



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 03:27 PM EDT

PDB ID : 6F2Y / pdb_00006f2y
Title : Crystal structure of ectonucleotide phosphodiesterase/pyrophosphatase-3 (NPP3) in complex with Ap4A
Authors : Dohler, C.; Zebisch, M.; Strater, N.
Deposited on : 2017-11-27
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

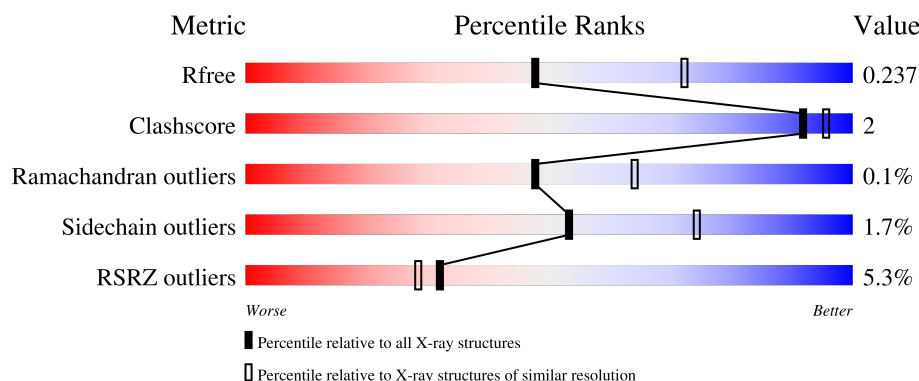
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	749	6% 89% 7%
1	B	749	4% 89% 7%
2	C	2	100%
2	D	2	50% 50%
2	E	2	50% 50%

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Mol	Chain	Length	Quality of chain
2	G	2	 50%50%
3	F	3	 33%67%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 12376 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 Ectonucleotide pyrophosphatase/phosphodiesterase family member 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	720	Total	C	N	O	S	0	0	0
			5795	3712	976	1074	33			
1	B	719	Total	C	N	O	S	0	0	0
			5789	3708	974	1074	33			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	136	ALA	-	expression tag	UNP P97675
A	137	GLU	-	expression tag	UNP P97675
A	138	THR	-	expression tag	UNP P97675
A	139	GLY	-	expression tag	UNP P97675
A	201	VAL	MET	variant	UNP P97675
A	206	ALA	THR	engineered mutation	UNP P97675
A	596	ASN	SER	variant	UNP P97675
A	597	ARG	GLY	variant	UNP P97675
A	876	GLY	-	expression tag	UNP P97675
A	877	THR	-	expression tag	UNP P97675
A	878	LYS	-	expression tag	UNP P97675
A	879	HIS	-	expression tag	UNP P97675
A	880	HIS	-	expression tag	UNP P97675
A	881	HIS	-	expression tag	UNP P97675
A	882	HIS	-	expression tag	UNP P97675
A	883	HIS	-	expression tag	UNP P97675
A	884	HIS	-	expression tag	UNP P97675
B	136	ALA	-	expression tag	UNP P97675
B	137	GLU	-	expression tag	UNP P97675
B	138	THR	-	expression tag	UNP P97675
B	139	GLY	-	expression tag	UNP P97675
B	201	VAL	MET	variant	UNP P97675
B	206	ALA	THR	engineered mutation	UNP P97675
B	596	ASN	SER	variant	UNP P97675

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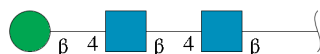
Chain	Residue	Modelled	Actual	Comment	Reference
B	597	ARG	GLY	variant	UNP P97675
B	876	GLY	-	expression tag	UNP P97675
B	877	THR	-	expression tag	UNP P97675
B	878	LYS	-	expression tag	UNP P97675
B	879	HIS	-	expression tag	UNP P97675
B	880	HIS	-	expression tag	UNP P97675
B	881	HIS	-	expression tag	UNP P97675
B	882	HIS	-	expression tag	UNP P97675
B	883	HIS	-	expression tag	UNP P97675
B	884	HIS	-	expression tag	UNP P97675

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



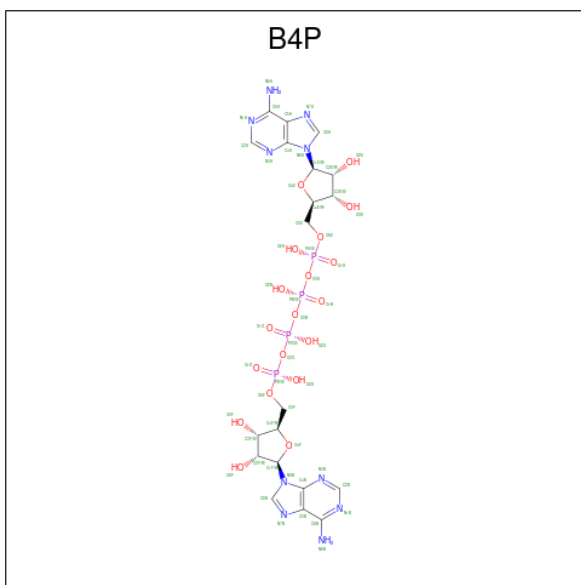
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 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
3	F	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 4 is BIS(ADENOSINE)-5'-TETRAPHOSPHATE (CCD ID: B4P) (formula: C₂₀H₂₈N₁₀O₁₉P₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0
			53	20	10	19	4	
4	B	1	Total	C	N	O	P	0
			53	20	10	19	4	

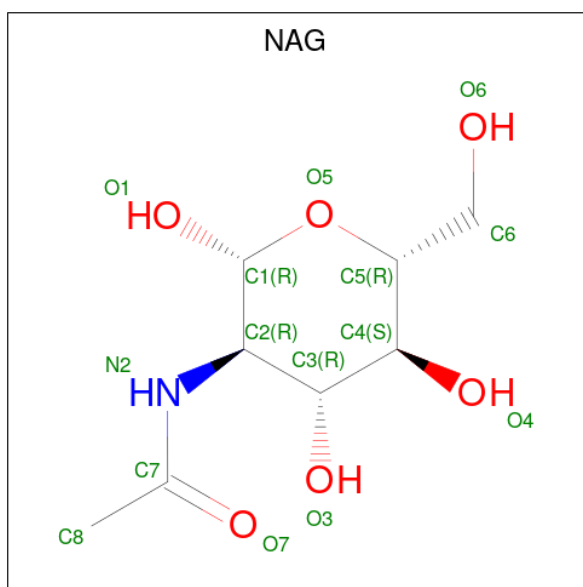
- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Zn	0	0
			2	2		
5	B	2	Total	Zn	0	0
			2	2		

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Ca	0	0
			1	1		
6	B	1	Total	Ca	0	0
			1	1		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

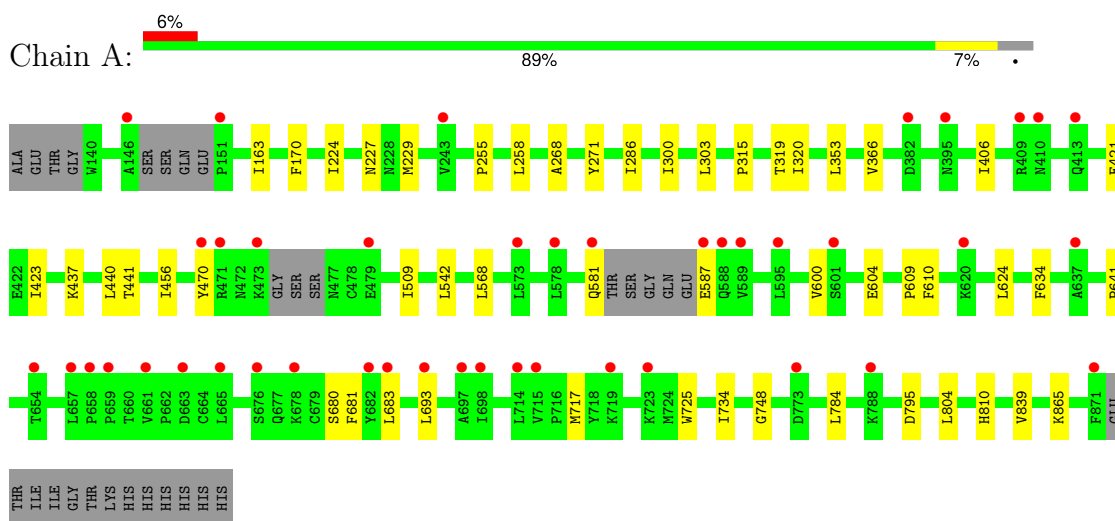
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	234	Total	O	0	0
			234	234		
8	B	197	Total	O	0	0
			197	197		

