



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 8, 2020 – 04:57 PM BST

PDB ID : 2HOX
Title : alliinase from allium sativum (garlic)
Authors : Shimon, L.J.W.; Rabinkov, A.; Wilcheck, M.; Mirelman, D.; Frolow, F.
Deposited on : 2006-07-17
Resolution : 1.40 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

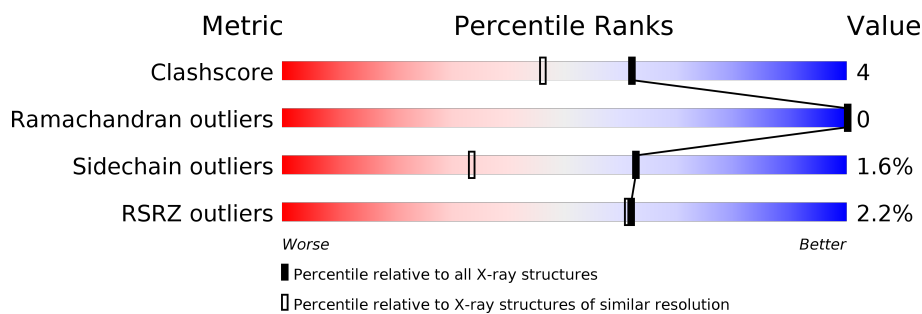
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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.



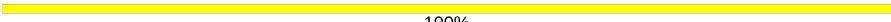
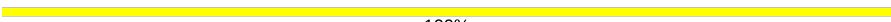
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)
RSRZ outliers	127900	1674 (1.40-1.40)

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 on 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	427	<div> <div>2%</div> <div>91%</div> <div>8%</div> </div>
1	B	427	<div> <div>2%</div> <div>93%</div> <div>6%</div> </div>
1	C	427	<div> <div>3%</div> <div>91%</div> <div>7%</div> </div>
1	D	427	<div> <div>2%</div> <div>91%</div> <div>9%</div> </div>
2	E	6	<div> <div>17%</div> <div>67%</div> <div>17%</div> </div>
3	F	2	<div> <div>50%</div> <div>50%</div> </div>
4	G	4	<div> <div>75%</div> <div>25%</div> </div>

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Mol	Chain	Length	Quality of chain
5	H	3	 100%
6	I	2	 100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	NAG	I	2	-	-	-	X
7	NAG	A	4500	X	-	-	-
7	NAG	A	507	-	-	-	X
7	NAG	B	503	-	-	-	X

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 16852 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.

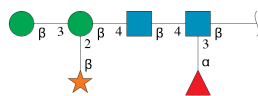
- Molecule 1 is a protein called Alliin lyase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	425	Total	C	N	O	S	0	1	0
			3436	2190	577	646	23			
1	B	427	Total	C	N	O	S	0	0	0
			3447	2197	582	645	23			
1	C	425	Total	C	N	O	S	0	1	0
			3445	2200	579	643	23			
1	D	427	Total	C	N	O	S	0	0	0
			3447	2197	582	645	23			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	176	ASP	ASN	SEE REMARK 999	UNP Q01594
B	176	ASP	ASN	SEE REMARK 999	UNP Q01594
C	176	ASP	ASN	SEE REMARK 999	UNP Q01594
D	176	ASP	ASN	SEE REMARK 999	UNP Q01594

- Molecule 2 is an oligosaccharide called beta-D-xylopyranose-(1-2)-[beta-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose.



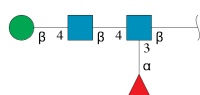
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	6	Total	C	N	O	0	0	0
			69	39	2	28			

- Molecule 3 is an oligosaccharide called alpha-L-fucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose.



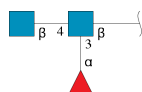
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	4	Total	C	N	O	0	0	0
			49	28	2	19			

- Molecule 5 is an oligosaccharide called alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose.



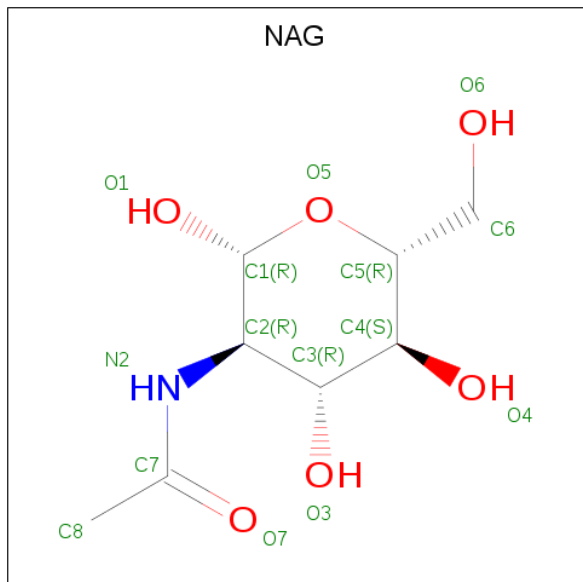
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	H	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 6 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
6	I	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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	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	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

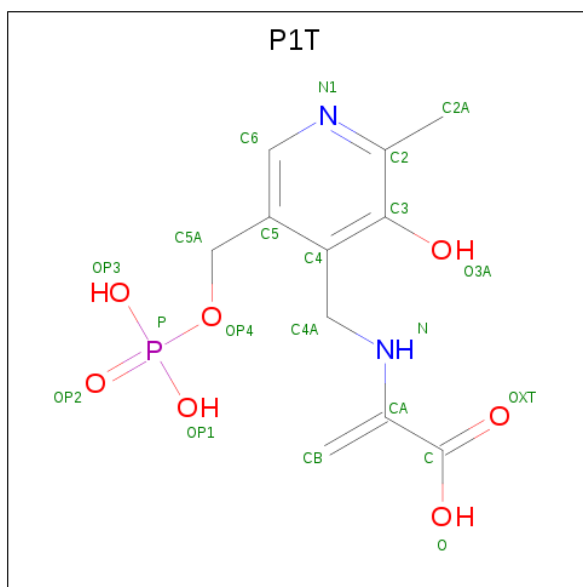
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Cl	0	0
			1	1		
8	A	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	D	1	Total Cl 1 1	0	0
8	C	1	Total Cl 1 1	0	0

- Molecule 9 is 2-[(3-HYDROXY-2-METHYL-5-[(PHOSPHONOOXY)METHYL]PYRIDIN-4-YL)METHYL)AMINO]ACRYLIC ACID (three-letter code: P1T) (formula: $C_{11}H_{15}N_2O_7P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C N O P 21 11 2 7 1	0	0
9	B	1	Total C N O P 21 11 2 7 1	0	0
9	C	1	Total C N O P 21 11 2 7 1	0	0
9	D	1	Total C N O P 21 11 2 7 1	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	752	Total O 752 752	0	0
10	B	685	Total O 685 685	0	0

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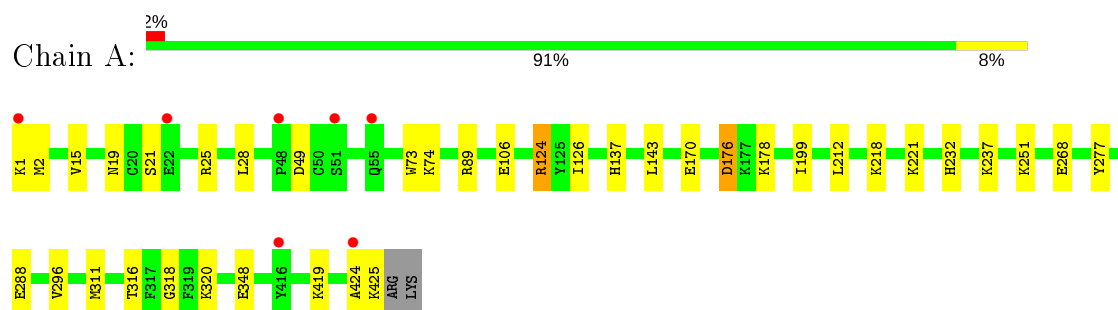
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	C	774	Total 774	O 774	0	0
10	D	458	Total 458	O 458	0	2

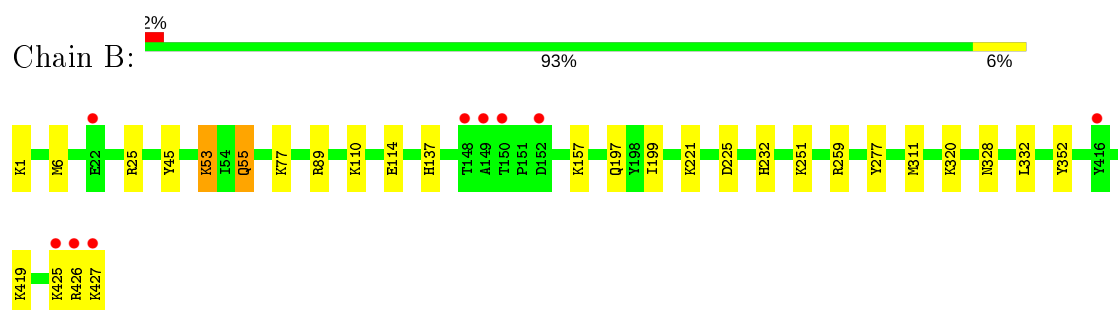
3 Residue-property plots [i](#)

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.

