



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 07:14 PM UTC

PDB ID : 6B9O / pdb_00006b9o
Title : Structure of GH 38 Jack Bean alpha-mannosidase
Authors : Howard, E.; Cousido-Siah, A.; Lepage, M.; Bodlenner, A.; Mitschler, A.; Meli, A.; De Riccardis, F.; Izzo, I.; Podjarny, A.; Compain, P.
Deposited on : 2017-10-11
Resolution : 1.84 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)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

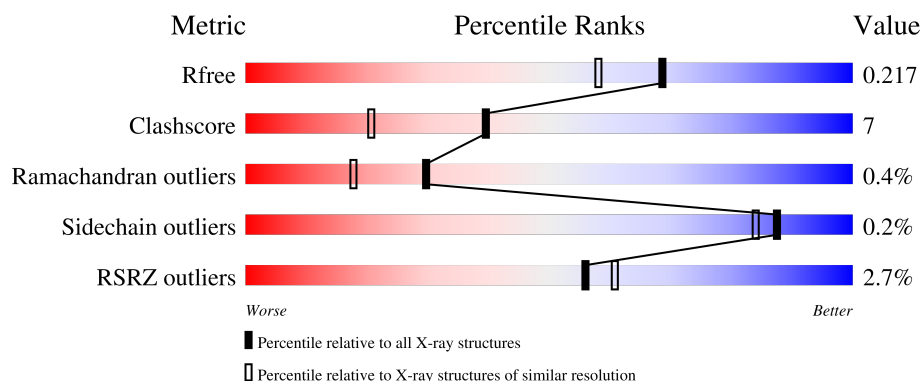
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.84 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	1296 (1.84-1.84)
Clashscore	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

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	981	3% 83% 12% 5%
1	B	981	3% 84% 12% .
2	C	12	17% 50% 33%
2	E	12	8% 75% 17%
3	D	2	50% 50%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	2	 50%50%

2 Entry composition [i](#)

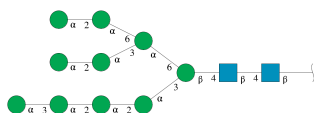
There are 5 unique types of molecules in this entry. The entry contains 17299 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Alpha-mannosidase from Canavalia ensiformis (jack bean).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	935	Total	C	N	O	S	0	10	0
			7561	4807	1288	1435	31			
1	B	937	Total	C	N	O	S	0	6	0
			7561	4805	1288	1437	31			

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]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
2	C	12	Total	C	N	O	0	1	0
			149	82	2	65			
2	E	12	Total	C	N	O	0	0	0
			138	76	2	60			

- Molecule 3 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
3	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

Continued on next page...

Continued from previous page...

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

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		
4	B	1	Total	Zn	0	0
			1	1		

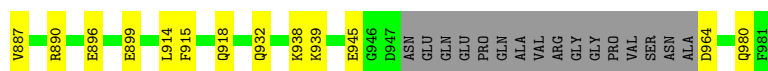
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	930	Total	O	0	3
			933	933		
5	B	898	Total	O	0	1
			899	899		

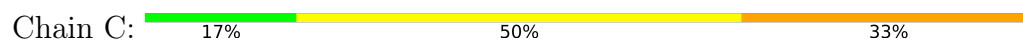
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

- Chain A:
-
- 3% 83% 12% 5%
- W1 R29 W28 V37 Q44 K95 N103 D110 Y116 E132 I137 F138 R139 I144 L157 E160 F168 E182 G208 G211 R221 Q228 K254 G266 F269 Y273 K274 E275 K290 Y304 K308 T314 I319 D320
- LEU THR LEU SER GLN LYS GLY GLU THR L570 F581 S582 S583 LEU G586 Q587 R590 M591 S594 D599 N605 S611 S612 Y619 S622 R628 P629 M630 G631 A628 D529 V530 Y531 P540 P541 W544 F548 E551 ALA THR GLY LYS ARG ASN ALA
- L669 Y670 K673 A676 E677 I678 E679 K707 R716 R726 W729 E732 K751 E756 R763 R782 M801 ASN LYS GLU TYR T806 R813 Y816 Y817 L818 P832 P633 P634 P635 P636 T637 VAL SER ARG S641 S642 E851 N852 G861 I862 D865 T878 L879 F880
- G885 L886 K887 L888 L889 R890 K908 K912 K913 L914 F915 A916 T917 Q918 K919 I920 E921 E922 Q932 E933 K934 S935 E936 S943 D947 ASN GLU GLN GLU PRO GLN ALA VAL ARG GLY GLY PRO VAL SER ASN ALA D964 P965 V966 Q980 F981