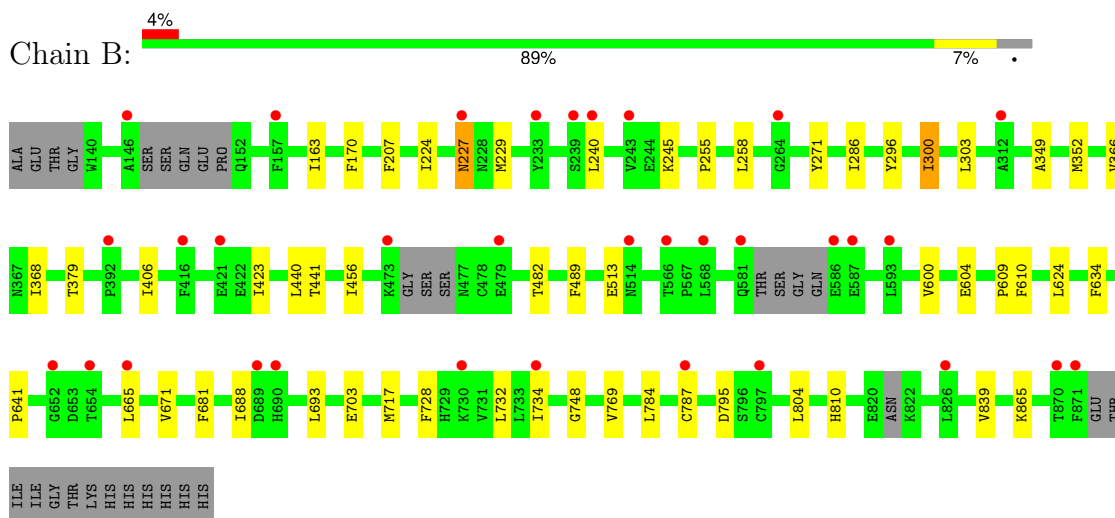
3 Residue-property plots

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.

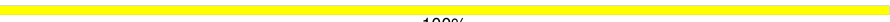
- Molecule 1: Ectonucleotide pyrophosphatase/phosphodiesterase family member 3



- Molecule 1: Ectonucleotide pyrophosphatase/phosphodiesterase family member 3



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

Chain C: 

MAG1
MAG2

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

Chain D:  50% 50%

MAG1
MAG2

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

Chain E:  50% 50%

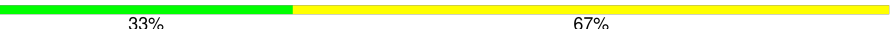
MAG1
MAG2

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

Chain G:  50% 50%

MAG1
MAG2

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

Chain F:  33% 67%

MAG1
MAG2
EMAG3

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.94Å 126.85Å 114.48Å 90.00° 97.54° 90.00°	Depositor
Resolution (Å)	48.24 – 2.40 48.24 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.7 (48.24-2.40) 98.7 (48.24-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 2.39Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.204 , 0.217 0.227 , 0.237	Depositor DCC
R_{free} test set	1617 reflections (1.95%)	wwPDB-VP
Wilson B-factor (Å ²)	45.6	Xtriage
Anisotropy	0.296	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 32.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12376	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 5.91% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, B4P, NAG, BMA, CA

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	0.70	0/5968	1.19	5/8124 (0.1%)
1	B	0.70	0/5960	1.21	8/8111 (0.1%)
All	All	0.70	0/11928	1.20	13/16235 (0.1%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	513	GLU	CA-C-N	7.30	130.38	120.38
1	B	513	GLU	C-N-CA	7.30	130.38	120.38
1	B	440	LEU	N-CA-C	-6.03	99.45	109.46
1	A	440	LEU	N-CA-C	-5.96	99.57	109.46
1	A	681	PHE	CA-CB-CG	5.91	119.71	113.80
1	B	681	PHE	CA-CB-CG	5.91	119.71	113.80
1	B	671	VAL	CA-C-N	5.22	128.08	120.51
1	B	671	VAL	C-N-CA	5.22	128.08	120.51
1	A	470	TYR	CA-C-N	5.07	127.03	120.44
1	A	470	TYR	C-N-CA	5.07	127.03	120.44
1	B	170	PHE	CA-CB-CG	5.05	118.86	113.80
1	B	489	PHE	CA-CB-CG	5.05	118.85	113.80
1	A	170	PHE	CA-CB-CG	5.02	118.82	113.80

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	5795	0	5586	18	0
1	B	5789	0	5575	19	0
2	C	28	0	25	0	0
2	D	28	0	25	0	0
2	E	28	0	25	0	0
2	G	28	0	25	0	0
3	F	39	0	34	0	0
4	A	53	0	24	0	0
4	B	53	0	24	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	28	0	26	0	0
7	B	70	0	65	0	0
8	A	234	0	0	0	0
8	B	197	0	0	0	0
All	All	12376	0	11434	37	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 2.

All (37) 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:255:PRO:HD2	1:B:258:LEU:HD12	1.85	0.58
1:A:255:PRO:HD2	1:A:258:LEU:HD12	1.85	0.57
1:B:634:PHE:HA	1:B:641:PRO:HA	1.89	0.55
1:A:634:PHE:HA	1:A:641:PRO:HA	1.89	0.54
1:B:163:ILE:HD12	1:B:366:VAL:HG11	1.91	0.52
1:A:163:ILE:HD12	1:A:366:VAL:HG11	1.91	0.51
1:B:688:ILE:HD11	1:B:769:VAL:HG13	1.93	0.49
1:B:379:THR:HG21	1:B:482:THR:HG22	1.94	0.49
1:A:717:MET:HA	1:A:810:HIS:NE2	2.28	0.48
1:A:839:VAL:HB	1:A:865:LYS:HA	1.95	0.48
1:B:839:VAL:HB	1:B:865:LYS:HA	1.95	0.48
1:A:784:LEU:HD12	1:A:804:LEU:HD23	1.96	0.47
1:B:784:LEU:HD12	1:B:804:LEU:HD23	1.97	0.47
1:B:224:ILE:HA	1:B:229:MET:HE1	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:ILE:HA	1:A:229:MET:HE1	1.98	0.46
1:A:268:ALA:HB2	1:A:315:PRO:HG2	1.98	0.46
1:B:296:TYR:O	1:B:300:ILE:HD12	2.15	0.46
1:B:717:MET:HA	1:B:810:HIS:NE2	2.30	0.46
1:B:240:LEU:HA	1:B:245:LYS:HG3	1.99	0.45
1:B:349:ALA:HA	1:B:352:MET:HE3	1.98	0.45
1:A:300:ILE:HD12	1:A:353:LEU:HB2	1.98	0.45
1:A:406:ILE:HG21	1:A:423:ILE:HG21	1.99	0.44
1:B:441:THR:HG21	1:B:456:ILE:HG22	1.99	0.44
1:A:441:THR:HG21	1:A:456:ILE:HG22	1.99	0.44
1:B:609:PRO:HB3	1:B:795:ASP:HA	2.00	0.44
1:A:609:PRO:HB3	1:A:795:ASP:HA	2.01	0.43
1:B:406:ILE:HG21	1:B:423:ILE:HG21	2.00	0.42
1:B:207:PHE:HB2	1:B:227:ASN:HD22	1.85	0.42
1:A:693:LEU:HD21	1:A:748:GLY:HA2	2.03	0.41
1:B:600:VAL:O	1:B:604:GLU:HG3	2.20	0.41
1:A:600:VAL:O	1:A:604:GLU:HG3	2.19	0.41
1:A:509:ILE:HD13	1:A:542:LEU:HD11	2.03	0.41
1:B:693:LEU:HD21	1:B:748:GLY:HA2	2.03	0.41
1:A:581:GLN:HE21	1:A:587:GLU:HB2	1.87	0.41
1:A:680:SER:HA	1:A:683:LEU:HD12	2.03	0.40
1:A:717:MET:HE1	1:A:725:TRP:CE2	2.56	0.40
1:B:728:PHE:HA	1:B:732:LEU:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	712/749 (95%)	684 (96%)	27 (4%)	1 (0%)	48 64
1	B	709/749 (95%)	682 (96%)	26 (4%)	1 (0%)	48 64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1421/1498 (95%)	1366 (96%)	53 (4%)	2 (0%)	48 64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	271	TYR
1	B	271	TYR

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	644/668 (96%)	633 (98%)	11 (2%)	53 74
1	B	643/668 (96%)	632 (98%)	11 (2%)	53 74
All	All	1287/1336 (96%)	1265 (98%)	22 (2%)	53 74

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	227	ASN
1	A	286	ILE
1	A	303	LEU
1	A	319	THR
1	A	320	ILE
1	A	421	GLU
1	A	437	LYS
1	A	568	LEU
1	A	610	PHE
1	A	624	LEU
1	A	734	ILE
1	B	227	ASN
1	B	286	ILE
1	B	300	ILE
1	B	303	LEU
1	B	368	ILE

