WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Aug 30, 2023 – 05:18 AM EDT

PDB ID	:	3NWD
Title	:	Glycoprotein B from Herpes simplex virus type 1, Y179S mutant, low-pH
Authors	:	Stampfer, S.D.; Lou, H.; Cohen, G.H.; Eisenberg, R.J.; Heldwein, E.E.
Deposited on	:	2010-07-09
Resolution	:	2.88 Å(reported)

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

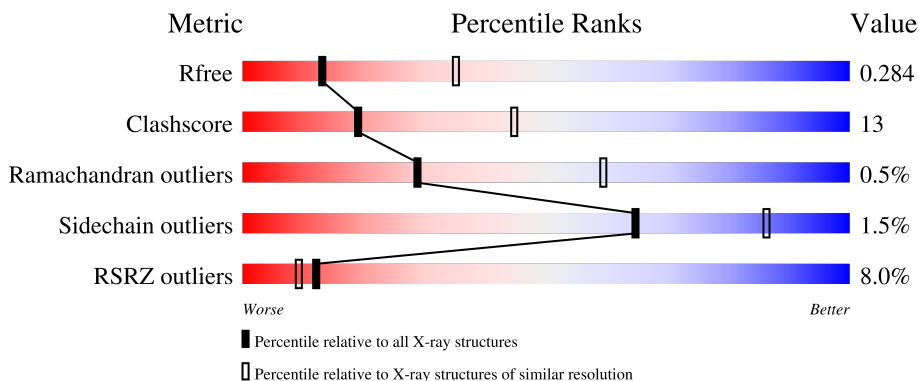|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.88 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	Percentile Ranks	Value
Rfree		0.284
Clashscore		13
Ramachandran outliers		0.5%
Sidechain outliers		1.5%
RSRZ outliers		8.0%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2691 (2.90-2.86)
Clashscore	141614	2947 (2.90-2.86)
Ramachandran outliers	138981	2868 (2.90-2.86)
Sidechain outliers	138945	2871 (2.90-2.86)
RSRZ outliers	127900	2629 (2.90-2.86)

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% 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	703	6% — 61% / 25% / · / 14%
1	B	703	7% — 60% / 24% / · / 15%
1	C	703	8% — 55% / 30% / 15%
1	D	703	6% — 65% / 21% / 14%
2	E	2	50% / 50%

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Mol	Chain	Length	Quality of chain
2	F	2	

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
2	NAG	E	1	X	-	-	-

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 19481 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 Envelope glycoprotein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	597	Total 4767	C 3000	N 835	O 910	S 22	0	1	0
1	A	606	Total 4843	C 3056	N 843	O 922	S 22	0	1	0
1	C	601	Total 4766	C 3003	N 831	O 910	S 22	0	0	0
1	D	606	Total 4829	C 3044	N 846	O 918	S 21	0	1	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	28	ASP	-	expression tag	UNP P06437
B	29	PRO	-	expression tag	UNP P06437
B	58	ALA	PRO	SEE REMARK 999	UNP P06437
B	179	SER	TYR	engineered mutation	UNP P06437
B	313	SER	THR	SEE REMARK 999	UNP P06437
B	443	LEU	GLN	SEE REMARK 999	UNP P06437
A	28	ASP	-	expression tag	UNP P06437
A	29	PRO	-	expression tag	UNP P06437
A	58	ALA	PRO	SEE REMARK 999	UNP P06437
A	179	SER	TYR	engineered mutation	UNP P06437
A	313	SER	THR	SEE REMARK 999	UNP P06437
A	443	LEU	GLN	SEE REMARK 999	UNP P06437
C	28	ASP	-	expression tag	UNP P06437
C	29	PRO	-	expression tag	UNP P06437
C	58	ALA	PRO	SEE REMARK 999	UNP P06437
C	179	SER	TYR	engineered mutation	UNP P06437
C	313	SER	THR	SEE REMARK 999	UNP P06437
C	443	LEU	GLN	SEE REMARK 999	UNP P06437
D	28	ASP	-	expression tag	UNP P06437
D	29	PRO	-	expression tag	UNP P06437
D	58	ALA	PRO	SEE REMARK 999	UNP P06437

