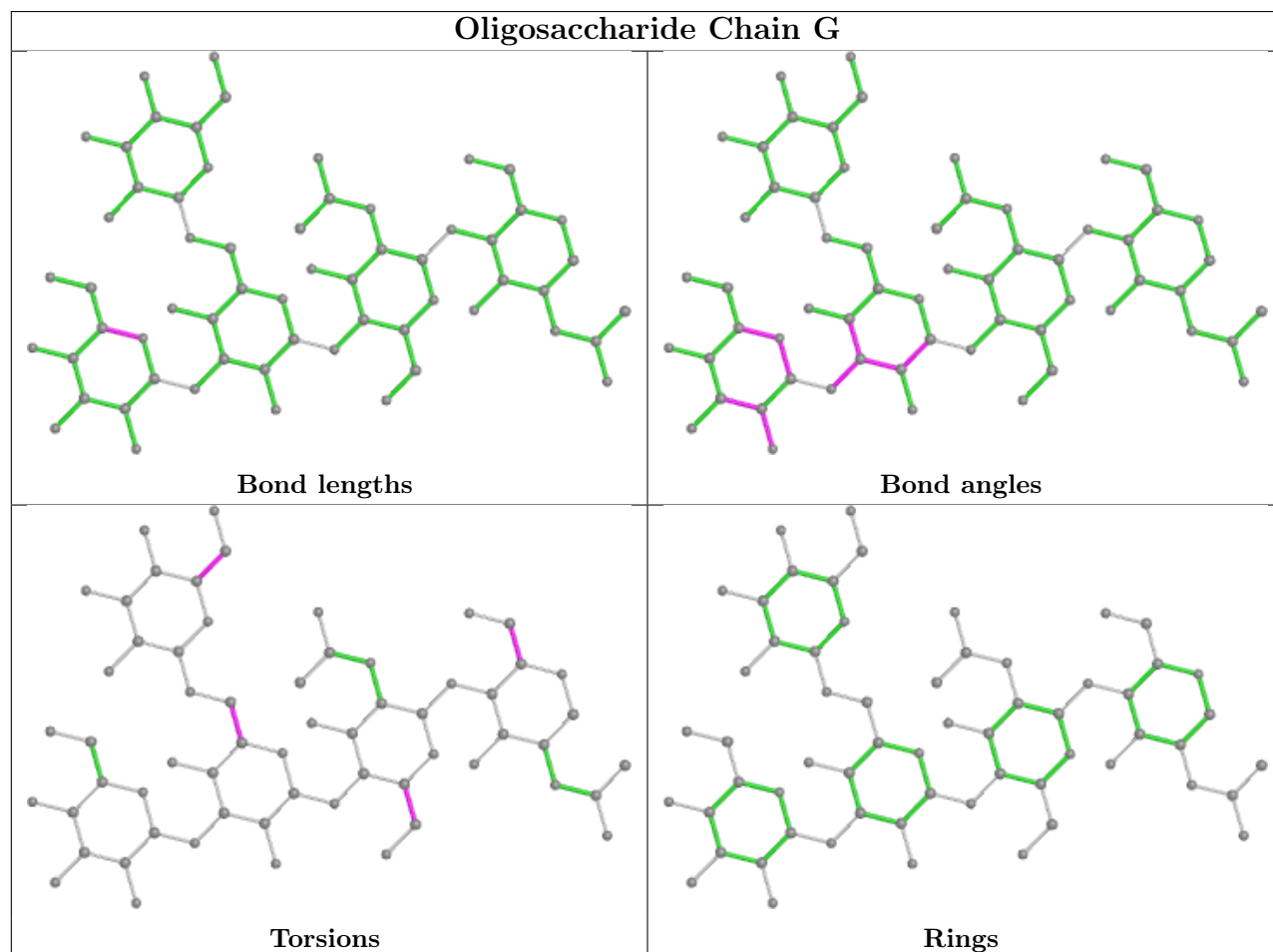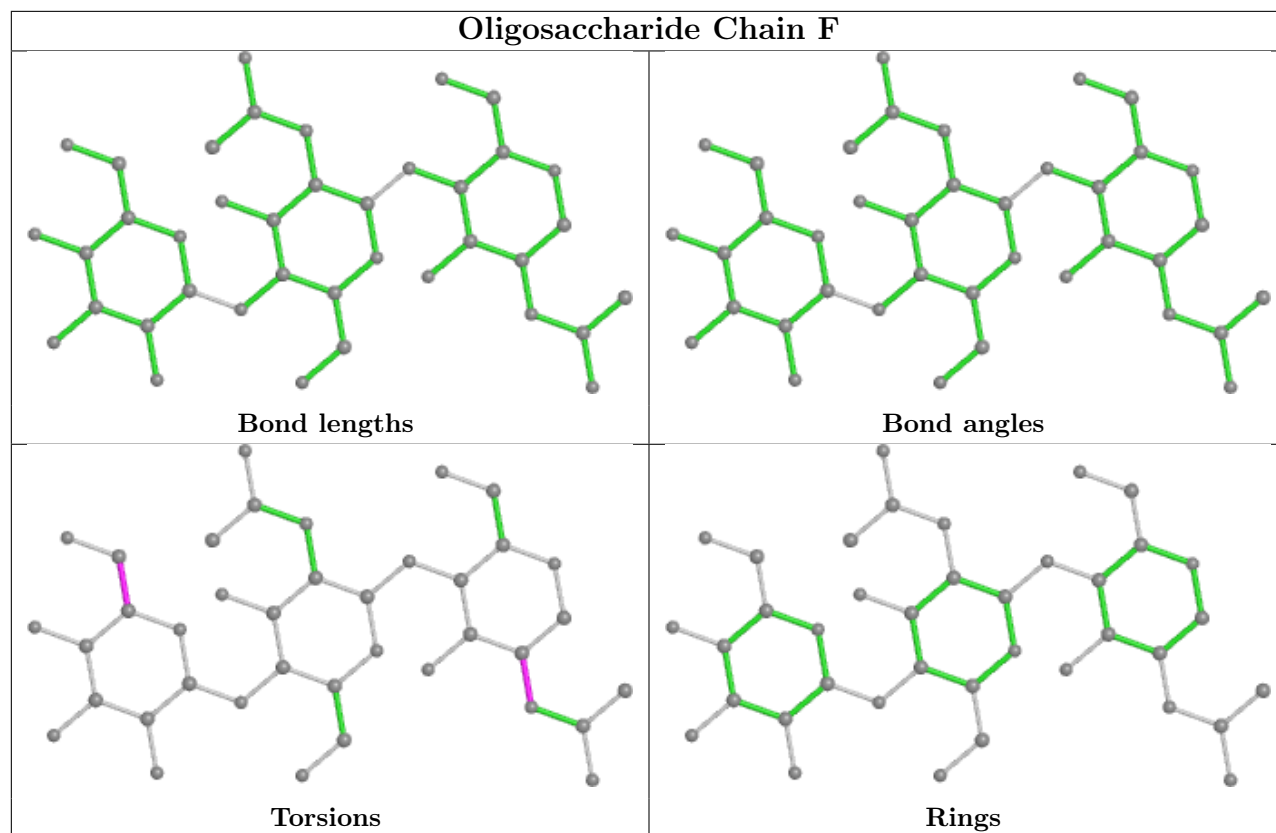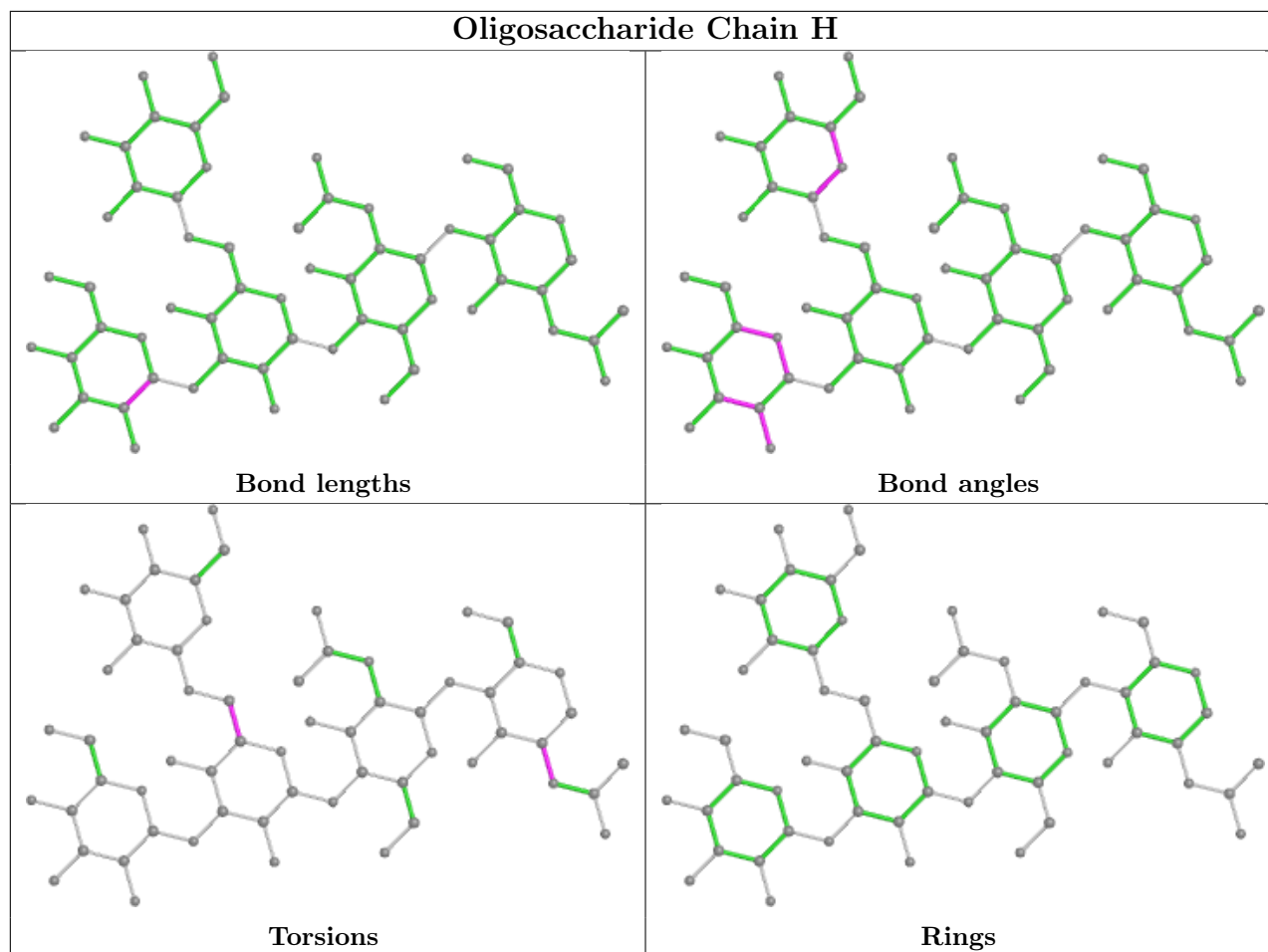
5.6 Ligand geometry ⓘ

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	A	803	1	14,14,15	0.64	1 (7%)	17,19,21	0.44	0
6	NAG	C	803	1	14,14,15	0.61	1 (7%)	17,19,21	0.44	0
6	NAG	C	802	1	14,14,15	0.21	0	17,19,21	0.59	0
6	NAG	A	801	1	14,14,15	0.22	0	17,19,21	0.78	0
6	NAG	C	801	1	14,14,15	0.22	0	17,19,21	0.78	0
6	NAG	A	802	1	14,14,15	0.23	0	17,19,21	0.58	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	A	803	1	-	4/6/23/26	0/1/1/1
6	NAG	C	803	1	-	4/6/23/26	0/1/1/1
6	NAG	C	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	C	801	1	-	1/6/23/26	0/1/1/1
6	NAG	A	802	1	-	2/6/23/26	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	2.16	1.55	1.52
6	C	803	NAG	C1-C2	2.06	1.55	1.52

There are no bond angle outliers.