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Mol	Chain	Res	Type
1	B	610	PHE
1	B	624	LEU
1	B	665	LEU
1	B	703	GLU
1	B	734	ILE
1	B	787	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	GLN
1	A	159	GLN
1	A	194	HIS
1	A	227	ASN
1	A	364	ASN
1	A	413	GLN
1	A	526	HIS
1	A	581	GLN
1	A	590	ASN
1	A	591	GLN
1	A	792	HIS
1	A	814	ASN
1	B	152	GLN
1	B	159	GLN
1	B	227	ASN
1	B	364	ASN
1	B	400	GLN
1	B	413	GLN
1	B	435	HIS
1	B	477	ASN
1	B	526	HIS
1	B	581	GLN
1	B	590	ASN
1	B	591	GLN
1	B	814	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 ⓘ

11 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	2,1	14,14,15	0.29	0	17,19,21	0.88	1 (5%)
2	NAG	C	2	2	14,14,15	0.30	0	17,19,21	0.78	1 (5%)
2	NAG	D	1	2,1	14,14,15	0.31	0	17,19,21	0.61	0
2	NAG	D	2	2	14,14,15	0.32	0	17,19,21	0.62	1 (5%)
2	NAG	E	1	2,1	14,14,15	0.31	0	17,19,21	0.77	0
2	NAG	E	2	2	14,14,15	0.31	0	17,19,21	0.58	1 (5%)
3	NAG	F	1	1,3	14,14,15	0.30	0	17,19,21	0.88	1 (5%)
3	NAG	F	2	3	14,14,15	0.30	0	17,19,21	0.77	1 (5%)
3	BMA	F	3	3	11,11,12	0.32	0	15,15,17	0.50	0
2	NAG	G	1	2,1	14,14,15	0.29	0	17,19,21	0.77	0
2	NAG	G	2	2	14,14,15	0.31	0	17,19,21	0.59	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	2,1	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	NAG	D	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	NAG	E	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1

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

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1	NAG	O5-C1-C2	-2.88	106.84	111.29
2	C	1	NAG	O5-C1-C2	-2.87	106.86	111.29
2	C	2	NAG	C1-O5-C5	2.86	116.02	112.19
3	F	2	NAG	C1-O5-C5	2.80	115.93	112.19
2	D	2	NAG	C1-O5-C5	2.12	115.02	112.19
2	G	2	NAG	C1-O5-C5	2.02	114.89	112.19
2	E	2	NAG	C1-O5-C5	2.01	114.89	112.19

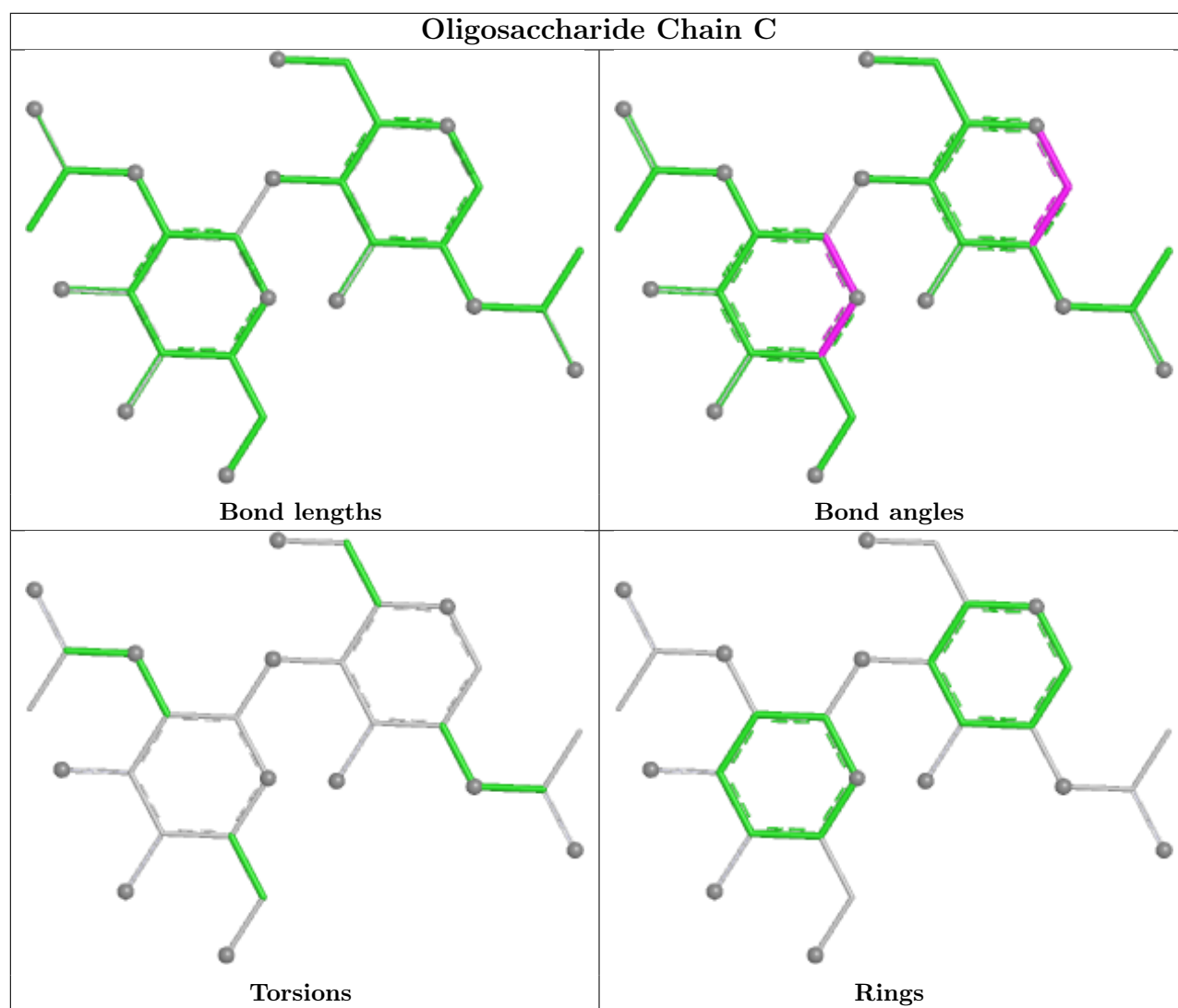
There are no chirality outliers.

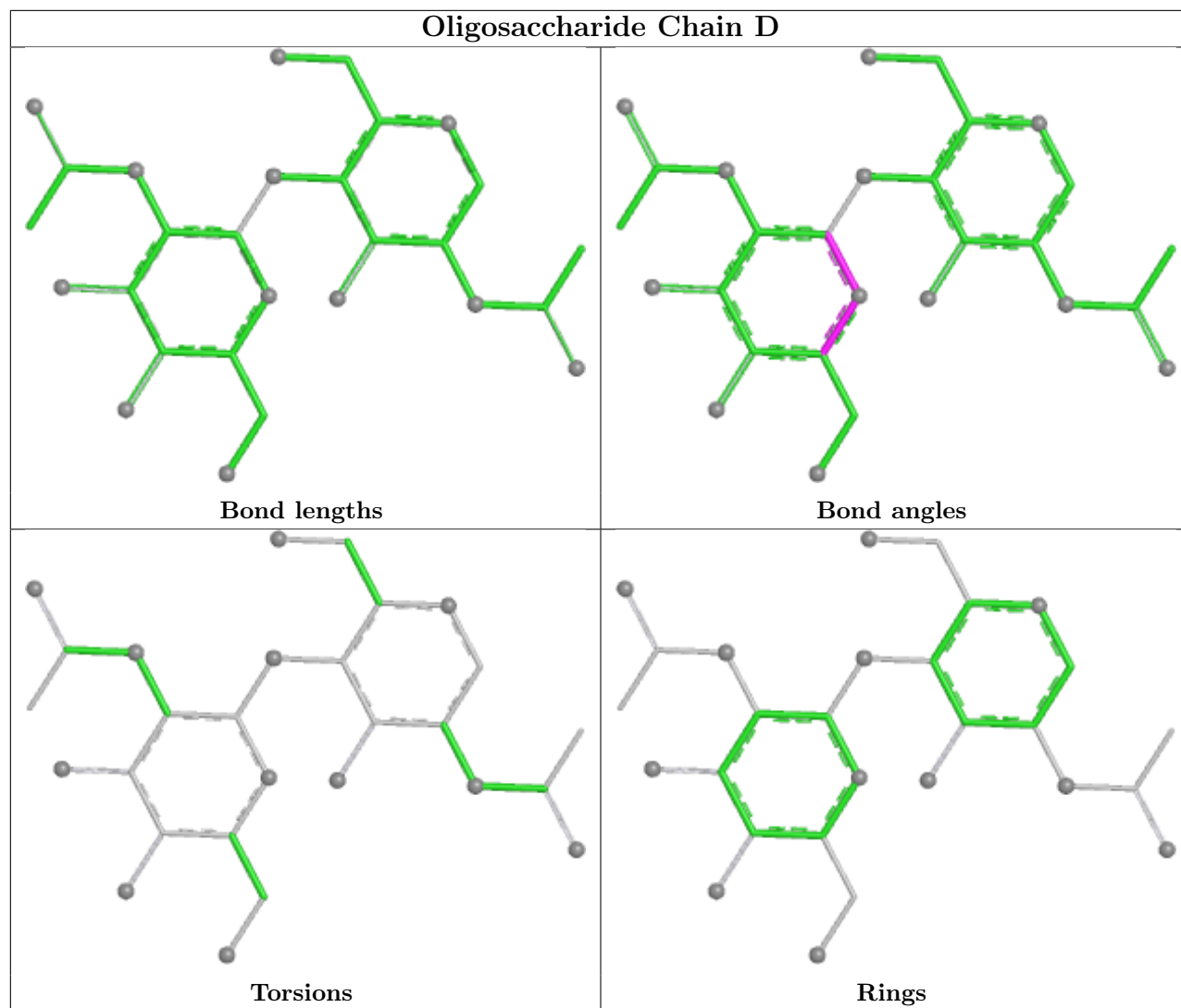
There are no torsion outliers.