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Chain	Residue	Modelled	Actual	Comment	Reference
D	179	SER	TYR	engineered mutation	UNP P06437
D	313	SER	THR	SEE REMARK 999	UNP P06437
D	443	LEU	GLN	SEE REMARK 999	UNP P06437

- Molecule 2 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
2	E	2	Total 28	C 16	N 2	O 10	0	0	0
2	F	2	Total 28	C 16	N 2	O 10	0	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
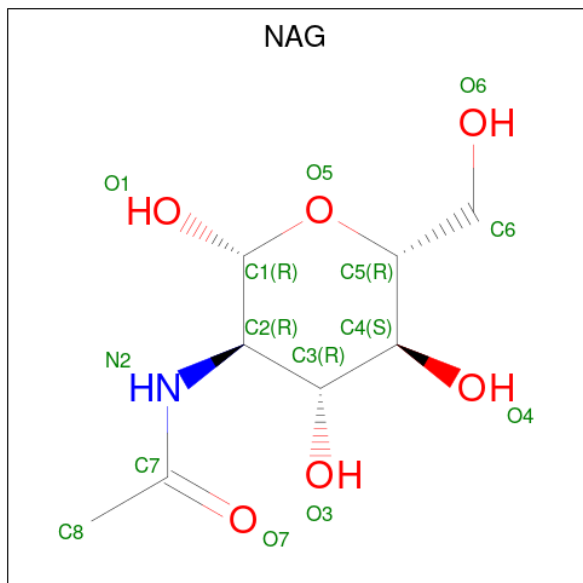
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total 14	C 8	N 1	O 5	0	0
3	B	1	Total 14	C 8	N 1	O 5	0	0

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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Cl 1	0	0
4	D	1	Total 1	Cl 1	0	0

- Molecule 5 is MESO-ERYTHRITOL (three-letter code: MRY) (formula: $C_4H_{10}O_4$).

MRY
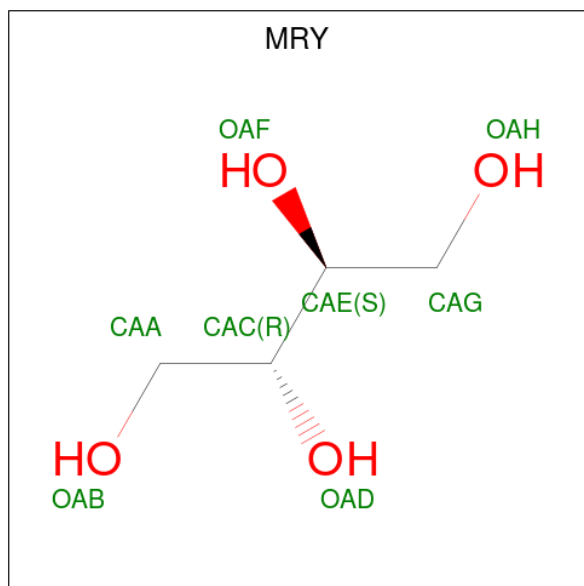
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			8	4	4		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	16	Total	O	0	0
			16	16		
6	A	25	Total	O	0	0
			25	25		
6	C	18	Total	O	0	0
			18	18		
6	D	25	Total	O	0	0
			25	25		

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: Envelope glycoprotein B

• Molecule 1: Envelope glycoprotein B

• Molecule 1: Envelope glycoprotein B

Chain C:

G615 Q616 L617 G618 E619 N620 N621 E622 L623 R624 L625 A629 I630 E631 P632 C633 T634 V635 G636 H637 R638 R639 Y640 F641 T642 V648 Y649 F650 E651 E652 Y653 H657 Q658 L659 D672 T690 E693 Y702 Q706 I723 HIS ALA ASP ALA ASN ALA ALA

• Molecule 1: Envelope glycoprotein B

Chain D:

ASP PRO ALA ALA PRO THR SER PRO GLY THR PRO GLY VAL ALA ALA ALA THR GLN ALA ALA ASN GLY GLY PRO ALA THR PRO PRO ALA PRO ALA LEU GLY ALA ALA PRO THR GLY ASP ALA PRO LYS PRO LYS LYS ASN LYS LYS PRO LYS ASN ASP PRO THR PRO PRO ARG PRO ALA GLY ASP ASN

