wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 11, 2024 – 03:18 PM EDT

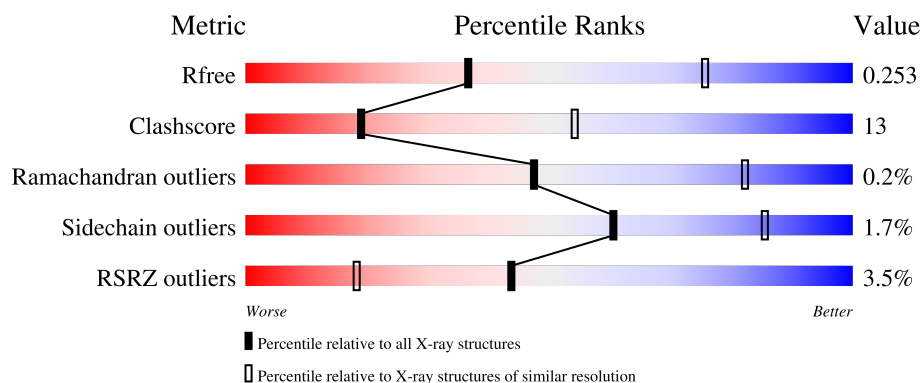|		
PDB ID	:	6MK0
Title	:	Integrin AlphaVBeta3 ectodomain bound to antagonist TDI-4161
Authors	:	van Agthoven, J.; Arnaout, M.A.
Deposited on	:	2018-09-24
Resolution	:	3.00 Å(reported)

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 3.00 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.
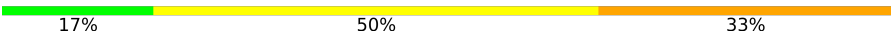
Metric	Percentile Ranks	Value
Rfree		0.253
Clashscore		13
Ramachandran outliers		0.2%
Sidechain outliers		1.7%
RSRZ outliers		3.5%

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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	954	% 73% 23% ·
2	B	687	7% 69% 30% ·
3	C	2	100%
3	E	2	100%
3	F	2	50% 50%

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Mol	Chain	Length	Quality of chain
3	G	2	50% 50%
4	D	6	17% 50% 33%
5	H	3	33% 67%

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
6	NAG	A	1013	-	-	-	X
6	NAG	B	701	-	-	-	X

2 Entry composition ⓘ

There are 9 unique types of molecules in this entry. The entry contains 12820 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 Integrin alpha-V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	920	Total 7163	C 4535	N 1216	O 1377	S 35	0	0	0

- Molecule 2 is a protein called Integrin beta-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	687	Total 5275	C 3239	N 900	O 1066	S 70	0	0	0

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

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

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-beta-D-mannopyranos e-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-be ta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.
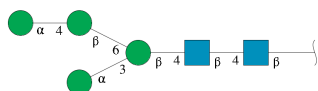
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.
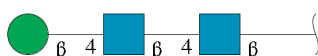
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	H	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
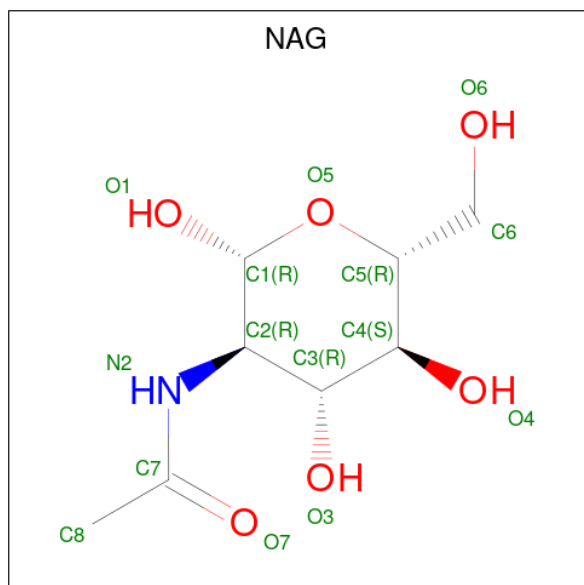
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 7 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	5	Total 5	Mn 5	0	0
7	B	3	Total 3	Mn 3	0	0

- Molecule 8 is (2S)-2-[(1,3-benzothiazole-2-carbonyl)amino]-4-{[5-(1,8-naphthyridin-2-yl)pe ntanoyl]amino}butanoic acid (three-letter code: JUY) (formula: $C_{25}H_{25}N_5O_4S$) (labeled as "Ligand of Interest" by depositor).
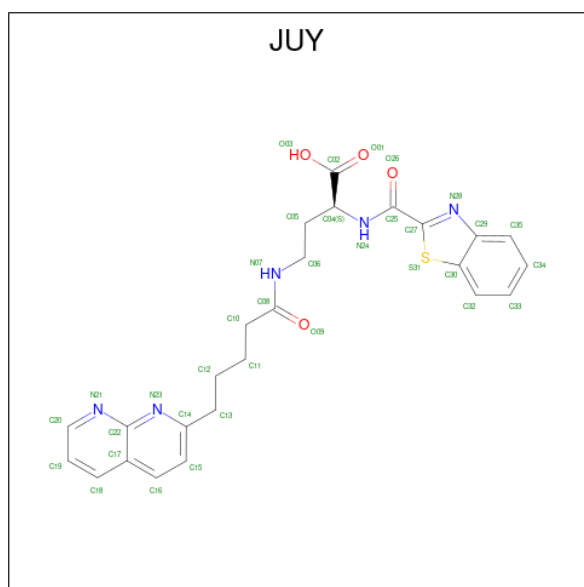
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total 35	C 25	N 5	O 4	S 1	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	4	Total 4	O 4	0	0

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: Integrin alpha-V

• Molecule 2: Integrin beta-3

D224 A229 D233 I236 R239 T249 I256 A257 L258 R261 D288 Y289 L292 M295 K298 L306 I307 F308 A309 V310 T311 E312 V315 N316 L317 Y318 Q319 N320 T328 T329 V330 L333 D336 S337 V340 I344 Y348 R352

V355 E356 L362 P363 E364 E365 L366 S367 L368 L375 E378 L383 K384 S385 C386 M387 G388 L389 K390 I399 V403 P407 I416 K417 P418 F421 L425 F431 D432 C435 Q438 A439 Q440 A441 E442 P443 N444 C448 N449 N450 G451 N452 G453 T454 F455 E456

C457 R461 C462 G463 P464 G465 W466 L467 G468 S469 Q470 C471 E472 C473 S474 E475 E476 D477 Y478 R479 P480 S481 Q482 Q483 D484 E485 C486 S487 P488 Q492 P493 V494 C495 S496 Q497 C501 L502 C503 G504 Q505 H509 S510 S511 D512 K515 K519 Y520 C521 E522 F526 S527 C528 V529

K532 M535 L574 R578 I589 Q590 P591 A607 K611 K618 T630 C631 N632 R633 S641 V642 K646 D647 K650 D651 A652 C655 T656 R666 F667 Q668 Y669 Y670 E671 D672 S673 S674 G675 K676 S677 V682 C687 P688 K689 G690

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

Chain C: 100%

NAG1 NAG2

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

Chain E: 100%

NAG1 NAG2

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

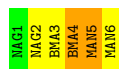Chain F: 50% 50%

NAG1 NAG2

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

Chain G: 50% 50%

NAG1 NAG2

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

NAG1 NAG2 BMA3 BMA4 MAN5 MAN6

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

Chain H:

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          33%                    67%
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NAG1 NAG2 BMA3

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	129.41Å 129.41Å 305.54Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.09 – 3.00 49.37 – 3.00	Depositor EDS
% Data completeness (in resolution range)	94.0 (49.09-3.00) 94.0 (49.37-3.00)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	3.23 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.222 , 0.253 0.221 , 0.253	Depositor DCC
R_{free} test set	2858 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	49.4	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 49.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	12820	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% 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: MAN, JUY, NAG, MN, 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	0.25	0/7319	0.46	0/9922
2	B	0.25	0/5370	0.49	0/7261
All	All	0.25	0/12689	0.47	0/17183