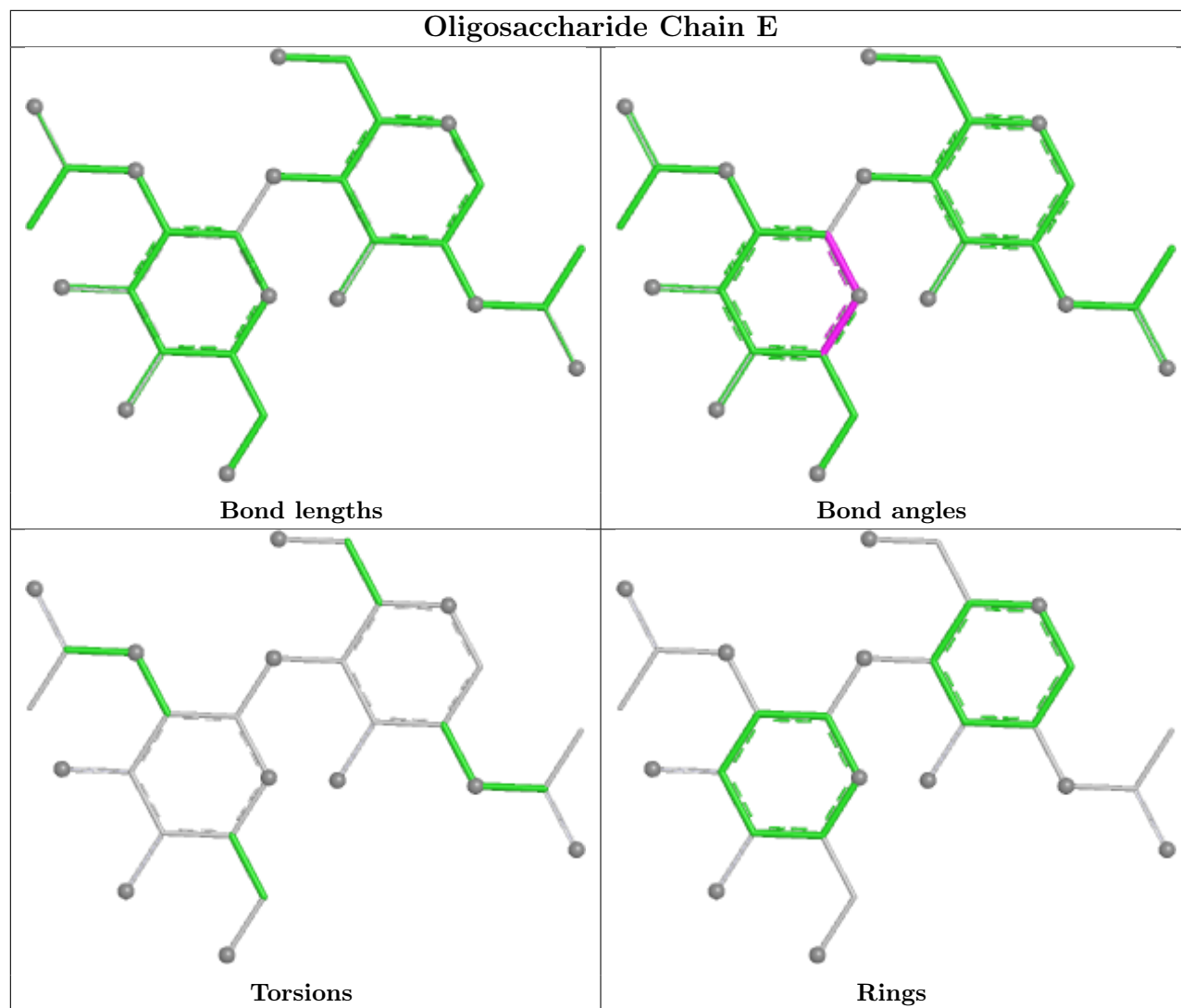
There are no ring outliers.

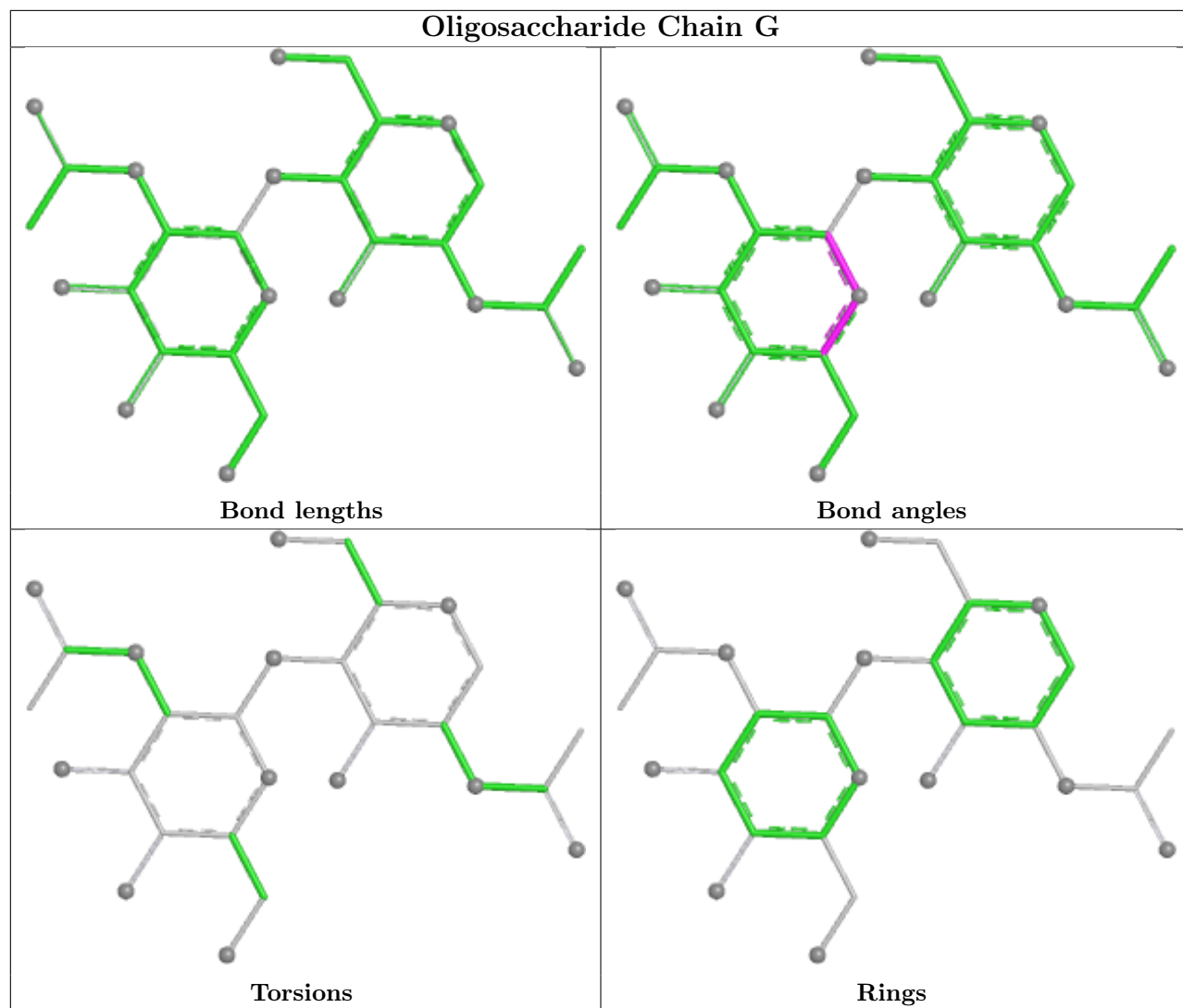
No monomer is involved in short contacts.