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	803	NAG	C1-C2-N2-C7
6	C	803	NAG	C1-C2-N2-C7
6	A	801	NAG	C3-C2-N2-C7
6	C	801	NAG	C3-C2-N2-C7
6	A	803	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	A	803	NAG	6	0
6	C	803	NAG	1	0
6	A	801	NAG	1	0
6	C	801	NAG	1	0

5.7 Other polymers ⓘ

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 ⓘ

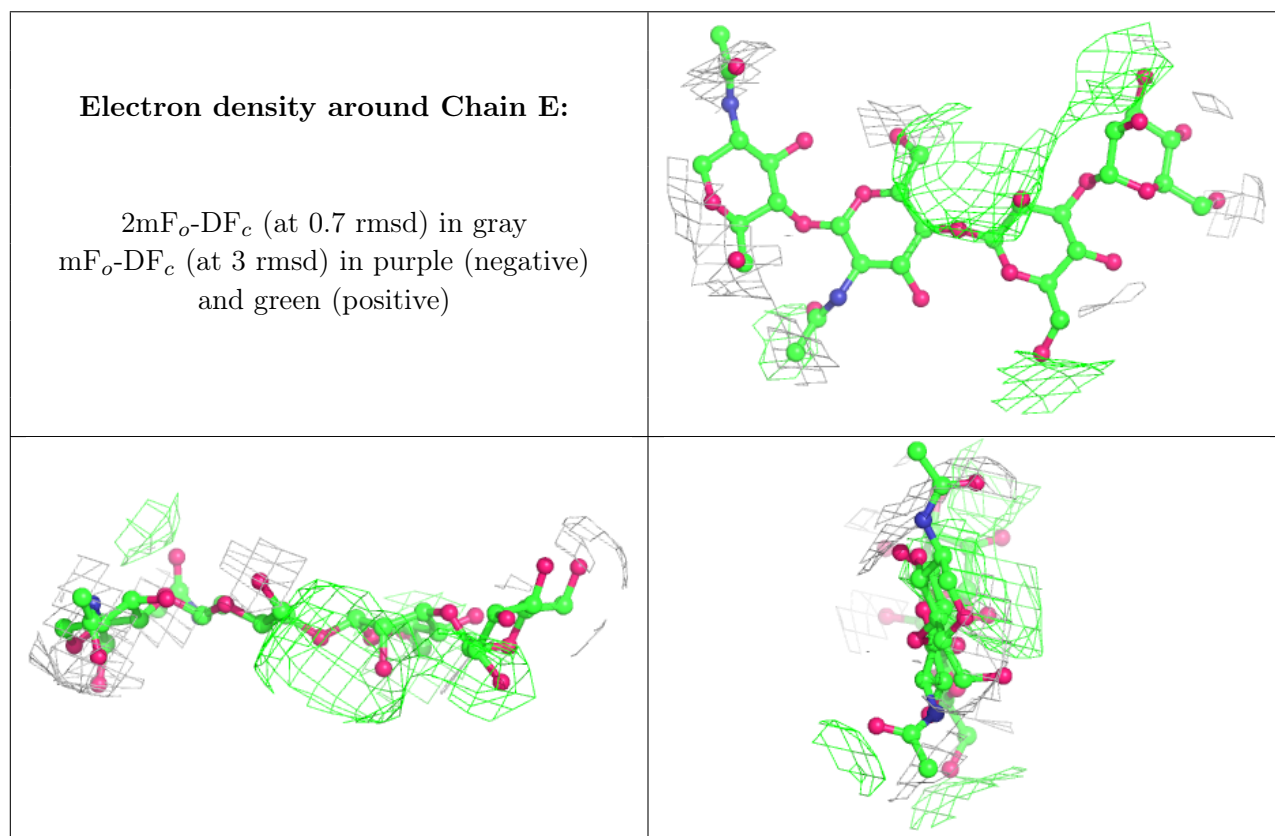Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3   Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (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)
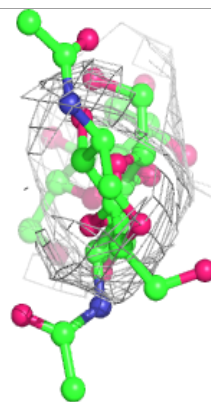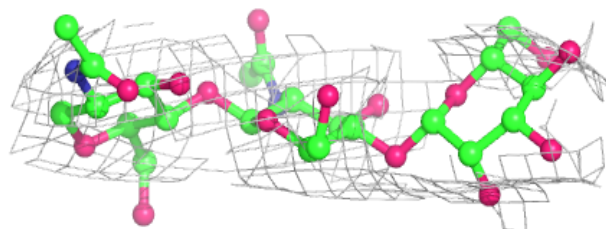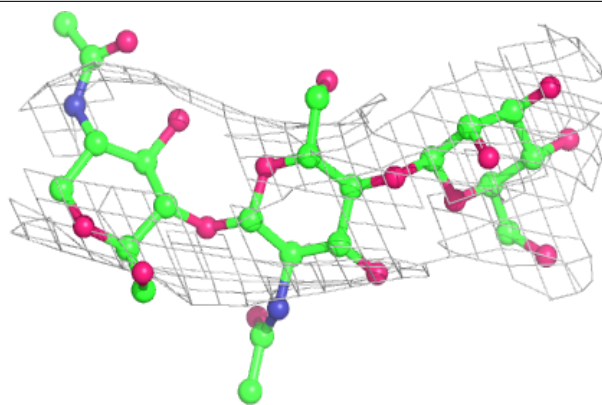
