



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 01:47 AM UTC

PDB ID : 4NDZ / pdb_00004ndz
Title : Structure of Maltose Binding Protein fusion to 2-O-Sulfotransferase with bound heptasaccharide and PAP
Authors : Liu, C.; Sheng, J.; Krahn, J.M.; Perera, L.; Xu, Y.; Hsieh, P.; Liu, J.; Pedersen, L.C.
Deposited on : 2013-10-28
Resolution : 3.45 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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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

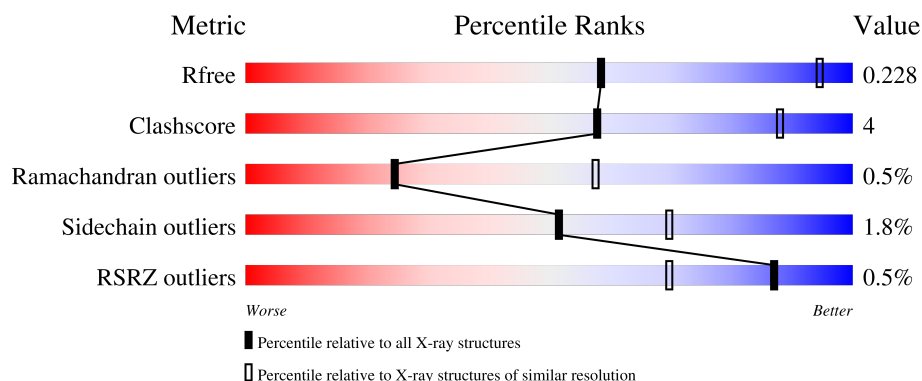
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.45 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.



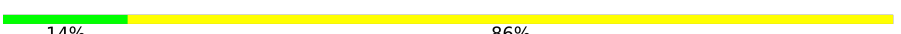
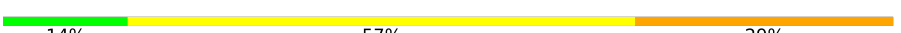
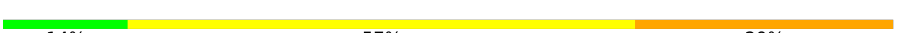
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1070 (3.50-3.42)
Clashscore	190562	1128 (3.50-3.42)
Ramachandran outliers	187476	1101 (3.50-3.42)
Sidechain outliers	187428	1102 (3.50-3.42)
RSRZ outliers	180081	1070 (3.50-3.42)

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	658	 38% 6% 56%
1	B	658	 2% 86% 13% ..
1	C	658	 86% 12% .
1	D	658	 86% 12% ..

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Mol	Chain	Length	Quality of chain
1	E	658	 86% 13% ..
1	F	658	 86% 13% ..
2	G	7	 14% 86%
2	I	7	 86% 14%
2	L	7	 14% 86%
2	N	7	 14% 57% 29%
2	P	7	 14% 57% 29%
3	H	2	 100%
3	J	2	 100%
3	K	2	 50% 50%
3	M	2	 50% 50%
3	O	2	 50% 50%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 28764 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 Maltose-binding periplasmic protein, Heparan sulfate 2-O-sulfotransferase 1 fusion.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	S	0	0	1
			2352	1522	399	422	9			
1	B	654	Total	C	N	O	S	0	0	1
			5136	3314	852	955	15			
1	C	655	Total	C	N	O	S	0	0	1
			5128	3311	848	955	14			
1	D	654	Total	C	N	O	S	0	0	1
			5136	3313	853	955	15			
1	E	654	Total	C	N	O	S	0	0	1
			5110	3298	842	955	15			
1	F	654	Total	C	N	O	S	0	1	0
			5124	3307	846	956	15			

There are 42 discrepancies between the modelled and reference sequences:

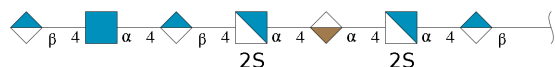
Chain	Residue	Modelled	Actual	Comment	Reference
A	359	ALA	GLU	engineered mutation	UNP P0AEX9
A	362	ALA	LYS	engineered mutation	UNP P0AEX9
A	363	ALA	ASP	engineered mutation	UNP P0AEX9
A	367	ASN	ARG	engineered mutation	UNP P0AEX9
A	368	ALA	-	linker	UNP P0AEX9
A	369	ALA	-	linker	UNP P0AEX9
A	370	ALA	-	linker	UNP P0AEX9
B	359	ALA	GLU	engineered mutation	UNP P0AEX9
B	362	ALA	LYS	engineered mutation	UNP P0AEX9
B	363	ALA	ASP	engineered mutation	UNP P0AEX9
B	367	ASN	ARG	engineered mutation	UNP P0AEX9
B	368	ALA	-	linker	UNP P0AEX9
B	369	ALA	-	linker	UNP P0AEX9
B	370	ALA	-	linker	UNP P0AEX9
C	359	ALA	GLU	engineered mutation	UNP P0AEX9
C	362	ALA	LYS	engineered mutation	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	363	ALA	ASP	engineered mutation	UNP P0AEX9
C	367	ASN	ARG	engineered mutation	UNP P0AEX9
C	368	ALA	-	linker	UNP P0AEX9
C	369	ALA	-	linker	UNP P0AEX9
C	370	ALA	-	linker	UNP P0AEX9
D	359	ALA	GLU	engineered mutation	UNP P0AEX9
D	362	ALA	LYS	engineered mutation	UNP P0AEX9
D	363	ALA	ASP	engineered mutation	UNP P0AEX9
D	367	ASN	ARG	engineered mutation	UNP P0AEX9
D	368	ALA	-	linker	UNP P0AEX9
D	369	ALA	-	linker	UNP P0AEX9
D	370	ALA	-	linker	UNP P0AEX9
E	359	ALA	GLU	engineered mutation	UNP P0AEX9
E	362	ALA	LYS	engineered mutation	UNP P0AEX9
E	363	ALA	ASP	engineered mutation	UNP P0AEX9
E	367	ASN	ARG	engineered mutation	UNP P0AEX9
E	368	ALA	-	linker	UNP P0AEX9
E	369	ALA	-	linker	UNP P0AEX9
E	370	ALA	-	linker	UNP P0AEX9
F	359	ALA	GLU	engineered mutation	UNP P0AEX9
F	362	ALA	LYS	engineered mutation	UNP P0AEX9
F	363	ALA	ASP	engineered mutation	UNP P0AEX9
F	367	ASN	ARG	engineered mutation	UNP P0AEX9
F	368	ALA	-	linker	UNP P0AEX9
F	369	ALA	-	linker	UNP P0AEX9
F	370	ALA	-	linker	UNP P0AEX9

- Molecule 2 is an oligosaccharide called beta-D-glucopyranuronic acid-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-4)-2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	7	Total	C	N	O	S	0	0	0
			92	44	3	43	2			
2	I	7	Total	C	N	O	S	0	0	0
			92	44	3	43	2			

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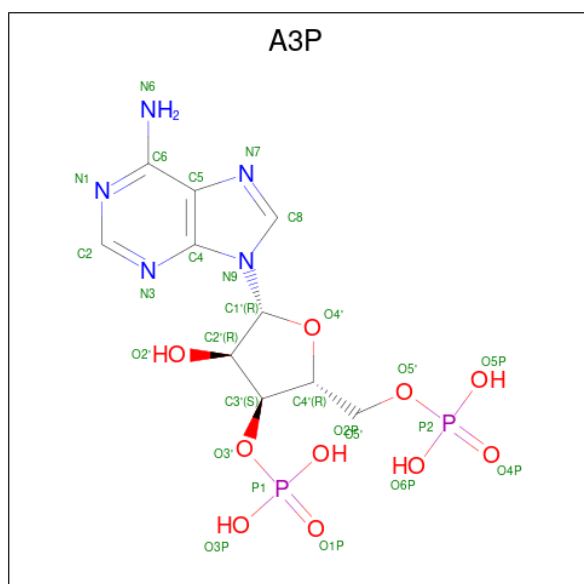
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	7	Total	C	N	O	S	0	0	0
			92	44	3	43	2			
2	N	7	Total	C	N	O	S	0	0	0
			92	44	3	43	2			
2	P	7	Total	C	N	O	S	0	0	0
			93	44	3	44	2			

- Molecule 3 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



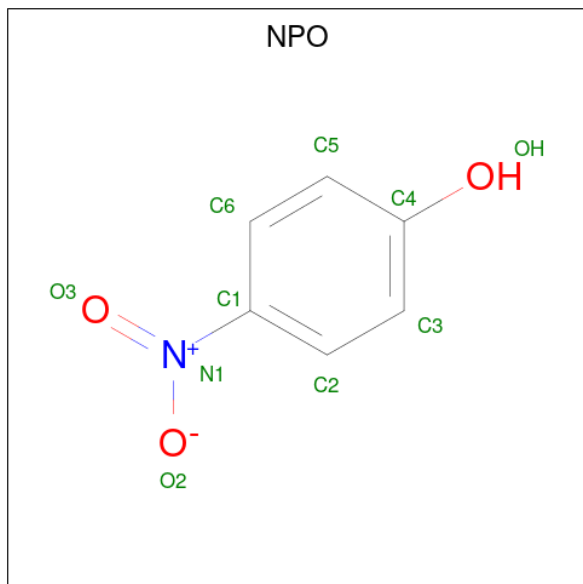
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	H	2	Total	C	O	0	0	0
			23	12	11			
3	J	2	Total	C	O	0	0	0
			23	12	11			
3	K	2	Total	C	O	0	0	0
			23	12	11			
3	M	2	Total	C	O	0	0	0
			23	12	11			
3	O	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 4 is ADENOSINE-3'-5'-DIPHOSPHATE (CCD ID: A3P) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 5 is P-NITROPHENOL (CCD ID: NPO) (formula: $C_6H_5NO_3$).

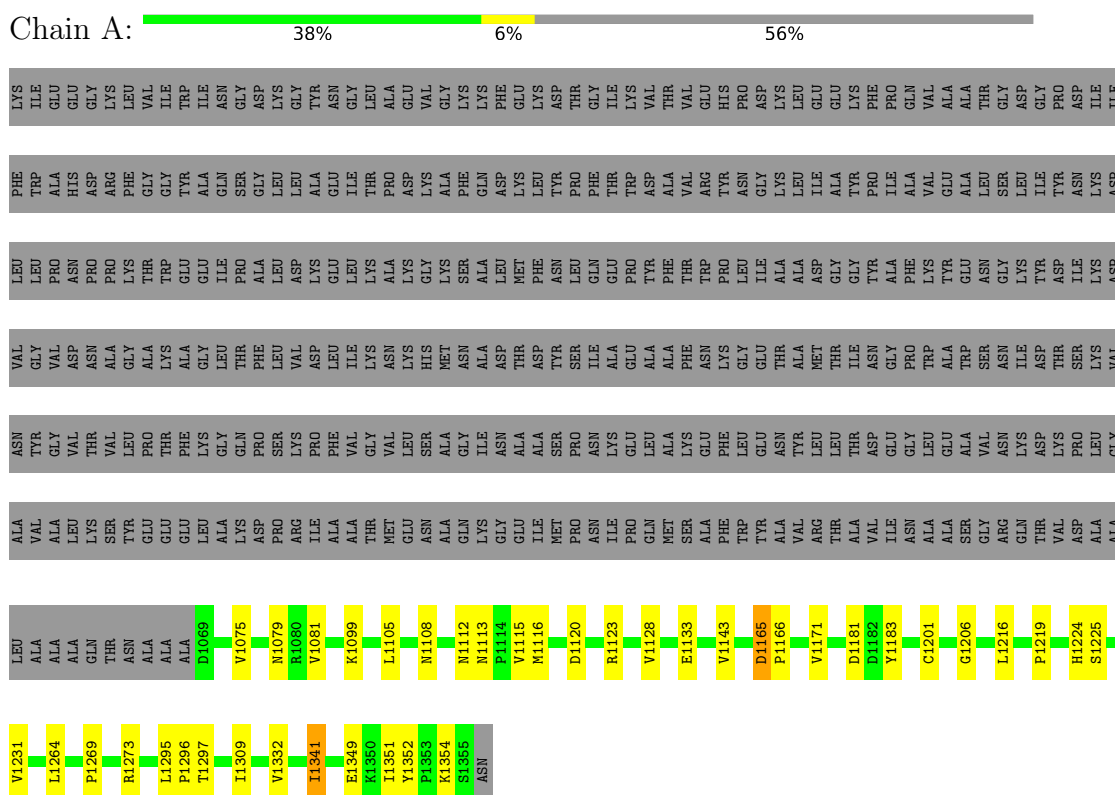


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			10	6	1	3		
5	B	1	Total	C	N	O	0	0
			10	6	1	3		
5	D	1	Total	C	N	O	0	0
			10	6	1	3		
5	E	1	Total	C	N	O	0	0
			10	6	1	3		

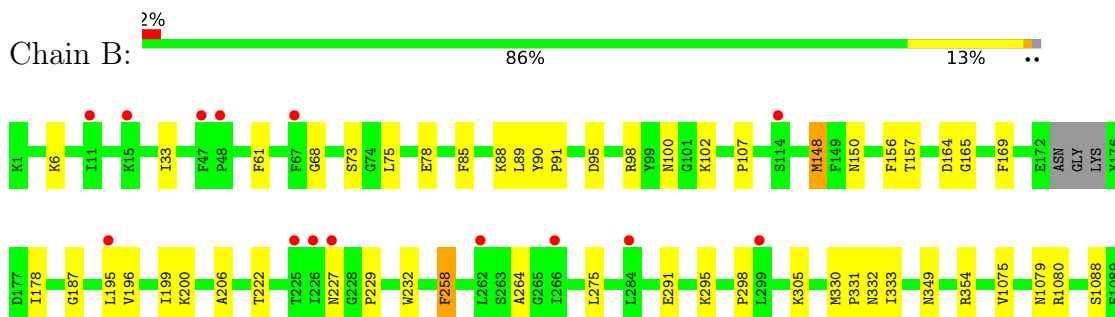
3 Residue-property plots

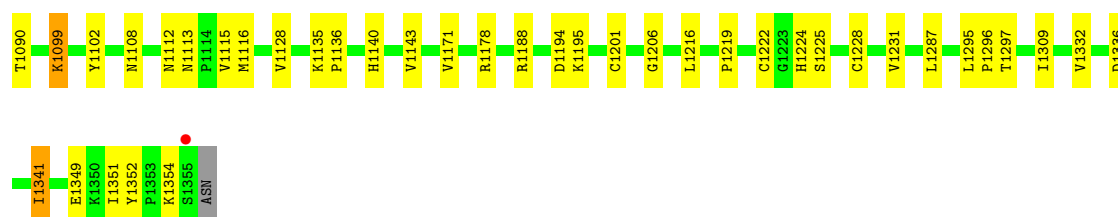
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Maltose-binding periplasmic protein, Heparan sulfate 2-O-sulfotransferase 1 fusion



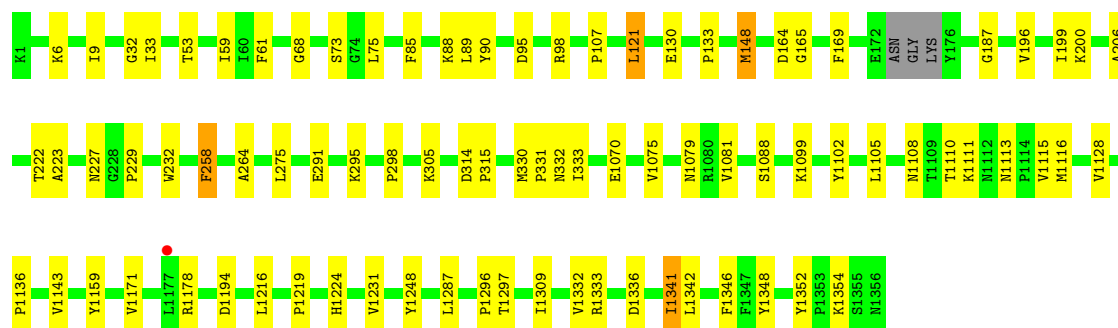
- Molecule 1: Maltose-binding periplasmic protein, Heparan sulfate 2-O-sulfotransferase 1 fusion





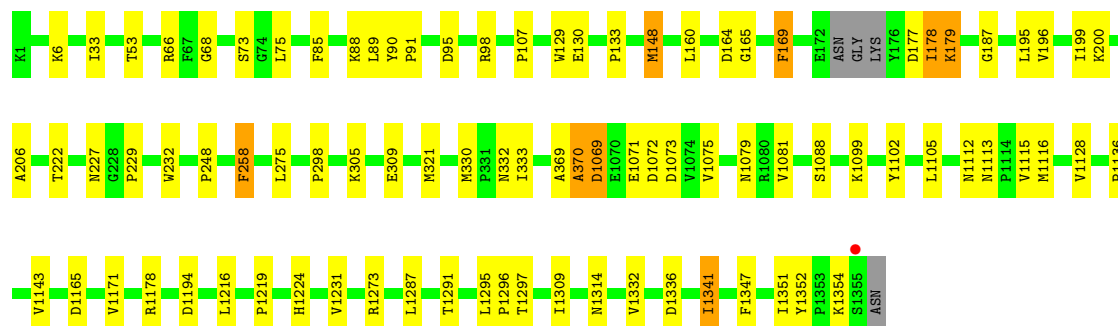
- Molecule 1: Maltose-binding periplasmic protein, Heparan sulfate 2-O-sulfotransferase 1 fusion

Chain C: 86% 12% .