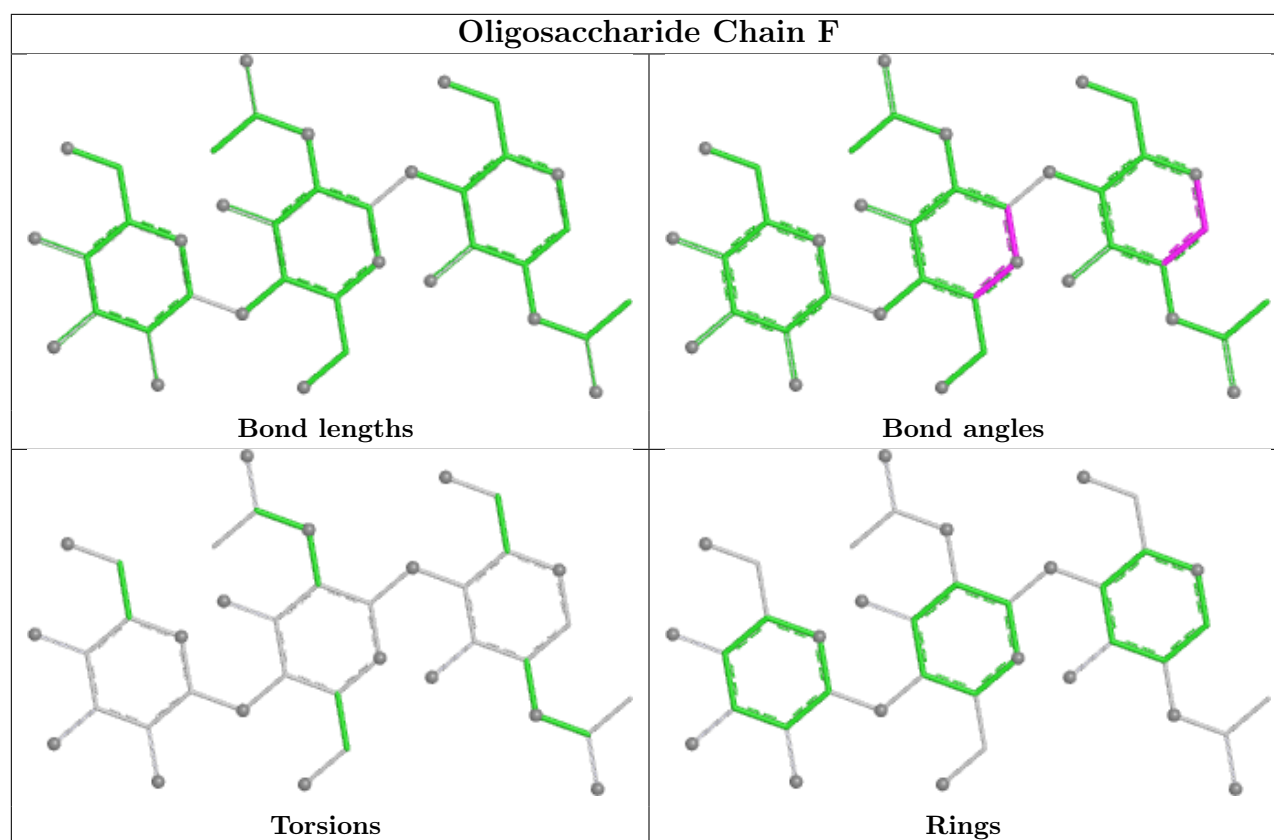
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 6 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	$\# Z > 2$
7	NAG	A	1007	1	14,14,15	0.30	0	17,19,21	0.74	1 (5%)
7	NAG	B	1012	1	14,14,15	0.33	0	17,19,21	0.61	0
7	NAG	B	1014	1	14,14,15	0.30	0	17,19,21	0.51	0
7	NAG	B	1013	1	14,14,15	0.33	0	17,19,21	0.54	0
4	B4P	A	1001	5	58,58,58	0.29	0	84,91,91	0.45	1 (1%)
7	NAG	B	1009	1	14,14,15	0.32	0	17,19,21	0.69	1 (5%)
7	NAG	A	1012	1	14,14,15	0.31	0	17,19,21	0.63	1 (5%)
4	B4P	B	1001	5	58,58,58	0.27	0	84,91,91	0.46	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	B	1008	1	14,14,15	0.30	0	17,19,21	0.67	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
7	NAG	A	1007	1	-	0/6/23/26	0/1/1/1
7	NAG	B	1012	1	-	0/6/23/26	0/1/1/1
7	NAG	B	1014	1	-	0/6/23/26	0/1/1/1
7	NAG	B	1013	1	-	0/6/23/26	0/1/1/1
4	B4P	A	1001	5	-	12/38/70/70	0/6/6/6
7	NAG	B	1009	1	-	0/6/23/26	0/1/1/1
7	NAG	A	1012	1	-	0/6/23/26	0/1/1/1
4	B4P	B	1001	5	-	8/38/70/70	0/6/6/6
7	NAG	B	1008	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	1009	NAG	C1-O5-C5	2.42	115.42	112.19
7	A	1007	NAG	C1-O5-C5	2.41	115.42	112.19
4	B	1001	B4P	PA-O5E-C5E	2.22	134.06	121.35
7	B	1008	NAG	C1-O5-C5	2.14	115.05	112.19
7	A	1012	NAG	C1-O5-C5	2.10	115.00	112.19
4	A	1001	B4P	PA-O5E-C5E	2.04	133.05	121.35

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1001	B4P	C5E-O5E-PA-O1A
4	A	1001	B4P	C5E-O5E-PA-O3A
4	B	1001	B4P	C5E-O5E-PA-O1A
4	B	1001	B4P	C5E-O5E-PA-O3A
4	B	1001	B4P	C5F-O5F-PD-O3G
4	B	1001	B4P	C5F-O5F-PD-O2D
4	A	1001	B4P	PB-O3A-PA-O1A

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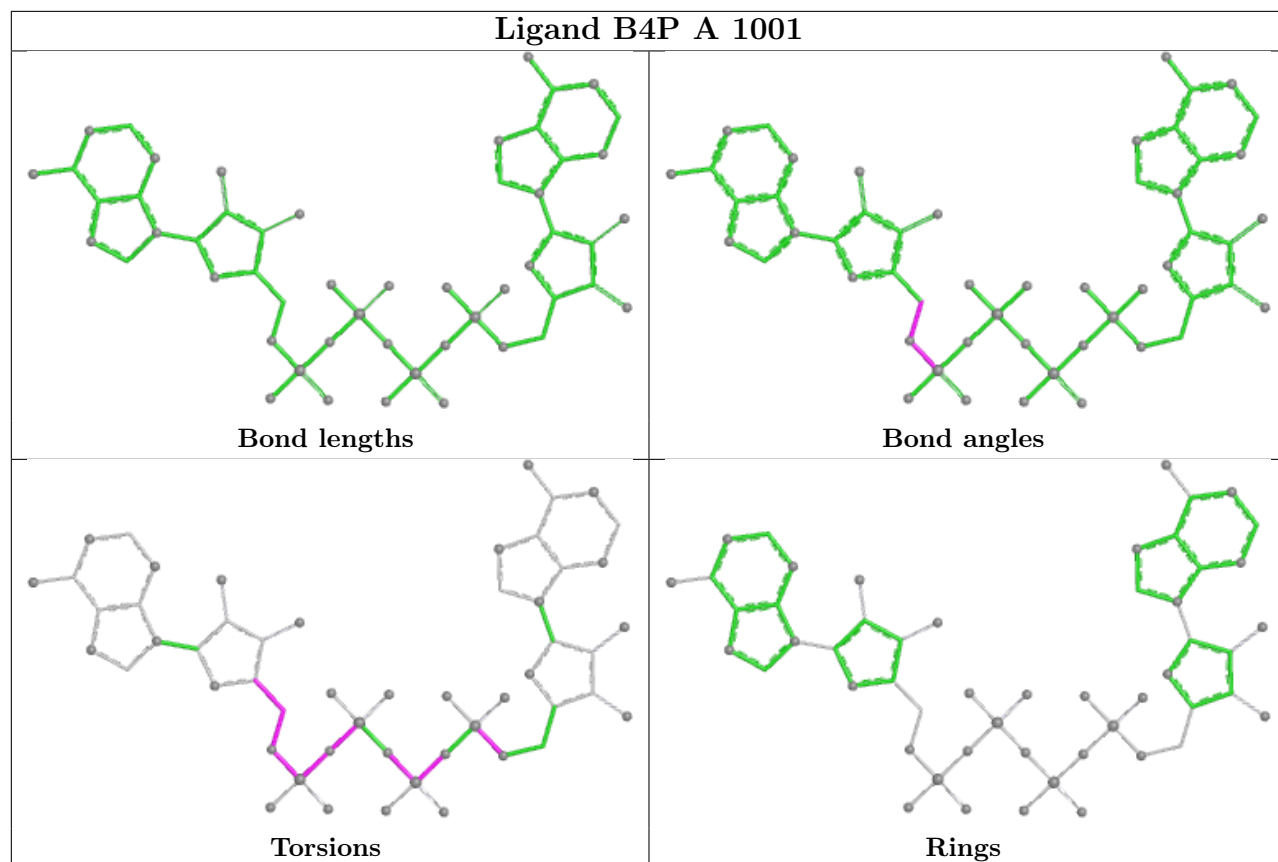
Mol	Chain	Res	Type	Atoms
4	B	1001	B4P	PB-O3B-PG-O1G
4	B	1001	B4P	PG-O3G-PD-O1D
4	A	1001	B4P	PB-O3A-PA-O5E
4	B	1001	B4P	PB-O3A-PA-O5E
4	A	1001	B4P	C3E-C4E-C5E-O5E
4	A	1001	B4P	C5F-O5F-PD-O3G
4	A	1001	B4P	C5F-O5F-PD-O1D
4	A	1001	B4P	C5F-O5F-PD-O2D
4	B	1001	B4P	C3E-C4E-C5E-O5E
4	A	1001	B4P	PA-O3A-PB-O2B
4	A	1001	B4P	PB-O3B-PG-O2G
4	A	1001	B4P	PD-O3G-PG-O2G
4	A	1001	B4P	C4E-C5E-O5E-PA