- Chain B:
-
- | Amino Acid | Category |
|------------|----------|
| M1 | Green |
| R358 | Green |
| LYS | Green |
| GLY | Green |
| A676 | Green |
| E677 | Green |
| THR | Green |
| ARG | Green |
| ASN | Green |
| G683 | Green |
| P684 | Green |
| W28 | Green |
| D62 | Green |
| H385 | Green |
| H386 | Green |
| D387 | Green |
| LEU | Green |
| THR | Green |
| SER | Green |
| D724 | Green |
| GLN | Green |
| L731 | Green |
| L744 | Green |
| L750 | Green |
| G573 | Green |
| K578 | Green |
| M579 | Green |
| S580 | Green |
| F581 | Green |
| S582 | Green |
| S583 | Green |
| L584 | Green |
| T585 | Green |
| D796 | Green |
| D797 | Green |
| F797 | Green |
| Q798 | Green |
| R799 | Green |
| T801 | Green |
| M801 | Green |
| ASN | Green |
| I600 | Green |
| W608 | Green |
| S611 | Green |
| R813 | Green |
| Y817 | Green |
| L818 | Green |
| S827 | Green |
| M841 | Green |
| N852 | Green |
| I862 | Green |
| Y863 | Green |
| M864 | Green |
| M867 | Green |
| T878 | Green |
| D884 | Green |
| GLN | Green |
| SER | Green |
| ALA | Green |
| ASP | Green |
| GLN | Green |
| C422 | Green |
| L423 | Green |
| K426 | Green |
| V467 | Green |
| S474 | Green |
| K475 | Green |
| K476 | Green |
| E477 | Green |
| D485 | Green |
| K526 | Green |
| D527 | Green |
| A528 | Green |
| D529 | Green |
| V530 | Green |
| Y531 | Green |
| K536 | Green |
| P540 | Green |
| P541 | Green |
| L542 | Green |
| G543 | Green |
| W544 | Green |
| Y545 | Green |
| S545 | Green |
| T546 | Green |
| A551 | Green |
| ALA | Green |
| THR | Green |
| CY | Green |
| K157 | Yellow |
| F168 | Yellow |
| R176 | Yellow |
| K180 | Yellow |
| A181 | Yellow |
| E182 | Yellow |
| K183 | Yellow |
| K193 | Yellow |
| G208 | Yellow |
| H209 | Yellow |
| T210 | Yellow |
| G211 | Yellow |
| Q228 | Yellow |
| T255 | Yellow |
| G266 | Yellow |
| Y273 | Yellow |
| A274 | Yellow |
| E275 | Yellow |
| K290 | Yellow |
| T314 | Yellow |
| R329 | Yellow |
| A342 | Yellow |
| L343 | Yellow |
| K344 | Yellow |
| D345 | Yellow |
| C432 | Grey |
| S433 | Grey |
| H443 | Grey |
| L570 | Grey |
| G573 | Grey |
| M579 | Grey |
| F581 | Grey |
| S582 | Grey |
| S583 | Grey |
| L584 | Grey |
| T585 | Grey |
| D796 | Grey |
| D797 | Grey |
| F797 | Grey |
| Q798 | Grey |
| R799 | Grey |
| T801 | Grey |
| M801 | Grey |
| ASN | Grey |
| I600 | Grey |
| W608 | Grey |
| S611 | Grey |
| R813 | Grey |
| Y817 | Grey |
| L818 | Grey |
| S827 | Grey |
| M841 | Grey |
| N852 | Grey |
| I862 | Grey |
| Y863 | Grey |
| M864 | Grey |
| M867 | Grey |
| T878 | Grey |
| D884 | Grey |
| GLN | Grey |
| SER | Grey |
| ALA | Grey |
| ASP | Grey |
| GLN | Grey |
| C422 | Grey |
| L423 | Grey |
| K426 | Grey |
| V467 | Grey |
| S474 | Grey |
| K475 | Grey |
| K476 | Grey |
| E477 | Grey |
| D485 | Grey |
| K526 | Grey |
| D527 | Grey |
| A528 | Grey |
| D529 | Grey |
| V530 | Grey |
| Y531 | Grey |
| K536 | Grey |
| P540 | Grey |
| P541 | Grey |
| L542 | Grey |
| G543 | Grey |
| W544 | Grey |
| Y545 | Grey |
| S545 | Grey |
| T546 | Grey |
| A551 | Grey |
| ALA | Grey |
| THR | Grey |
| CY | Grey |



- Molecule 2: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]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



- Molecule 2: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]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



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.31Å 119.67Å 277.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.55 – 1.84 49.55 – 1.84	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.55-1.84) 99.4 (49.55-1.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 1.84Å)	Xtriage
Refinement program	PHENIX 1.11.1 _2575	Depositor
R, R_{free}	0.175 , 0.216 0.176 , 0.217	Depositor DCC
R_{free} test set	9670 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	23.3	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 35.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17299	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% 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, BMA, ZN, 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	0.36	0/7777	0.55	1/10540 (0.0%)
1	B	0.35	0/7767	0.54	1/10528 (0.0%)
All	All	0.35	0/15544	0.55	2/21068 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	157	LEU	CA-CB-CG	-5.89	95.69	116.30
1	A	157	LEU	CA-CB-CG	-5.65	96.53	116.30

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	7561	0	7318	97	0
1	B	7561	0	7298	100	0
2	C	149	0	125	8	0
2	E	138	0	115	5	0
3	D	28	0	25	0	0
3	F	28	0	25	1	0
4	A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
5	A	933	0	0	40	2
5	B	899	0	0	52	2
All	All	17299	0	14906	204	2

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 7.

The worst 5 of 204 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:B:541:PRO:O	1:B:862:ILE:CD1	2.06	1.03
1:B:541:PRO:O	1:B:862:ILE:HD13	1.64	0.97
1:B:813:ARG:H	2:E:1:NAG:H81	1.40	0.84
1:B:632:GLN:NE2	1:B:633:PRO:O	2.13	0.81
1:B:329:ARG:NH2	5:B:1102:HOH:O	2.15	0.80

All (2) 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)
5:A:1365:HOH:O	5:B:1804:HOH:O[1_655]	1.93	0.27
5:A:1365:HOH:O	5:B:1133:HOH:O[1_655]	2.19	0.01

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	931/981 (95%)	894 (96%)	34 (4%)	3 (0%)	36 25
1	B	931/981 (95%)	893 (96%)	34 (4%)	4 (0%)	30 18

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1862/1962 (95%)	1787 (96%)	68 (4%)	7 (0%)	30 18

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	586	GLY
1	A	28	TRP
1	B	28	TRP
1	B	208	GLY
1	B	103	ASN

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	823/849 (97%)	820 (100%)	3 (0%)	84 78
1	B	821/849 (97%)	820 (100%)	1 (0%)	88 85
All	All	1644/1698 (97%)	1640 (100%)	4 (0%)	87 84

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

Mol	Chain	Res	Type
1	A	228	GLN
1	A	818[A]	LEU
1	A	818[B]	LEU
1	B	182	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	223	ASN
1	B	313	GLN
1	B	932	GLN
1	B	605	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	632	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 ⓘ