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
2	B	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	453	GLY	Peptide
2	B	472	GLU	Peptide
2	B	479	ARG	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	7163	0	6978	153	0
2	B	5275	0	5003	168	1
3	C	28	0	25	1	0
3	E	28	0	25	0	0
3	F	28	0	25	0	0
3	G	28	0	25	1	0
4	D	72	0	61	3	0
5	H	39	0	34	6	0
6	A	70	0	65	6	0
6	B	42	0	39	2	0
7	A	5	0	0	0	0
7	B	3	0	0	0	0
8	B	35	0	0	1	0
9	B	4	0	0	0	0
All	All	12820	0	12280	327	1

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 327 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:492:GLN:HB2	2:B:493:PRO:HD2	1.43	0.98
1:A:938:ILE:HG13	1:A:939:GLU:H	1.35	0.91
5:H:2:NAG:H3	5:H:2:NAG:H83	1.55	0.86
6:A:1012:NAG:H83	6:A:1012:NAG:H3	1.57	0.85
1:A:940:ASP:O	1:A:941:ILE:HG13	1.76	0.85

All (1) 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:77:SER:OG	2:B:641:SER:O[5_555]	2.05	0.15

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	916/954 (96%)	838 (92%)	77 (8%)	1 (0%)	51	85
2	B	685/687 (100%)	579 (84%)	103 (15%)	3 (0%)	34	72
All	All	1601/1641 (98%)	1417 (88%)	180 (11%)	4 (0%)	47	82

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	450	ASN
2	B	453	GLY
1	A	940	ASP
2	B	443	PRO

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	780/809 (96%)	771 (99%)	9 (1%)	71	90
2	B	610/610 (100%)	596 (98%)	14 (2%)	50	80
All	All	1390/1419 (98%)	1367 (98%)	23 (2%)	60	85

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	474	SER
2	B	503	CYS
2	B	486	CYS
2	B	509	HIS
1	A	622	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	C	1	1,3	14,14,15	0.27	0	17,19,21	0.42	0
3	NAG	C	2	3	14,14,15	0.23	0	17,19,21	0.40	0
4	NAG	D	1	1,4	14,14,15	0.39	0	17,19,21	0.41	0
4	NAG	D	2	4	14,14,15	0.26	0	17,19,21	0.45	0
4	BMA	D	3	4	11,11,12	0.59	0	15,15,17	0.83	0
4	BMA	D	4	4	11,11,12	0.89	0	15,15,17	0.91	1 (6%)
4	MAN	D	5	4	11,11,12	1.54	2 (18%)	15,15,17	2.16	5 (33%)
4	MAN	D	6	4	11,11,12	1.29	2 (18%)	15,15,17	1.09	1 (6%)
3	NAG	E	1	1,3	14,14,15	0.23	0	17,19,21	0.39	0
3	NAG	E	2	3	14,14,15	0.19	0	17,19,21	0.45	0
3	NAG	F	1	1,3	14,14,15	0.21	0	17,19,21	0.40	0
3	NAG	F	2	3	14,14,15	0.42	0	17,19,21	0.69	1 (5%)
3	NAG	G	1	2,3	14,14,15	0.34	0	17,19,21	0.48	0
3	NAG	G	2	3	14,14,15	0.49	0	17,19,21	0.66	1 (5%)
5	NAG	H	1	2,5	14,14,15	0.27	0	17,19,21	0.47	0
5	NAG	H	2	5	14,14,15	0.27	0	17,19,21	0.57	0
5	BMA	H	3	5	11,11,12	1.00	0	15,15,17	2.92	6 (40%)

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	C	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
4	NAG	D	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	BMA	D	3	4	-	2/2/19/22	0/1/1/1
4	BMA	D	4	4	-	1/2/19/22	1/1/1/1
4	MAN	D	5	4	-	2/2/19/22	0/1/1/1
4	MAN	D	6	4	-	0/2/19/22	0/1/1/1
3	NAG	E	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	E	2	3	-	4/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	NAG	G	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	4/6/23/26	0/1/1/1
5	NAG	H	1	2,5	-	2/6/23/26	0/1/1/1
5	NAG	H	2	5	-	5/6/23/26	0/1/1/1
5	BMA	H	3	5	-	1/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	5	MAN	C1-C2	4.26	1.61	1.52
4	D	6	MAN	O5-C1	-2.63	1.39	1.43
4	D	5	MAN	O5-C1	2.51	1.47	1.43
4	D	6	MAN	C2-C3	2.35	1.56	1.52

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	3	BMA	C1-C2-C3	5.98	117.02	109.67
5	H	3	BMA	C1-O5-C5	5.54	119.70	112.19
4	D	5	MAN	C1-O5-C5	5.52	119.67	112.19
5	H	3	BMA	O3-C3-C2	5.04	119.64	109.99
4	D	5	MAN	C1-C2-C3	3.84	114.38	109.67

There are no chirality outliers.

5 of 37 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1	NAG	C4-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
4	D	5	MAN	O5-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	4	BMA	C1-C2-C3-C4-C5-O5

8 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	2	NAG	1	0
3	C	1	NAG	1	0
3	C	2	NAG	1	0
4	D	2	NAG	1	0
4	D	3	BMA	1	0
4	D	5	MAN	2	0
4	D	4	BMA	1	0
5	H	2	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 C