ALA THR VAL ALA ALA GLY HIS ALA THR LEU ARG GLU HIS LEU ARG ASP I104 K105 A106 E107 N108 F113 Y114 V115 C116 P117 P118 P119 T120 G121 V124 E138 G139 E144 G145 I146 F150 A155 P156 Y164 Y165 K166 D167 W174 F175 G176 H177 R178 F182 R189

A190 P191 K200 V206 C207 R208 S209 L218 F223 H224 R225 D226 E233 L234 K235 H248 T249 T250 D251 L252 K253 Y254 R258 V259 E260 A261 PHE HIS R264 Y265 V269 N270 C271 S280 F287 F294 F300 S307 A315 A327 A336 T340

N343 F350 A353 W356 R360 P361 M375 L376 R377 F384 F385 F386 S392 T393 T394 T397 Y402 P403 D408 L409 C412 K415 A420 I424 F425 Y429 N430 H433 I434 G437 Q438 P439 Q440 A444 Y452 Q453 P454 L455 L456 S457 N458

A461 E467 H468 E471 Q472 S473 P476 P477 ASN PRO THR PRO PRO PRO PRO GLY ALA SER ALA ASN ALA SER V492 T498 I501 E502 F503 L506 Q507 F508 N511 R515 G522 L531 E535 N540 R543 N546 A549 I550 A551 S552 V553

S560 A561 R562 M568 A569 T572 C573 V574 P575 V576 A577 A578 D579 N580 V581 I582 V583 Q584 I589 S590 S591 R592 P593 C596 Y597 S598 R599 P600 L601 V602 S603 F604 R605 Y606 Q609 L612 V613 Q616 L617 G618 E619 E622 L623 R624 L625 T626 R627 D628 A629 I630 G636

H637 R638 R639 Y640 F641 T642 F643 Y647 F650 Q658 L659 S660 R661 A662 D663 T690 E693 H724 A725 ASP ALA ASN ALA ALA

• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluc opyranose

Chain E:

NAG1 NAG2

• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluc opyranose

Chain F:

NAG1 NAG2

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α, β, γ	117.76Å 117.76Å 318.56Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.56 – 2.88 48.56 – 2.88	Depositor EDS
% Data completeness (in resolution range)	88.0 (48.56-2.88) 88.0 (48.56-2.88)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.32 (at 2.86Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.238 , 0.283 0.235 , 0.284	Depositor DCC
R_{free} test set	5310 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å^2)	64.3	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 48.9	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.020 for -h,-k,l 0.468 for h,-h-k,-l 0.022 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	19481	wwPDB-VP
Average B, all atoms (Å^2)	86.0	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 73.43 % 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 1.8395e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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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: NAG, CL, MRY

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	0.21	0/4966	0.39	0/6757
1	B	0.22	0/4879	0.38	0/6631
1	C	0.22	0/4880	0.38	0/6639
1	D	0.22	0/4948	0.38	0/6731
All	All	0.22	0/19673	0.38	0/26758

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	4843	0	4604	113	0
1	B	4767	0	4540	123	0
1	C	4766	0	4514	144	0
1	D	4829	0	4602	111	0
2	E	28	0	25	2	0
2	F	28	0	25	3	0
3	A	42	0	39	0	0
3	B	28	0	26	0	0
3	C	42	0	39	0	0

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PROTEIN DATA BANK

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	14	0	13	0	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
5	C	8	0	10	1	0
6	A	25	0	0	0	0
6	B	16	0	0	0	0
6	C	18	0	0	1	0
6	D	25	0	0	0	0
All	All	19481	0	18437	491	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 13.

The worst 5 of 491 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:183:MET:H	1:A:184:GLY:HA3	1.20	1.05
1:A:183:MET:N	1:A:184:GLY:HA3	1.88	0.88
1:B:259:VAL:HG22	1:B:260:GLU:H	1.45	0.82
1:C:256:PRO:HD3	1:C:266:GLY:HA2	1.64	0.79
1:D:403:PRO:HG3	1:D:476:PRO:HB3	1.65	0.79

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	603/703 (86%)	543 (90%)	56 (9%)	4 (1%)	22	52
1	B	590/703 (84%)	523 (89%)	64 (11%)	3 (0%)	29	59
1	C	595/703 (85%)	532 (89%)	58 (10%)	5 (1%)	19	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	601/703 (86%)	548 (91%)	52 (9%)	1 (0%)	47	76
All	All	2389/2812 (85%)	2146 (90%)	230 (10%)	13 (0%)	29	59