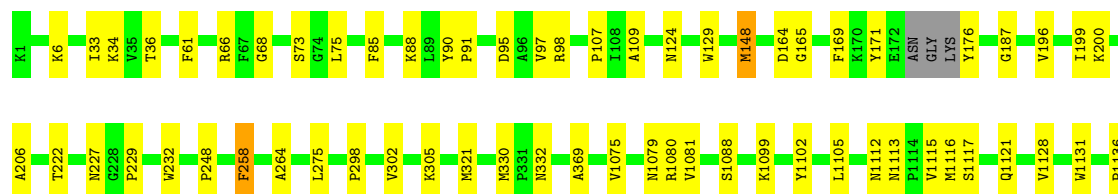
- Molecule 1: Maltose-binding periplasmic protein, Heparan sulfate 2-O-sulfotransferase 1 fusion

Chain D: 86% 12% ..



- Molecule 1: Maltose-binding periplasmic protein, Heparan sulfate 2-O-sulfotransferase 1 fusion

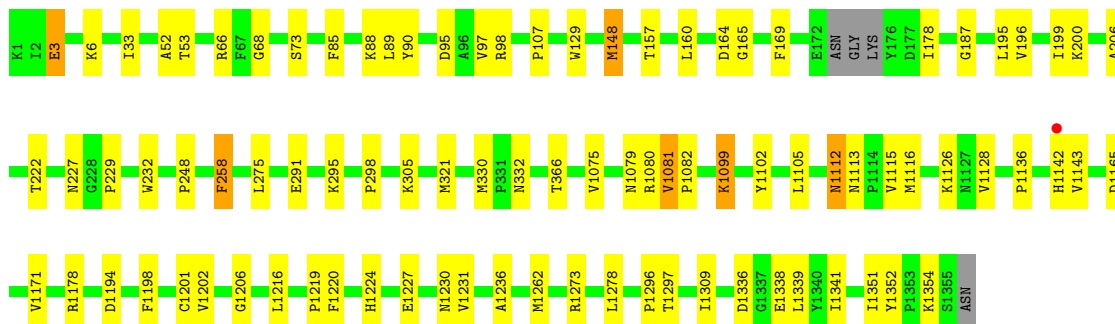
Chain E: 86% 13% ..





- Molecule 1: Maltose-binding periplasmic protein, Heparan sulfate 2-O-sulfotransferase 1 fusion

Chain F: 86% 13% ..



- Molecule 2: beta-D-glucopyranuronic acid-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-4)-2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid

Chain G: 14% 86%



- Molecule 2: beta-D-glucopyranuronic acid-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-4)-2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid

Chain I: 86% 14%



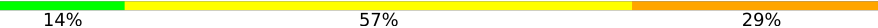
- Molecule 2: beta-D-glucopyranuronic acid-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-4)-2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid

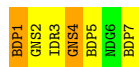
Chain L: 14% 86%



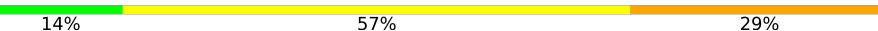
- Molecule 2: beta-D-glucopyranuronic acid-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-4)-2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid

a-L-idopyranuronic acid-(1-4)-2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid

Chain N:  14% 57% 29%

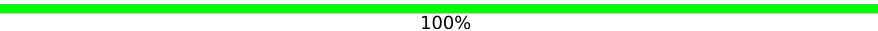


- Molecule 2: beta-D-glucopyranuronic acid-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-4)-2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid

Chain P:  14% 57% 29%

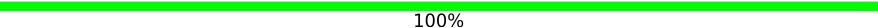


- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain H:  100%



- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain J:  100%



- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain K:  50% 50%



- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain M:  50% 50%



- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain O:  50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	155.72Å 170.69Å 183.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.66 – 3.45 49.66 – 3.45	Depositor EDS
% Data completeness (in resolution range)	98.5 (49.66-3.45) 91.0 (49.66-3.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.08 (at 3.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.176 , 0.228 0.180 , 0.228	Depositor DCC
R_{free} test set	1962 reflections (3.01%)	wwPDB-VP
Wilson B-factor (Å ²)	88.5	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 129.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	28764	wwPDB-VP
Average B, all atoms (Å ²)	138.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.94% 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: GNS, IDR, NPO, A3P, BDP, GLC, NDG

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	0.48	0/2416	0.78	4/3270 (0.1%)
1	B	0.39	0/5267	0.74	0/7153
1	C	0.38	0/5259	0.75	2/7144 (0.0%)
1	D	0.39	0/5267	0.75	5/7152 (0.1%)
1	E	0.39	0/5241	0.76	6/7123 (0.1%)
1	F	0.38	0/5256	0.74	4/7142 (0.1%)
All	All	0.39	0/28706	0.75	21/38984 (0.1%)

There are no bond length outliers.

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	1081	VAL	CA-C-N	6.27	126.64	119.93
1	F	1081	VAL	C-N-CA	6.27	126.64	119.93
1	A	1165	ASP	CA-C-N	6.02	125.50	119.24
1	A	1165	ASP	C-N-CA	6.02	125.50	119.24
1	C	1081	VAL	CA-C-N	5.84	126.18	119.93

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	2352	0	2265	21	0
1	B	5136	0	4988	51	0
1	C	5128	0	4973	43	0
1	D	5136	0	4988	46	0
1	E	5110	0	4933	49	0
1	F	5124	0	4950	53	0
2	G	92	0	54	0	0
2	I	92	0	54	2	0
2	L	92	0	54	0	0
2	N	92	0	54	2	0
2	P	93	0	56	2	0
3	H	23	0	21	0	0
3	J	23	0	21	0	0
3	K	23	0	21	1	0
3	M	23	0	21	1	0
3	O	23	0	21	1	0
4	A	27	0	11	0	0
4	B	27	0	11	0	0
4	C	27	0	11	0	0
4	D	27	0	11	0	0
4	E	27	0	11	0	0
4	F	27	0	11	0	0
5	A	10	0	4	0	0
5	B	10	0	4	0	0
5	D	10	0	4	0	0
5	E	10	0	4	0	0
All	All	28764	0	27556	251	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 4.

The worst 5 of 251 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:D:369:ALA:O	1:D:1069:ASP:N	2.24	0.71
1:E:1131:TRP:NE1	1:F:366:THR:HG21	2.08	0.68
1:E:1131:TRP:CD1	1:F:366:THR:HG21	2.30	0.66
1:D:1071:GLU:O	1:D:1073:ASP:N	2.30	0.65
1:A:1120:ASP:OD1	1:A:1123:ARG:NH1	2.31	0.63

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	285/658 (43%)	272 (95%)	13 (5%)	0	100	100
1	B	650/658 (99%)	616 (95%)	31 (5%)	3 (0%)	24	57
1	C	651/658 (99%)	619 (95%)	28 (4%)	4 (1%)	21	53
1	D	650/658 (99%)	614 (94%)	30 (5%)	6 (1%)	14	46
1	E	650/658 (99%)	619 (95%)	28 (4%)	3 (0%)	24	57
1	F	651/658 (99%)	619 (95%)	29 (4%)	3 (0%)	24	57
All	All	3537/3948 (90%)	3359 (95%)	159 (4%)	19 (0%)	24	57

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	370	ALA
1	D	1072	ASP
1	E	369	ALA
1	B	1336	ASP
1	B	169	PHE

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	245/548 (45%)	239 (98%)	6 (2%)	43	65
1	B	524/548 (96%)	515 (98%)	9 (2%)	53	70
1	C	522/548 (95%)	515 (99%)	7 (1%)	61	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	524/548 (96%)	513 (98%)	11 (2%)	47	66
1	E	519/548 (95%)	511 (98%)	8 (2%)	57	72
1	F	521/548 (95%)	511 (98%)	10 (2%)	50	68
All	All	2855/3288 (87%)	2804 (98%)	51 (2%)	51	70

5 of 51 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	1112	ASN
1	E	258	PHE
1	F	1297	THR
1	D	1273	ARG
1	D	1341	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	1330	HIS
1	E	1113	ASN
1	E	1106	HIS
1	E	1127	ASN
1	C	365	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 ⓘ

45 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	BDP	G	1	2,5	12,12,13	2.67	8 (66%)	14,17,19	1.00	0
2	GNS	G	2	2	15,15,16	2.48	8 (53%)	17,22,24	2.36	3 (17%)
2	IDR	G	3	2	12,12,13	2.52	6 (50%)	14,17,19	1.18	2 (14%)
2	GNS	G	4	2	15,15,16	2.30	8 (53%)	17,22,24	2.47	4 (23%)
2	BDP	G	5	2	12,12,13	2.49	5 (41%)	14,17,19	1.05	0
2	NDG	G	6	2	14,14,15	0.58	0	17,19,21	0.52	0
2	BDP	G	7	2	12,12,13	2.55	6 (50%)	14,17,19	0.93	1 (7%)
3	GLC	H	1	3	12,12,12	0.52	0	17,17,17	0.63	0
3	GLC	H	2	3	11,11,12	0.61	0	15,15,17	0.59	0
2	BDP	I	1	2,5	12,12,13	2.73	8 (66%)	14,17,19	0.85	0
2	GNS	I	2	2	15,15,16	2.43	6 (40%)	17,22,24	2.31	3 (17%)
2	IDR	I	3	2	12,12,13	2.49	6 (50%)	14,17,19	1.25	2 (14%)
2	GNS	I	4	2	15,15,16	2.48	8 (53%)	17,22,24	2.50	4 (23%)
2	BDP	I	5	2	12,12,13	2.50	6 (50%)	14,17,19	1.04	0
2	NDG	I	6	2	14,14,15	0.56	0	17,19,21	0.64	0
2	BDP	I	7	2	12,12,13	2.59	6 (50%)	14,17,19	0.73	0
3	GLC	J	1	3	12,12,12	0.51	0	17,17,17	0.59	0
3	GLC	J	2	3	11,11,12	0.58	0	15,15,17	0.62	0
3	GLC	K	1	3	12,12,12	0.51	0	17,17,17	0.61	0
3	GLC	K	2	3	11,11,12	0.64	0	15,15,17	0.61	0
2	BDP	L	1	2,5	12,12,13	2.50	6 (50%)	14,17,19	1.02	0
2	GNS	L	2	2	15,15,16	2.48	8 (53%)	17,22,24	2.41	5 (29%)
2	IDR	L	3	2	12,12,13	2.48	6 (50%)	14,17,19	1.10	2 (14%)
2	GNS	L	4	2	15,15,16	2.43	6 (40%)	17,22,24	2.60	4 (23%)
2	BDP	L	5	2	12,12,13	2.42	5 (41%)	14,17,19	0.99	0
2	NDG	L	6	2	14,14,15	0.48	0	17,19,21	0.67	0
2	BDP	L	7	2	12,12,13	2.52	5 (41%)	14,17,19	0.99	0
3	GLC	M	1	3	12,12,12	0.52	0	17,17,17	0.63	0
3	GLC	M	2	3	11,11,12	0.64	0	15,15,17	0.73	0
2	BDP	N	1	2,5	12,12,13	2.58	7 (58%)	14,17,19	0.97	0
2	GNS	N	2	2	15,15,16	2.45	8 (53%)	17,22,24	2.48	3 (17%)
2	IDR	N	3	2	12,12,13	2.43	6 (50%)	14,17,19	1.14	1 (7%)
2	GNS	N	4	2	15,15,16	2.34	7 (46%)	17,22,24	2.50	3 (17%)
2	BDP	N	5	2	12,12,13	2.56	5 (41%)	14,17,19	0.88	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NDG	N	6	2	14,14,15	0.57	0	17,19,21	0.51	0
2	BDP	N	7	2	12,12,13	2.56	7 (58%)	14,17,19	0.81	0
3	GLC	O	1	3	12,12,12	0.50	0	17,17,17	0.64	0
3	GLC	O	2	3	11,11,12	0.63	0	15,15,17	0.54	0
2	BDP	P	1	2	13,13,13	2.22	4 (30%)	18,19,19	1.46	1 (5%)
2	GNS	P	2	2	15,15,16	2.44	8 (53%)	17,22,24	2.58	3 (17%)
2	IDR	P	3	2	12,12,13	2.42	6 (50%)	14,17,19	1.15	2 (14%)
2	GNS	P	4	2	15,15,16	2.36	7 (46%)	17,22,24	2.47	3 (17%)
2	BDP	P	5	2	12,12,13	2.54	5 (41%)	14,17,19	0.92	0
2	NDG	P	6	2	14,14,15	0.55	0	17,19,21	0.51	0
2	BDP	P	7	2	12,12,13	2.52	6 (50%)	14,17,19	0.90	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BDP	G	1	2,5	-	0/4/21/24	0/1/1/1
2	GNS	G	2	2	-	0/7/24/27	0/1/1/1
2	IDR	G	3	2	-	2/4/21/24	0/1/1/1
2	GNS	G	4	2	-	1/7/24/27	0/1/1/1
2	BDP	G	5	2	-	0/4/21/24	0/1/1/1
2	NDG	G	6	2	-	0/6/23/26	0/1/1/1
2	BDP	G	7	2	-	2/4/21/24	0/1/1/1
3	GLC	H	1	3	-	0/2/22/22	0/1/1/1
3	GLC	H	2	3	-	0/2/19/22	0/1/1/1
2	BDP	I	1	2,5	-	0/4/21/24	0/1/1/1
2	GNS	I	2	2	-	0/7/24/27	0/1/1/1
2	IDR	I	3	2	-	2/4/21/24	0/1/1/1
2	GNS	I	4	2	-	1/7/24/27	0/1/1/1
2	BDP	I	5	2	-	0/4/21/24	0/1/1/1
2	NDG	I	6	2	-	3/6/23/26	0/1/1/1
2	BDP	I	7	2	-	2/4/21/24	0/1/1/1
3	GLC	J	1	3	-	0/2/22/22	0/1/1/1
3	GLC	J	2	3	-	0/2/19/22	0/1/1/1
3	GLC	K	1	3	-	0/2/22/22	0/1/1/1
3	GLC	K	2	3	-	0/2/19/22	0/1/1/1
2	BDP	L	1	2,5	-	0/4/21/24	0/1/1/1
2	GNS	L	2	2	-	0/7/24/27	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	IDR	L	3	2	-	2/4/21/24	0/1/1/1
2	GNS	L	4	2	-	1/7/24/27	0/1/1/1
2	BDP	L	5	2	-	0/4/21/24	0/1/1/1
2	NDG	L	6	2	-	2/6/23/26	0/1/1/1
2	BDP	L	7	2	-	1/4/21/24	0/1/1/1
3	GLC	M	1	3	-	0/2/22/22	0/1/1/1
3	GLC	M	2	3	-	0/2/19/22	0/1/1/1
2	BDP	N	1	2,5	-	0/4/21/24	0/1/1/1
2	GNS	N	2	2	-	1/7/24/27	0/1/1/1
2	IDR	N	3	2	-	3/4/21/24	0/1/1/1
2	GNS	N	4	2	-	1/7/24/27	0/1/1/1
2	BDP	N	5	2	-	1/4/21/24	0/1/1/1
2	NDG	N	6	2	-	0/6/23/26	0/1/1/1
2	BDP	N	7	2	-	2/4/21/24	0/1/1/1
3	GLC	O	1	3	-	0/2/22/22	0/1/1/1
3	GLC	O	2	3	-	0/2/19/22	0/1/1/1
2	BDP	P	1	2	-	0/4/24/24	0/1/1/1
2	GNS	P	2	2	-	0/7/24/27	0/1/1/1
2	IDR	P	3	2	-	3/4/21/24	0/1/1/1
2	GNS	P	4	2	-	1/7/24/27	0/1/1/1
2	BDP	P	5	2	-	0/4/21/24	0/1/1/1
2	NDG	P	6	2	-	0/6/23/26	0/1/1/1
2	BDP	P	7	2	-	1/4/21/24	0/1/1/1