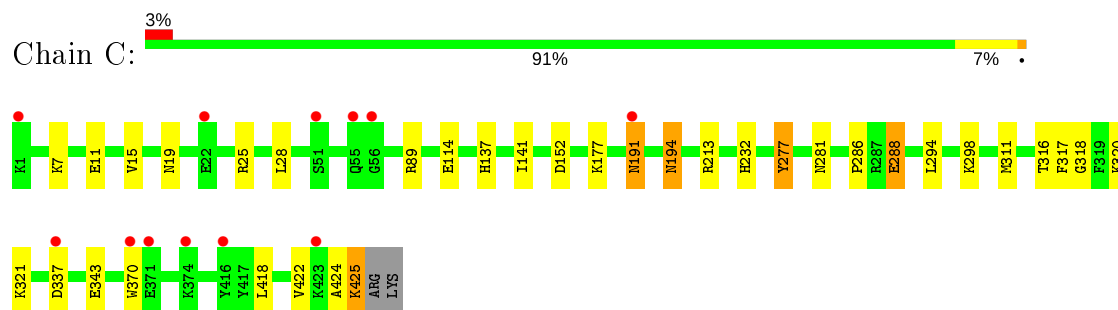
- Molecule 1: Alliin lyase 1



- Molecule 1: Alliin lyase 1

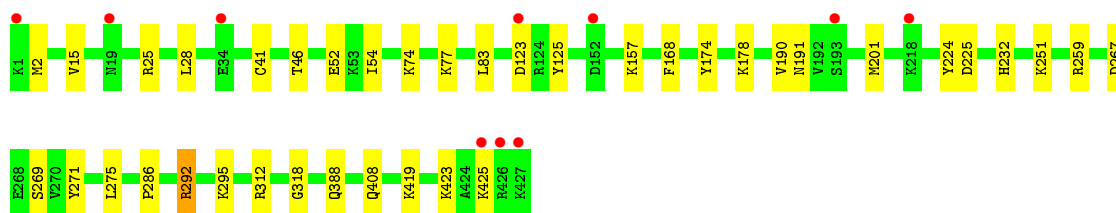


- Molecule 1: Alliin lyase 1



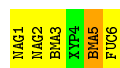
- Molecule 1: Alliin lyase 1





- Molecule 2: beta-D-xylopyranose-(1-2)-[beta-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 17% 67% 17%



- Molecule 3: alpha-L-fucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 50% 50%



- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G: 75% 25%



- Molecule 5: alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H: 100%



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I: 100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.67Å 126.89Å 102.66Å 90.00° 97.30° 90.00°	Depositor
Resolution (Å)	46.10 – 1.40 46.11 – 1.40	Depositor EDS
% Data completeness (in resolution range)	96.5 (46.10-1.40) 96.4 (46.11-1.40)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 1.39Å)	Xtriage
Refinement program	REFMAC 5.2.0013	Depositor
R, R_{free}	0.167 , 0.205 0.177 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	16.1	Xtriage
Anisotropy	0.132	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 52.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	16852	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% 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: XYP, BMA, NAG, CL, P1T, FUC

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	0.87	2/3525 (0.1%)	0.86	2/4772 (0.0%)
1	B	0.87	2/3536 (0.1%)	0.87	2/4785 (0.0%)
1	C	0.87	3/3543 (0.1%)	0.84	2/4793 (0.0%)
1	D	0.87	2/3536 (0.1%)	0.84	1/4785 (0.0%)
All	All	0.87	9/14140 (0.1%)	0.85	7/19135 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	224	TYR	CE2-CZ	-6.82	1.29	1.38
1	C	277	TYR	CE1-CZ	-6.80	1.29	1.38
1	A	277	TYR	CE1-CZ	-6.28	1.30	1.38
1	C	277	TYR	CD2-CE2	5.96	1.48	1.39
1	A	288	GLU	CB-CG	-5.71	1.41	1.52

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	259	ARG	NE-CZ-NH2	7.51	124.06	120.30
1	B	89	ARG	NE-CZ-NH2	-7.07	116.77	120.30
1	C	89	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	C	213	ARG	NE-CZ-NH2	-5.90	117.35	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	124	ARG	NE-CZ-NH2	-5.73	117.43	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	424	ALA	Peptide

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	3436	0	3325	28	0
1	B	3447	0	3347	19	0
1	C	3445	0	3360	40	0
1	D	3447	0	3347	31	0
2	E	69	0	51	2	0
3	F	24	0	22	0	0
4	G	49	0	43	1	0
5	H	38	0	34	0	0
6	I	28	0	25	0	0
7	A	42	0	39	1	0
7	B	42	0	39	4	0
7	C	28	0	26	1	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
9	A	21	0	11	2	0
9	B	21	0	11	3	0
9	C	21	0	11	0	0
9	D	21	0	12	4	0
10	A	752	0	0	14	1
10	B	685	0	0	7	2
10	C	774	0	0	17	1
10	D	458	0	0	11	0
All	All	16852	0	13703	123	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 4.

The worst 5 of 123 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:41:CYS:SG	10:D:6250:HOH:O	1.94	1.21
1:C:277:TYR:CE2	10:C:6486:HOH:O	1.98	1.12
1:C:277:TYR:CZ	10:C:6486:HOH:O	2.02	1.09
1:B:328:ASN:HD21	7:B:502:NAG:C1	1.78	0.95
1:B:137:HIS:HD2	10:B:6599:HOH:O	1.49	0.94

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)
10:B:6436:HOH:O	10:C:6361:HOH:O[1_455]	1.99	0.21
10:A:6664:HOH:O	10:B:6132:HOH:O[2_645]	2.11	0.09

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	424/427 (99%)	411 (97%)	13 (3%)	0	100	100
1	B	425/427 (100%)	413 (97%)	12 (3%)	0	100	100
1	C	426/427 (100%)	414 (97%)	12 (3%)	0	100	100
1	D	425/427 (100%)	412 (97%)	13 (3%)	0	100	100
All	All	1700/1708 (100%)	1650 (97%)	50 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	374/375 (100%)	369 (99%)	5 (1%)	69	42
1	B	375/375 (100%)	366 (98%)	9 (2%)	49	16
1	C	376/375 (100%)	369 (98%)	7 (2%)	57	25
1	D	375/375 (100%)	371 (99%)	4 (1%)	73	50
All	All	1500/1500 (100%)	1475 (98%)	25 (2%)	62	31

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	425	LYS
1	B	427	LYS
1	D	178	LYS
1	B	426	ARG
1	C	7	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	381	GLN
1	B	386	ASN
1	D	137	HIS
1	B	328	ASN
1	D	191	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

17 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	NAG	E	1	1,2	14,14,15	0.67	0	17,19,21	1.60	4 (23%)
2	NAG	E	2	2	14,14,15	0.39	0	17,19,21	1.17	2 (11%)
2	BMA	E	3	2	11,11,12	0.57	0	15,15,17	1.28	1 (6%)
2	XYP	E	4	2	9,9,10	0.81	0	10,12,14	0.85	0
2	BMA	E	5	2	11,11,12	0.94	1 (9%)	15,15,17	5.30	5 (33%)
2	FUC	E	6	2	10,10,11	0.53	0	14,14,16	1.47	3 (21%)
3	NAG	F	1	1,3	14,14,15	0.49	0	17,19,21	1.92	1 (5%)
3	FUC	F	2	3	10,10,11	0.33	0	14,14,16	0.53	0
4	NAG	G	1	1,4	14,14,15	0.72	0	17,19,21	1.12	1 (5%)
4	NAG	G	2	4	14,14,15	0.69	1 (7%)	17,19,21	1.61	5 (29%)
4	BMA	G	3	4	11,11,12	0.62	0	15,15,17	1.11	1 (6%)
4	FUC	G	4	4	10,10,11	0.54	0	14,14,16	1.28	2 (14%)
5	NAG	H	1	1,5	14,14,15	0.53	0	17,19,21	1.29	1 (5%)
5	FUC	H	2	5	10,10,11	0.41	0	14,14,16	0.85	1 (7%)
5	NAG	H	3	5	14,14,15	0.70	1 (7%)	17,19,21	0.76	0
6	NAG	I	1	1,6	14,14,15	0.71	0	17,19,21	1.16	2 (11%)
6	NAG	I	2	6	14,14,15	0.61	0	17,19,21	1.28	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	BMA	E	3	2	-	0/2/19/22	0/1/1/1
2	XYP	E	4	2	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BMA	E	5	2	-	0/2/19/22	0/1/1/1
2	FUC	E	6	2	-	-	0/1/1/1
3	NAG	F	1	1,3	-	2/6/23/26	0/1/1/1
3	FUC	F	2	3	-	-	0/1/1/1
4	NAG	G	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	BMA	G	3	4	-	2/2/19/22	0/1/1/1
4	FUC	G	4	4	-	-	0/1/1/1
5	NAG	H	1	1,5	-	0/6/23/26	0/1/1/1
5	FUC	H	2	5	-	-	0/1/1/1
5	NAG	H	3	5	-	0/6/23/26	0/1/1/1
6	NAG	I	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	I	2	6	-	1/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	5	BMA	O5-C1	-2.60	1.39	1.43
5	H	3	NAG	O5-C1	-2.21	1.40	1.43
4	G	2	NAG	O5-C1	-2.03	1.40	1.43

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	5	BMA	C1-C2-C3	-15.02	91.20	109.67
2	E	5	BMA	C1-O5-C5	-12.48	95.28	112.19
3	F	1	NAG	C1-O5-C5	6.80	121.41	112.19
2	E	5	BMA	O2-C2-C1	4.19	117.72	109.15
2	E	3	BMA	O3-C3-C4	-3.77	101.64	110.35