Bond lengths

Bond angles

Torsions

Rings

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 D

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain H

Bond lengths

Bond angles

Torsions

Rings
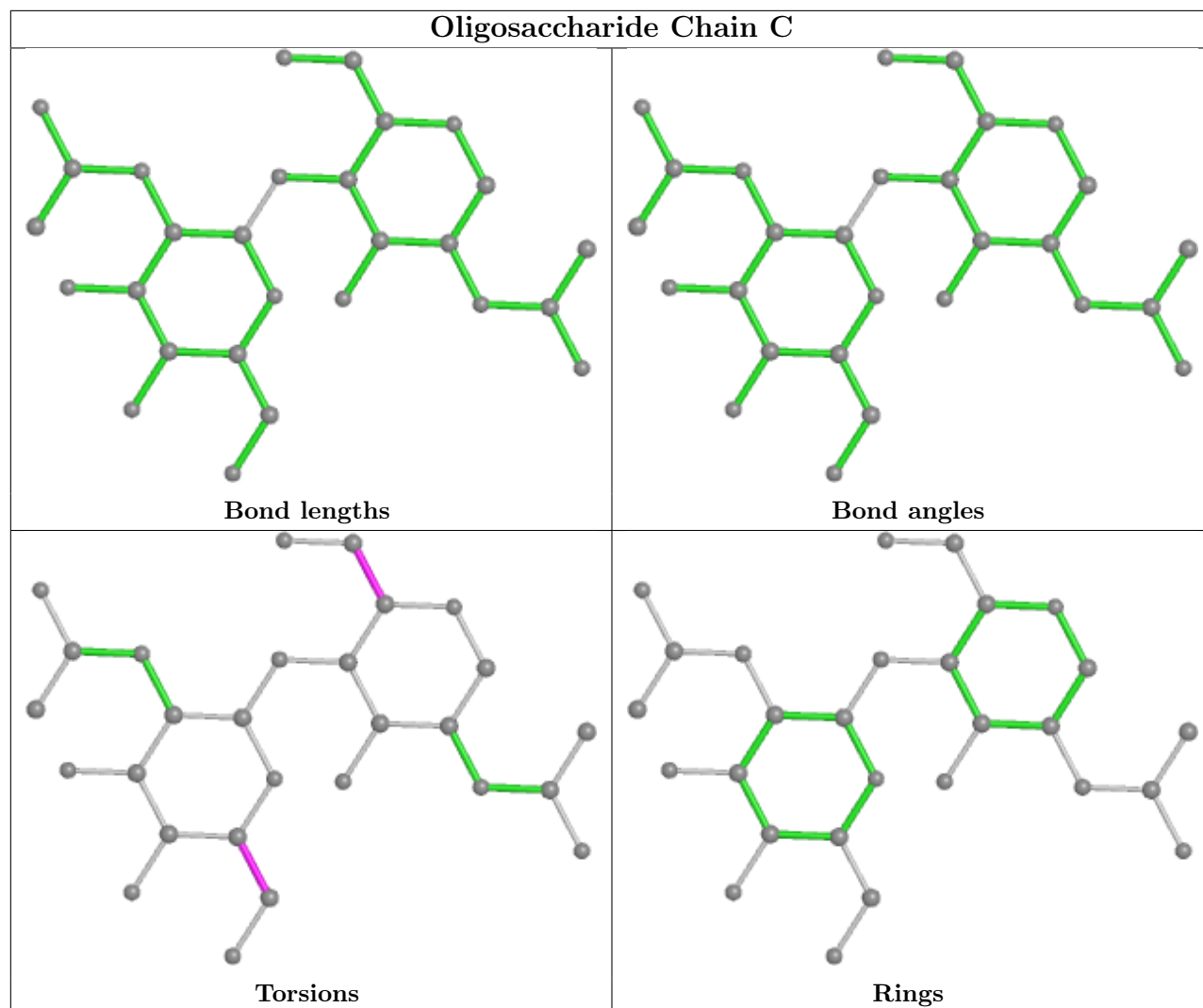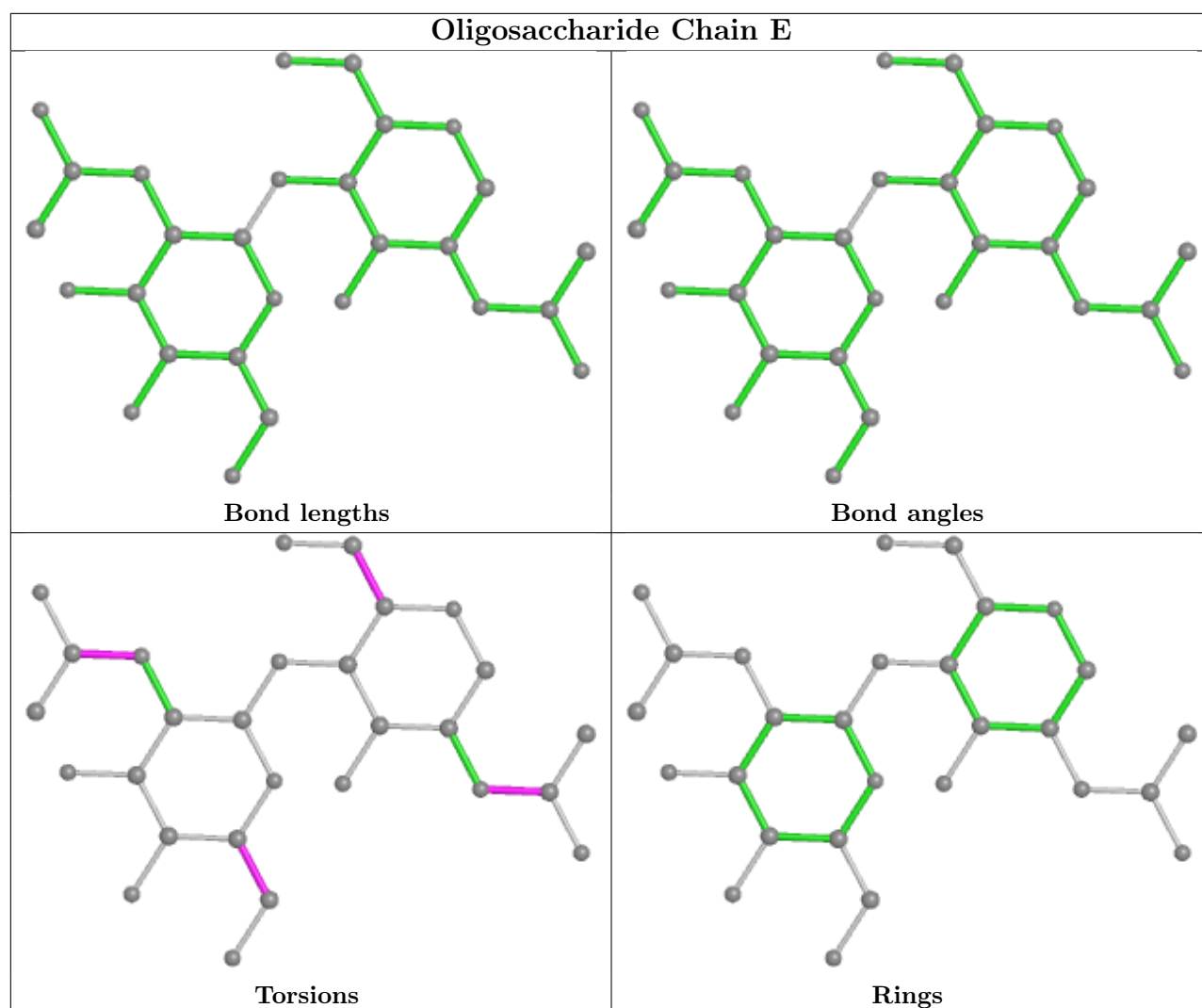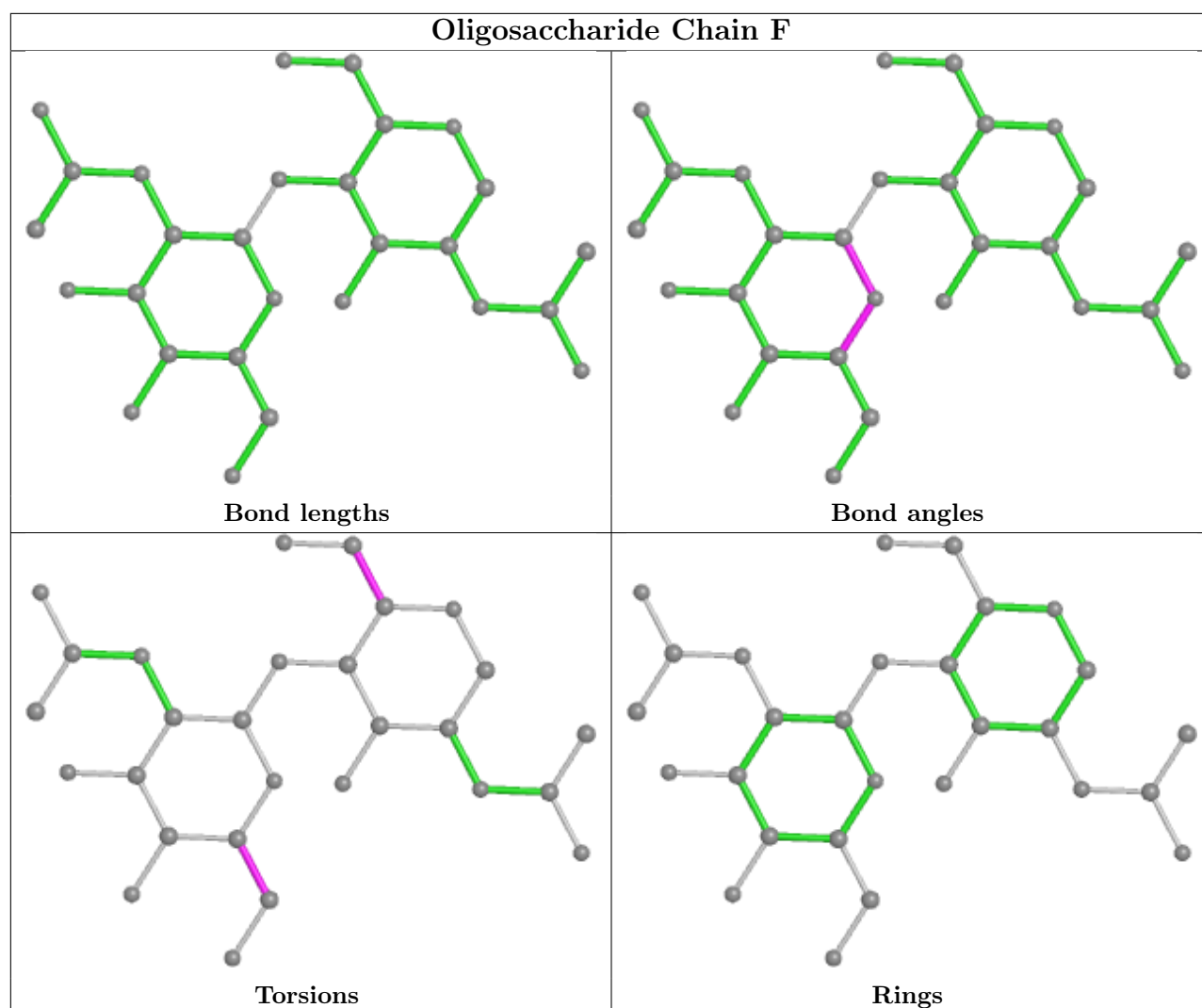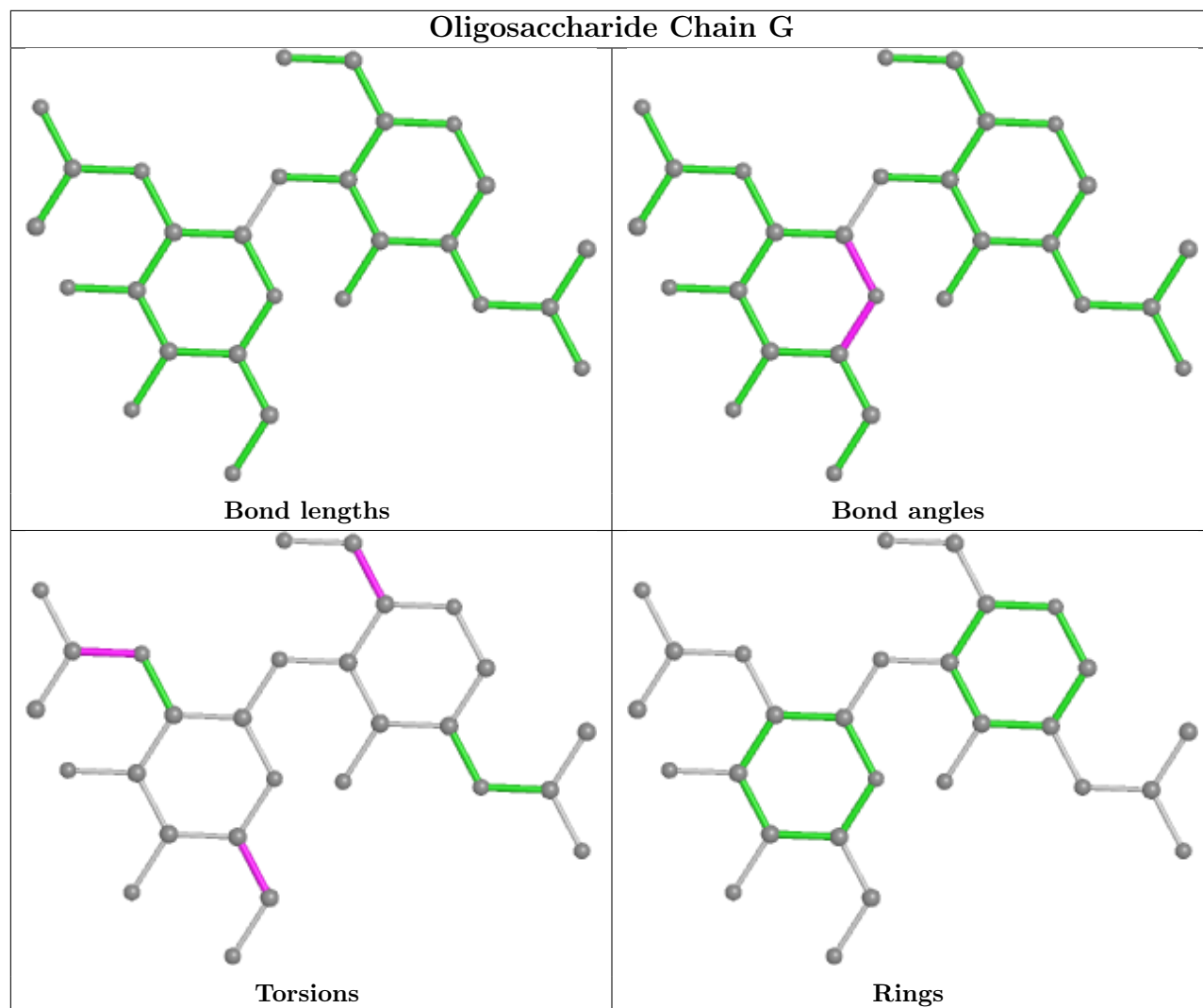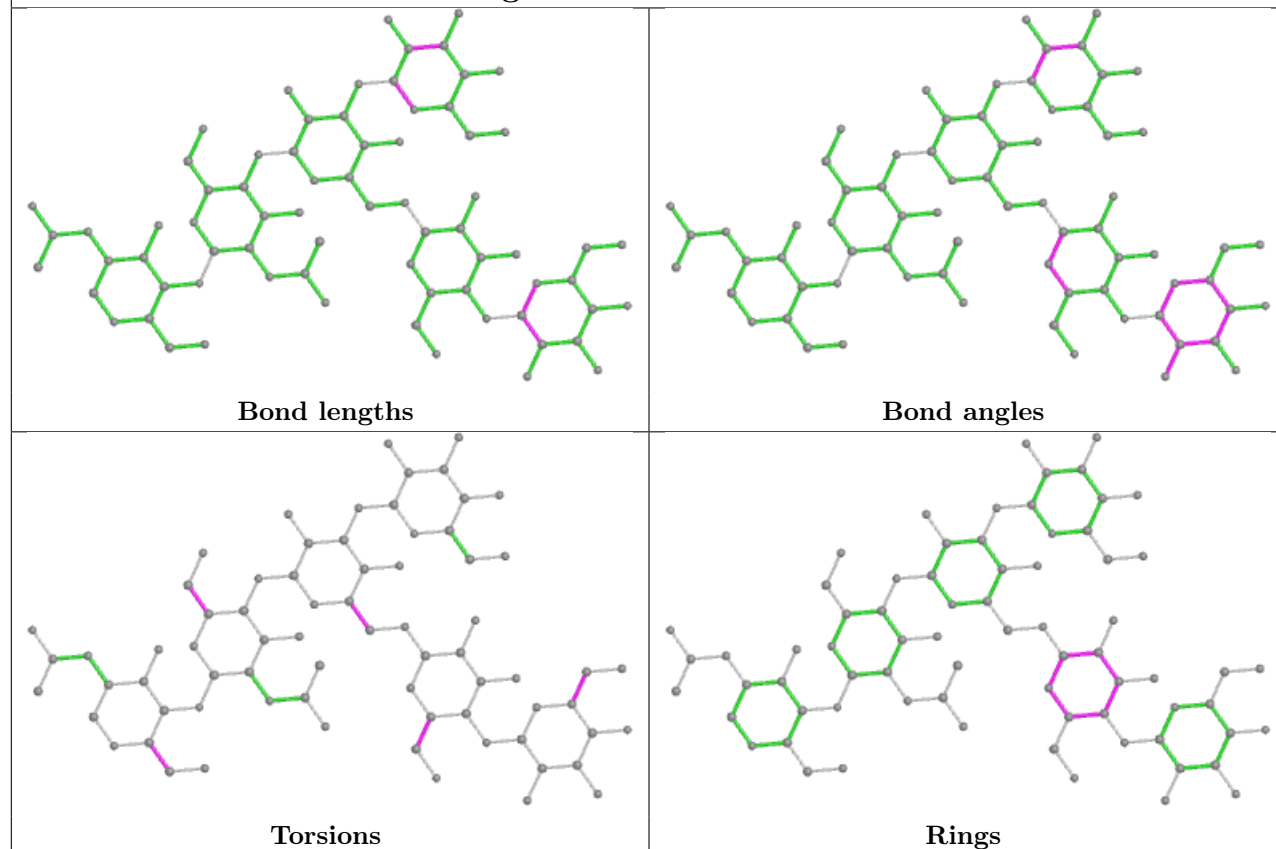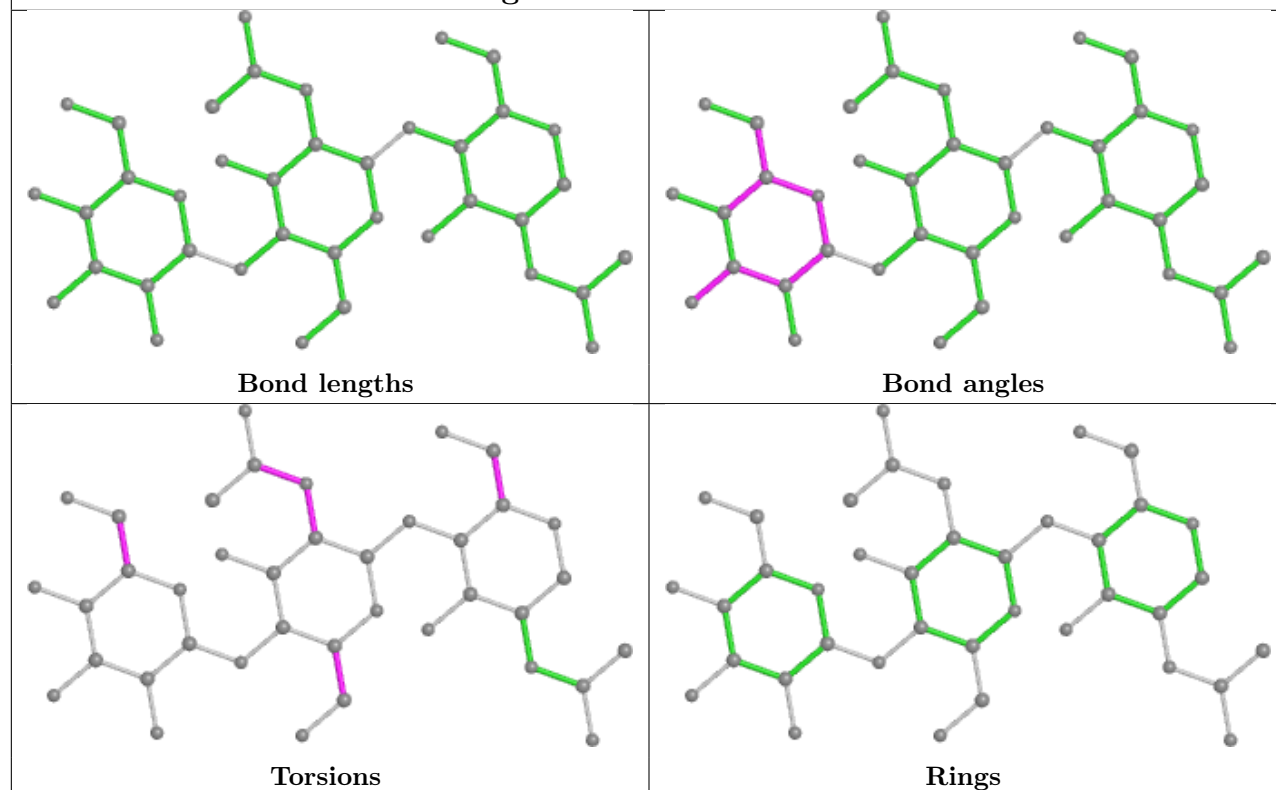
5.6 Ligand geometry ⓘ