The worst 5 of 193 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	5	BDP	O6A-C6	5.50	1.38	1.22
2	I	1	BDP	O6A-C6	5.50	1.38	1.22
2	N	3	IDR	O6A-C6	5.45	1.38	1.22
2	P	1	BDP	O6A-C6	5.44	1.38	1.22
2	L	3	IDR	O6A-C6	5.44	1.38	1.22

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	4	GNS	O2S-S1-O3S	-7.67	103.30	120.36
2	L	4	GNS	O2S-S1-O3S	-7.64	103.37	120.36
2	N	4	GNS	O2S-S1-O3S	-7.60	103.45	120.36
2	L	2	GNS	O2S-S1-O3S	-7.30	104.11	120.36
2	I	4	GNS	O2S-S1-O3S	-7.29	104.15	120.36

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

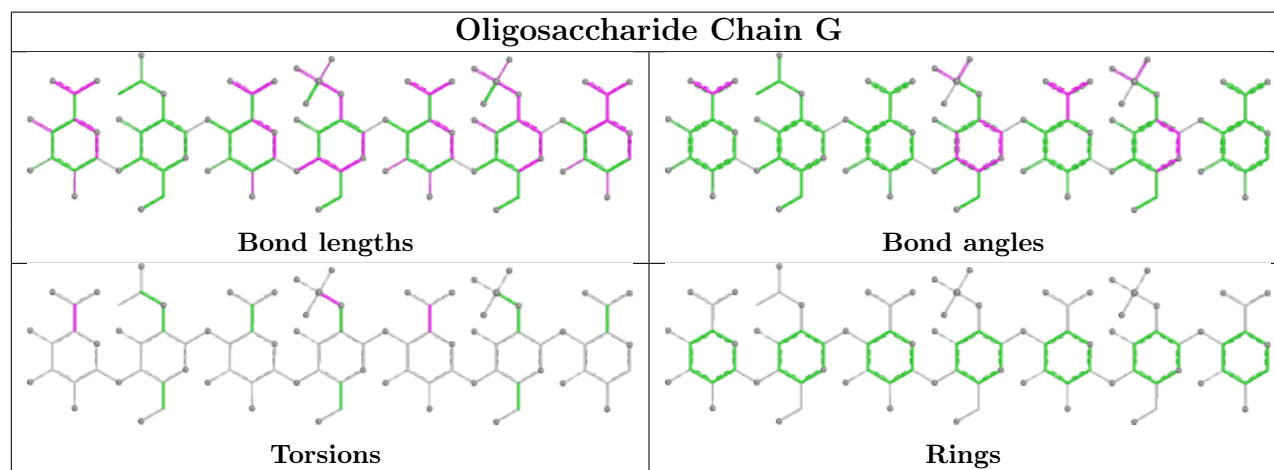
Mol	Chain	Res	Type	Atoms
2	G	3	IDR	C4-C5-C6-O6A
2	G	3	IDR	C4-C5-C6-O6B
2	I	3	IDR	C4-C5-C6-O6A
2	I	3	IDR	C4-C5-C6-O6B
2	L	3	IDR	C4-C5-C6-O6A

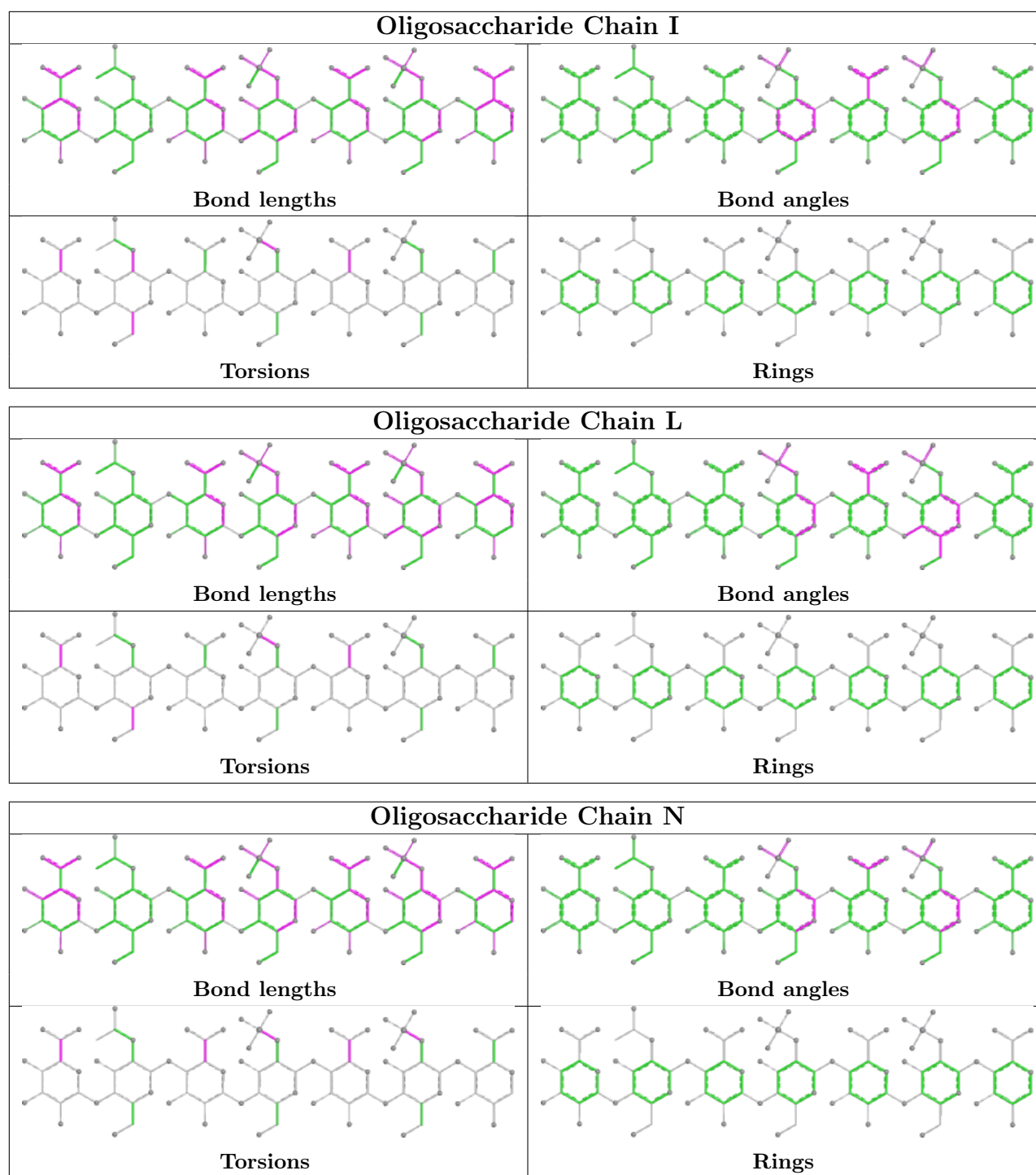
There are no ring outliers.

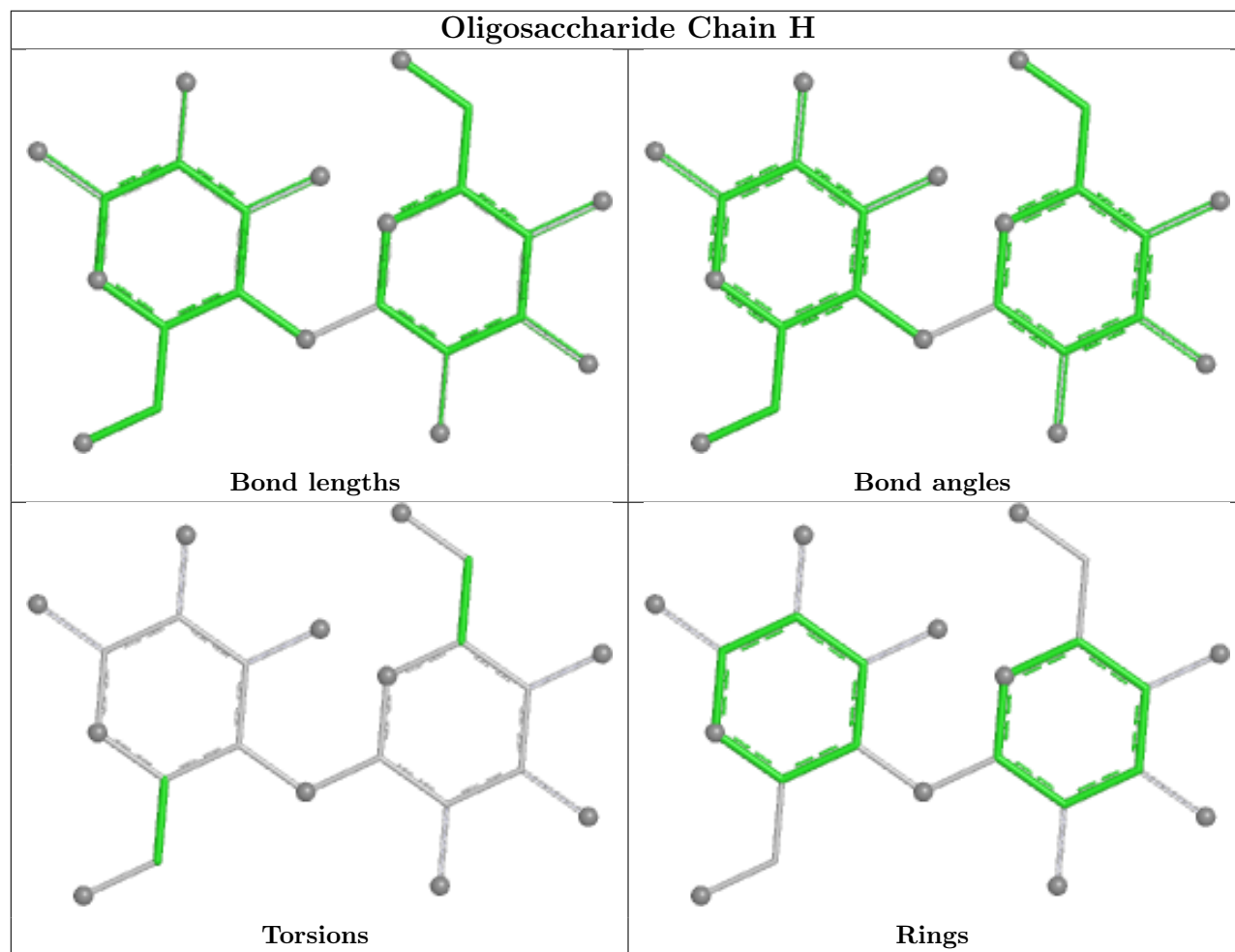
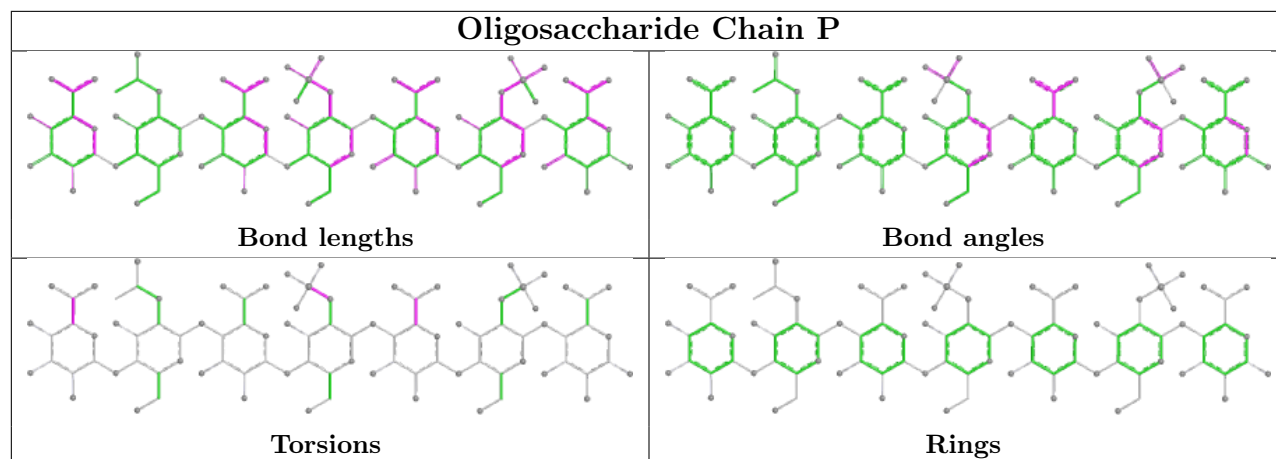
9 monomers are involved in 9 short contacts:

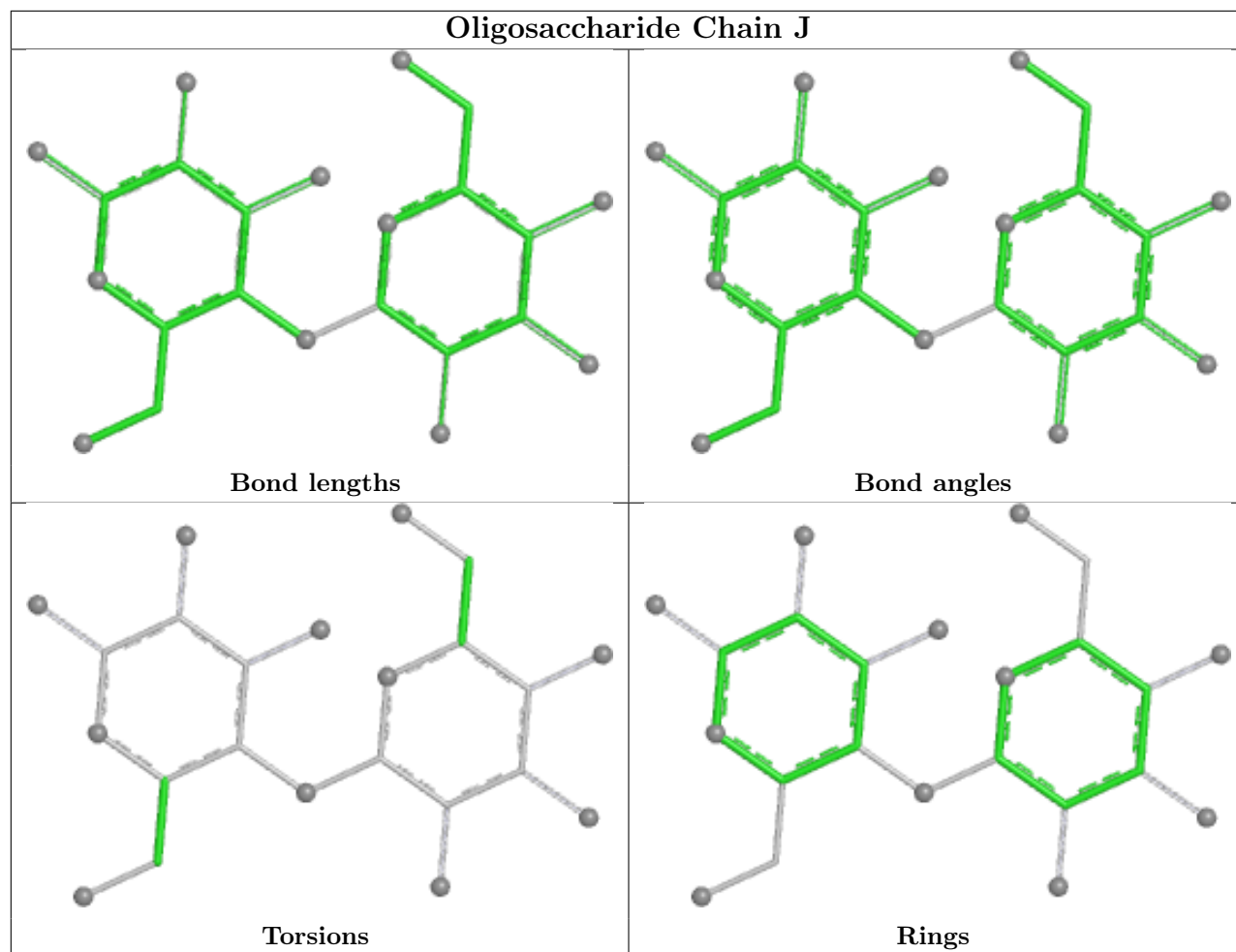
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	2	GLC	1	0
3	O	2	GLC	1	0
2	P	1	BDP	1	0
2	I	4	GNS	1	0
2	N	4	GNS	1	0
2	I	6	NDG	1	0
2	P	4	GNS	1	0
3	K	2	GLC	1	0
2	N	1	BDP	1	0

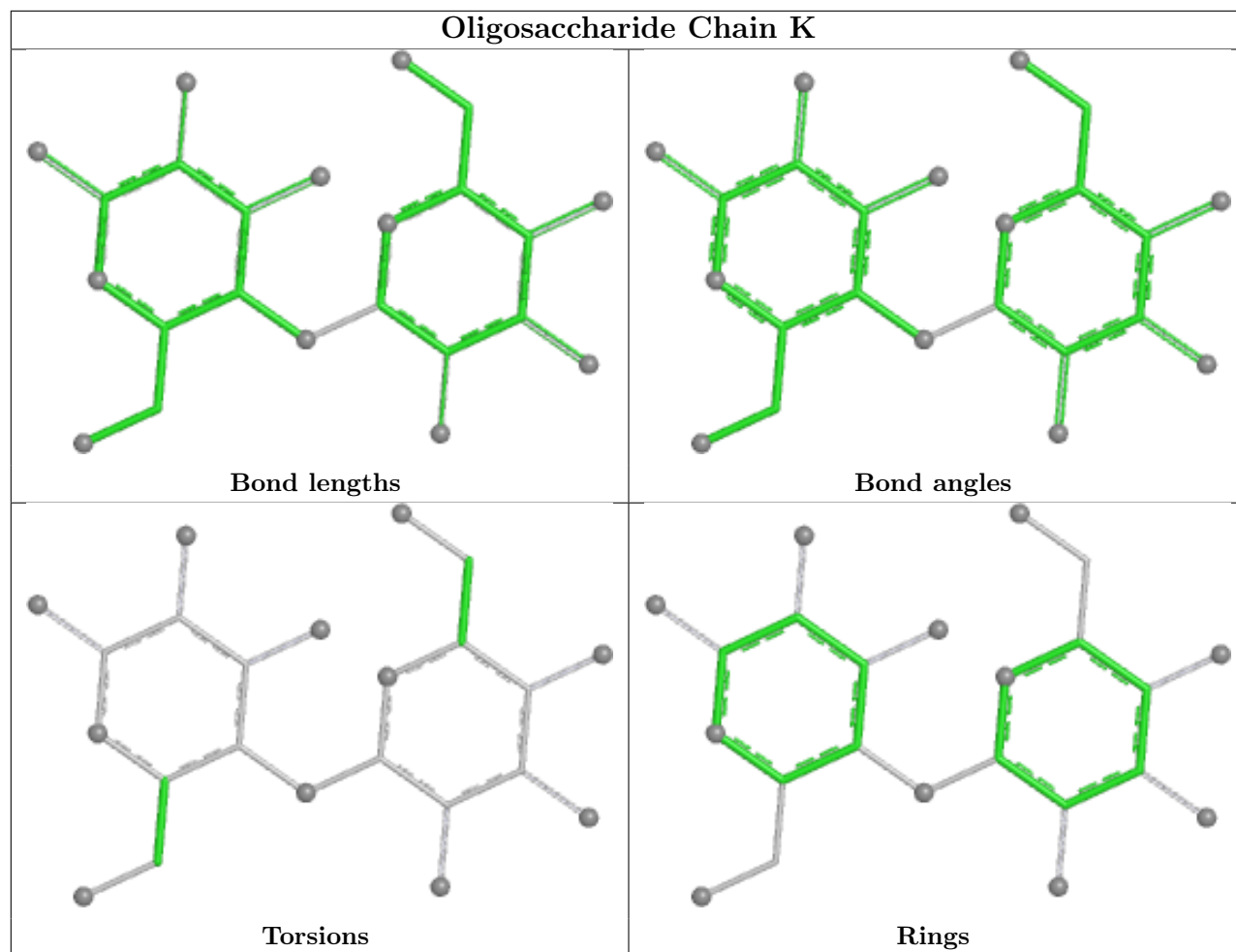
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

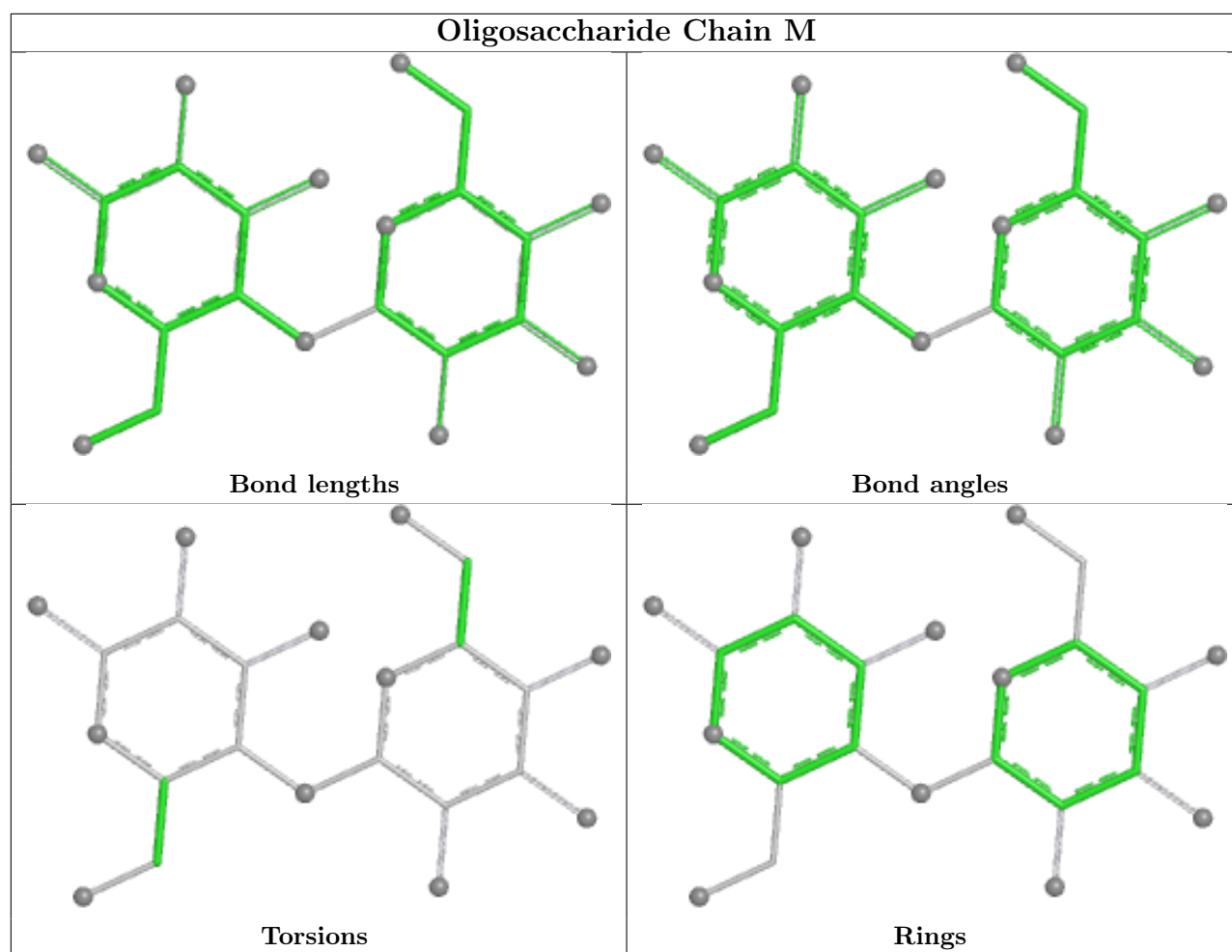


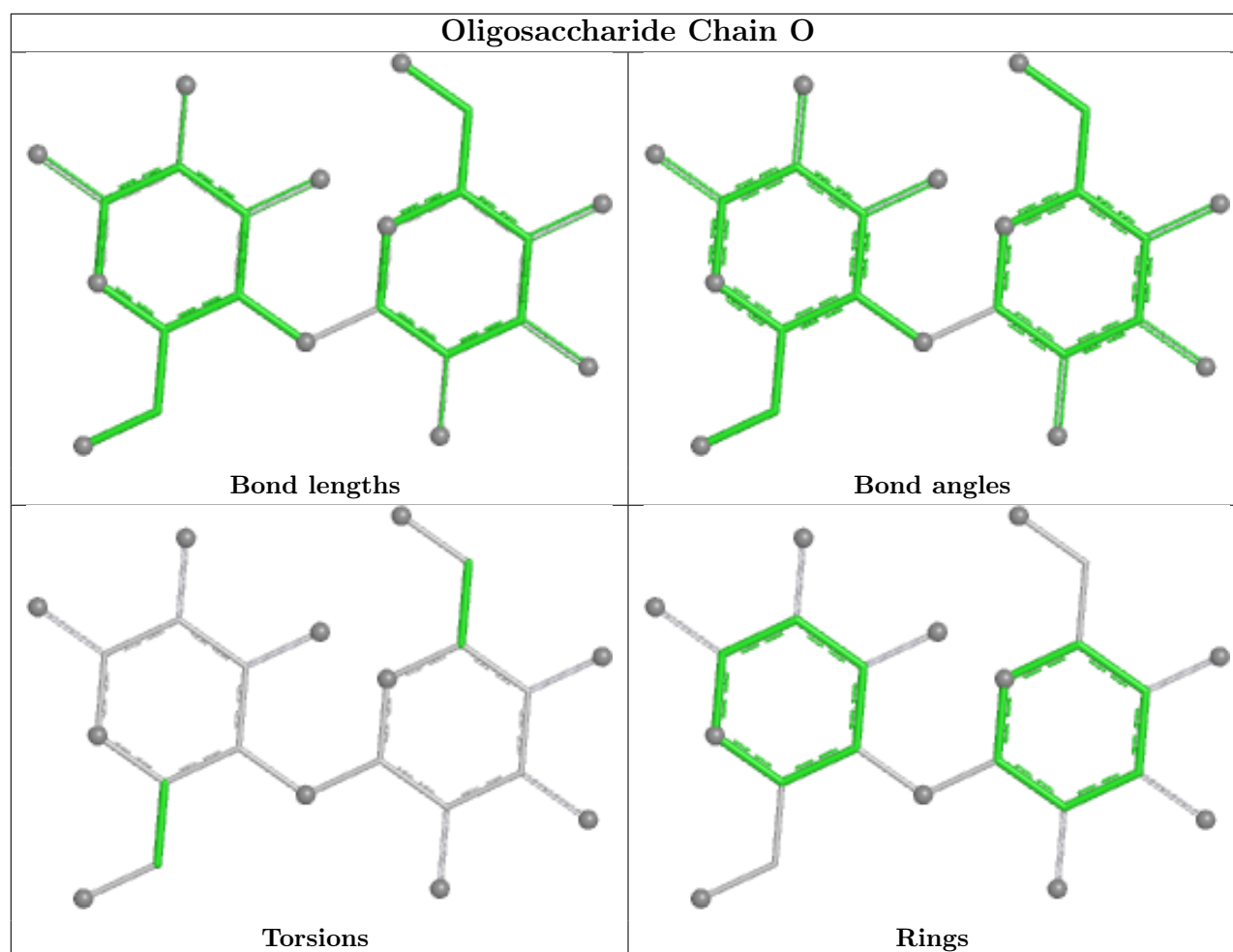












5.6 Ligand geometry [i](#)

10 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
5	NPO	E	2011	2	10,10,10	0.46	0	11,13,13	0.54	0
4	A3P	F	2003	-	29,29,29	2.90	13 (44%)	44,45,45	1.74	8 (18%)
5	NPO	D	2011	2	10,10,10	0.47	0	11,13,13	0.56	0
4	A3P	A	2003	-	29,29,29	2.87	15 (51%)	44,45,45	1.81	8 (18%)
4	A3P	E	2003	-	29,29,29	2.89	13 (44%)	44,45,45	1.81	8 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	A3P	C	2003	-	29,29,29	2.89	14 (48%)	44,45,45	1.81	8 (18%)
4	A3P	B	2003	-	29,29,29	2.82	13 (44%)	44,45,45	1.75	8 (18%)
5	NPO	A	2011	2	10,10,10	0.53	0	11,13,13	0.89	1 (9%)
5	NPO	B	2011	2	10,10,10	0.51	0	11,13,13	0.74	0
4	A3P	D	2003	-	29,29,29	2.82	13 (44%)	44,45,45	1.78	8 (18%)

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
5	NPO	E	2011	2	-	0/2/4/4	0/1/1/1
4	A3P	F	2003	-	-	1/15/31/31	0/3/3/3
5	NPO	D	2011	2	-	0/2/4/4	0/1/1/1
4	A3P	A	2003	-	-	0/15/31/31	0/3/3/3
4	A3P	E	2003	-	-	0/15/31/31	0/3/3/3
4	A3P	C	2003	-	-	0/15/31/31	0/3/3/3
4	A3P	B	2003	-	-	0/15/31/31	0/3/3/3
5	NPO	A	2011	2	-	0/2/4/4	0/1/1/1
5	NPO	B	2011	2	-	0/2/4/4	0/1/1/1
4	A3P	D	2003	-	-	0/15/31/31	0/3/3/3

The worst 5 of 81 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	2003	A3P	C8-N7	6.16	1.43	1.31
4	E	2003	A3P	C8-N7	6.13	1.43	1.31
4	A	2003	A3P	C8-N7	6.13	1.43	1.31
4	B	2003	A3P	C8-N7	6.10	1.43	1.31
4	F	2003	A3P	C8-N7	6.05	1.43	1.31

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2003	A3P	C5-C4-N3	-5.47	119.18	126.72
4	C	2003	A3P	C5-C4-N3	-5.42	119.25	126.72
4	E	2003	A3P	C5-C4-N3	-5.36	119.34	126.72
4	D	2003	A3P	C5-C4-N3	-5.30	119.42	126.72
4	F	2003	A3P	C5-C4-N3	-5.08	119.72	126.72

There are no chirality outliers.