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

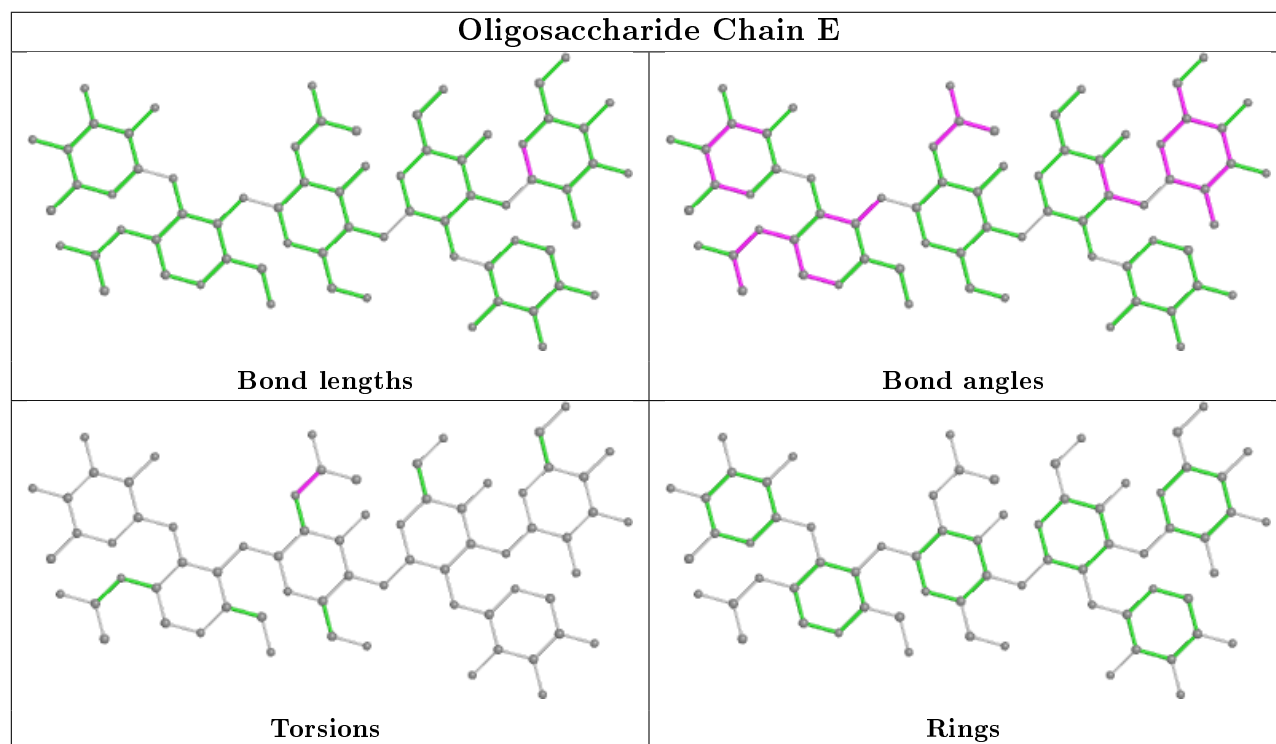
Mol	Chain	Res	Type	Atoms
4	G	3	BMA	O5-C5-C6-O6
4	G	2	NAG	C8-C7-N2-C2
4	G	3	BMA	C4-C5-C6-O6
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2

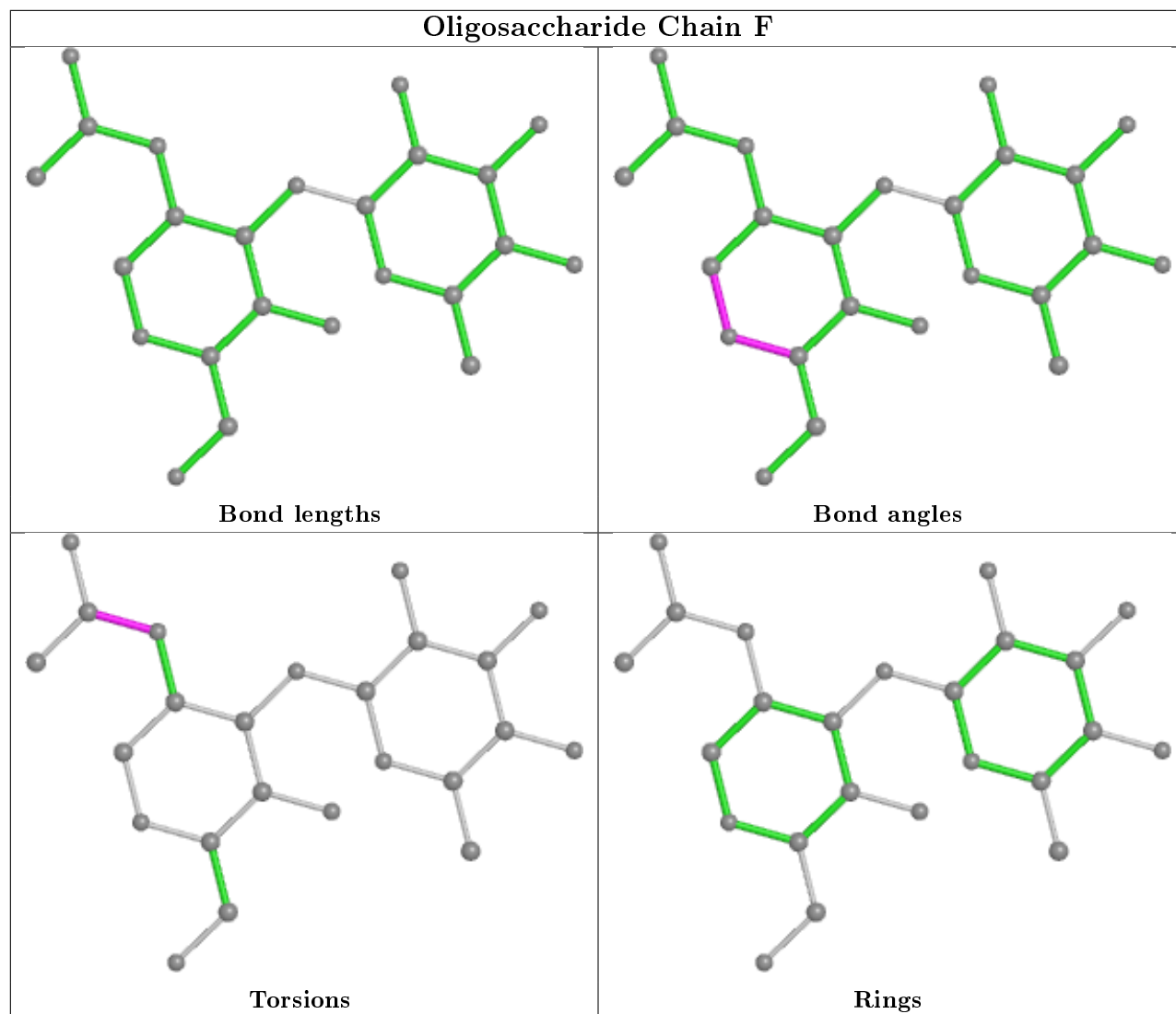
There are no ring outliers.

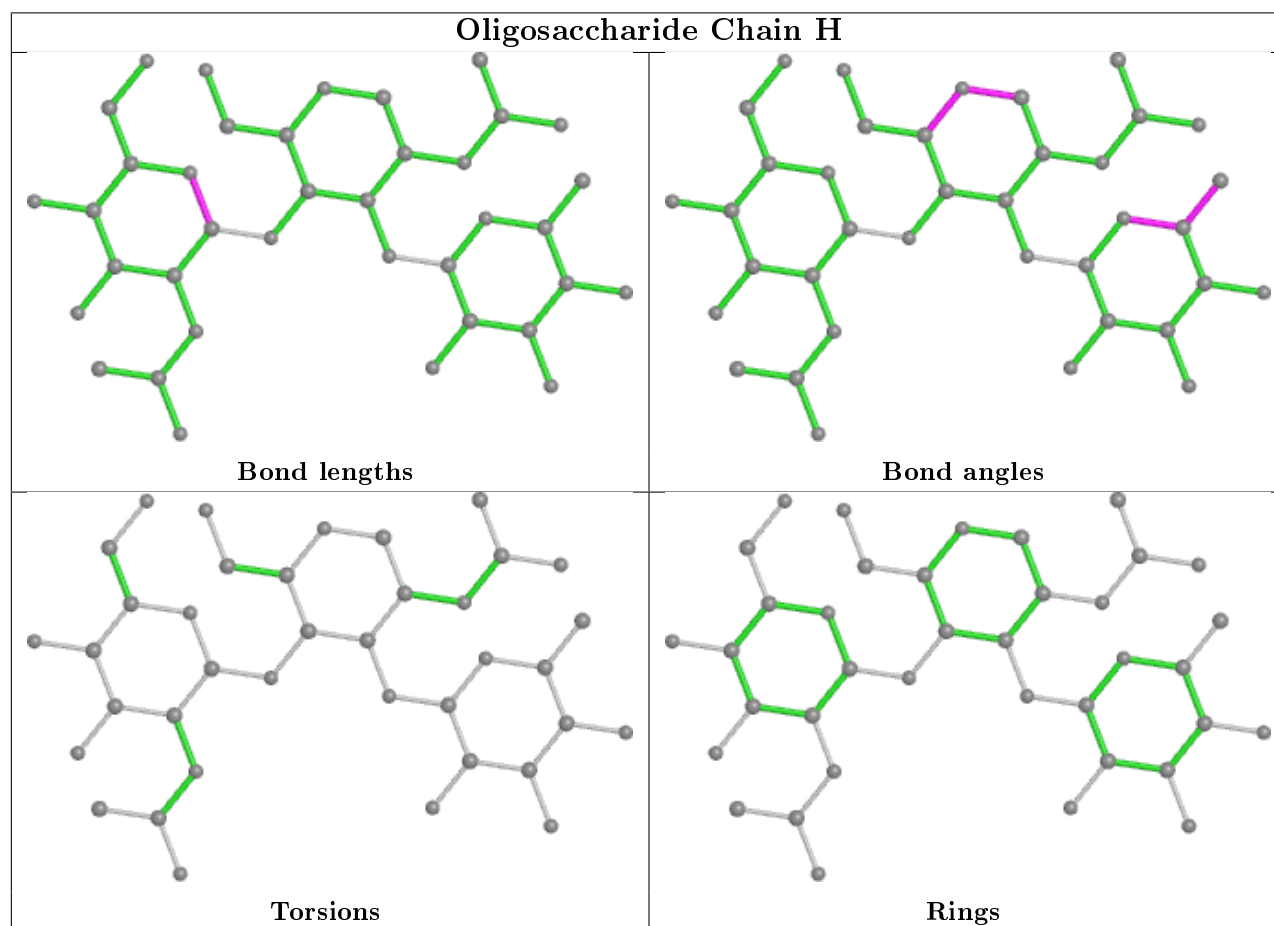
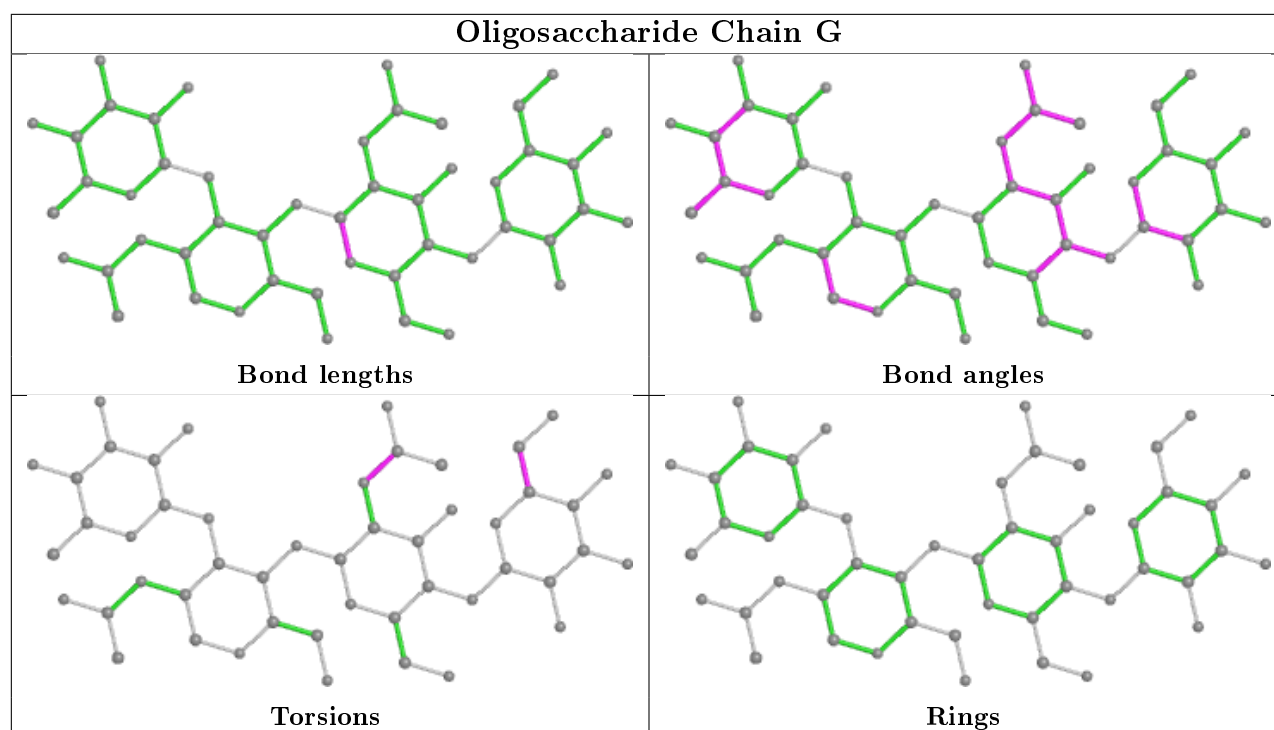
2 monomers are involved in 3 short contacts:

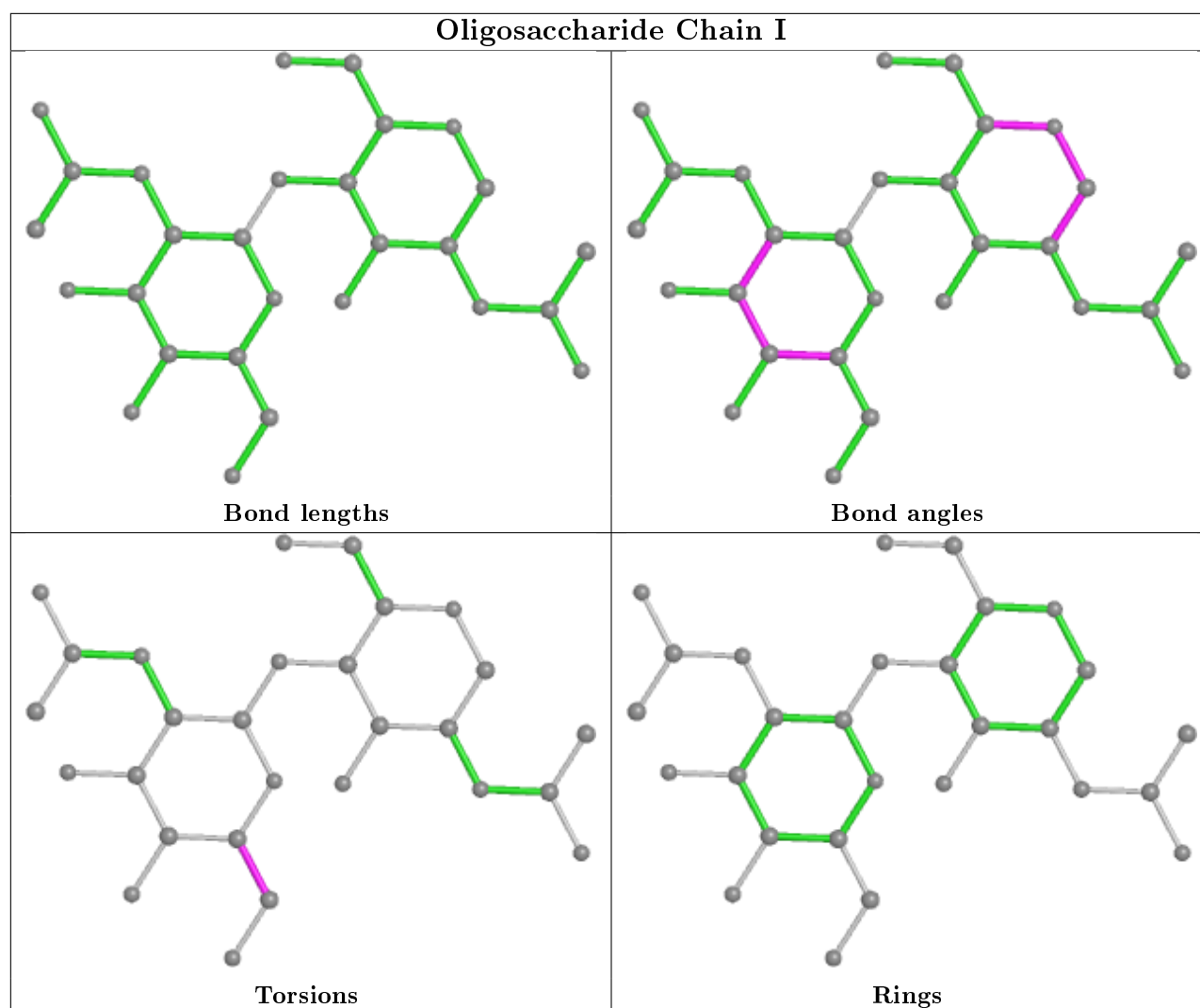
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	1	NAG	1	0
2	E	5	BMA	2	0

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 ⓘ

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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	506	1	14,14,15	0.46	0	17,19,21	0.76	0
7	NAG	B	3500	1	14,14,15	0.57	0	17,19,21	1.21	1 (5%)
7	NAG	C	505	-	14,14,15	0.70	0	17,19,21	1.53	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	P1T	B	6002	-	18,21,21	2.52	5 (27%)	23,30,30	2.23	7 (30%)
7	NAG	B	503	-	14,14,15	0.49	0	17,19,21	0.91	0
9	P1T	C	6003	-	18,21,21	2.69	5 (27%)	23,30,30	1.89	5 (21%)
7	NAG	A	4500	1	14,14,15	0.40	0	17,19,21	1.75	2 (11%)
7	NAG	C	504	1	14,14,15	0.52	0	17,19,21	0.96	0
7	NAG	A	507	-	14,14,15	0.48	0	17,19,21	1.31	2 (11%)
9	P1T	D	6004	-	18,21,21	2.53	3 (16%)	23,30,30	2.14	9 (39%)
7	NAG	B	502	-	14,14,15	0.54	0	17,19,21	1.52	3 (17%)
9	P1T	A	6001	-	18,21,21	2.41	5 (27%)	23,30,30	2.23	9 (39%)

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	506	1	-	0/6/23/26	0/1/1/1
7	NAG	B	3500	1	-	2/6/23/26	0/1/1/1
7	NAG	C	505	-	-	4/6/23/26	0/1/1/1
9	P1T	B	6002	-	-	3/10/15/15	0/1/1/1
7	NAG	B	503	-	-	4/6/23/26	0/1/1/1
9	P1T	C	6003	-	-	4/10/15/15	0/1/1/1
7	NAG	A	4500	1	1/1/5/7	2/6/23/26	0/1/1/1
7	NAG	C	504	1	-	0/6/23/26	0/1/1/1
7	NAG	A	507	-	-	3/6/23/26	0/1/1/1
9	P1T	D	6004	-	-	4/10/15/15	0/1/1/1
7	NAG	B	502	-	-	0/6/23/26	0/1/1/1
9	P1T	A	6001	-	-	6/10/15/15	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	6003	P1T	C4A-N	-8.57	1.29	1.46
9	A	6001	P1T	C4A-N	-8.56	1.29	1.46
9	D	6004	P1T	C4A-N	-8.29	1.29	1.46
9	B	6002	P1T	C4A-N	-7.94	1.30	1.46
9	C	6003	P1T	C3-C2	4.13	1.45	1.40

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	4500	NAG	C1-O5-C5	6.25	120.65	112.19
9	B	6002	P1T	C4A-C4-C5	5.29	125.59	119.71
9	D	6004	P1T	C6-C5-C4	4.56	121.35	118.12
9	A	6001	P1T	C4A-C4-C5	4.45	124.65	119.71
9	C	6003	P1T	C4-C4A-N	4.41	120.24	111.22