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	259	VAL
1	B	413	ILE
1	A	238	ASN
1	C	429	TYR
1	B	106	ALA

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	517/593 (87%)	505 (98%)	12 (2%)	50	79
1	B	509/593 (86%)	501 (98%)	8 (2%)	62	85
1	C	506/593 (85%)	501 (99%)	5 (1%)	76	91
1	D	514/593 (87%)	509 (99%)	5 (1%)	76	91
All	All	2046/2372 (86%)	2016 (98%)	30 (2%)	65	86

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	323	ASP
1	D	384	PHE
1	A	401	GLU
1	D	625	LEU
1	C	631	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	468	HIS
1	D	472	GLN
1	A	620	ASN
1	C	140	GLN
1	C	270	ASN

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 ⓘ

4 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	0.62	0	17,19,21	1.09	1 (5%)
2	NAG	E	2	2	14,14,15	0.48	0	17,19,21	0.70	0
2	NAG	F	1	1,2	14,14,15	0.55	0	17,19,21	1.46	4 (23%)
2	NAG	F	2	2	14,14,15	0.52	0	17,19,21	0.84	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	1/1/5/7	3/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	F	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	F	2	2	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	1	NAG	C2-N2-C7	-3.44	118.00	122.90
2	F	1	NAG	C1-O5-C5	2.54	115.63	112.19
2	F	1	NAG	O7-C7-C8	-2.45	117.51	122.06
2	E	1	NAG	C2-N2-C7	2.41	126.34	122.90
2	F	1	NAG	O7-C7-N2	2.28	126.15	121.95