29 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	C	1	1,2	14,14,15	0.84	1 (7%)	17,19,21	0.80	1 (5%)
2	MAN	C	10	2	11,11,12	0.74	0	15,15,17	1.03	1 (6%)
2	MAN	C	11	2	11,11,12	1.05	1 (9%)	15,15,17	1.29	2 (13%)
2	MAN	C	12	2	11,11,12	0.55	0	15,15,17	1.03	1 (6%)
2	NAG	C	2	2	14,14,15	0.63	0	17,19,21	0.81	1 (5%)
2	BMA	C	3	2	11,11,12	0.86	0	15,15,17	0.92	0
2	MAN	C	4	2	11,11,12	0.82	0	15,15,17	1.10	1 (6%)
2	MAN	C	5	2	11,11,12	0.77	0	15,15,17	1.02	0
2	MAN	C	6[A]	2	11,11,12	1.59	3 (27%)	15,15,17	1.66	3 (20%)
2	MAN	C	6[B]	2	11,11,12	1.98	2 (18%)	15,15,17	2.06	4 (26%)
2	MAN	C	7	2	11,11,12	1.90	3 (27%)	15,15,17	1.56	4 (26%)
2	MAN	C	8	2	11,11,12	0.72	0	15,15,17	1.24	2 (13%)
2	MAN	C	9	2	11,11,12	0.69	0	15,15,17	1.09	2 (13%)
3	NAG	D	1	1,3	14,14,15	0.36	0	17,19,21	0.72	0
3	NAG	D	2	3	14,14,15	0.34	0	17,19,21	1.99	2 (11%)

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	0.66	0	17,19,21	0.77	1 (5%)
2	MAN	E	10	2	11,11,12	0.95	1 (9%)	15,15,17	1.16	1 (6%)
2	MAN	E	11	2	11,11,12	0.85	0	15,15,17	1.10	1 (6%)
2	MAN	E	12	2	11,11,12	0.73	0	15,15,17	0.88	1 (6%)
2	NAG	E	2	2	14,14,15	0.65	0	17,19,21	0.82	1 (5%)
2	BMA	E	3	2	11,11,12	0.63	0	15,15,17	0.98	0
2	MAN	E	4	2	11,11,12	0.78	0	15,15,17	1.06	1 (6%)
2	MAN	E	5	2	11,11,12	0.62	0	15,15,17	1.13	2 (13%)
2	MAN	E	6	2	11,11,12	1.05	0	15,15,17	1.32	2 (13%)
2	MAN	E	7	2	11,11,12	1.59	1 (9%)	15,15,17	1.30	2 (13%)
2	MAN	E	8	2	11,11,12	0.78	0	15,15,17	1.16	2 (13%)
2	MAN	E	9	2	11,11,12	0.86	1 (9%)	15,15,17	1.25	2 (13%)
3	NAG	F	1	1,3	14,14,15	1.52	2 (14%)	17,19,21	1.38	1 (5%)
3	NAG	F	2	3	14,14,15	1.30	2 (14%)	17,19,21	1.42	1 (5%)

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	C	1	1,2	-	4/6/23/26	0/1/1/1
2	MAN	C	10	2	-	0/2/19/22	0/1/1/1
2	MAN	C	11	2	-	0/2/19/22	0/1/1/1
2	MAN	C	12	2	-	0/2/19/22	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	MAN	C	4	2	-	0/2/19/22	0/1/1/1
2	MAN	C	5	2	-	0/2/19/22	0/1/1/1
2	MAN	C	6[A]	2	-	2/2/19/22	0/1/1/1
2	MAN	C	6[B]	2	-	2/2/19/22	0/1/1/1
2	MAN	C	7	2	-	0/2/19/22	0/1/1/1
2	MAN	C	8	2	-	0/2/19/22	0/1/1/1
2	MAN	C	9	2	-	0/2/19/22	0/1/1/1
3	NAG	D	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	2/6/23/26	0/1/1/1
2	MAN	E	10	2	-	2/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	E	11	2	-	0/2/19/22	0/1/1/1
2	MAN	E	12	2	-	0/2/19/22	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	BMA	E	3	2	-	0/2/19/22	0/1/1/1
2	MAN	E	4	2	-	1/2/19/22	0/1/1/1
2	MAN	E	5	2	-	0/2/19/22	0/1/1/1
2	MAN	E	6	2	-	2/2/19/22	0/1/1/1
2	MAN	E	7	2	-	0/2/19/22	0/1/1/1
2	MAN	E	8	2	-	0/2/19/22	0/1/1/1
2	MAN	E	9	2	-	0/2/19/22	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	7	MAN	C2-C3	5.28	1.60	1.52
2	E	7	MAN	C2-C3	4.64	1.59	1.52
3	F	1	NAG	O5-C1	4.56	1.51	1.43
3	F	2	NAG	O5-C1	4.36	1.51	1.43
2	C	6[B]	MAN	C2-C3	4.23	1.59	1.52

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2	NAG	C1-O5-C5	7.43	122.14	112.19
3	F	2	NAG	C1-O5-C5	5.57	119.65	112.19
2	C	6[B]	MAN	C2-C3-C4	5.43	120.41	110.86
3	F	1	NAG	C1-O5-C5	5.32	119.32	112.19
2	C	6[A]	MAN	C1-O5-C5	4.29	117.93	112.19