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	A	4500	NAG	C1

5 of 32 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	503	NAG	C8-C7-N2-C2
7	B	503	NAG	O7-C7-N2-C2
7	A	507	NAG	C8-C7-N2-C2
7	A	507	NAG	O7-C7-N2-C2
9	A	6001	P1T	C5A-OP4-P-OP3

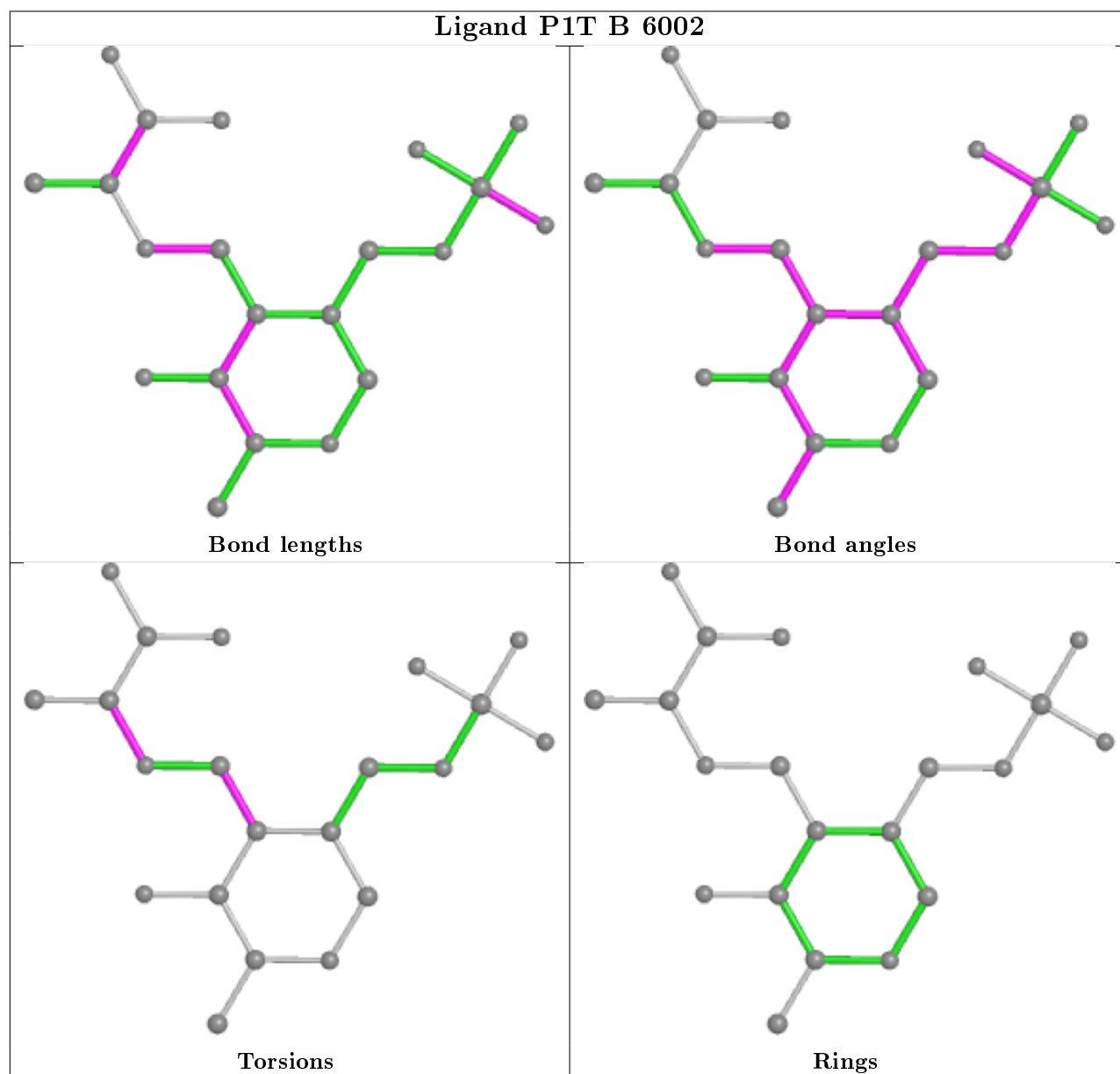
There are no ring outliers.

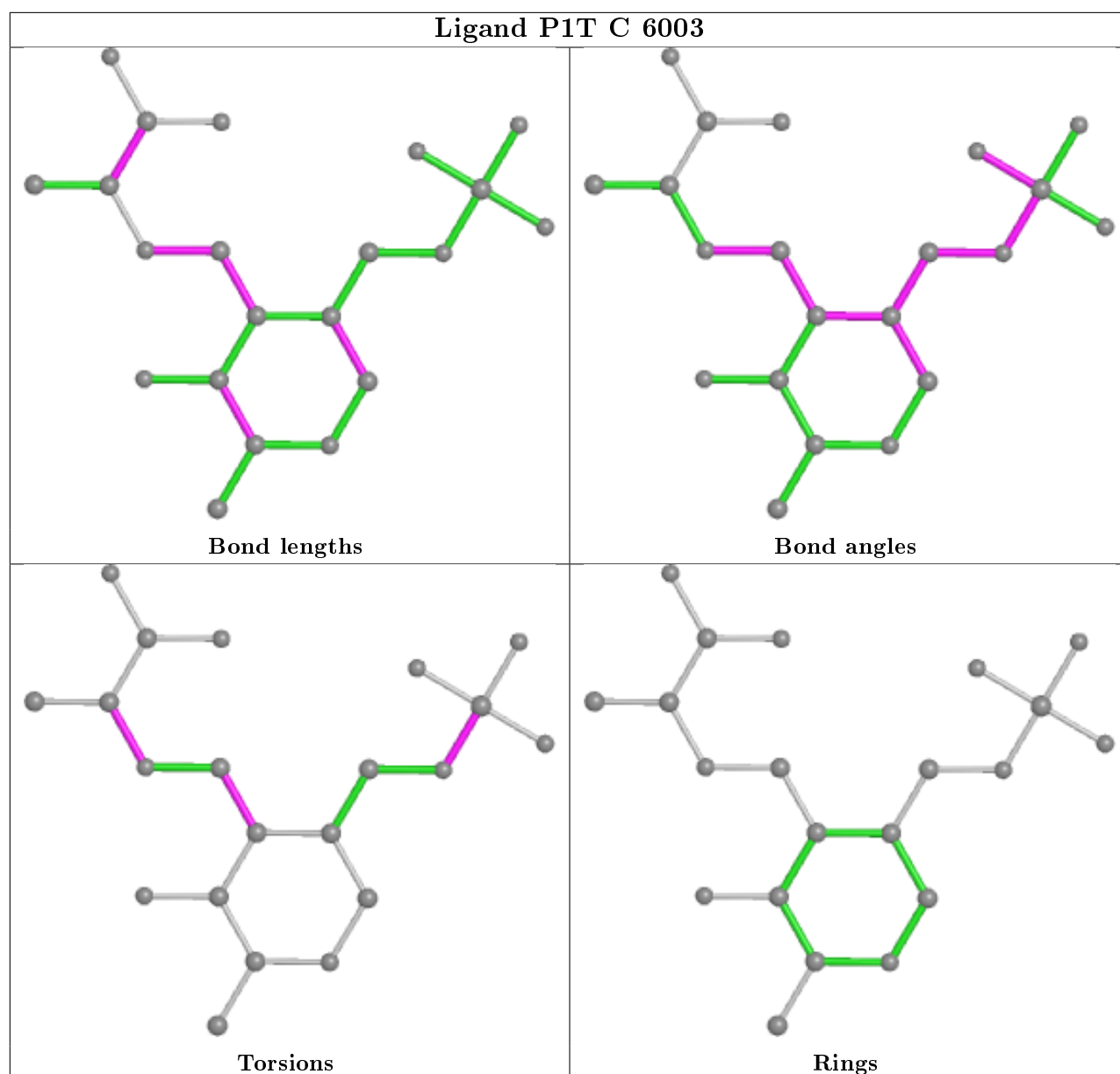
8 monomers are involved in 15 short contacts:

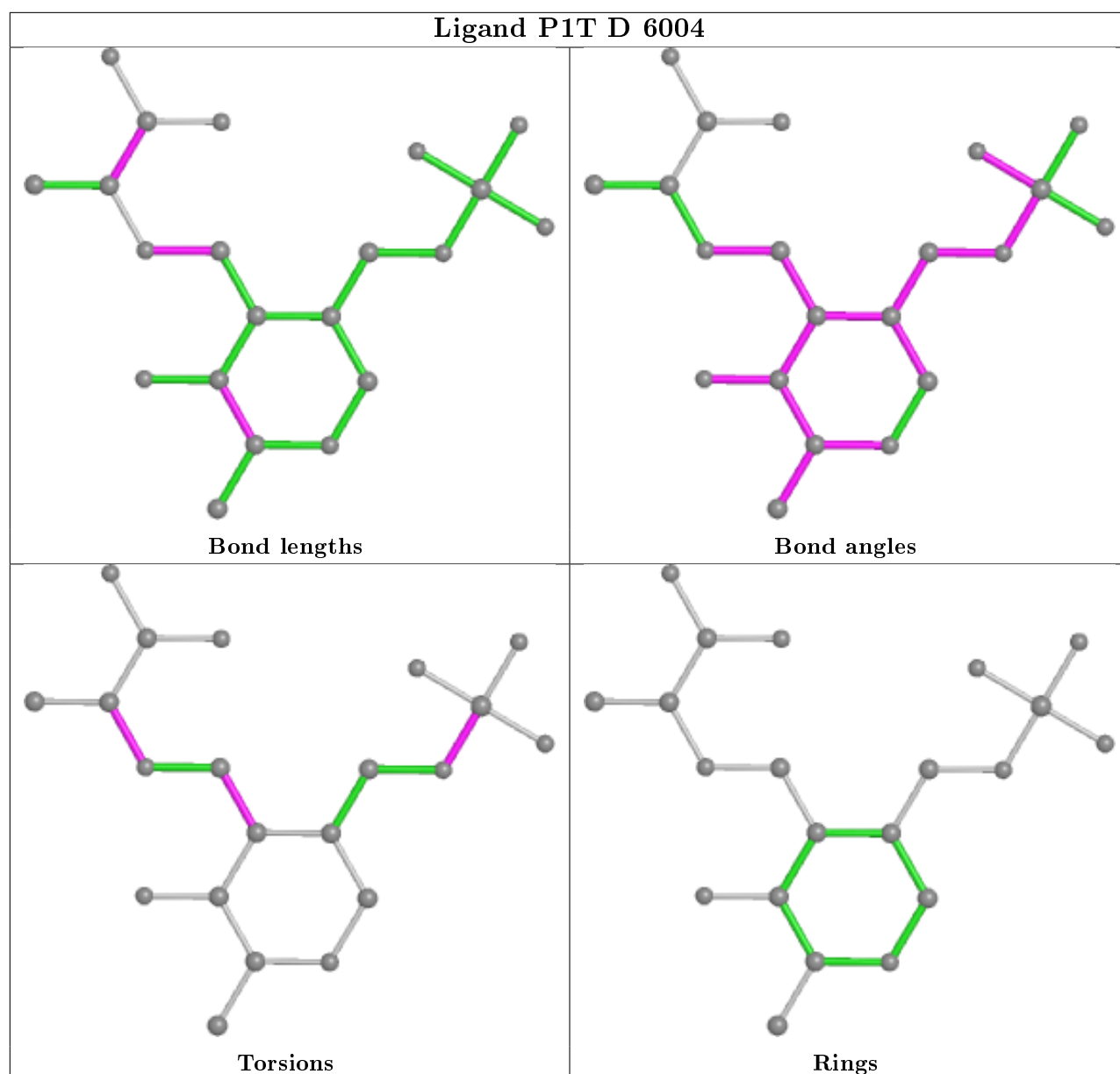
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	3500	NAG	1	0
7	C	505	NAG	1	0
9	B	6002	P1T	3	0
7	A	4500	NAG	1	0
7	C	504	NAG	1	0
9	D	6004	P1T	4	0
7	B	502	NAG	3	0
9	A	6001	P1T	2	0

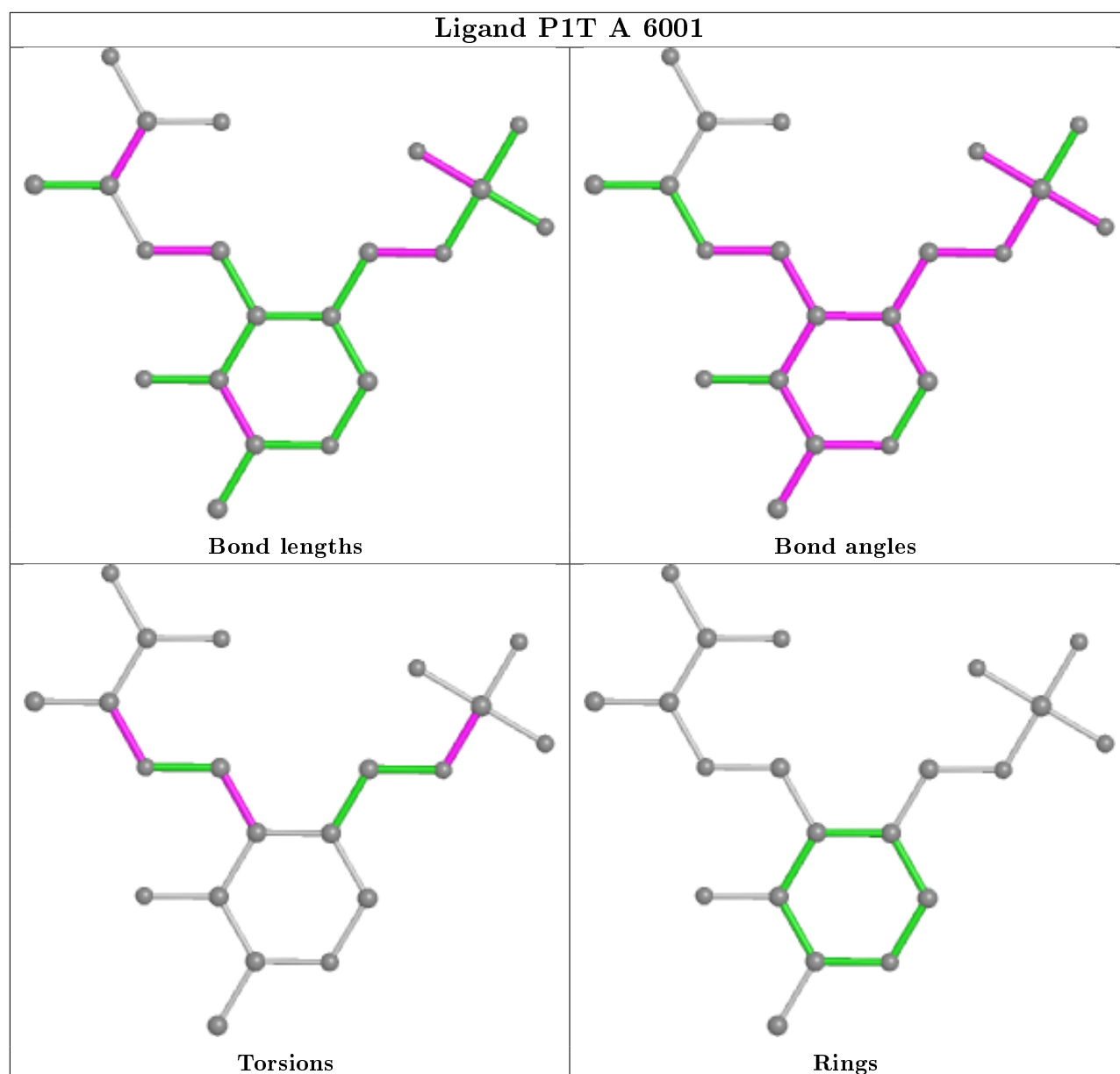
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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	425/427 (99%)	-0.15	7 (1%) 72 71	10, 19, 37, 53	1 (0%)
1	B	427/427 (100%)	-0.14	9 (2%) 63 63	11, 18, 35, 65	1 (0%)
1	C	425/427 (99%)	-0.17	12 (2%) 53 52	10, 18, 33, 52	0
1	D	427/427 (100%)	-0.13	10 (2%) 60 60	11, 18, 36, 69	0
All	All	1704/1708 (99%)	-0.15	38 (2%) 62 61	10, 18, 36, 69	2 (0%)

The worst 5 of 38 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	427	LYS	7.7
1	D	427	LYS	7.6
1	A	1	LYS	6.9
1	D	152	ASP	5.9
1	B	425	LYS	4.9

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.

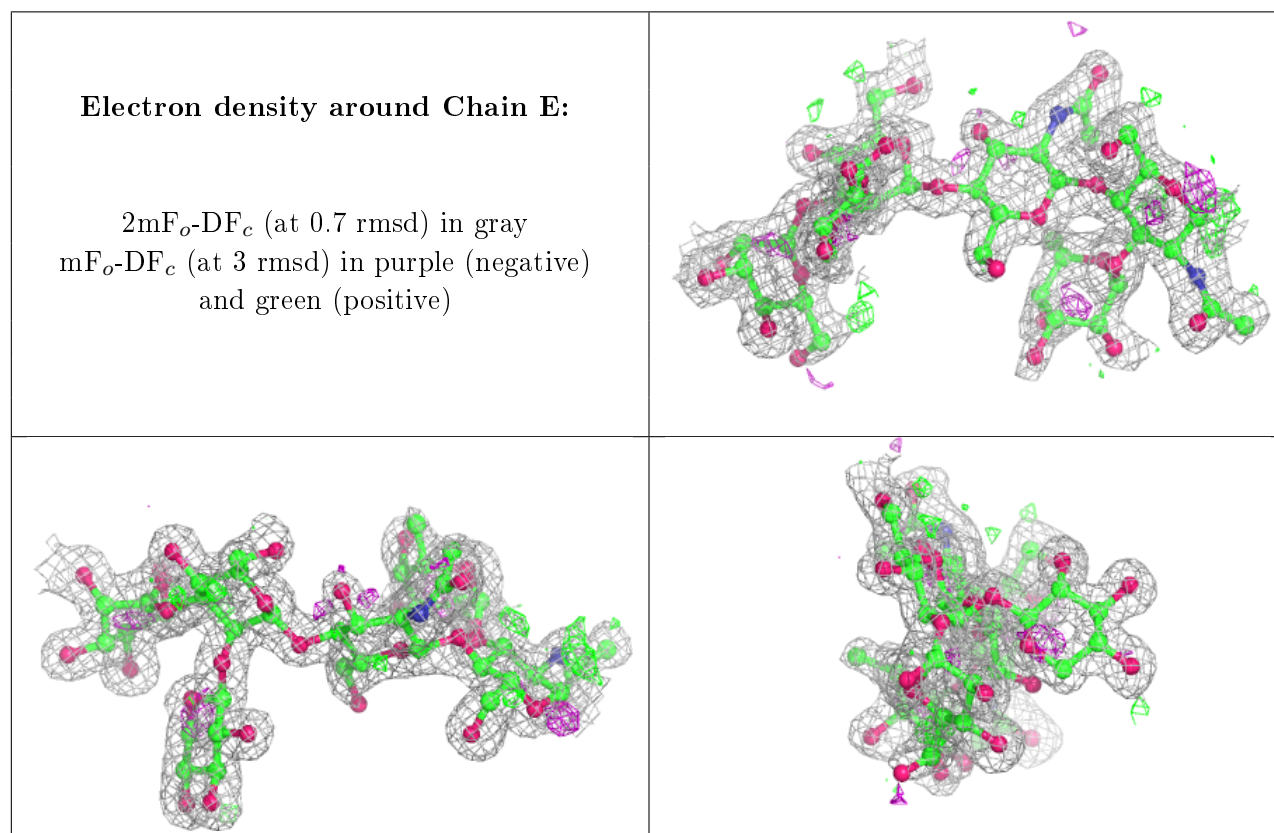
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	BMA	G	3	11/12	0.37	0.23	69,71,74,76	0
6	NAG	I	2	14/15	0.46	0.44	68,72,75,76	0