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	E	1	NAG	C1

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1	NAG	C3-C2-N2-C7
2	F	1	NAG	C8-C7-N2-C2
2	F	1	NAG	O7-C7-N2-C2
2	E	1	NAG	C4-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1	NAG	2	0
2	F	1	NAG	3	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
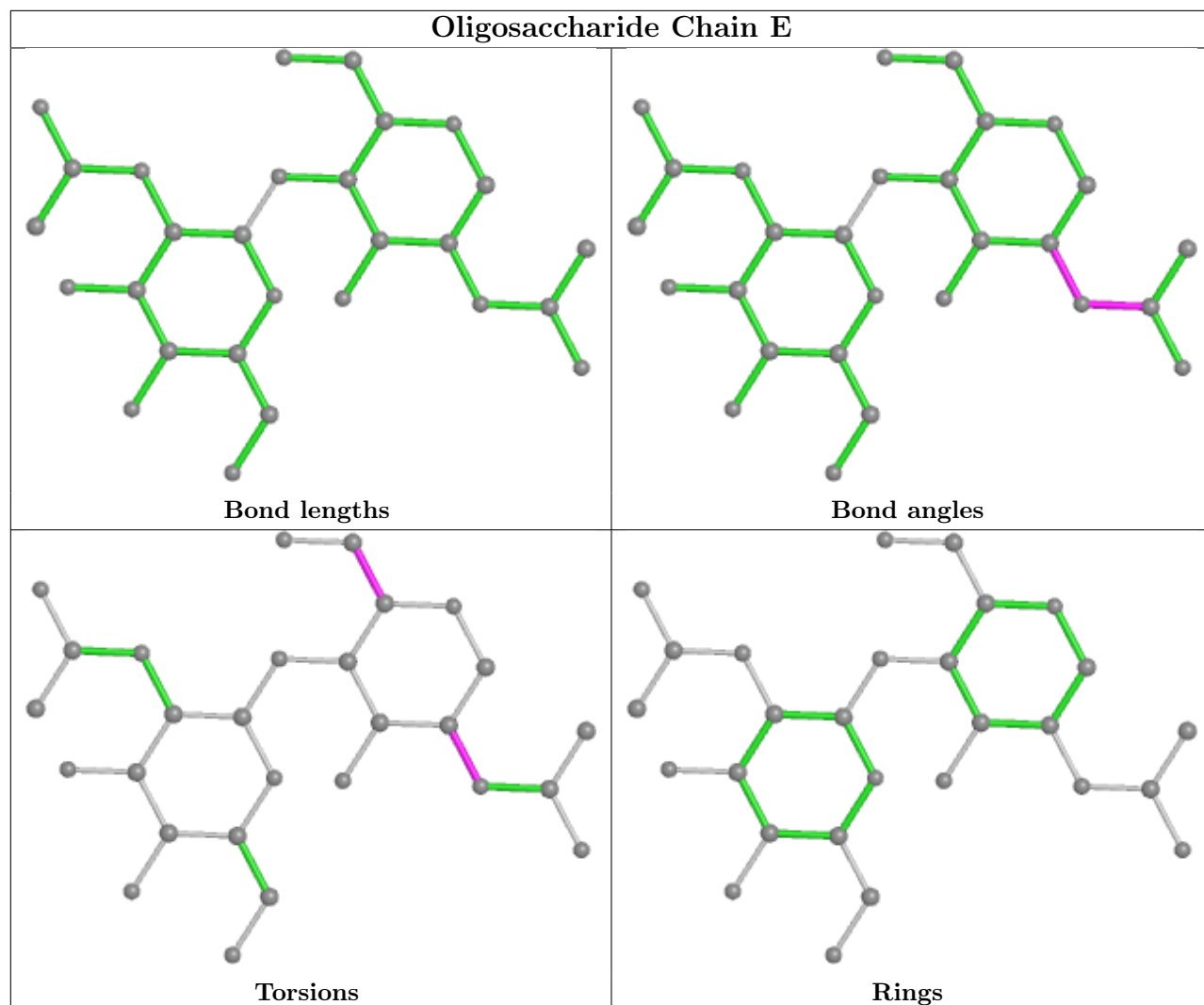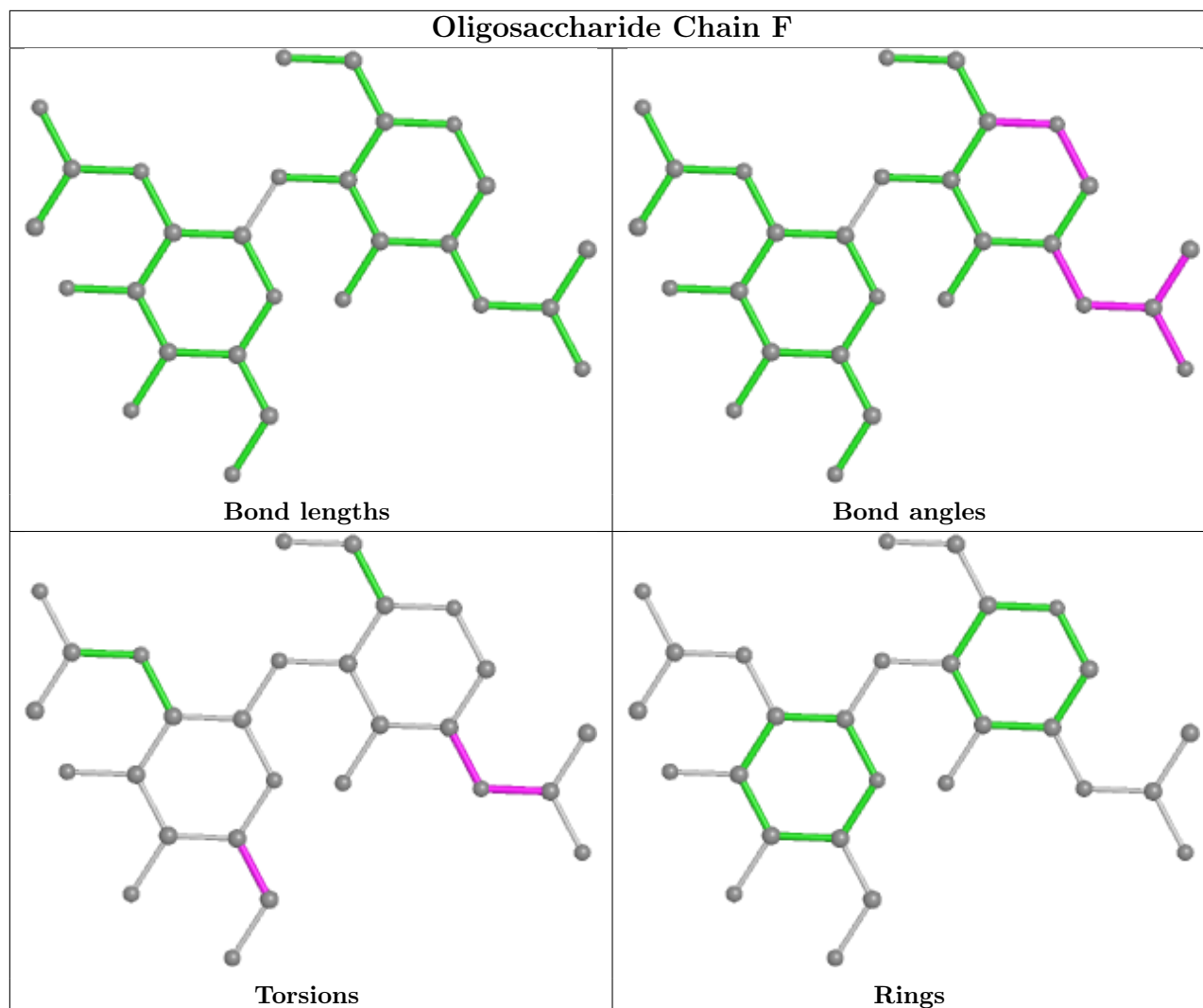
5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
3	NAG	B	1430	1	14,14,15	0.59	0	17,19,21	1.30	2 (11%)
5	MRY	C	2001	-	7,7,7	0.38	0	8,8,8	0.34	0
3	NAG	D	1398	1	14,14,15	0.56	0	17,19,21	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	NAG	A	1141	1	14,14,15	0.51	0	17,19,21	0.71	0
3	NAG	A	1430	1	14,14,15	0.56	0	17,19,21	0.92	1 (5%)
3	NAG	C	1430	1	14,14,15	0.48	0	17,19,21	1.16	1 (5%)
3	NAG	B	1398	1	14,14,15	0.55	0	17,19,21	0.64	0
3	NAG	A	1674	1	14,14,15	0.52	0	17,19,21	0.64	0
3	NAG	C	1674	1	14,14,15	0.53	0	17,19,21	0.63	0
3	NAG	C	1141	1	14,14,15	0.54	0	17,19,21	0.62	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
3	NAG	B	1430	1	-	4/6/23/26	0/1/1/1
5	MRY	C	2001	-	-	0/8/8/8	-
3	NAG	D	1398	1	-	3/6/23/26	0/1/1/1
3	NAG	A	1141	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1430	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1430	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1398	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1674	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1674	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1141	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1430	NAG	C1-O5-C5	3.27	116.63	112.19
3	B	1430	NAG	O5-C1-C2	3.19	116.33	111.29
3	B	1430	NAG	C1-O5-C5	2.82	116.02	112.19
3	A	1430	NAG	C1-O5-C5	2.36	115.39	112.19