There are no ring outliers.

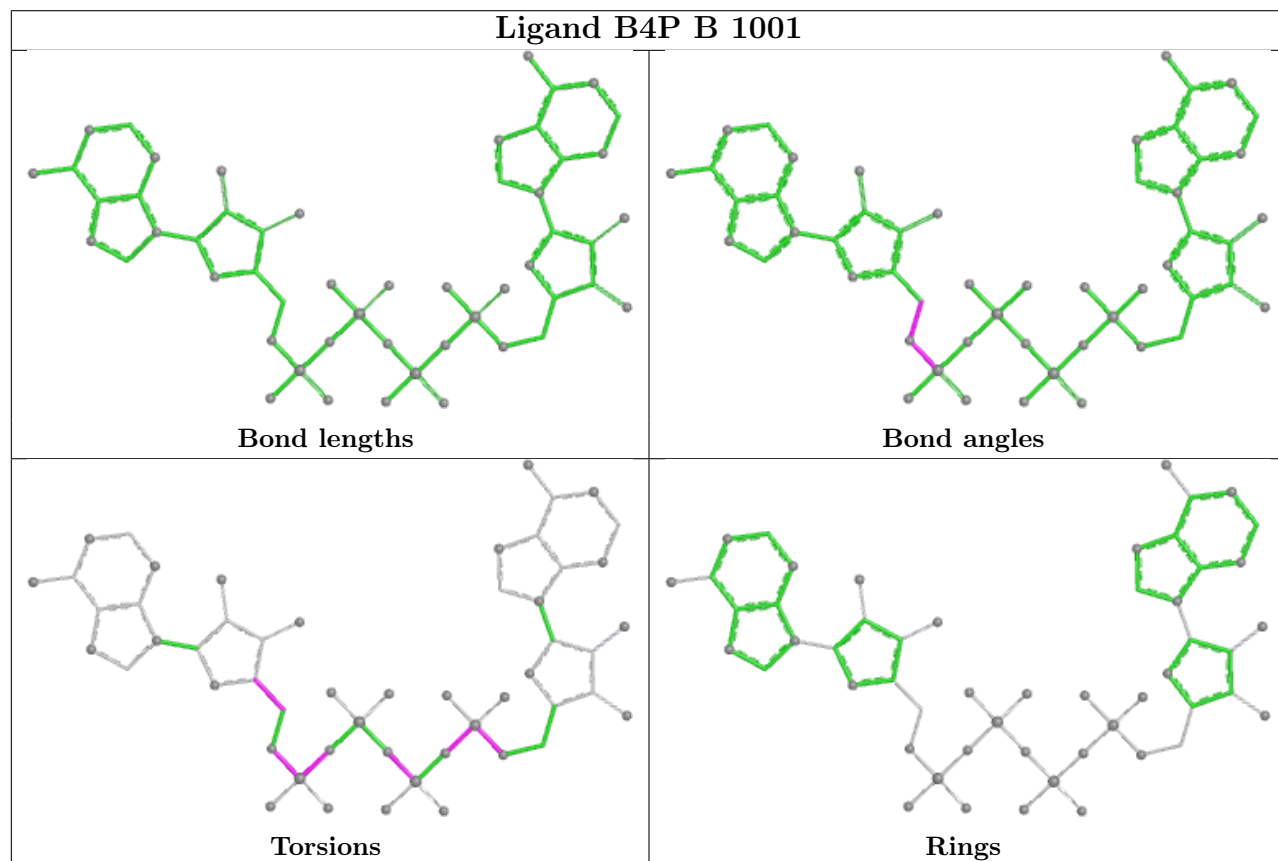
No monomer is involved in short contacts.

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 than 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 B4P A 1001



Ligand B4P B 1001



5.7 Other polymers [i](#)

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

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	720/749 (96%)	0.56	43 (5%) 27 24	33, 53, 89, 138	1 (0%)
1	B	719/749 (95%)	0.57	33 (4%) 37 33	36, 54, 83, 122	1 (0%)
All	All	1439/1498 (96%)	0.57	76 (5%) 32 28	33, 53, 86, 138	2 (0%)

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	683	LEU	5.3
1	A	657	LEU	5.1
1	A	470	TYR	3.8
1	B	146	ALA	3.8
1	A	413	GLN	3.6
1	B	479	GLU	3.5
1	A	682	TYR	3.5
1	A	146	ALA	3.5
1	A	151	PRO	3.5
1	A	587	GLU	3.2
1	A	773	ASP	3.2
1	A	658	PRO	3.2
1	B	871	PHE	3.1
1	A	395	ASN	3.1
1	B	797	CYS	3.0
1	A	581	GLN	3.0
1	A	637	ALA	2.9
1	A	479	GLU	2.9
1	B	243	VAL	2.9
1	B	734	ILE	2.8
1	A	382	ASP	2.8
1	B	514	ASN	2.8
1	A	659	PRO	2.8
1	A	243	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	578	LEU	2.7
1	A	665	LEU	2.7
1	A	697	ALA	2.7
1	B	730	LYS	2.7
1	A	788	LYS	2.7
1	A	678	LYS	2.6
1	A	698	ILE	2.6
1	B	233	TYR	2.6
1	B	473	LYS	2.6
1	B	312	ALA	2.6
1	A	714	LEU	2.6
1	A	471	ARG	2.5
1	A	663	ASP	2.5
1	B	157	PHE	2.5
1	A	661	VAL	2.5
1	A	654	THR	2.5
1	A	601	SER	2.5
1	A	871	PHE	2.5
1	A	676	SER	2.5
1	B	652	GLY	2.4
1	A	620	LYS	2.4
1	A	595	LEU	2.3
1	B	568	LEU	2.3
1	A	589	VAL	2.3
1	A	410	ASN	2.3
1	A	588	GLN	2.3
1	B	787	CYS	2.3
1	B	240	LEU	2.3
1	B	593	LEU	2.3
1	B	587	GLU	2.3
1	B	566	THR	2.2
1	B	826	LEU	2.2
1	B	581	GLN	2.2
1	B	586	GLU	2.2
1	B	227	ASN	2.2
1	B	870	THR	2.2
1	B	392	PRO	2.2
1	A	715	VAL	2.2
1	A	723	LYS	2.2
1	B	654	THR	2.2
1	B	665	LEU	2.2
1	B	239	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	473	LYS	2.1
1	B	690	HIS	2.1
1	A	409	ARG	2.1
1	B	689	ASP	2.1
1	A	573	LEU	2.1
1	B	421	GLU	2.1
1	A	719	LYS	2.1
1	B	416	PHE	2.0
1	B	264	GLY	2.0
1	A	693	LEU	2.0

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](#)