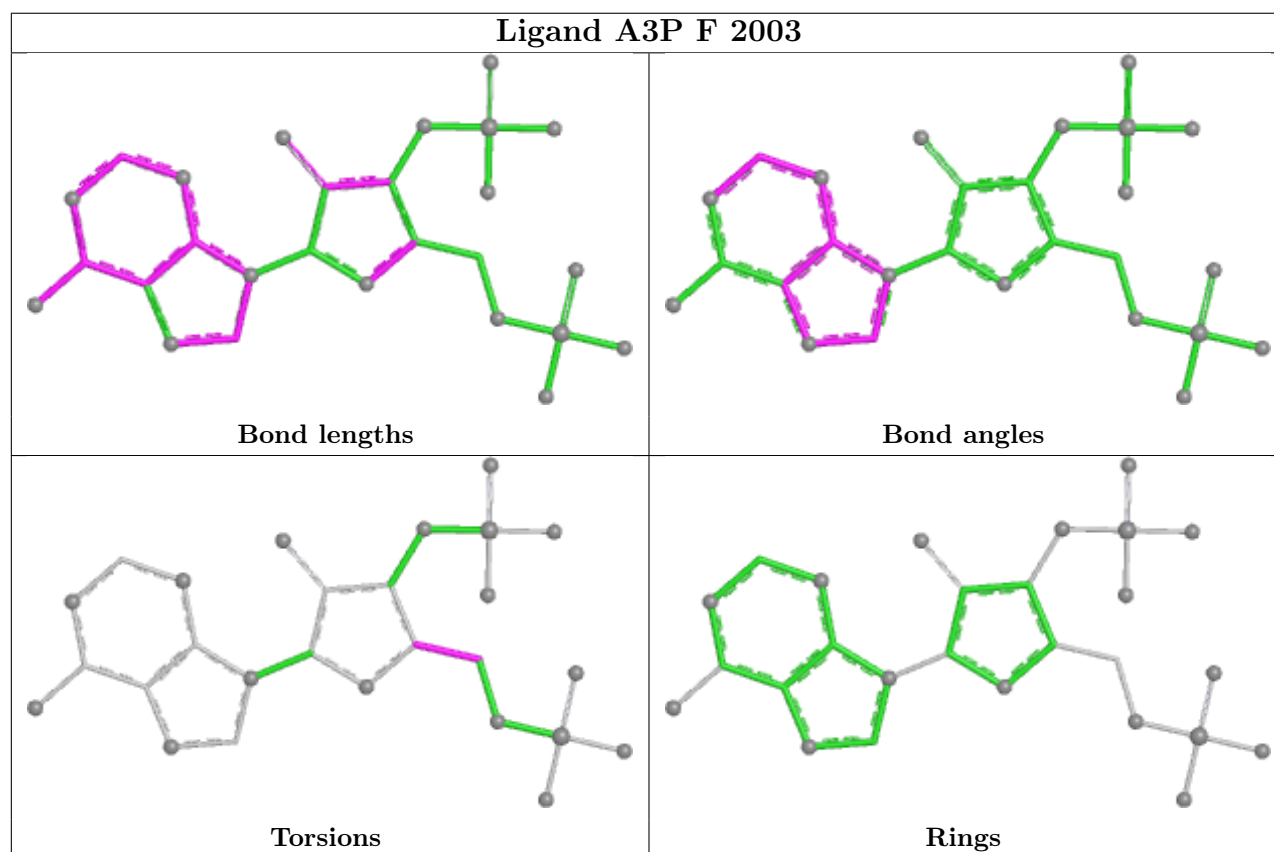
All (1) torsion outliers are listed below:

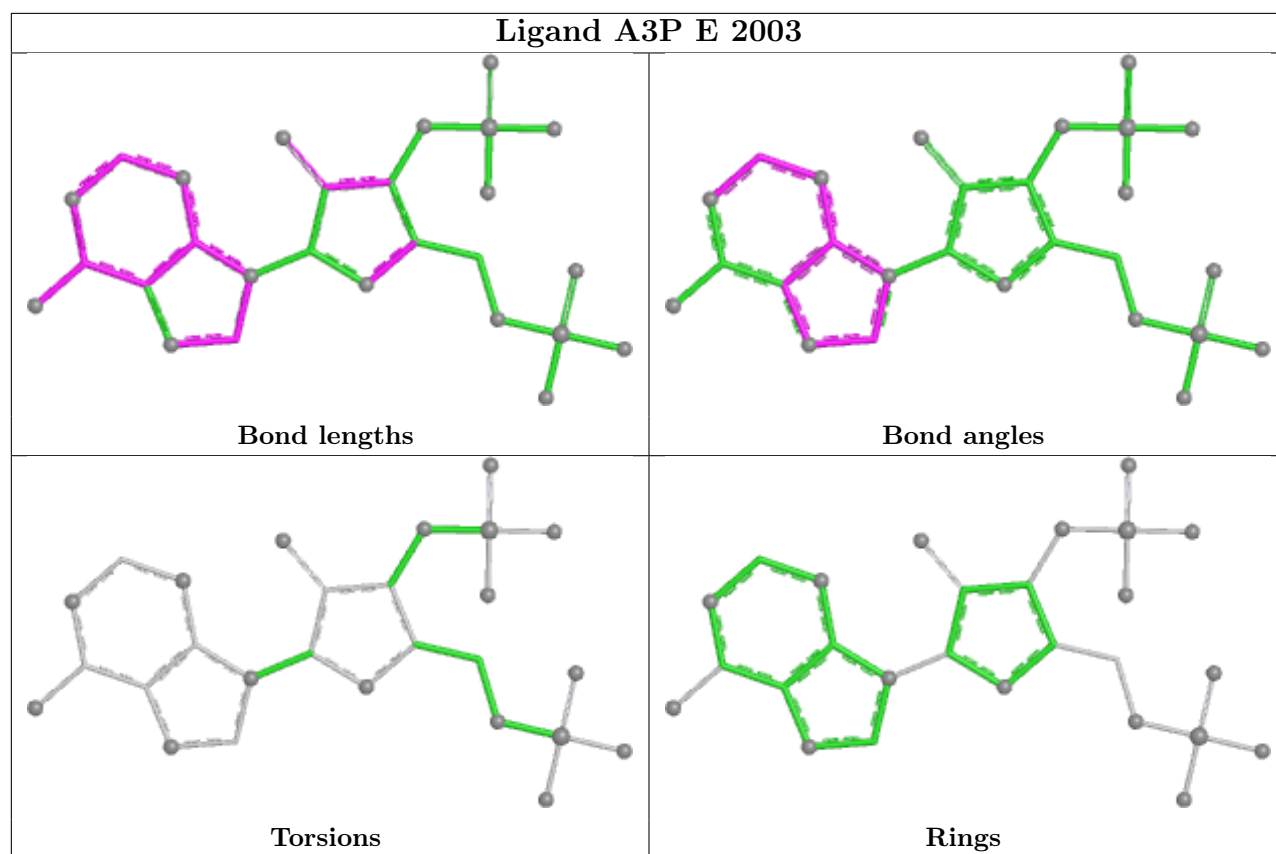
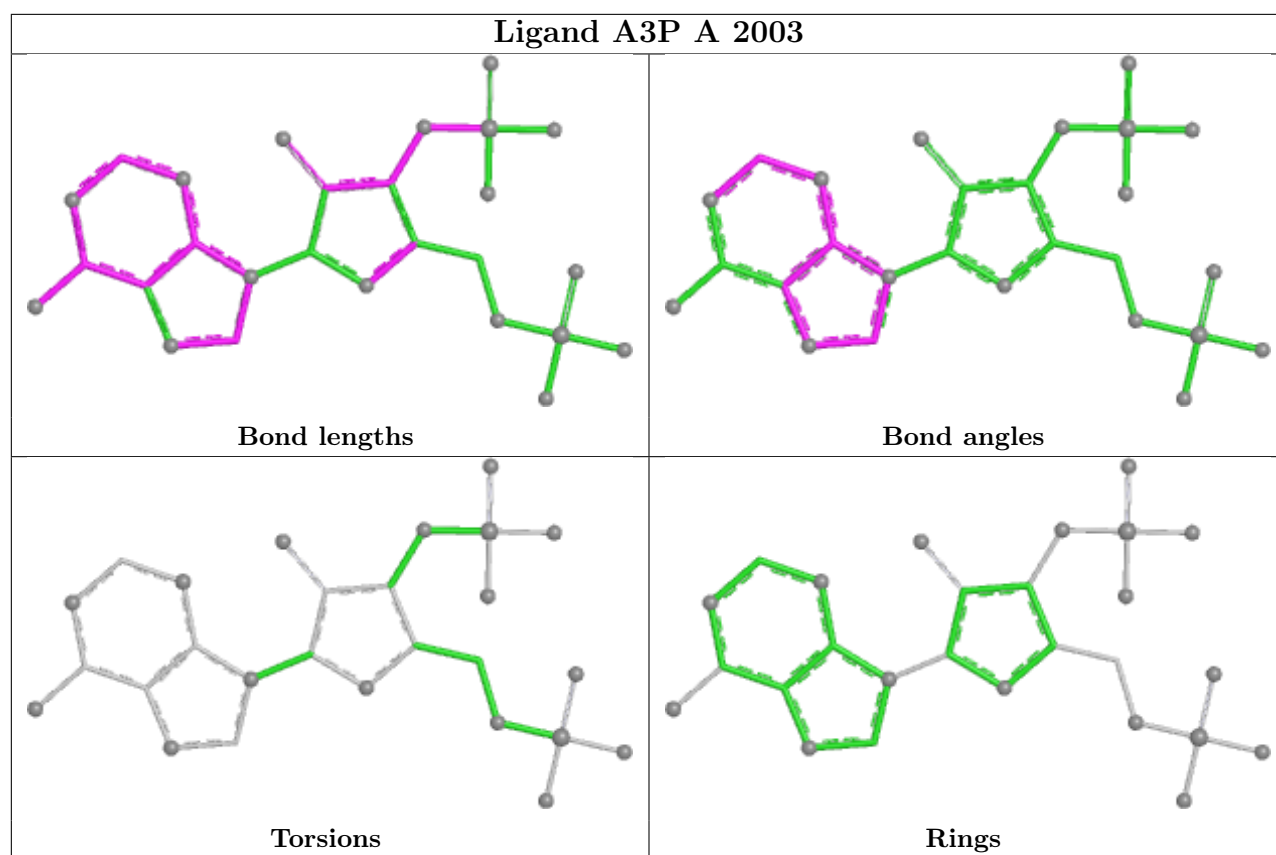
Mol	Chain	Res	Type	Atoms
4	F	2003	A3P	C3'-C4'-C5'-O5'

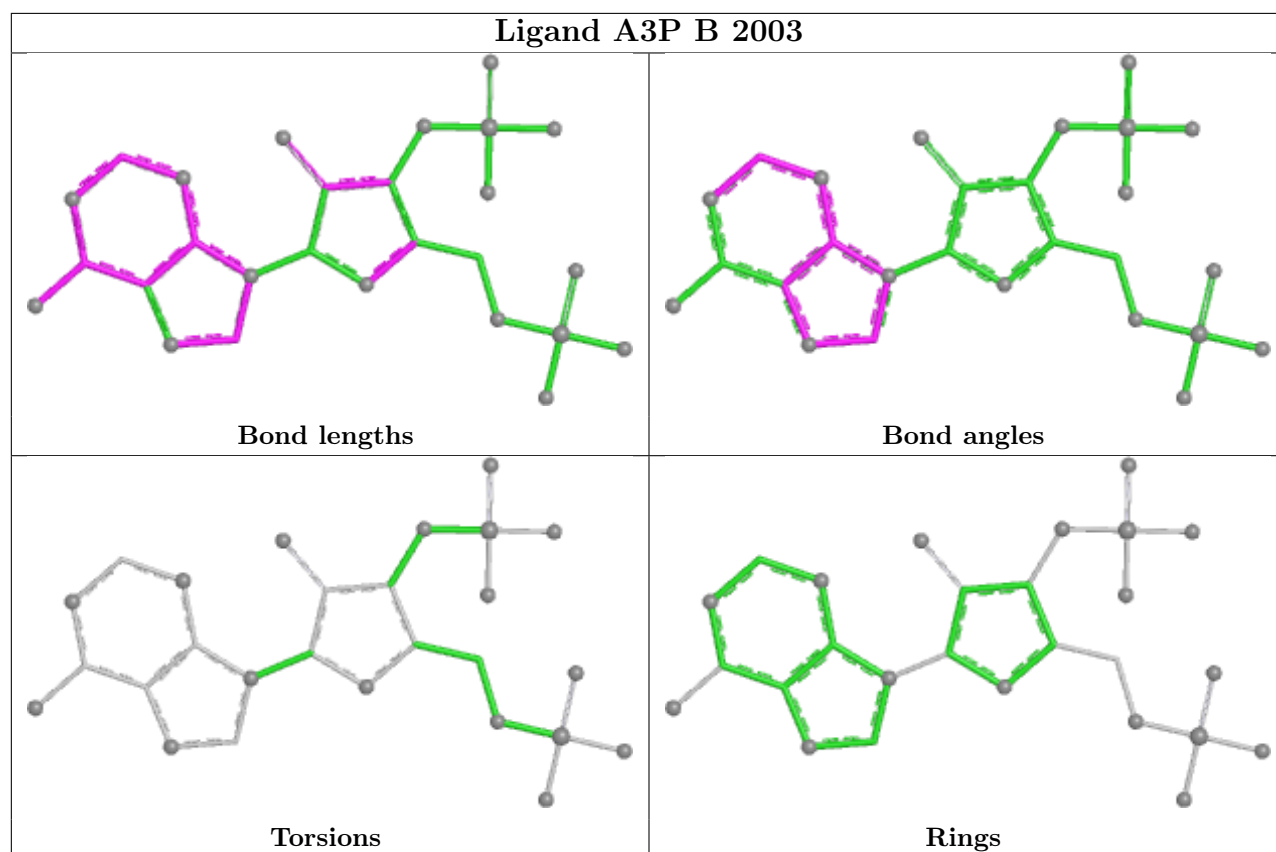
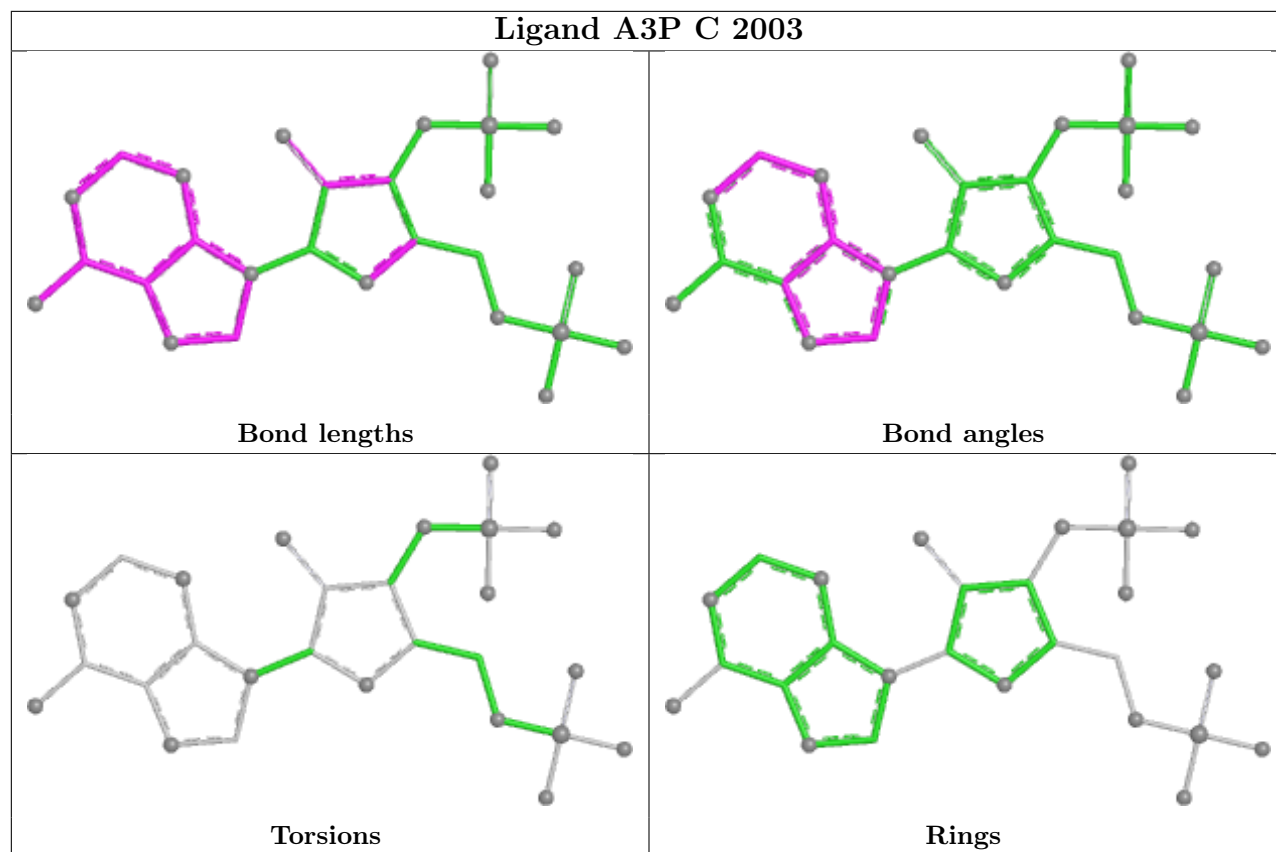
There are no ring outliers.