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1430	NAG	C3-C2-N2-C7
3	B	1430	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	B	1430	NAG	O7-C7-N2-C2
3	C	1141	NAG	C3-C2-N2-C7
3	C	1141	NAG	C8-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	2001	MRY	1	0

5.7   Other polymers ⓘ

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 ⓘ

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	606/703 (86%)	0.48	42 (6%)	16	13	20, 66, 145, 550	0
1	B	597/703 (84%)	0.70	52 (8%)	10	7	23, 71, 174, 550	0
1	C	601/703 (85%)	0.60	53 (8%)	10	7	20, 76, 176, 550	0
1	D	606/703 (86%)	0.58	45 (7%)	14	11	22, 65, 151, 550	0
All	All	2410/2812 (85%)	0.59	192 (7%)	12	9	20, 69, 164, 550	0

The worst 5 of 192 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	600	PRO	23.9
1	C	595	ALA	22.8
1	D	600	PRO	16.5
1	B	612	LEU	15.9
1	D	604	PHE	14.1

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.
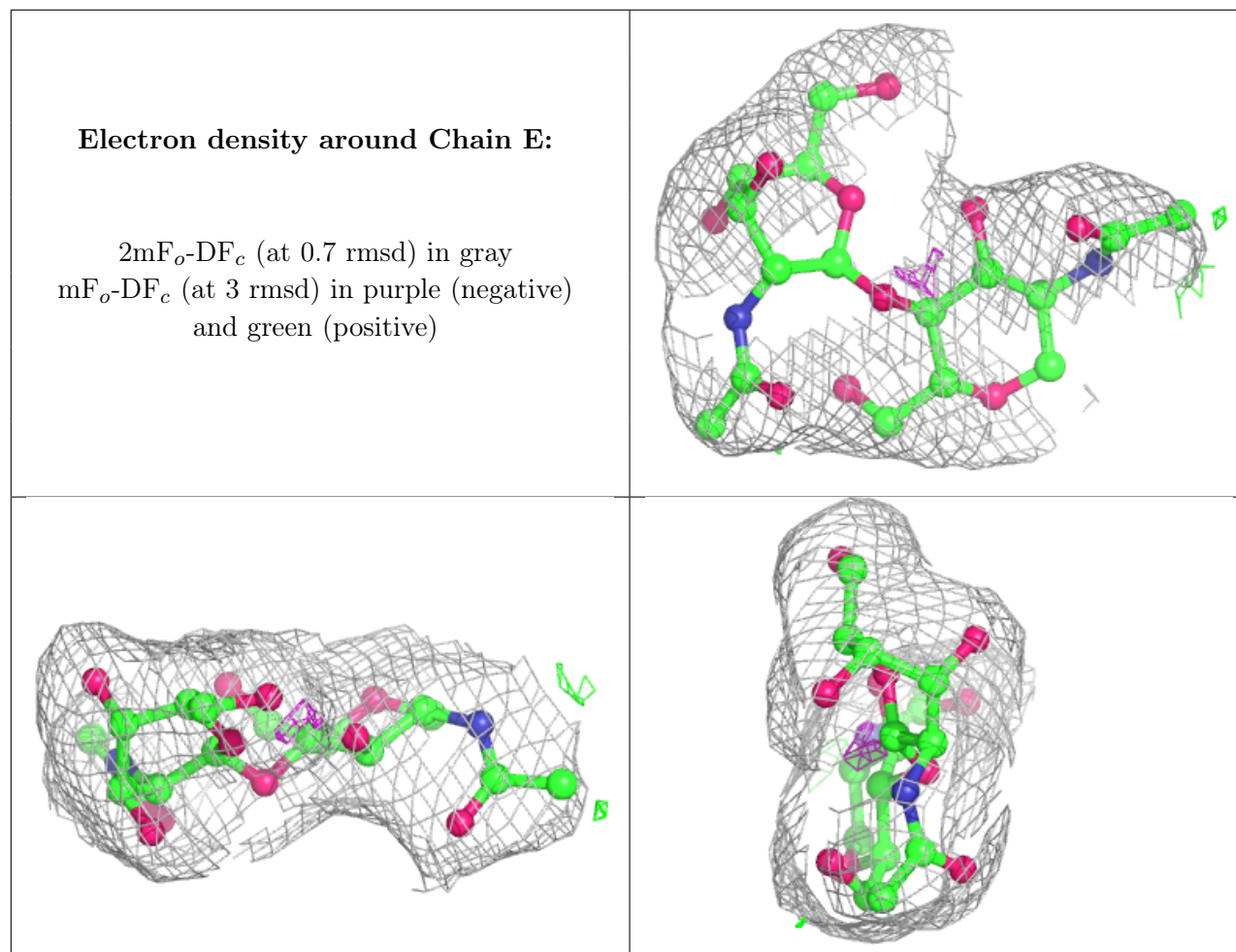
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	E	1	14/15	0.91	0.10	104,104,104,104	0