Electron density around Chain G:

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)
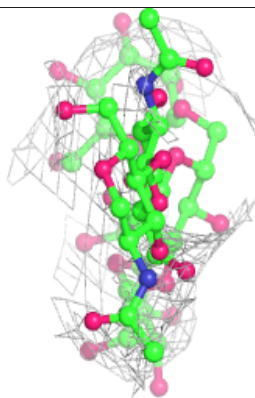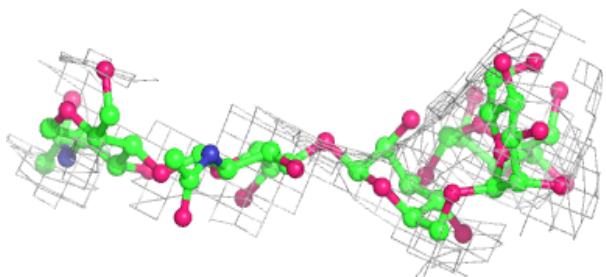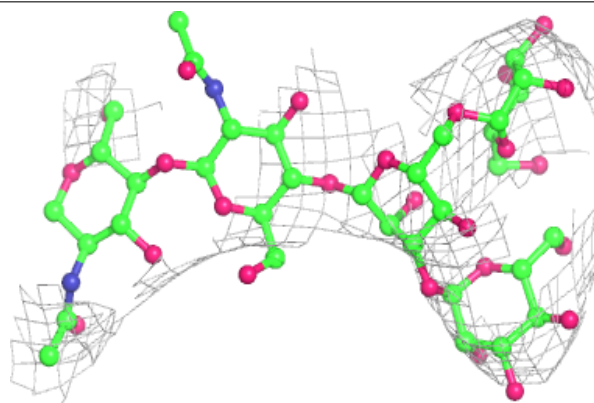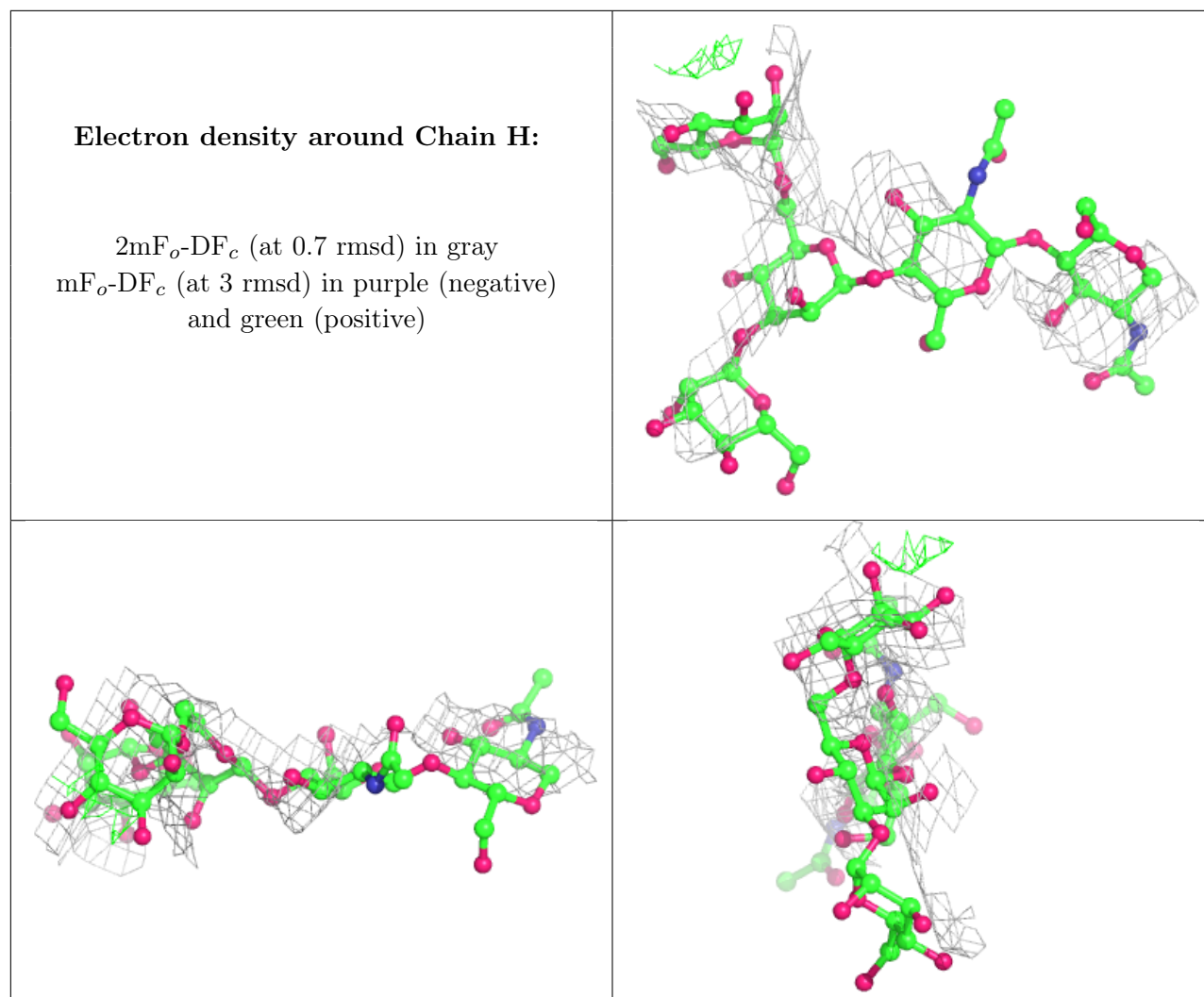
6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.