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

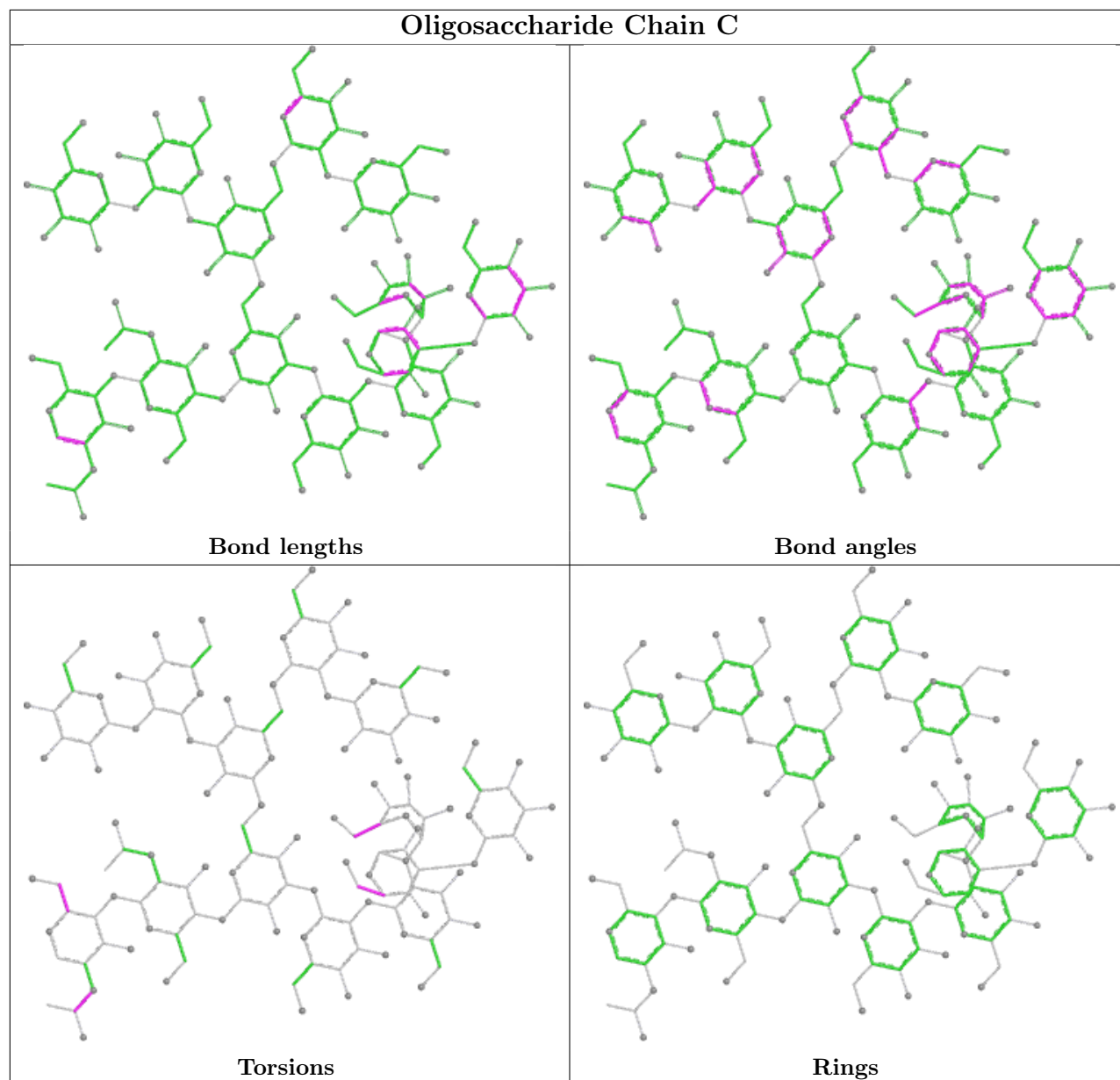
Mol	Chain	Res	Type	Atoms
2	C	6[A]	MAN	O5-C5-C6-O6
2	C	6[B]	MAN	C4-C5-C6-O6
2	C	6[B]	MAN	O5-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
2	C	6[A]	MAN	C4-C5-C6-O6

There are no ring outliers.

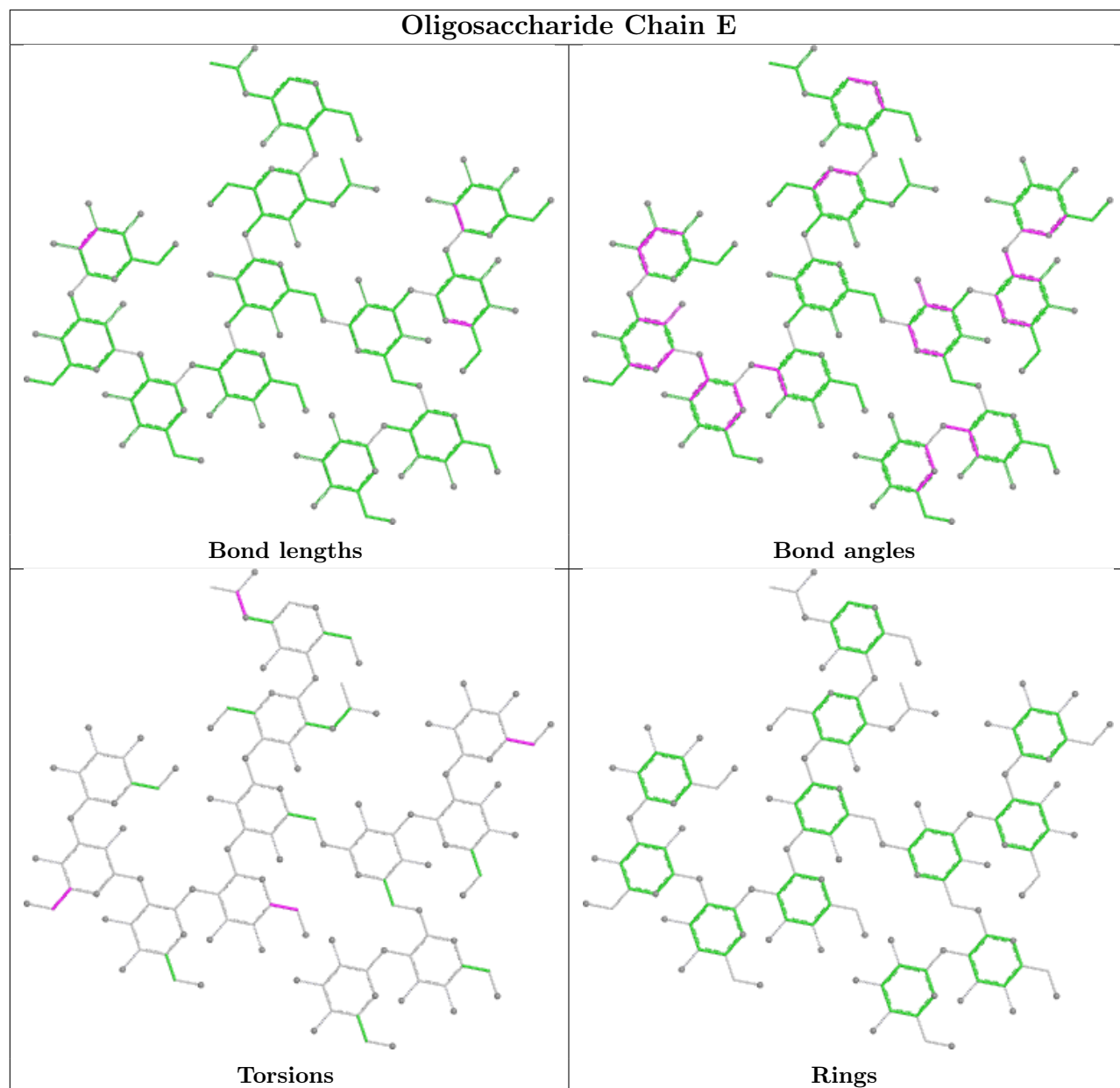
8 monomers are involved in 14 short contacts:

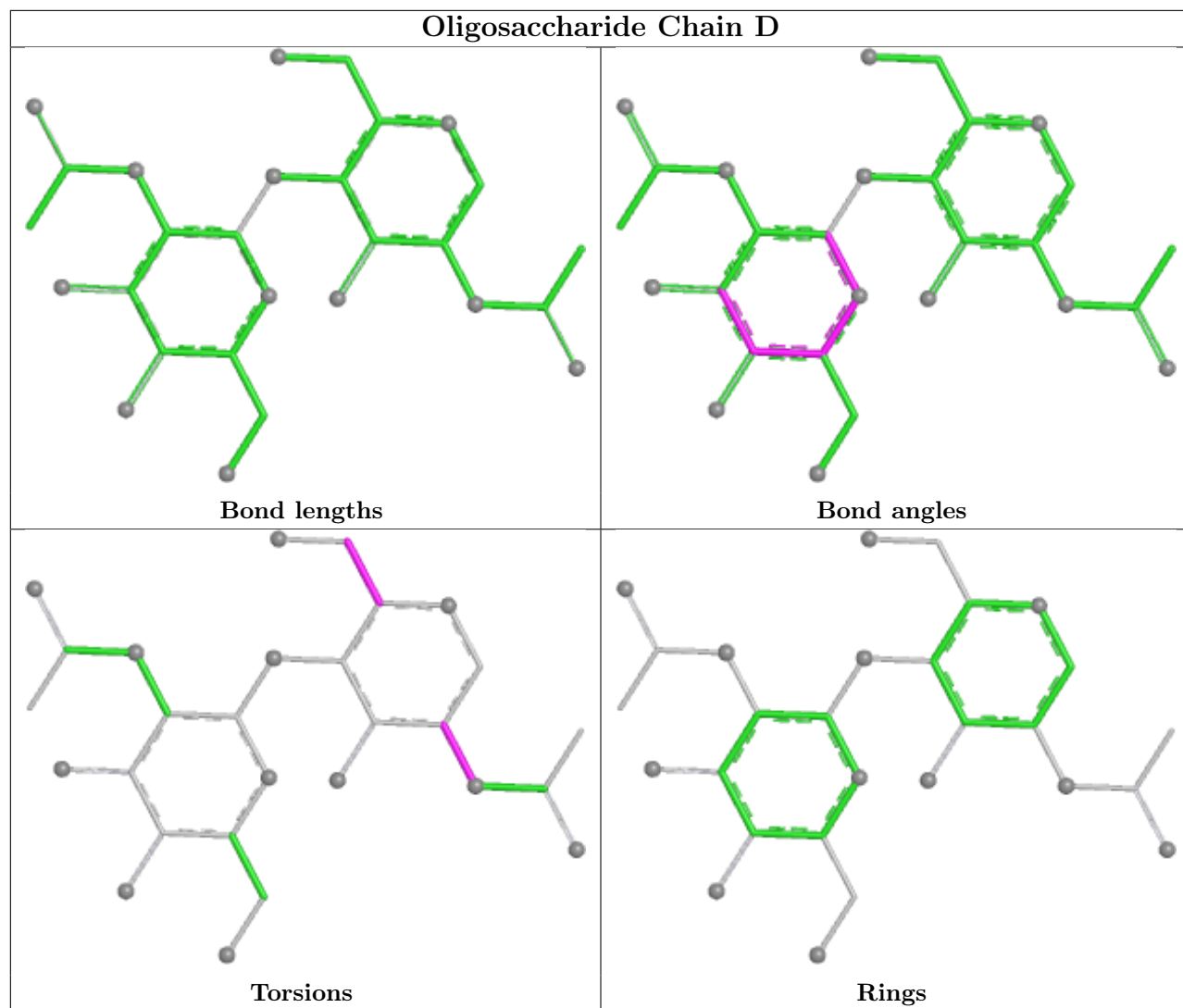
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	NAG	3	0
3	F	1	NAG	1	0
2	C	7	MAN	1	0
2	E	1	NAG	3	0
2	C	6[B]	MAN	1	0
2	E	2	NAG	2	0
2	C	6[A]	MAN	1	0
2	C	2	NAG	3	0