2	NAG	F	2	14/15	0.92	0.14	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	E	2	14/15	0.94	0.09	89,89,89,89	0
2	NAG	F	1	14/15	0.96	0.12	77,77,77,77	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.
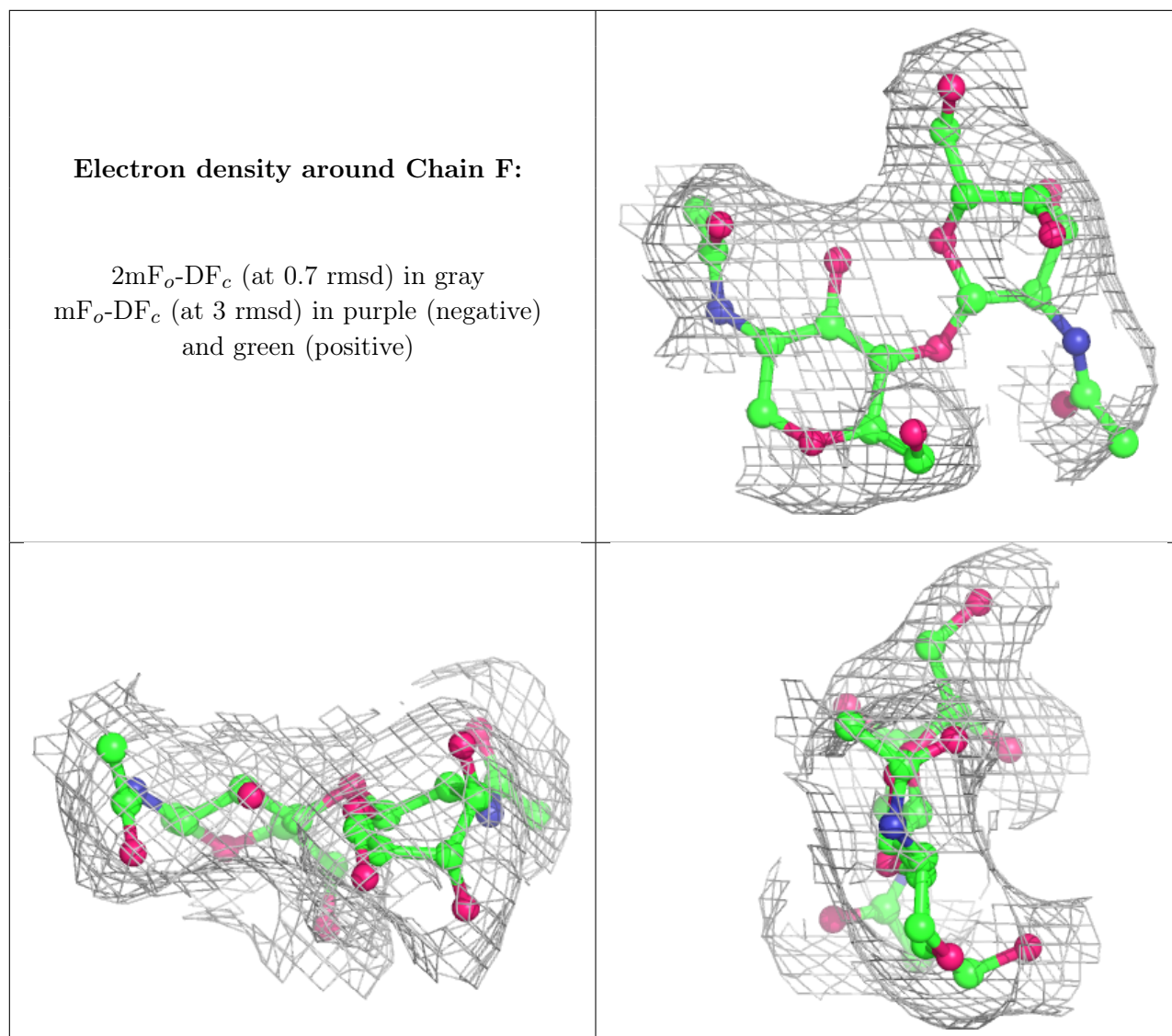
Electron density around Chain E:

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)

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
3	NAG	A	1430	14/15	0.81	0.18	118,118,118,118	0
3	NAG	C	1141	14/15	0.81	0.26	113,113,113,113	0
3	NAG	C	1430	14/15	0.84	0.17	117,117,117,117	0
3	NAG	B	1430	14/15	0.85	0.20	117,117,117,117	0
3	NAG	D	1398	14/15	0.88	0.16	87,87,87,87	0
3	NAG	C	1674	14/15	0.89	0.12	77,77,77,77	0
4	CL	A	2	1/1	0.89	0.11	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	B	1398	14/15	0.90	0.14	92,92,92,92	0
4	CL	D	1	1/1	0.90	0.15	59,59,59,59	0
3	NAG	A	1674	14/15	0.92	0.14	89,89,89,89	0
3	NAG	A	1141	14/15	0.94	0.25	120,120,120,120	0
5	MRY	C	2001	8/8	0.95	0.17	69,69,69,69	0

6.5 Other polymers ⓘ

There are no such residues in this entry.