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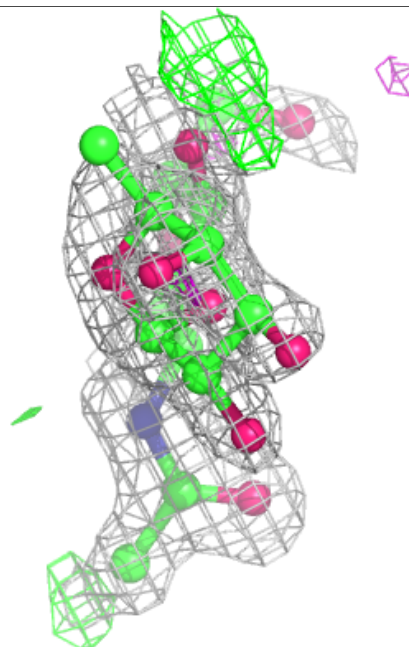
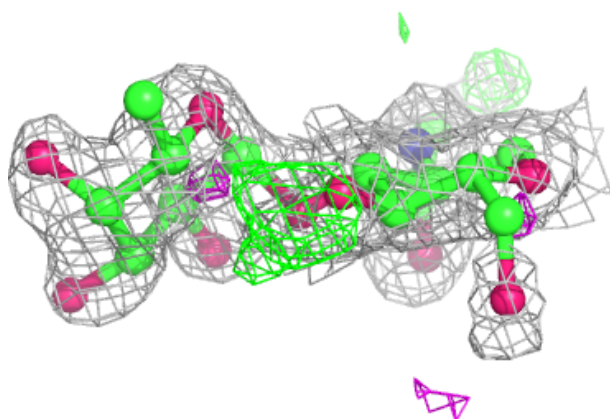
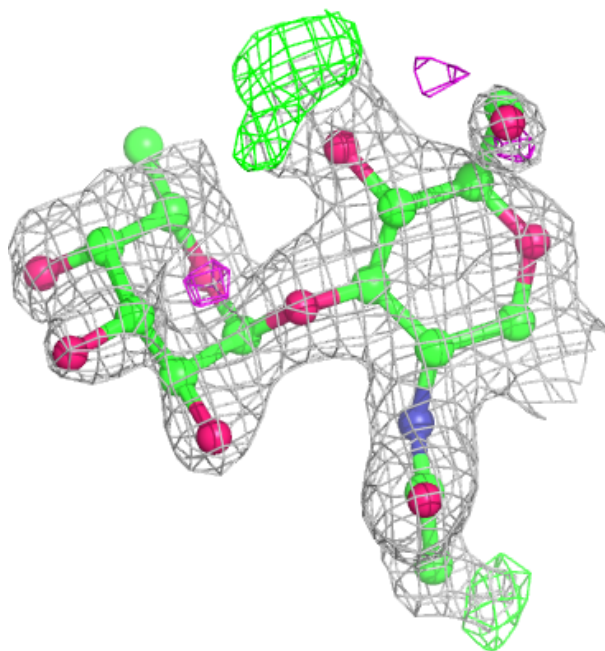
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	E	1	14/15	0.76	0.16	26,32,36,36	0
2	FUC	E	6	10/11	0.76	0.19	39,44,50,50	0
5	NAG	H	3	14/15	0.80	0.23	40,46,48,54	0
6	NAG	I	1	14/15	0.82	0.24	31,38,54,61	0
3	NAG	F	1	14/15	0.84	0.17	32,40,48,51	0
3	FUC	F	2	10/11	0.85	0.20	46,51,55,56	0
5	NAG	H	1	14/15	0.86	0.14	28,33,38,39	0
2	NAG	E	2	14/15	0.87	0.15	26,31,47,50	0
2	BMA	E	5	11/12	0.91	0.14	20,23,33,43	0
5	FUC	H	2	10/11	0.91	0.17	36,41,50,52	0
4	FUC	G	4	10/11	0.92	0.09	24,29,32,33	0
4	NAG	G	2	14/15	0.92	0.14	30,36,51,60	0
4	NAG	G	1	14/15	0.93	0.08	24,27,33,34	0
2	XYP	E	4	9/10	0.94	0.15	20,21,22,24	0
2	BMA	E	3	11/12	0.95	0.14	18,23,31,39	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.



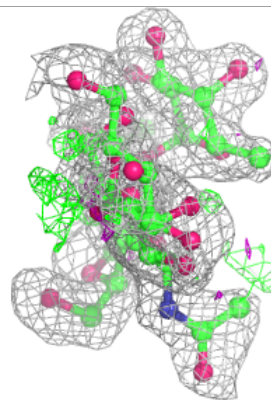
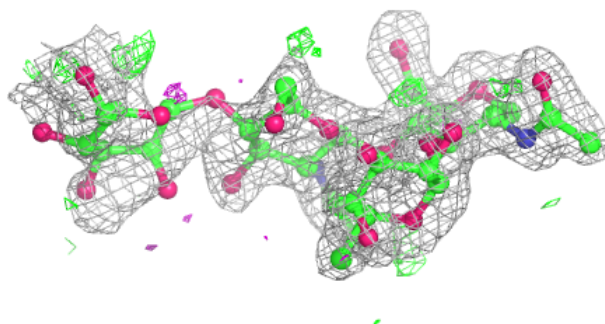
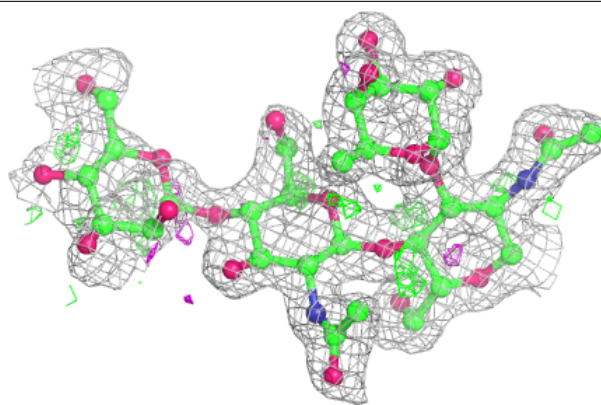
Electron density around Chain F:

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



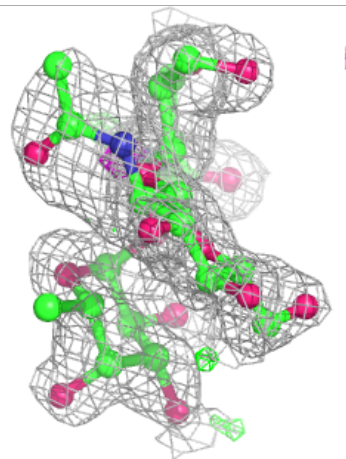
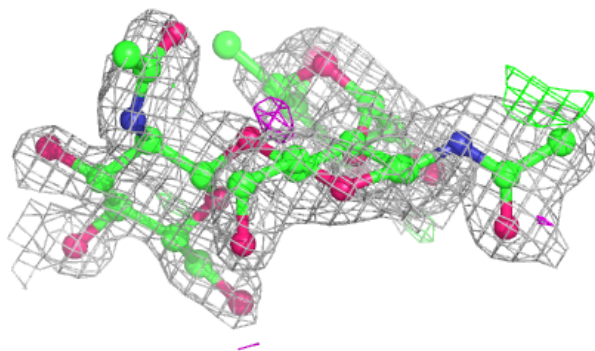
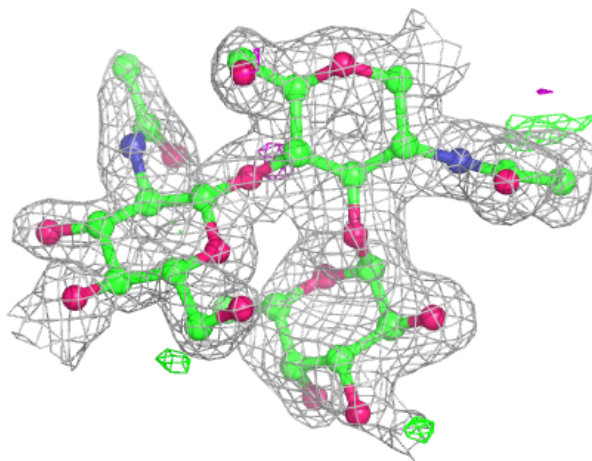
Electron density around Chain G:

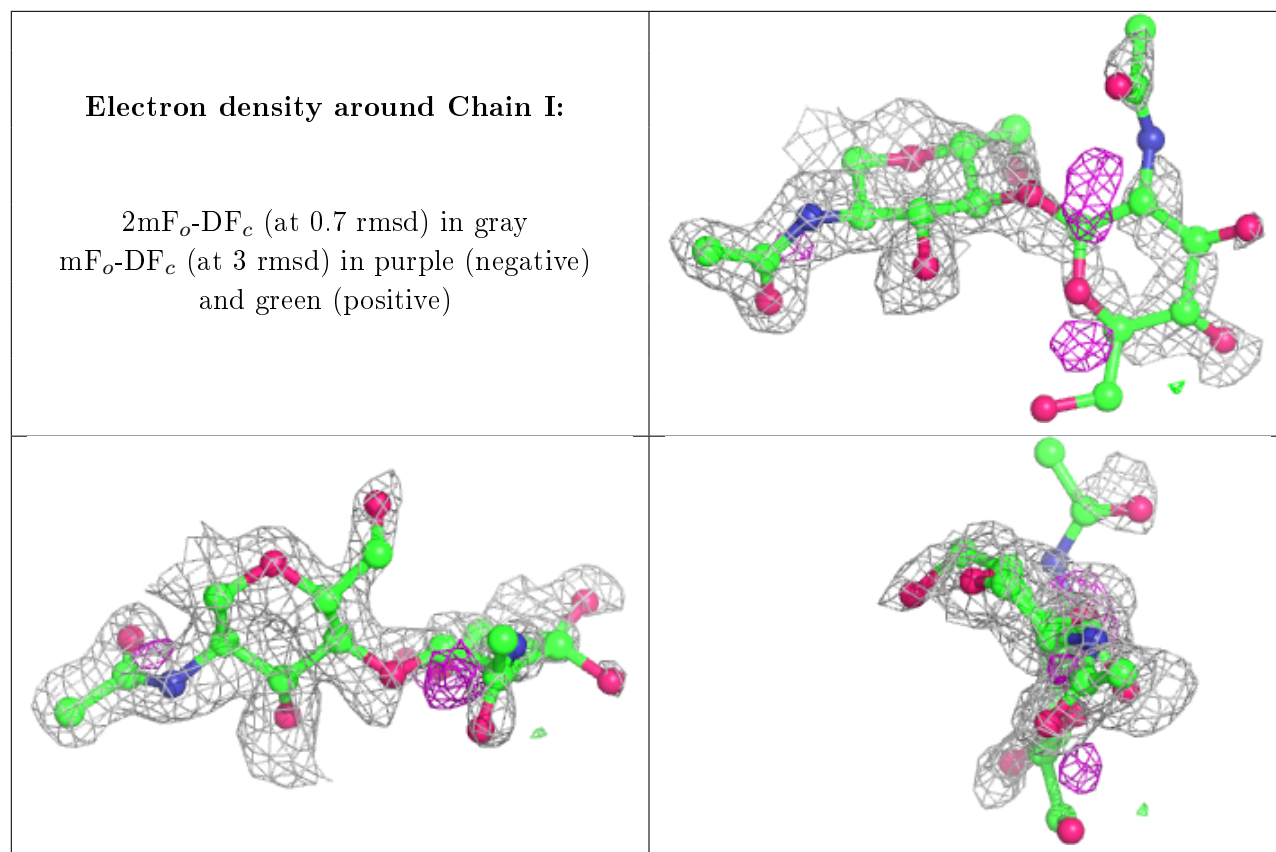
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain H:

$2mF_o-DF_c$ (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	503	14/15	-0.04	0.60	128,132,132,133	0
7	NAG	A	507	14/15	0.42	0.41	104,110,112,113	0
7	NAG	A	4500	14/15	0.48	0.36	64,70,79,80	0
7	NAG	C	505	14/15	0.54	0.32	73,82,84,84	0
7	NAG	B	502	14/15	0.67	0.21	48,59,69,69	0
7	NAG	B	3500	14/15	0.85	0.21	42,52,55,59	0
7	NAG	A	506	14/15	0.88	0.15	32,42,55,61	0
7	NAG	C	504	14/15	0.91	0.14	27,33,44,44	0
9	P1T	D	6004	21/21	0.96	0.09	12,17,25,27	0
9	P1T	C	6003	21/21	0.97	0.08	13,17,25,28	0
9	P1T	B	6002	21/21	0.97	0.09	12,17,24,25	0
9	P1T	A	6001	21/21	0.97	0.09	13,17,29,29	0
8	CL	D	5004	1/1	0.99	0.06	15,15,15,15	0
8	CL	B	5002	1/1	0.99	0.07	16,16,16,16	0

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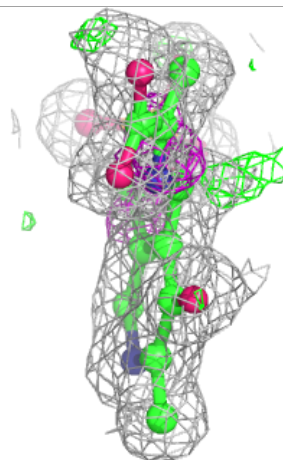
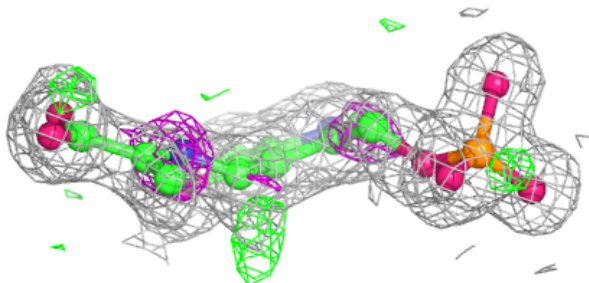
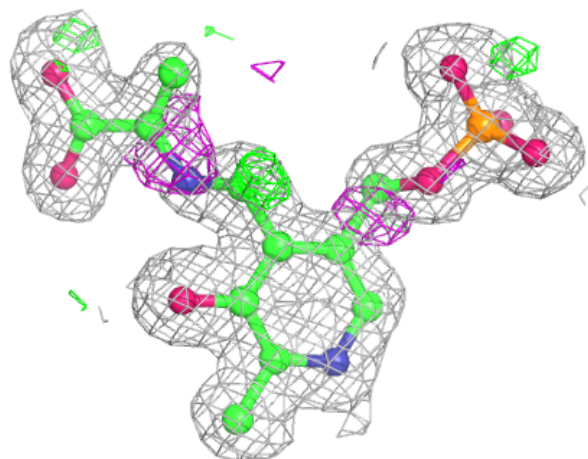
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	CL	C	5003	1/1	1.00	0.07	13,13,13,13	0
8	CL	A	5001	1/1	1.00	0.06	12,12,12,12	0

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.

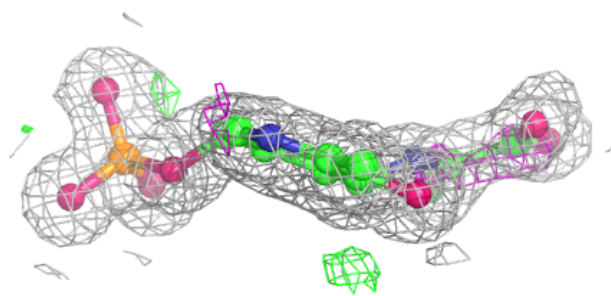
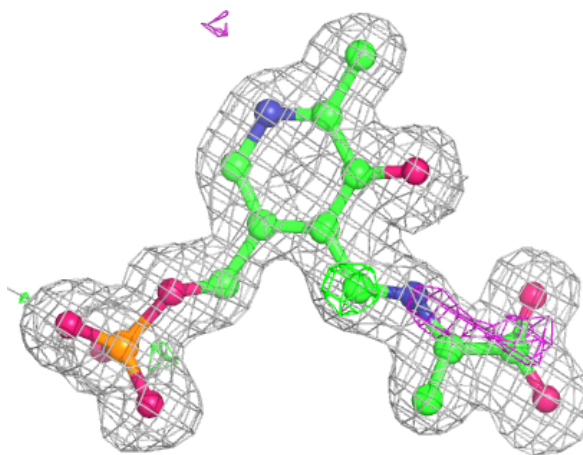
Electron density around P1T D 6004:

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



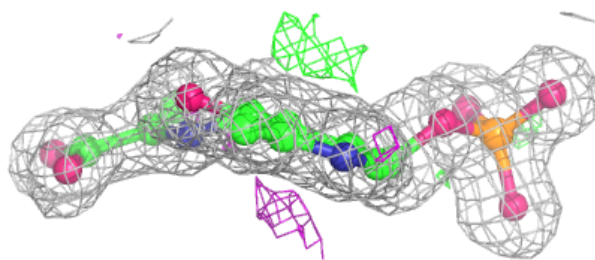
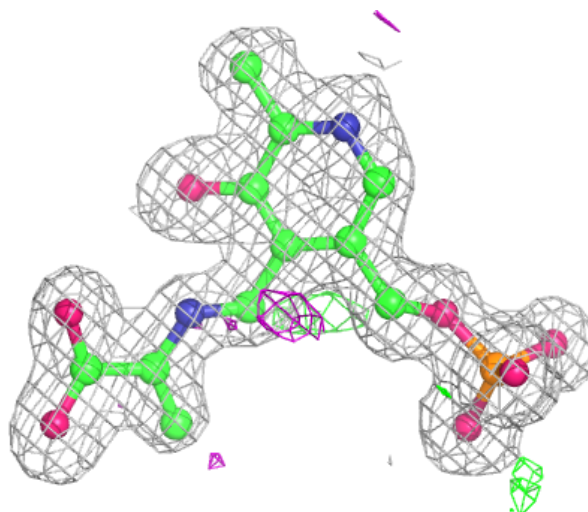
Electron density around P1T C 6003:

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



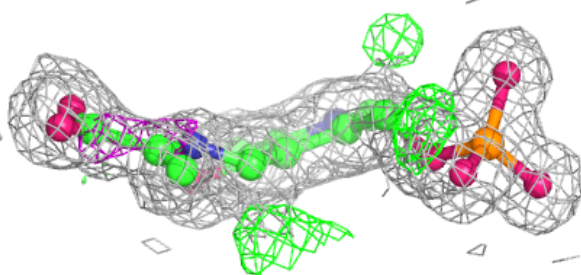
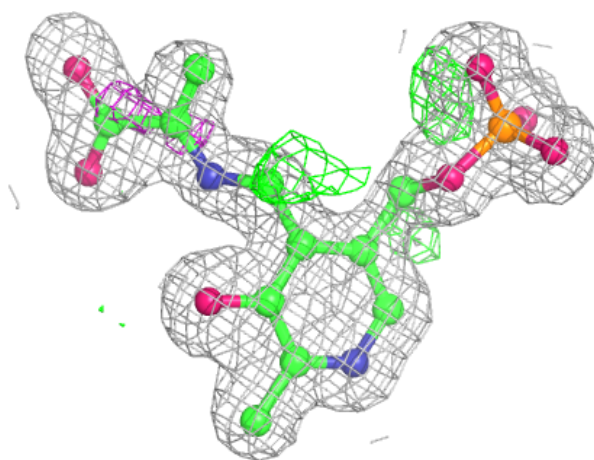
Electron density around P1T B 6002:

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



Electron density around P1T A 6001:

$2mF_o-DF_c$ (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.