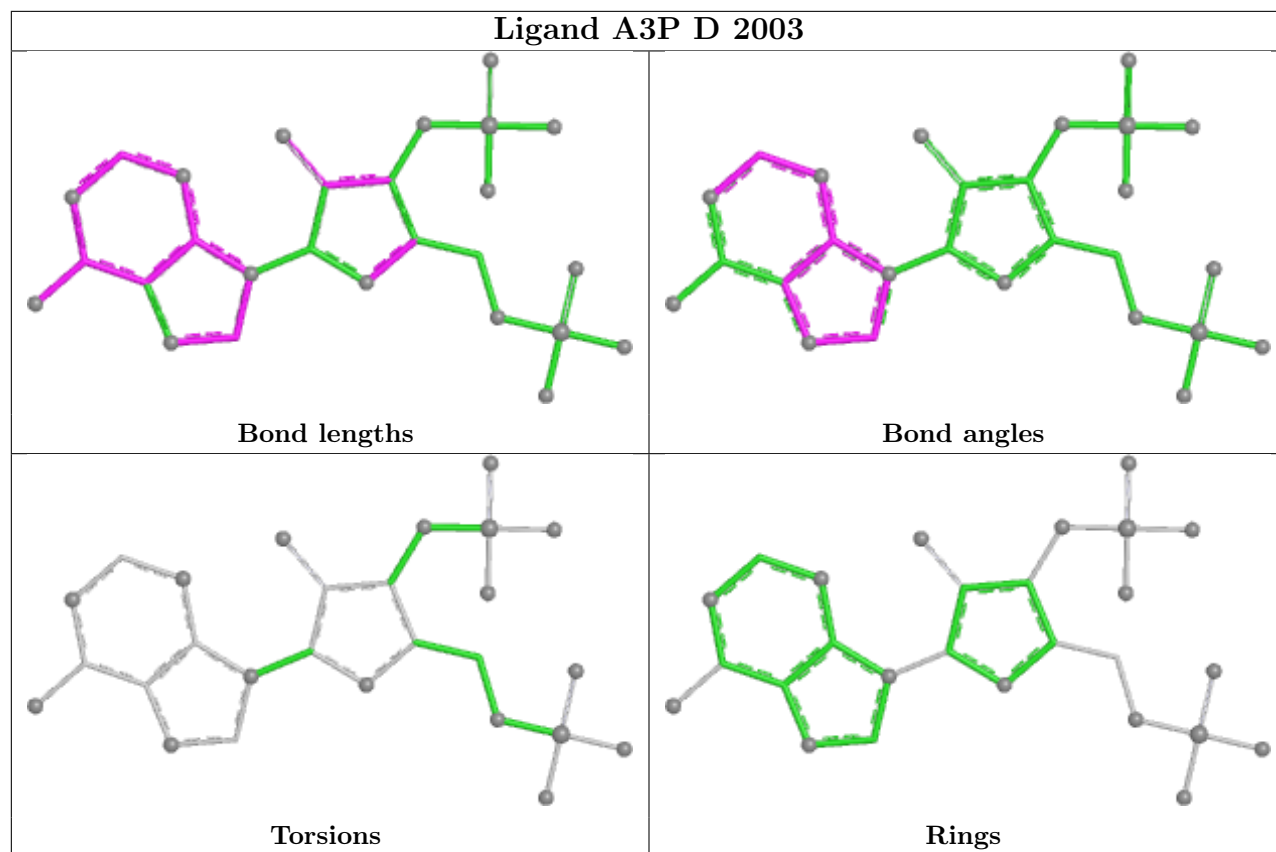
No monomer is involved in short contacts.

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.









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 [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	287/658 (43%)	-0.61	0 100 100	48, 83, 133, 185	0
1	B	654/658 (99%)	-0.21	15 (2%) 61 38	54, 196, 294, 399	0
1	C	655/658 (99%)	-0.49	1 (0%) 91 83	63, 129, 207, 293	0
1	D	654/658 (99%)	-0.52	1 (0%) 91 83	54, 128, 195, 252	0
1	E	654/658 (99%)	-0.58	1 (0%) 91 83	58, 122, 191, 274	0
1	F	654/658 (99%)	-0.48	1 (0%) 91 83	39, 170, 263, 333	1 (0%)
All	All	3558/3948 (90%)	-0.47	19 (0%) 87 70	39, 127, 250, 399	1 (0%)

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	1355	SER	4.6
1	B	11	ILE	4.0
1	B	1355	SER	3.7
1	B	226	ILE	3.3
1	D	1355	SER	2.9

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.

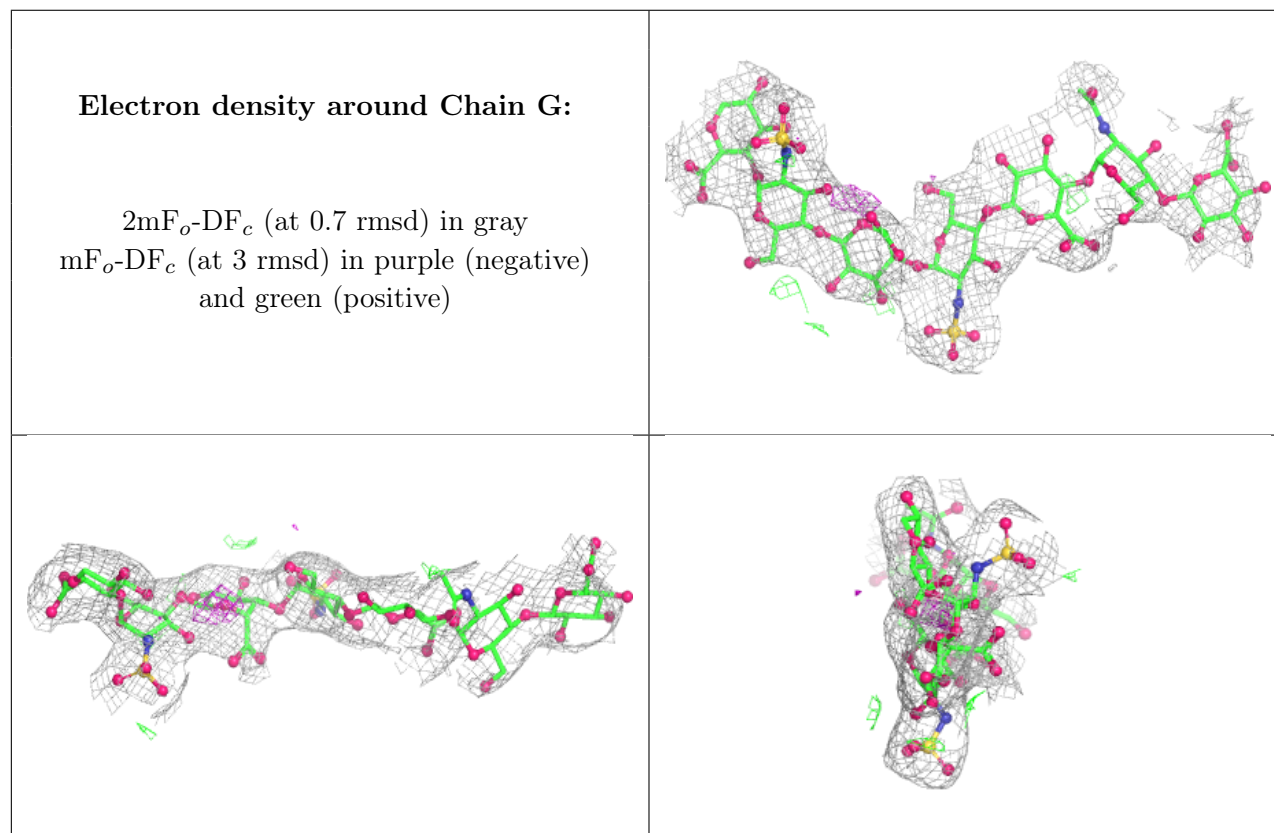
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GLC	H	1	12/12	0.32	0.15	197,218,230,239	0
2	NDG	P	6	14/15	0.53	0.09	145,173,202,210	0
2	BDP	N	7	12/13	0.55	0.08	186,205,213,218	0
2	BDP	P	5	12/13	0.60	0.09	136,206,212,214	0
2	BDP	P	7	12/13	0.69	0.07	195,218,230,230	0
2	BDP	P	1	13/13	0.72	0.10	120,143,173,179	0
2	BDP	G	7	12/13	0.73	0.08	179,197,225,229	0
2	BDP	N	5	12/13	0.75	0.09	145,194,213,217	0
3	GLC	O	1	12/12	0.75	0.08	165,176,181,186	0
2	BDP	N	1	12/13	0.76	0.09	146,191,216,218	0
2	BDP	I	5	12/13	0.76	0.08	108,137,152,153	0
3	GLC	H	2	11/12	0.76	0.09	218,235,256,257	0
2	BDP	L	7	12/13	0.76	0.09	172,199,213,219	0
2	NDG	N	6	14/15	0.79	0.07	139,188,202,212	0
2	BDP	I	7	12/13	0.80	0.06	148,161,172,176	0
2	BDP	L	5	12/13	0.81	0.07	126,144,163,173	0
2	NDG	L	6	14/15	0.81	0.07	104,145,162,178	0
3	GLC	K	1	12/12	0.82	0.09	135,142,153,154	0
2	BDP	G	5	12/13	0.85	0.08	95,130,153,167	0
2	IDR	P	3	12/13	0.86	0.16	142,162,187,200	0
2	NDG	I	6	14/15	0.88	0.06	109,128,158,160	0
2	IDR	L	3	12/13	0.89	0.11	103,126,151,165	0
2	GNS	P	2	15/16	0.89	0.14	177,183,197,203	0
2	IDR	I	3	12/13	0.91	0.11	100,112,121,124	0
3	GLC	O	2	11/12	0.91	0.06	149,166,181,185	0
2	GNS	N	4	15/16	0.93	0.08	123,144,168,187	0
2	IDR	G	3	12/13	0.93	0.10	68,88,103,113	0
2	NDG	G	6	14/15	0.93	0.05	107,132,150,170	0
3	GLC	K	2	11/12	0.93	0.06	92,109,127,127	0
3	GLC	M	1	12/12	0.93	0.09	88,98,112,113	0
2	GNS	N	2	15/16	0.93	0.09	150,164,191,196	0
2	IDR	N	3	12/13	0.93	0.10	128,148,209,213	0
2	BDP	I	1	12/13	0.94	0.08	77,94,107,109	0
2	BDP	L	1	12/13	0.94	0.06	103,127,150,155	0
3	GLC	J	1	12/12	0.94	0.08	95,124,137,149	0
2	GNS	P	4	15/16	0.94	0.08	112,150,186,198	0
3	GLC	M	2	11/12	0.96	0.06	79,95,124,133	0
2	BDP	G	1	12/13	0.96	0.07	68,93,105,108	0
2	GNS	L	2	15/16	0.96	0.09	100,120,139,152	0
2	GNS	G	2	15/16	0.97	0.07	63,75,99,100	0
2	GNS	L	4	15/16	0.97	0.06	88,117,142,145	0
3	GLC	J	2	11/12	0.97	0.04	93,97,110,112	0
2	GNS	I	2	15/16	0.98	0.05	84,89,108,118	0

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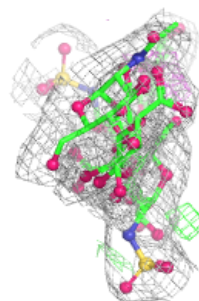
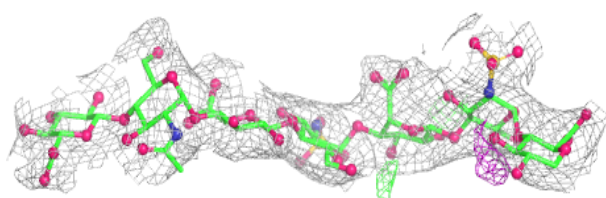
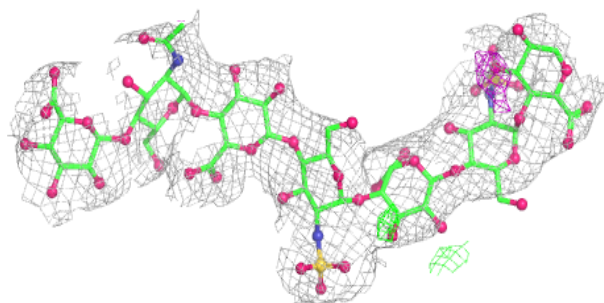
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GNS	I	4	15/16	0.98	0.05	79,93,110,133	0
2	GNS	G	4	15/16	0.99	0.04	72,78,98,101	0

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.