Of 17 ligands modelled in this entry, 8 are monoatomic - leaving 9 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	$\#\|Z\| > 2$
8	JUY	B	712	7	37,38,38	2.99	14 (37%)	44,51,51	2.51	16 (36%)
6	NAG	A	1016	1	14,14,15	0.26	0	17,19,21	0.38	0
6	NAG	B	711	2	14,14,15	0.30	0	17,19,21	0.40	0
6	NAG	A	1012	1	14,14,15	0.19	0	17,19,21	0.59	0
6	NAG	B	701	2	14,14,15	0.41	0	17,19,21	0.69	1 (5%)
6	NAG	A	1003	1	14,14,15	0.35	0	17,19,21	0.78	1 (5%)
6	NAG	B	702	2	14,14,15	0.31	0	17,19,21	0.41	0
6	NAG	A	1017	1	14,14,15	0.26	0	17,19,21	0.38	0
6	NAG	A	1013	1	14,14,15	0.31	0	17,19,21	0.36	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
8	JUY	B	712	7	-	4/21/25/25	0/4/4/4
6	NAG	A	1016	1	-	0/6/23/26	0/1/1/1
6	NAG	B	711	2	-	0/6/23/26	0/1/1/1
6	NAG	A	1012	1	-	3/6/23/26	0/1/1/1
6	NAG	B	701	2	-	0/6/23/26	0/1/1/1
6	NAG	A	1003	1	-	3/6/23/26	0/1/1/1
6	NAG	B	702	2	-	1/6/23/26	0/1/1/1
6	NAG	A	1017	1	-	3/6/23/26	0/1/1/1
6	NAG	A	1013	1	-	1/6/23/26	0/1/1/1

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	712	JUY	C19-C18	8.88	1.57	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	712	JUY	C20-N21	7.25	1.47	1.32
8	B	712	JUY	C22-N21	6.41	1.45	1.37
8	B	712	JUY	C27-S31	6.20	1.82	1.73
8	B	712	JUY	C19-C20	6.11	1.55	1.37

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	712	JUY	C14-N23-C22	6.94	120.80	117.51
8	B	712	JUY	C18-C17-C22	6.18	122.48	117.75
8	B	712	JUY	C27-N28-C29	5.80	115.27	103.78
8	B	712	JUY	C19-C20-N21	-5.27	115.86	123.94
8	B	712	JUY	C18-C19-C20	-3.91	113.90	118.93

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1003	NAG	O5-C5-C6-O6
6	A	1003	NAG	C4-C5-C6-O6
6	A	1012	NAG	C8-C7-N2-C2
6	A	1012	NAG	O7-C7-N2-C2
6	A	1017	NAG	C8-C7-N2-C2

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	712	JUY	1	0
6	B	711	NAG	1	0
6	A	1012	NAG	4	0
6	A	1003	NAG	2	0
6	B	702	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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand JUY B 712