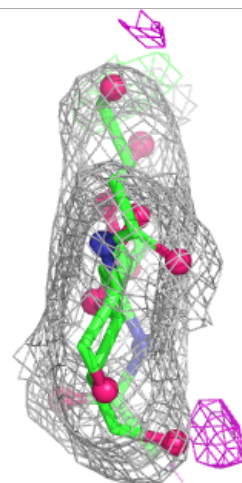
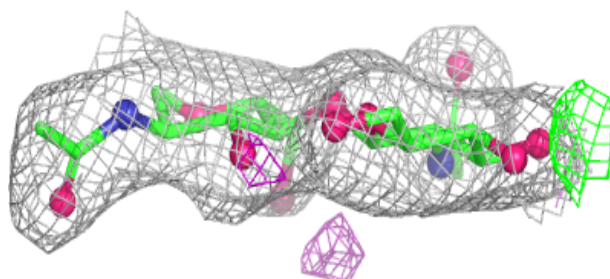
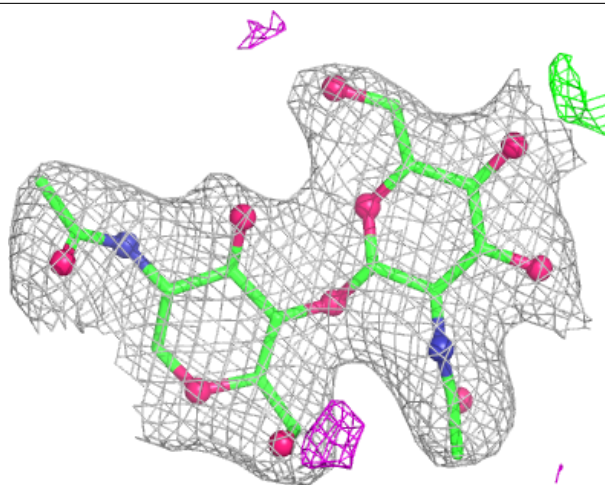
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	BMA	F	3	11/12	0.73	0.12	86,88,88,88	0
2	NAG	D	2	14/15	0.78	0.15	69,69,71,71	0
2	NAG	G	2	14/15	0.84	0.14	60,62,65,65	0
2	NAG	D	1	14/15	0.85	0.14	63,64,67,67	0
3	NAG	F	2	14/15	0.87	0.13	81,82,84,85	0
2	NAG	C	2	14/15	0.87	0.10	60,64,66,66	0
3	NAG	F	1	14/15	0.89	0.12	75,77,78,80	0
2	NAG	E	2	14/15	0.89	0.10	55,58,59,60	0
2	NAG	C	1	14/15	0.89	0.11	59,61,62,64	0
2	NAG	E	1	14/15	0.96	0.08	43,45,47,51	0
2	NAG	G	1	14/15	0.96	0.09	49,52,55,58	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.

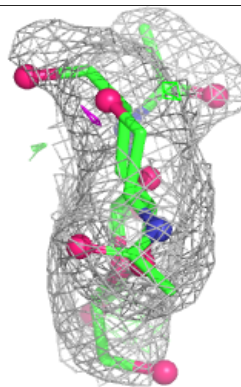
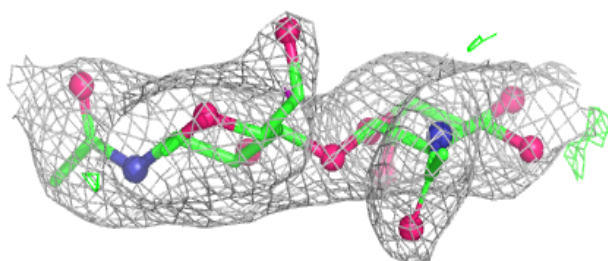
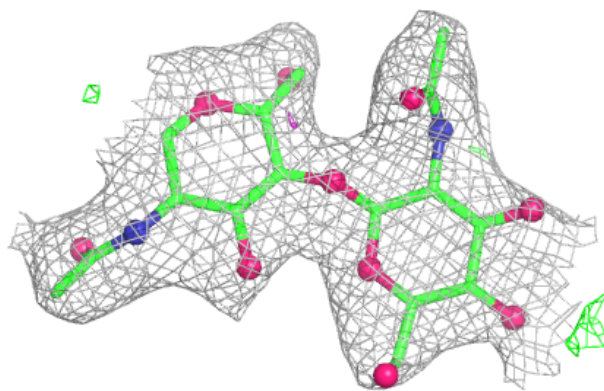
Electron density around Chain C:

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



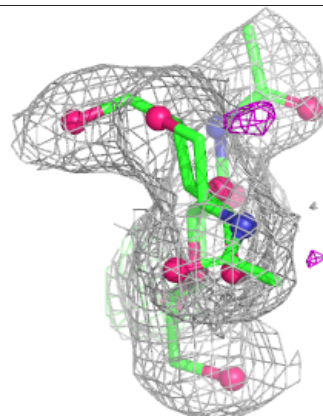
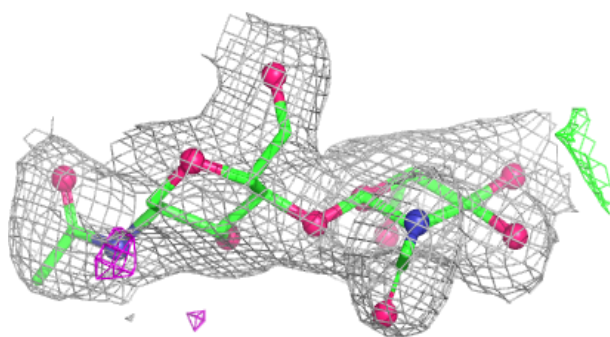
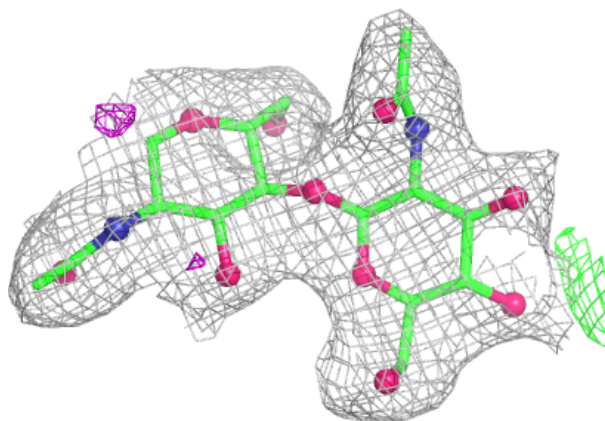
Electron density around Chain D:

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

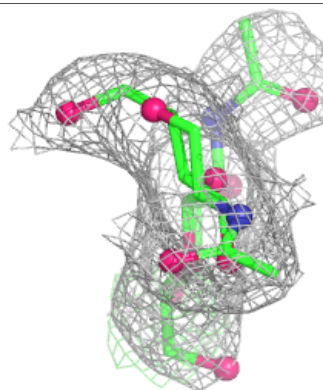
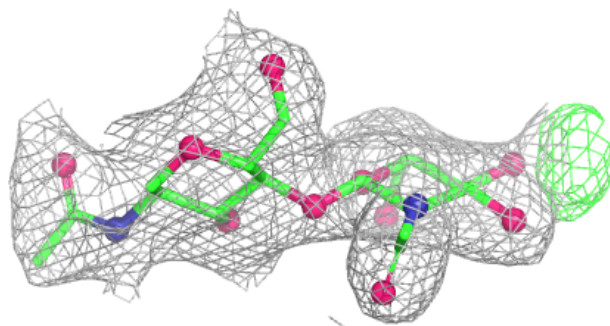
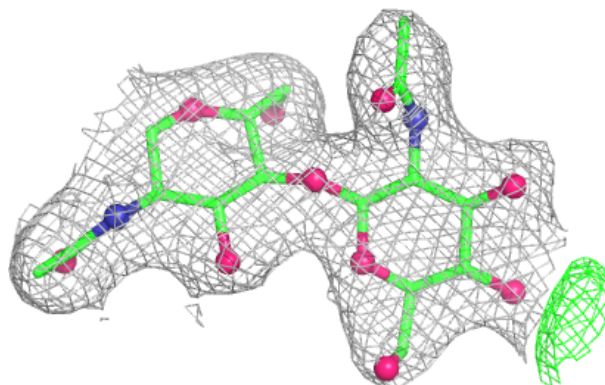