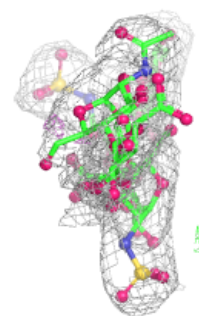
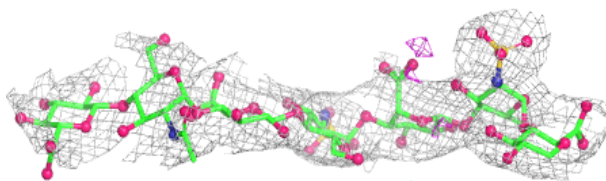
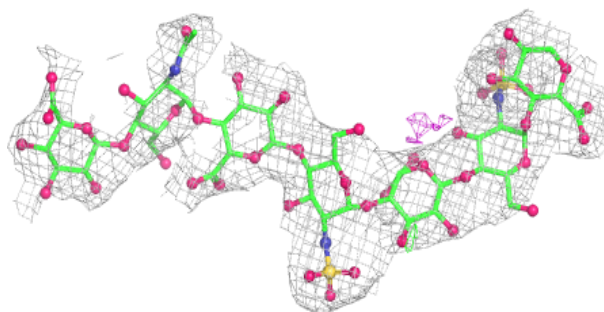


Electron density around Chain I:

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

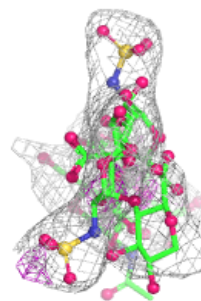
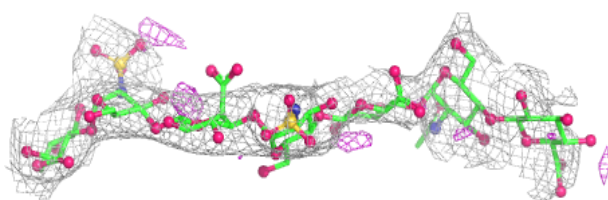
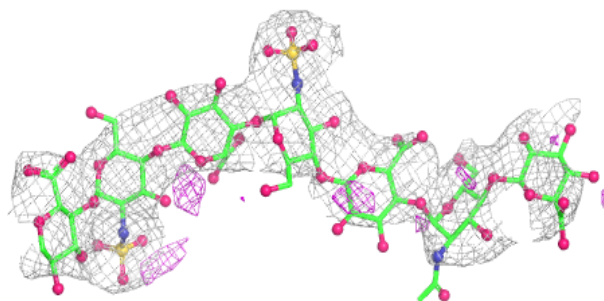
**Electron density around Chain L:**

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

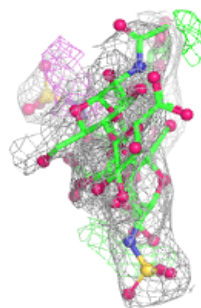
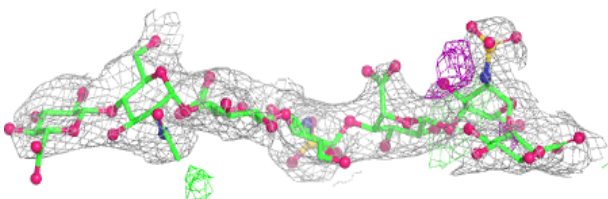
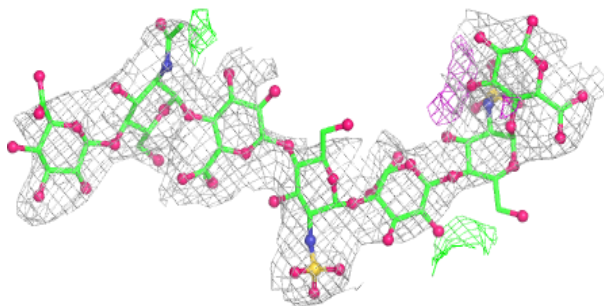


Electron density around Chain N:

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

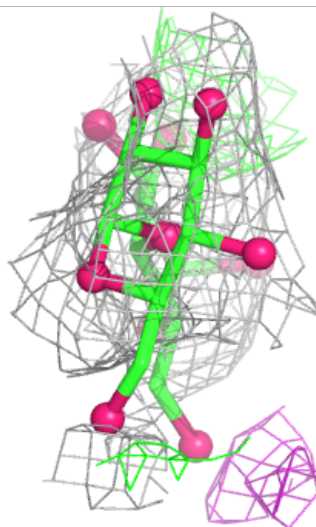
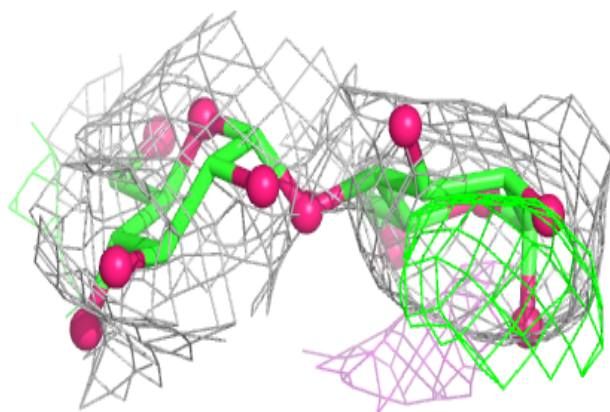
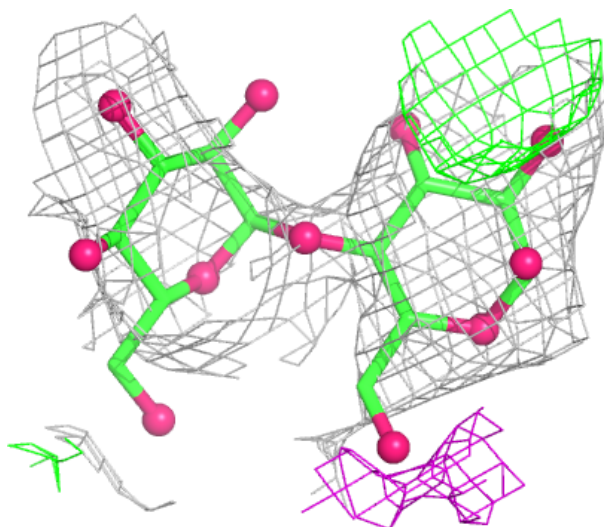
**Electron density around Chain P:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



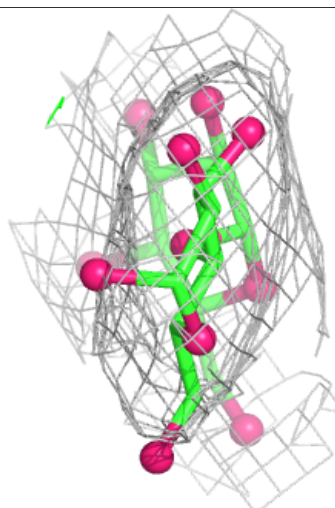
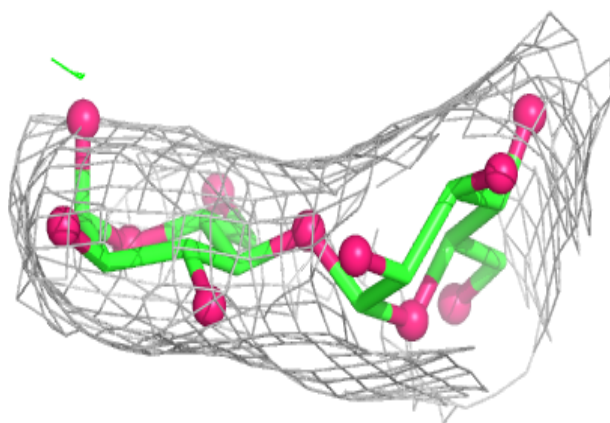
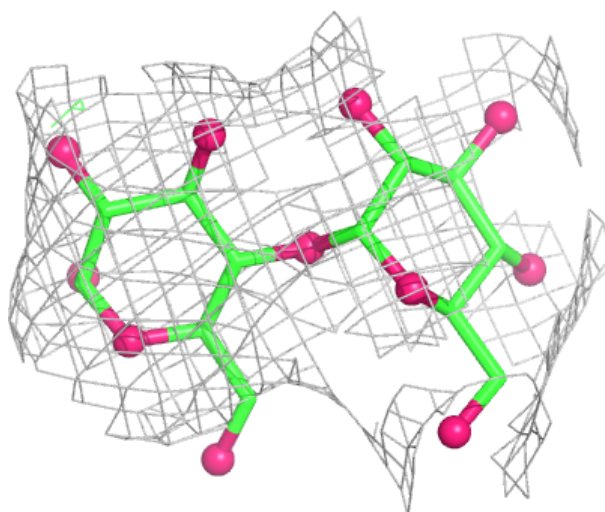
Electron density around Chain H:

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



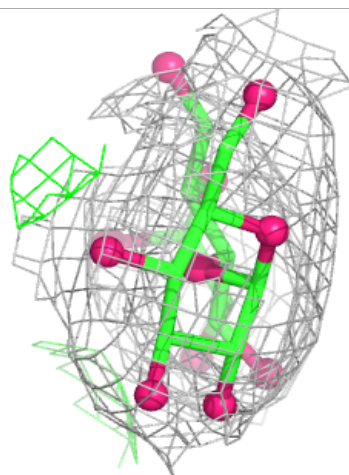
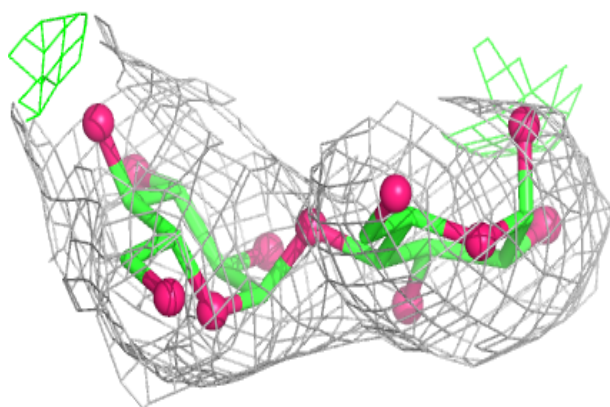
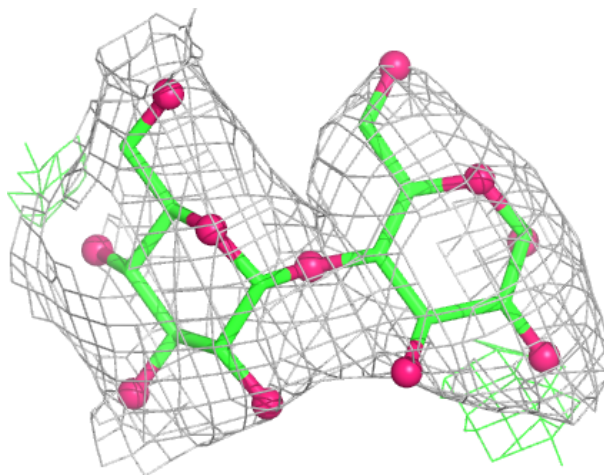
Electron density around Chain J:

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



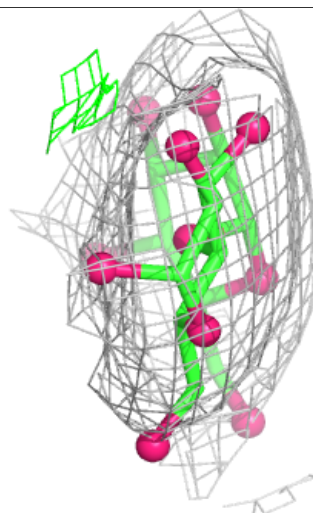
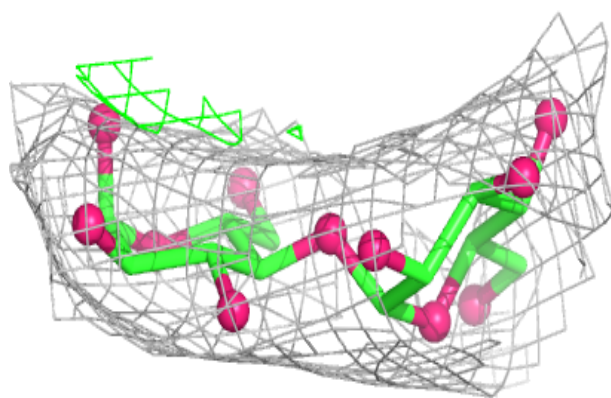
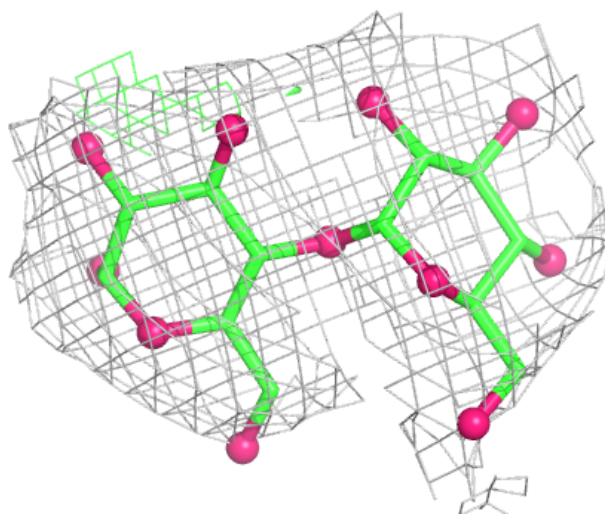
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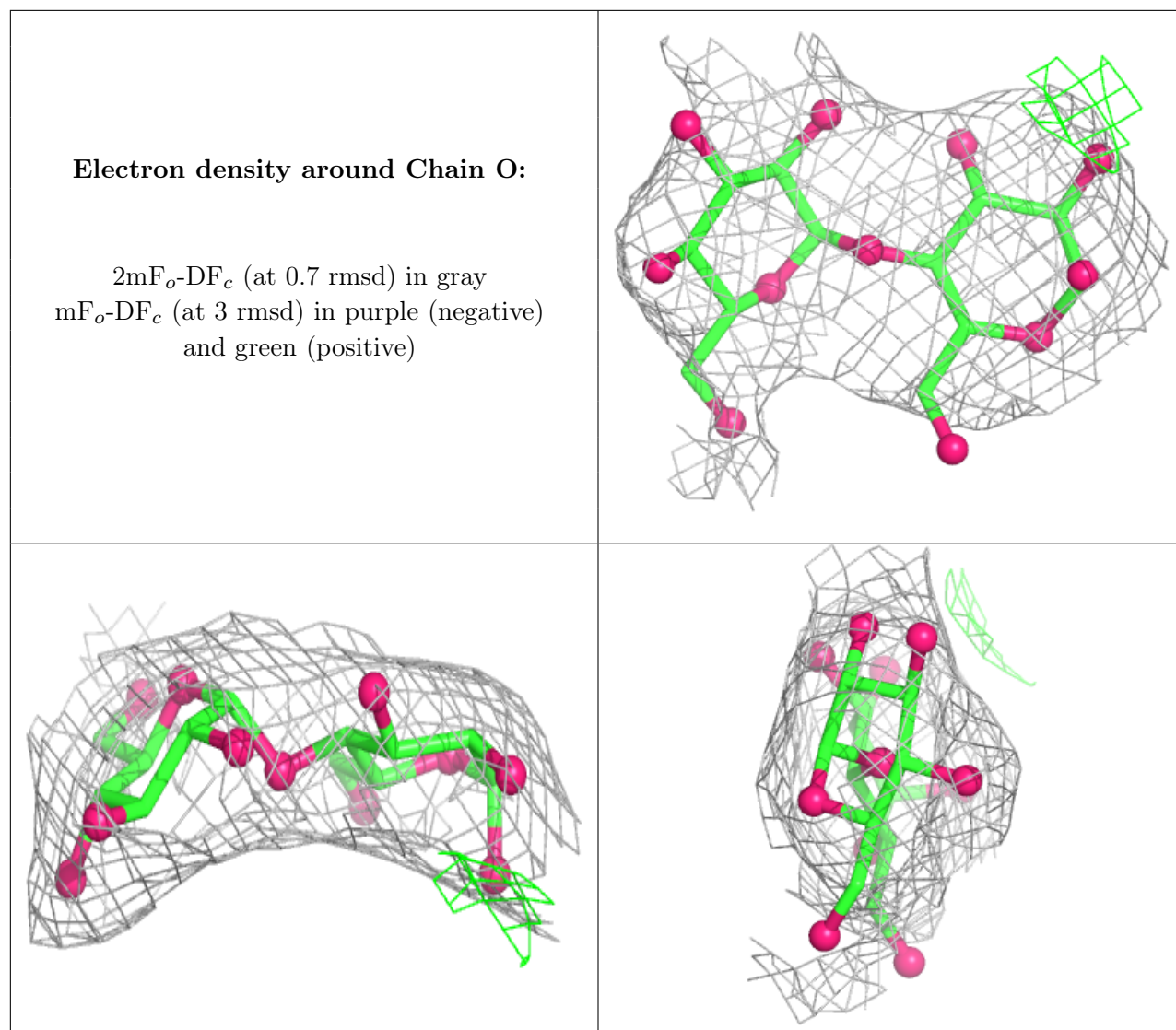
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain M:

$2mF_o-DF_c$ (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(Å ²)	Q<0.9
5	NPO	A	2011	10/10	0.85	0.09	103,138,146,154	0
5	NPO	E	2011	10/10	0.86	0.10	157,172,185,189	0
5	NPO	D	2011	10/10	0.93	0.07	159,170,199,200	0
5	NPO	B	2011	10/10	0.93	0.06	105,120,169,173	0
4	A3P	F	2003	27/27	0.95	0.06	67,89,104,115	0
4	A3P	C	2003	27/27	0.96	0.06	74,106,135,145	0
4	A3P	D	2003	27/27	0.96	0.06	57,83,108,112	0

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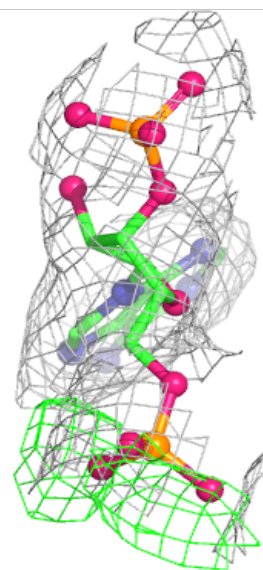
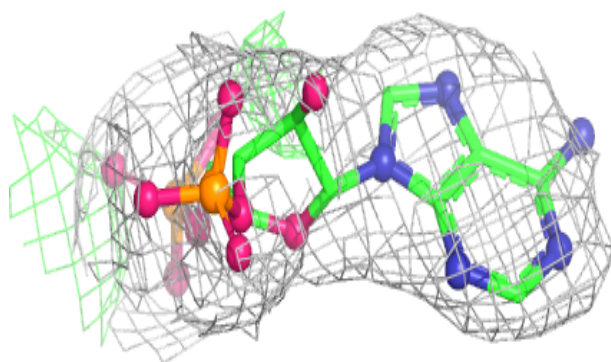
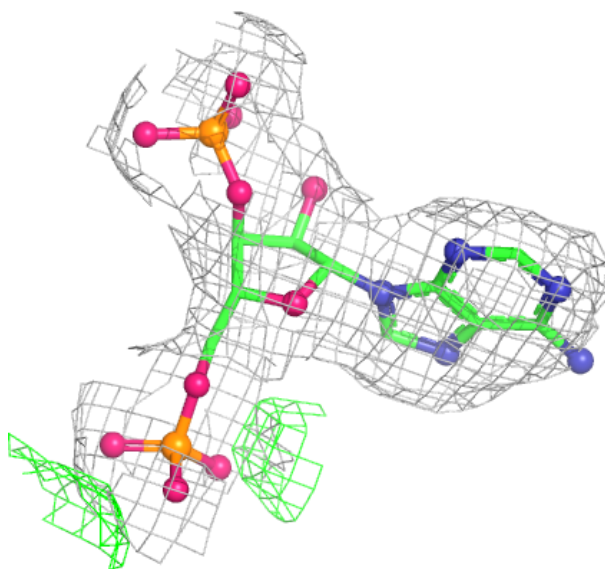
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	A3P	E	2003	27/27	0.96	0.06	80,104,114,119	0
4	A3P	B	2003	27/27	0.96	0.06	66,80,103,148	0
4	A3P	A	2003	27/27	0.97	0.06	53,68,87,93	0

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.

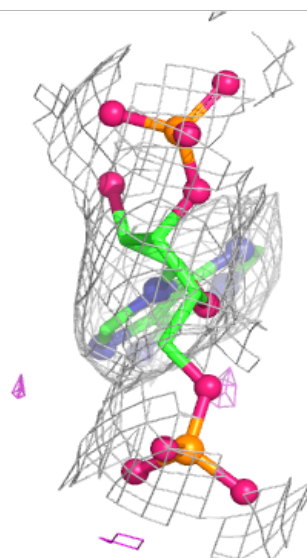
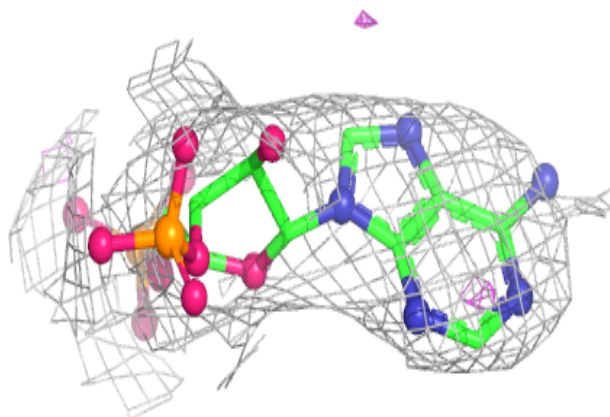
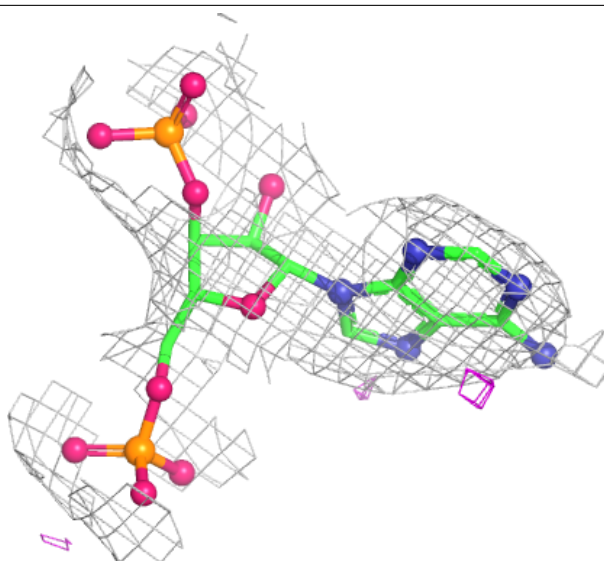
Electron density around A3P F 2003:

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



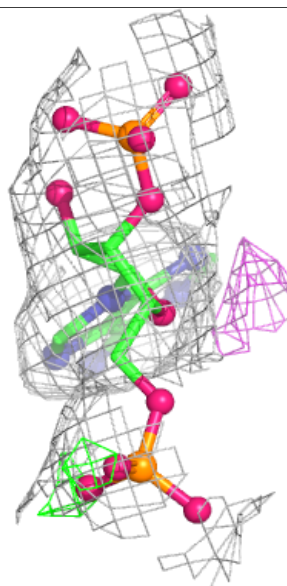
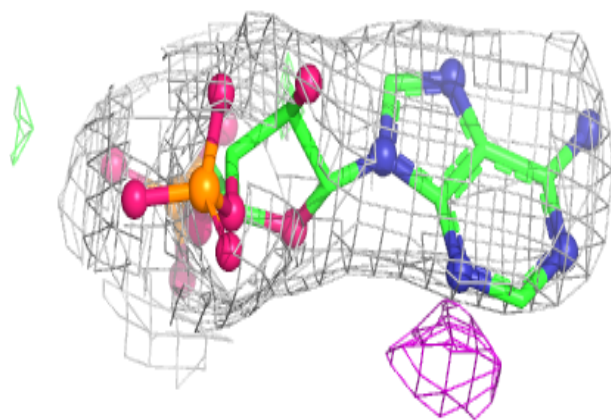
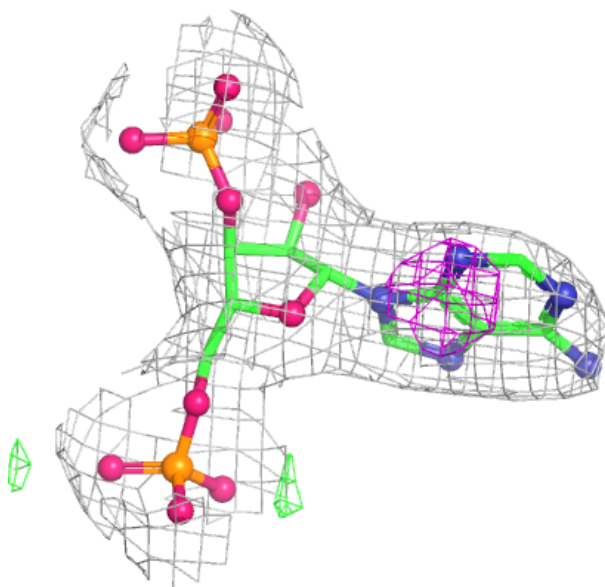
Electron density around A3P C 2003:

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and green (positive)



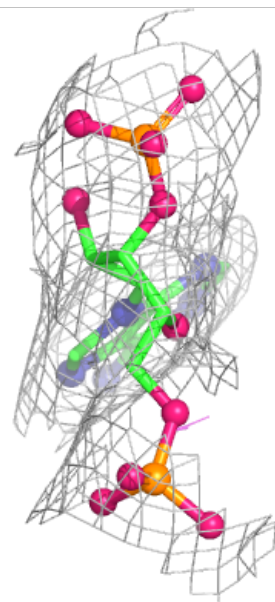
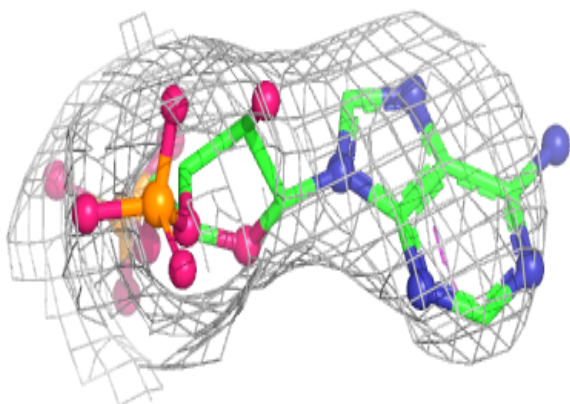
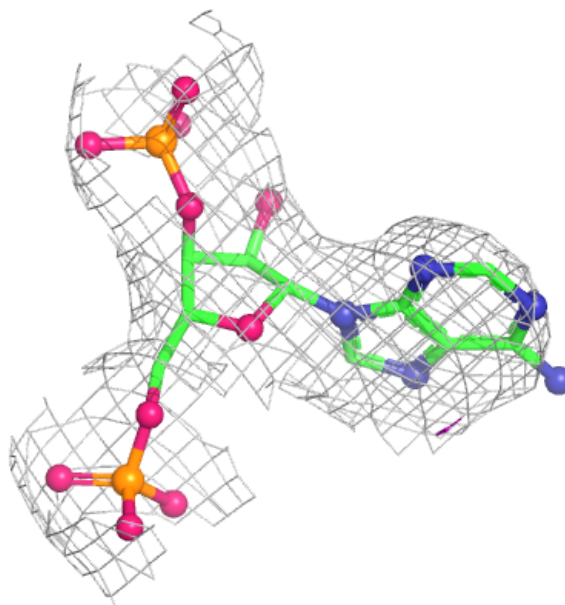
Electron density around A3P D 2003:

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



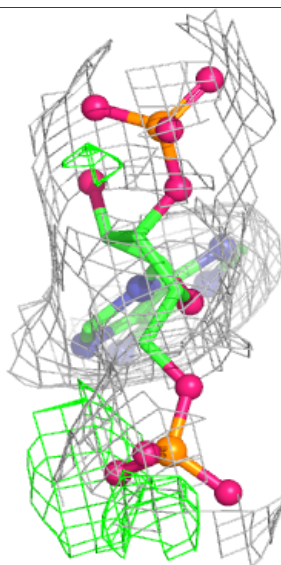
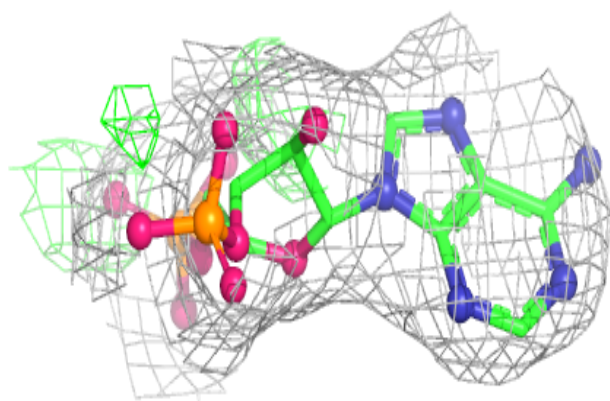
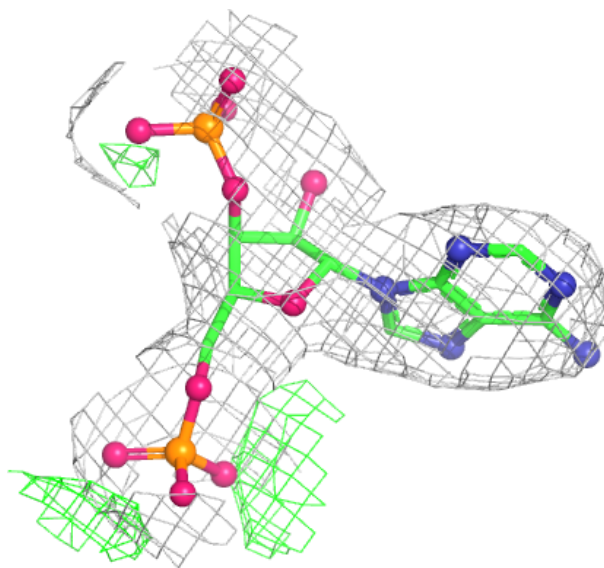
Electron density around A3P E 2003:

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



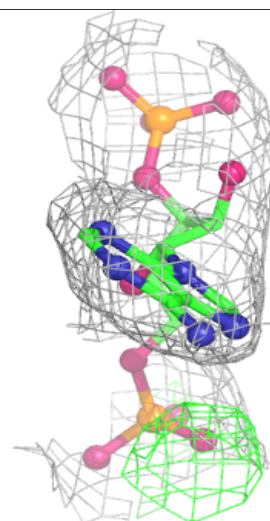
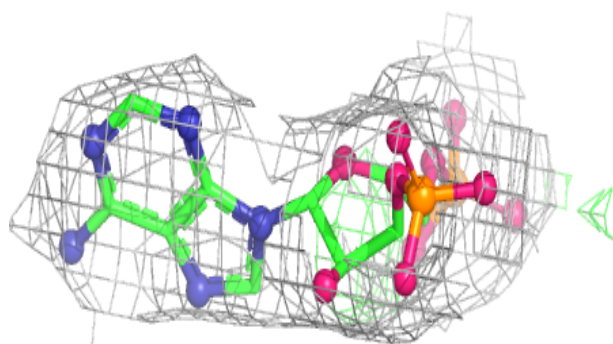
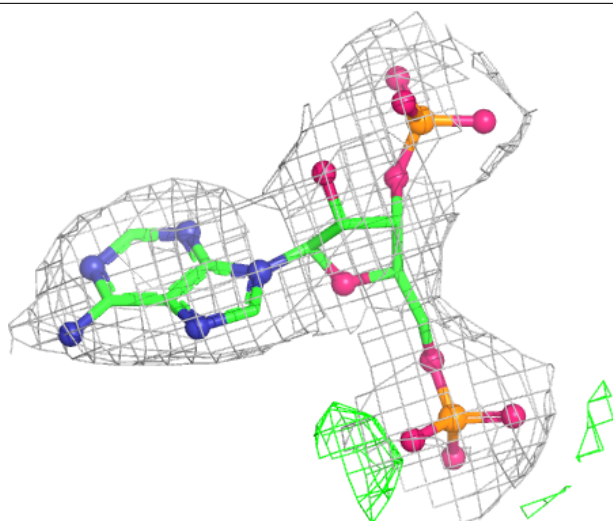
Electron density around A3P B 2003:

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



Electron density around A3P A 2003:

$2mF_o-DF_c$ (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.