Bond lengths   Bond angles

Torsions   Rings
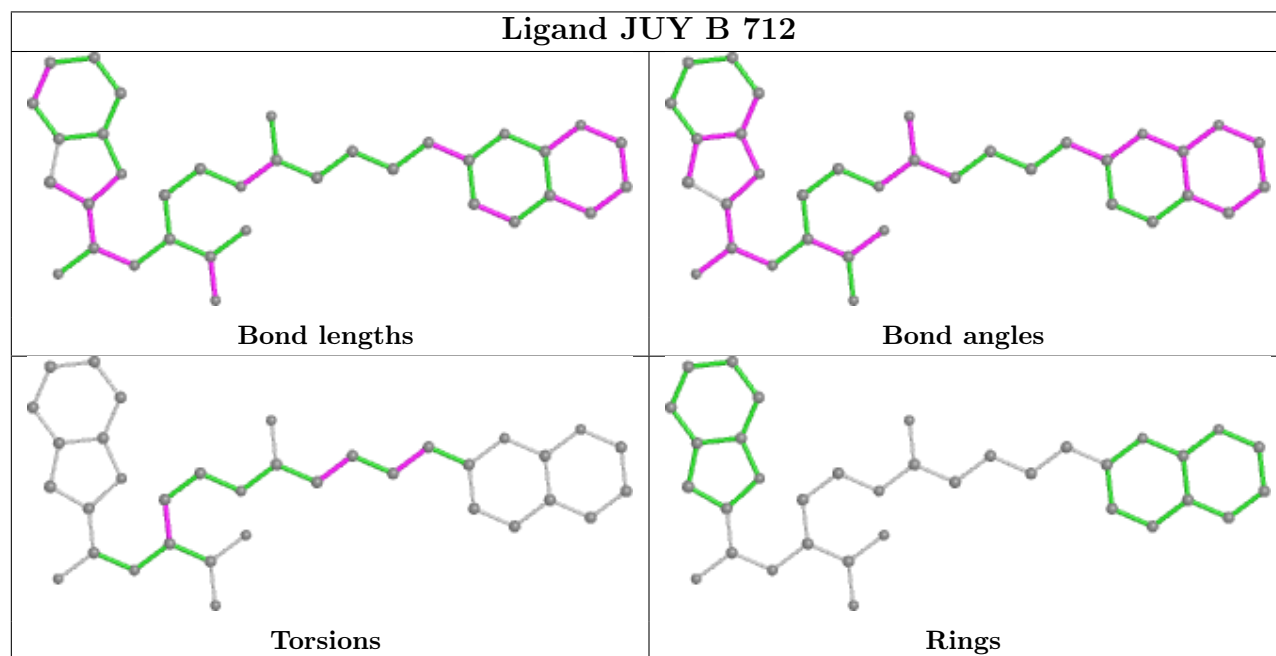
5.7 Other polymers ⓘ

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	920/954 (96%)	-0.22	7 (0%)	86	65	17, 44, 91, 121	0
2	B	687/687 (100%)	0.16	50 (7%)	15	4	21, 56, 133, 165	1 (0%)
All	All	1607/1641 (97%)	-0.06	57 (3%)	44	18	17, 50, 119, 165	1 (0%)

The worst 5 of 57 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	466	TRP	10.1
2	B	36	PRO	9.8
2	B	441	ALA	8.4
2	B	29	GLU	7.3
2	B	482	GLN	7.3

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.
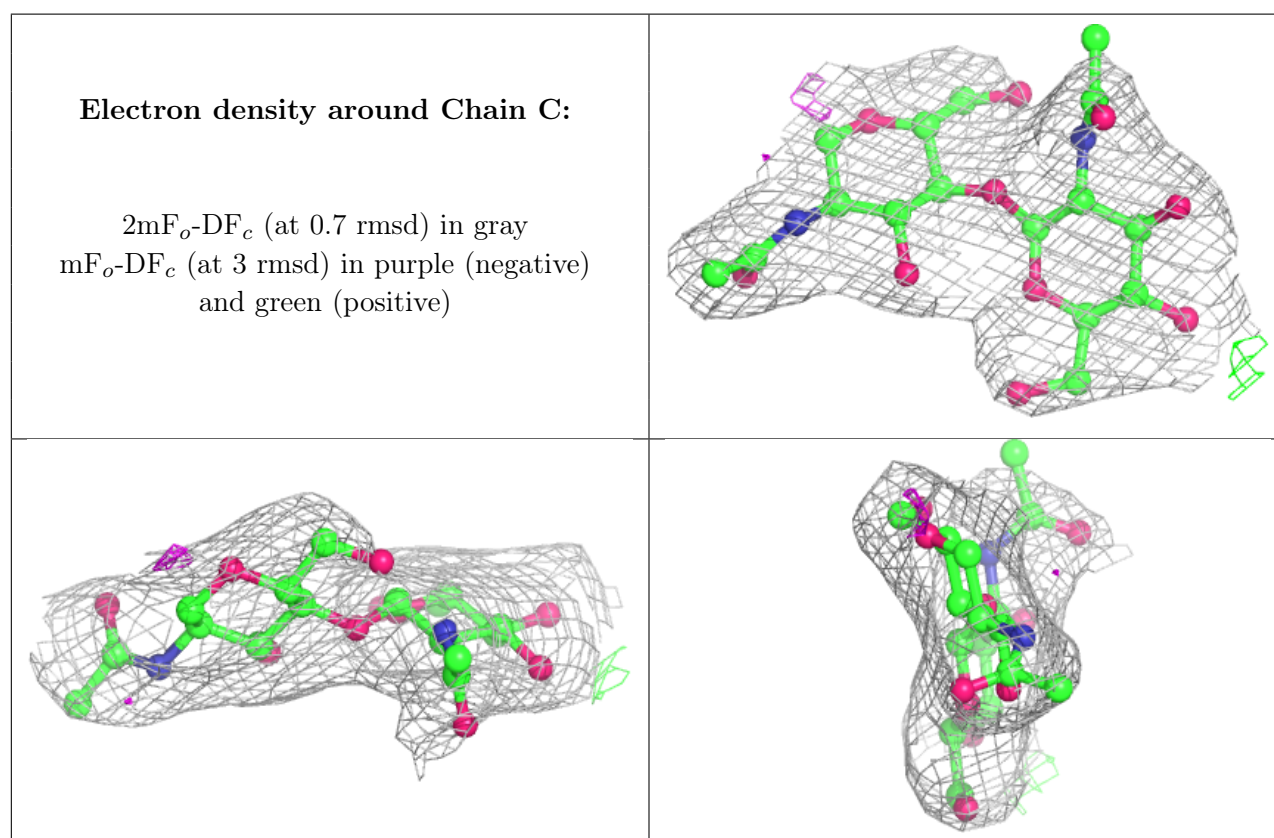
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	G	2	14/15	0.75	0.30	92,108,113,118	0
3	NAG	F	2	14/15	0.80	0.40	60,84,95,99	0
4	BMA	D	4	11/12	0.80	0.19	58,71,78,80	0
3	NAG	E	2	14/15	0.83	0.30	58,83,90,92	0
3	NAG	F	1	14/15	0.84	0.29	48,71,78,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	BMA	H	3	11/12	0.84	0.21	60,78,88,91	0
4	MAN	D	6	11/12	0.85	0.25	64,72,87,89	0
5	NAG	H	2	14/15	0.88	0.30	84,96,112,112	0
3	NAG	G	1	14/15	0.88	0.14	46,64,80,82	0
3	NAG	E	1	14/15	0.89	0.23	32,55,78,79	0
4	MAN	D	5	11/12	0.90	0.19	47,64,75,79	0
3	NAG	C	2	14/15	0.92	0.15	39,54,61,73	0
5	NAG	H	1	14/15	0.95	0.18	43,52,71,76	0
4	BMA	D	3	11/12	0.95	0.09	46,54,70,80	0
3	NAG	C	1	14/15	0.95	0.16	4,24,51,55	0
4	NAG	D	2	14/15	0.96	0.14	13,36,54,71	0
4	NAG	D	1	14/15	0.97	0.13	5,24,42,51	0

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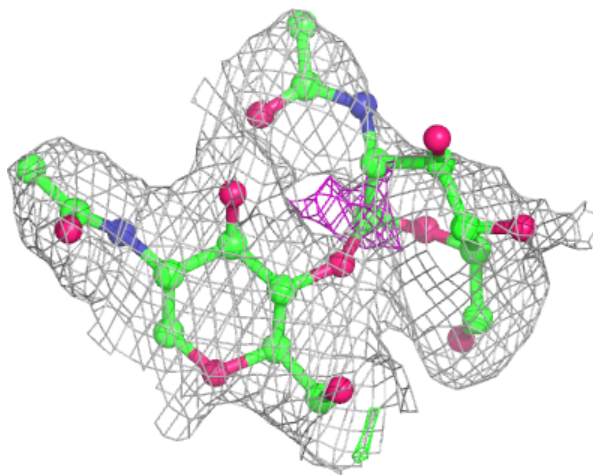