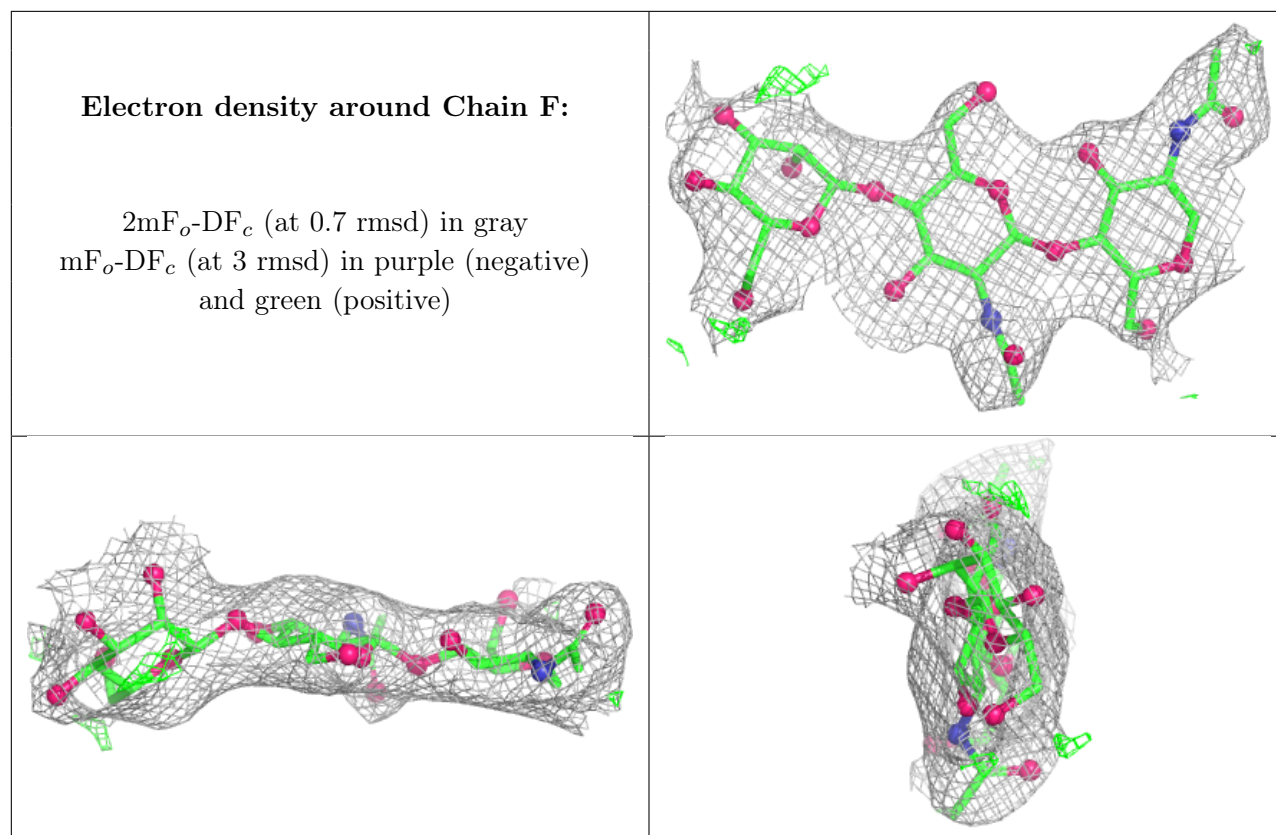
Electron density around Chain E:

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

**Electron density around Chain G:**

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





6.4 Ligands ⓘ

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	NAG	B	1013	14/15	0.69	0.16	96,97,99,99	0
7	NAG	A	1012	14/15	0.72	0.14	89,90,91,91	0
7	NAG	B	1014	14/15	0.72	0.14	81,81,82,82	0
7	NAG	B	1012	14/15	0.73	0.16	89,90,92,92	0
7	NAG	B	1009	14/15	0.78	0.13	74,76,77,77	0
7	NAG	A	1007	14/15	0.83	0.11	59,61,63,64	0
4	B4P	B	1001	53/53	0.85	0.15	58,88,112,112	0
7	NAG	B	1008	14/15	0.86	0.14	67,70,73,73	0
4	B4P	A	1001	53/53	0.89	0.13	49,69,81,82	0
6	CA	A	1004	1/1	0.98	0.03	51,51,51,51	0
5	ZN	B	1002	1/1	0.98	0.05	67,67,67,67	0
6	CA	B	1004	1/1	0.99	0.03	38,38,38,38	0
5	ZN	A	1002	1/1	0.99	0.05	55,55,55,55	0
5	ZN	B	1003	1/1	1.00	0.02	44,44,44,44	0

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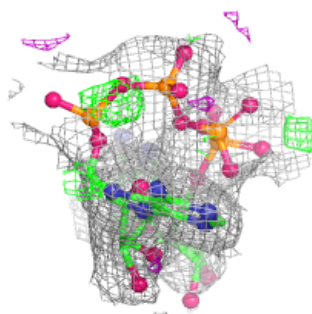
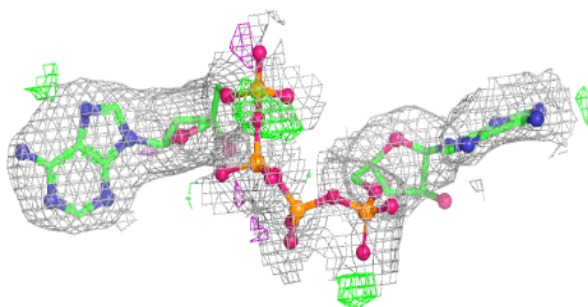
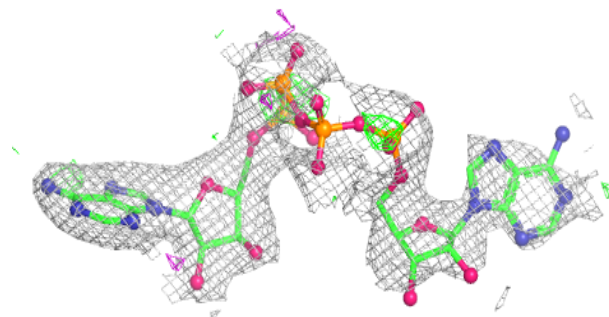
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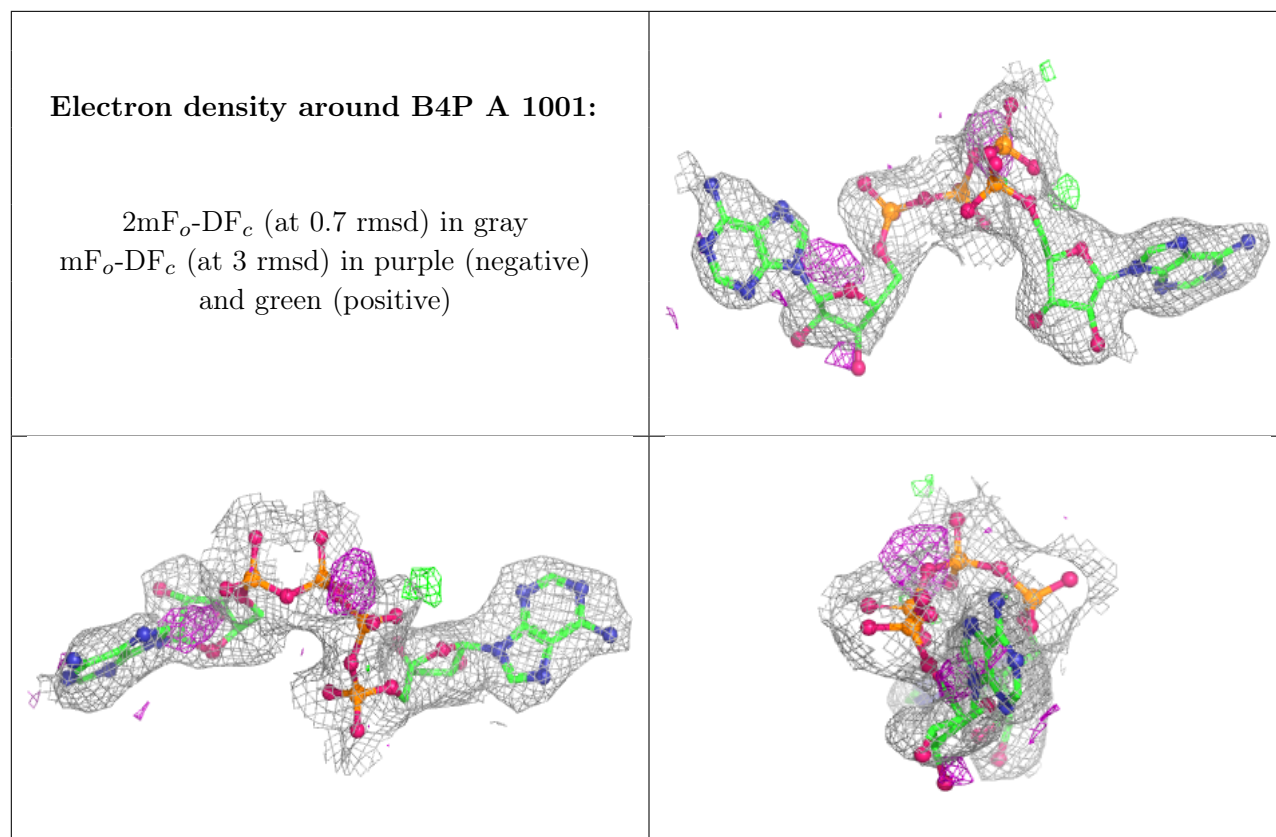
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	ZN	A	1003	1/1	1.00	0.04	44,44,44,44	0

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 B4P B 1001:

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 [i](#)

There are no such residues in this entry.