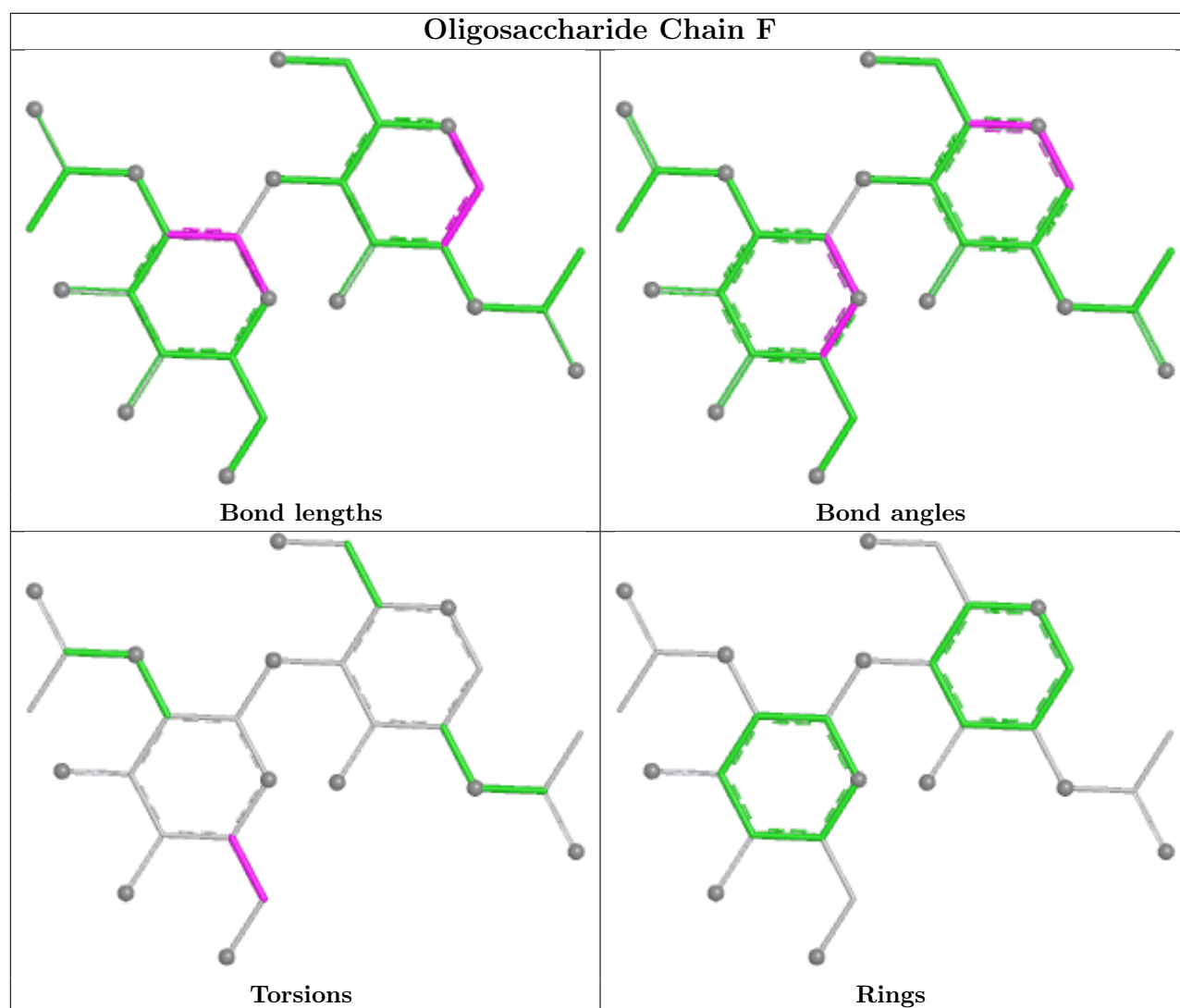
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



Oligosaccharide Chain E







5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	935/981 (95%)	-0.24	25 (2%) 56 61	8, 24, 48, 79	10 (1%)
1	B	937/981 (95%)	-0.13	26 (2%) 55 60	9, 26, 51, 103	6 (0%)
All	All	1872/1962 (95%)	-0.18	51 (2%) 56 61	8, 25, 50, 103	16 (0%)

The worst 5 of 51 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	917	THR	4.9
1	A	570	LEU	4.7
1	B	636	HIS	4.4
1	B	570	LEU	4.3
1	B	805	TYR	4.3

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
3	NAG	F	2	14/15	0.21	0.24	100,133,145,147	0
3	NAG	F	1	14/15	0.24	0.20	88,106,117,130	0
3	NAG	D	2	14/15	0.33	0.22	76,87,94,95	0
3	NAG	D	1	14/15	0.69	0.14	56,64,74,79	0
2	MAN	C	6[A]	11/12	0.73	0.18	43,46,48,49	11

Continued on next page...