Electron density around Chain C:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
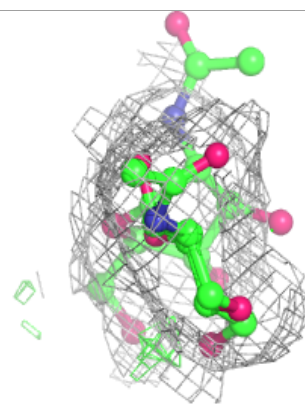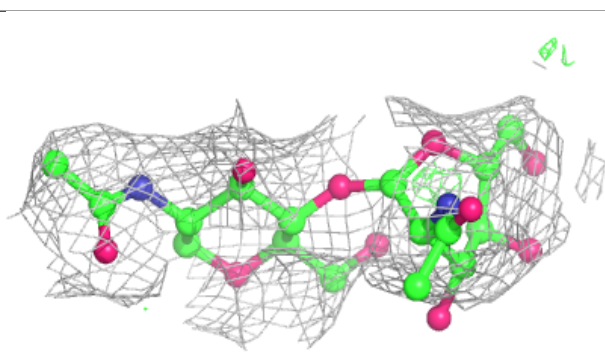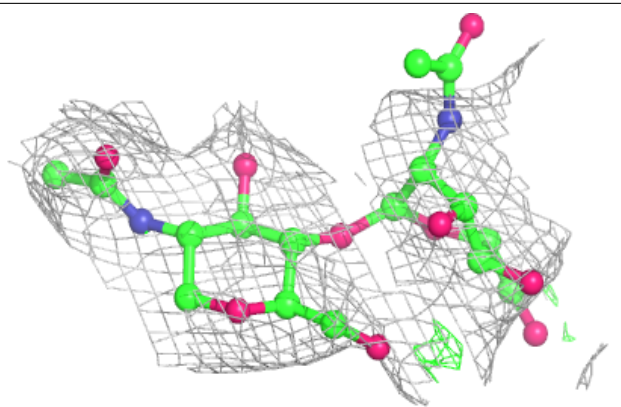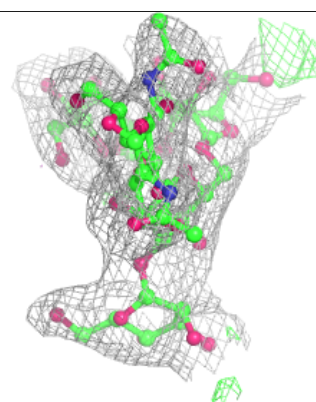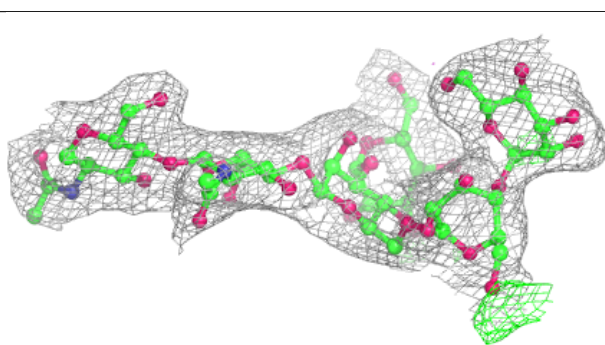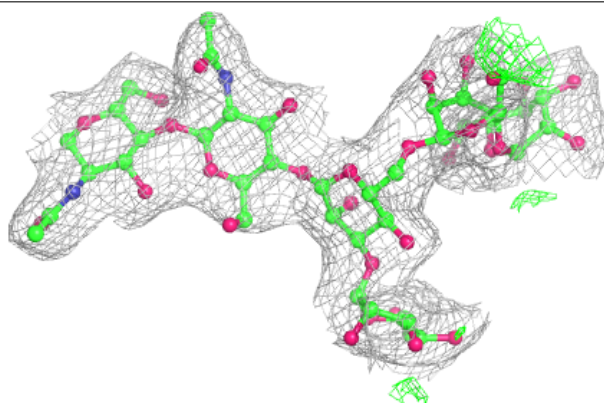and green (positive)

Electron density around Chain E:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
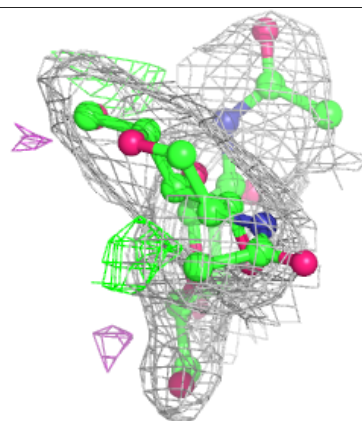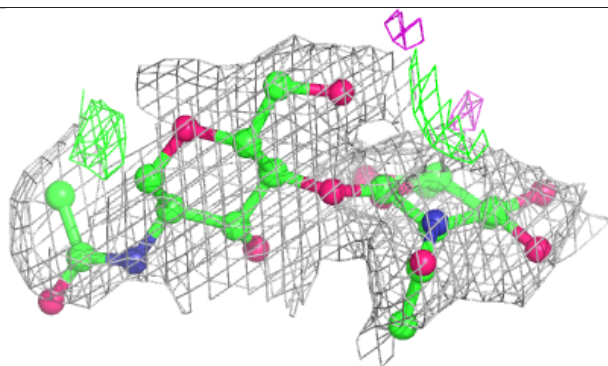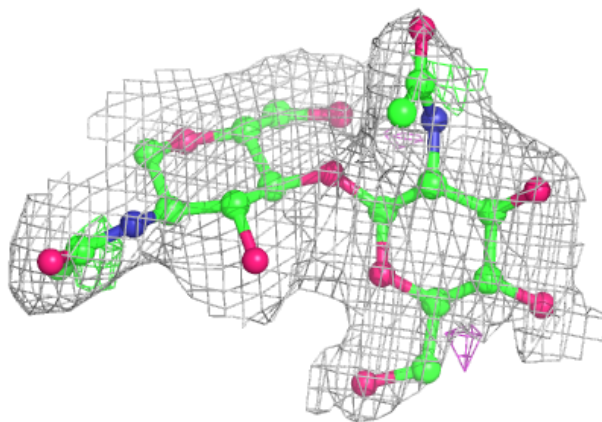
Electron density around Chain F:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
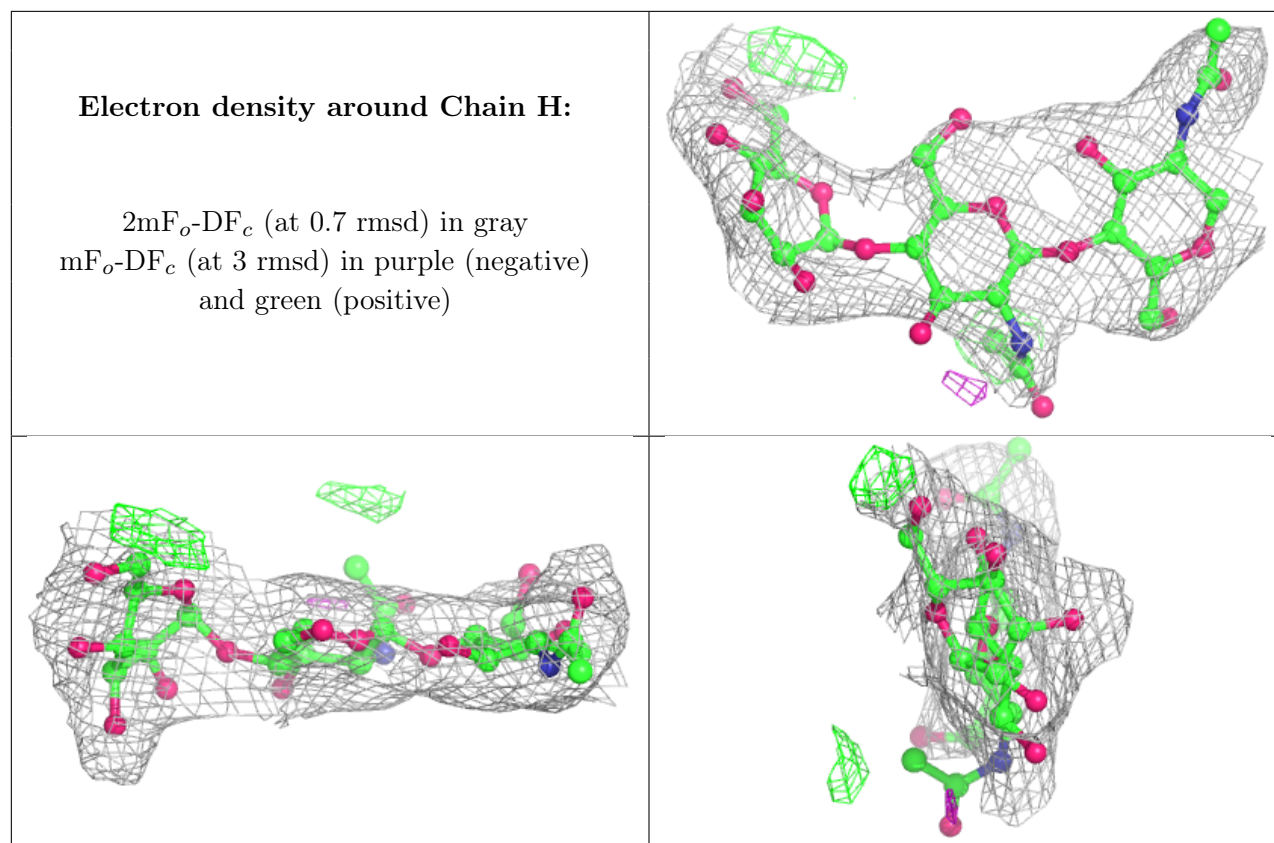mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
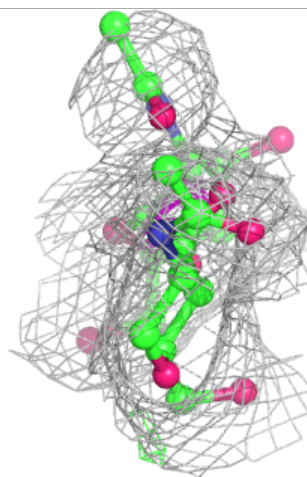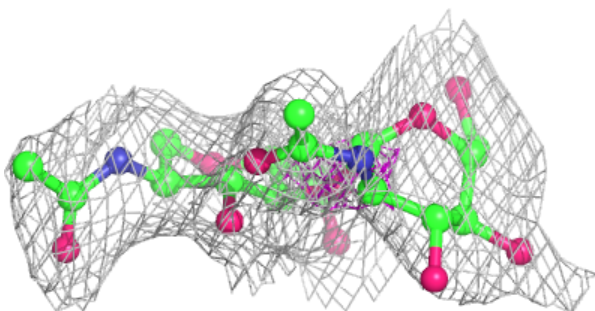
Electron density around Chain G:

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

Electron density around Chain D:

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

Electron density around Chain H:

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

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.
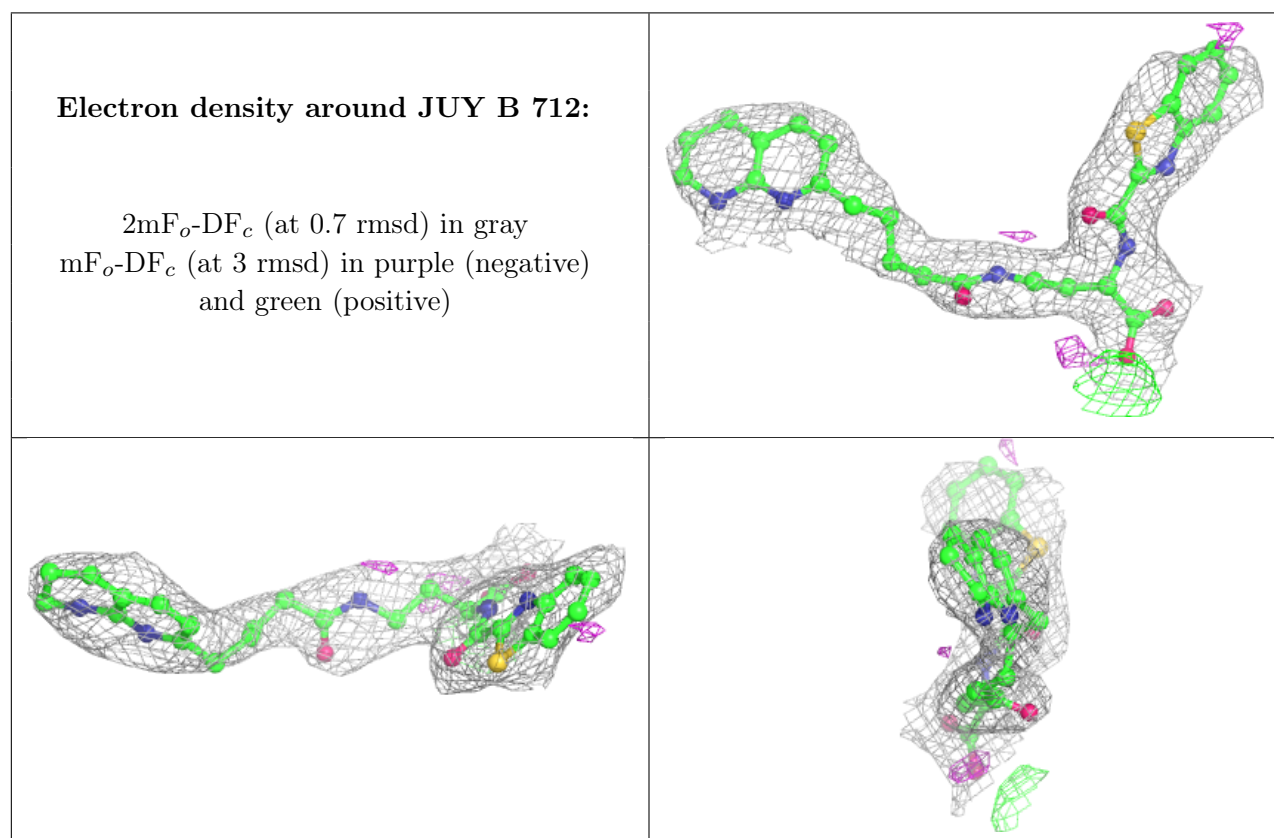
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
7	MN	B	709	1/1	0.30	0.31	210,210,210,210	0
6	NAG	A	1013	14/15	0.50	0.48	55,96,103,103	0
6	NAG	B	701	14/15	0.73	0.41	68,88,99,101	0
7	MN	B	708	1/1	0.75	0.28	80,80,80,80	0
6	NAG	B	711	14/15	0.79	0.28	58,68,81,86	0
6	NAG	A	1012	14/15	0.81	0.18	51,72,88,90	0
6	NAG	B	702	14/15	0.88	0.18	56,73,91,103	0
6	NAG	A	1003	14/15	0.88	0.19	52,69,79,79	0
7	MN	A	1018	1/1	0.89	0.15	99,99,99,99	0
7	MN	A	1020	1/1	0.89	0.16	76,76,76,76	0
6	NAG	A	1016	14/15	0.91	0.17	18,60,65,77	0
8	JUY	B	712	35/35	0.92	0.20	15,49,78,146	0
6	NAG	A	1017	14/15	0.94	0.17	30,52,73,75	0
7	MN	A	1019	1/1	0.96	0.29	178,178,178,178	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
7	MN	A	1021	1/1	0.97	0.17	105,105,105,105	0
7	MN	A	1022	1/1	0.98	0.17	83,83,83,83	0
7	MN	B	710	1/1	0.99	0.19	46,46,46,46	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around JUY B 712:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.