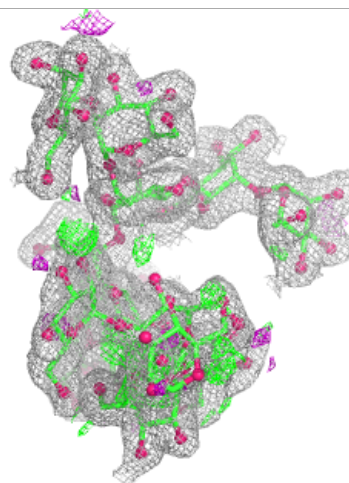
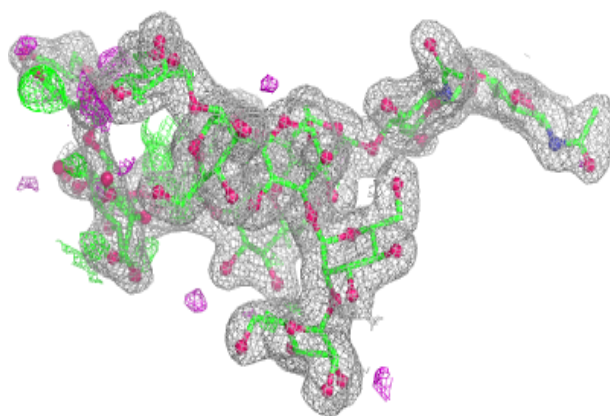
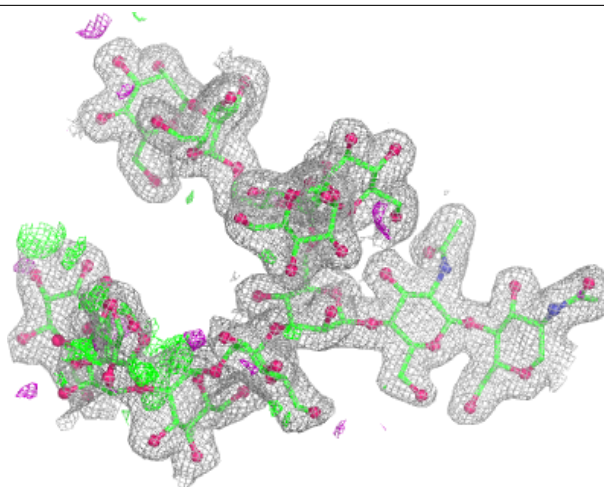
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MAN	C	6[B]	11/12	0.73	0.18	45,47,50,50	11
2	MAN	E	6	11/12	0.75	0.15	49,53,58,61	0
2	MAN	C	7	11/12	0.84	0.13	31,43,48,52	0
2	MAN	C	5	11/12	0.86	0.10	27,38,43,44	0
2	MAN	E	7	11/12	0.88	0.13	29,46,52,61	0
2	MAN	E	5	11/12	0.89	0.10	24,39,46,47	0
2	MAN	E	10	11/12	0.89	0.10	34,39,43,45	0
2	MAN	C	4	11/12	0.92	0.09	26,31,40,42	0
2	MAN	E	4	11/12	0.93	0.09	24,30,37,41	0
2	MAN	E	9	11/12	0.94	0.08	28,32,36,37	0
2	MAN	C	10	11/12	0.94	0.07	28,31,38,44	0
2	NAG	E	1	14/15	0.94	0.08	21,24,28,39	0
2	NAG	C	2	14/15	0.95	0.07	21,24,33,38	0
2	NAG	E	2	14/15	0.95	0.07	15,22,31,38	0
2	NAG	C	1	14/15	0.96	0.07	21,24,28,34	0
2	MAN	C	12	11/12	0.97	0.05	17,18,20,21	0
2	MAN	E	8	11/12	0.97	0.05	17,20,24,24	0
2	MAN	C	9	11/12	0.97	0.05	25,25,30,30	0
2	BMA	C	3	11/12	0.97	0.04	18,18,23,24	0
2	MAN	E	12	11/12	0.98	0.05	15,17,20,22	0
2	MAN	C	8	11/12	0.98	0.04	17,19,22,25	0
2	BMA	E	3	11/12	0.98	0.05	18,22,27,29	0
2	MAN	C	11	11/12	0.98	0.04	17,20,24,25	0
2	MAN	E	11	11/12	0.98	0.04	18,21,24,26	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.

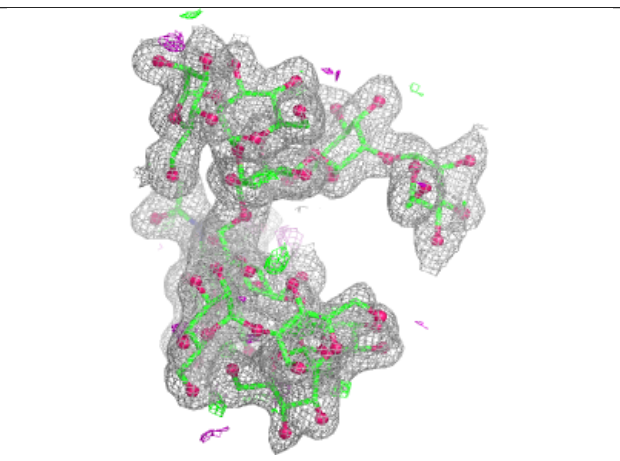
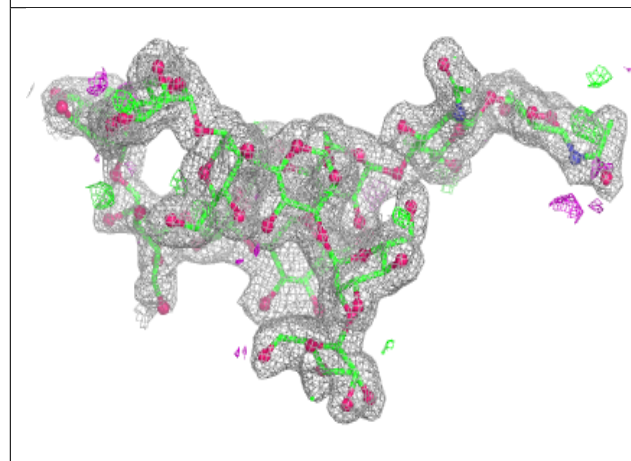
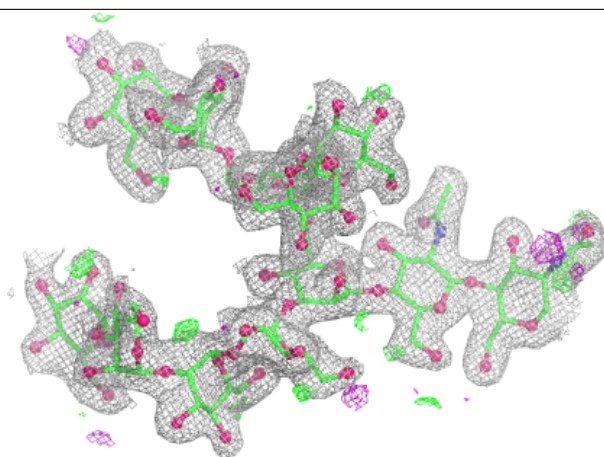
Electron density around Chain C:

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



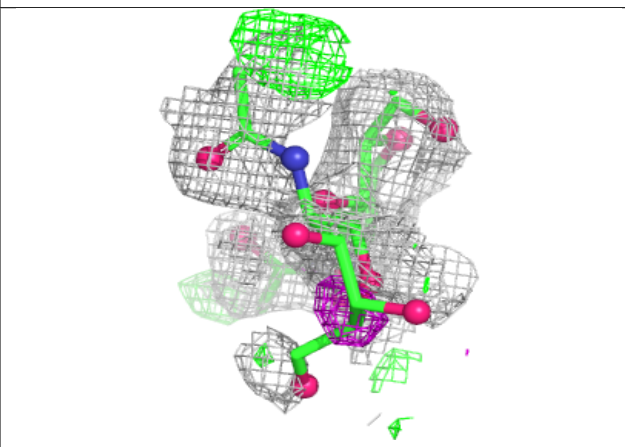
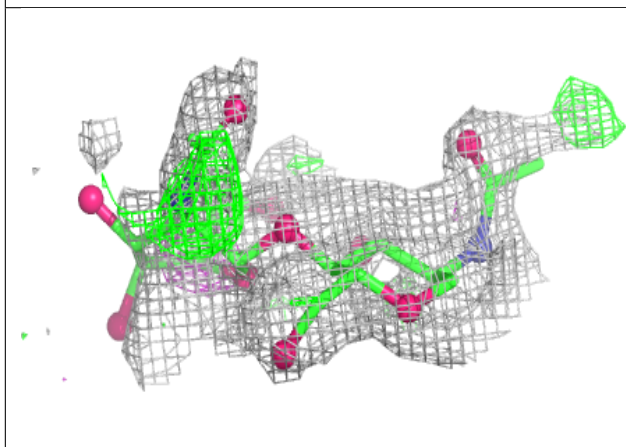
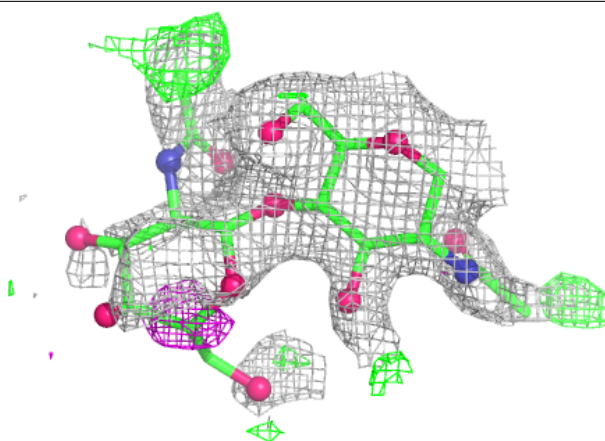
Electron density around Chain E:

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

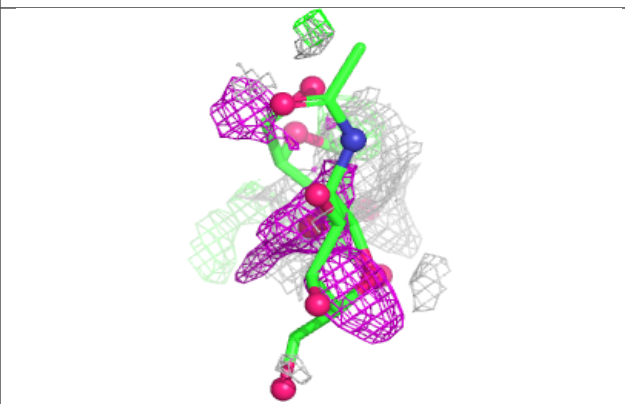
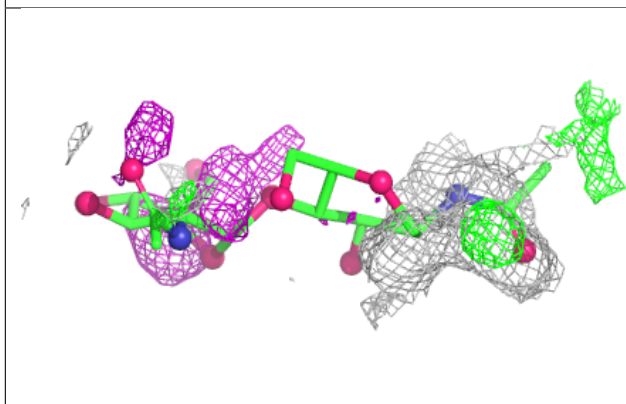
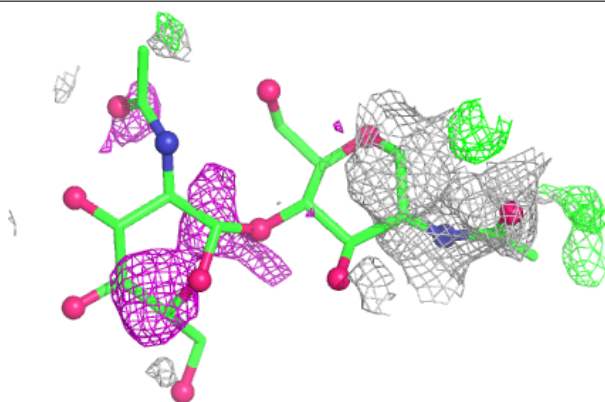


Electron density around Chain D:

$2mF_o - DF_c$ (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 [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($\text{\AA}^2$)	Q<0.9
4	ZN	A	1001	1/1	1.00	0.02	16,16,16,16	0
4	ZN	B	1001	1/1	1.00	0.01	17,17,17,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.