



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 05:02 PM UTC

PDB ID : 6VJ7 / pdb_00006vj7
Title : Crystal structure of red kidney bean purple acid phosphatase in complex with adenosine 5'-(beta,gamma imido)triphosphate
Authors : Feder, D.; Schenk, G.; Guddat, L.W.; McGeary, R.P.; Mitic, N.; Furtado, A.; Schulz, B.L.; Henry, R.J.; Schmidt, S.
Deposited on : 2020-01-15
Resolution : 2.60 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
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

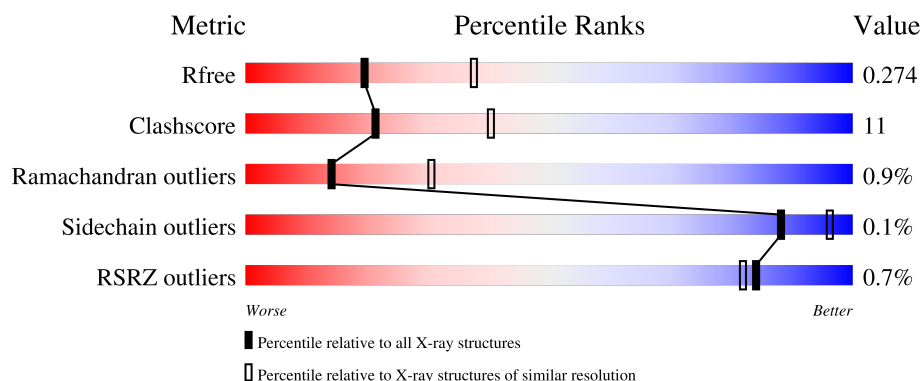
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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.



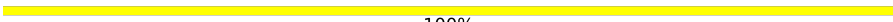
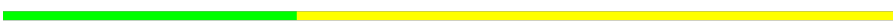
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	426	% 80% 19% .
1	B	426	74% 25%
1	C	426	81% 18% .
1	D	426	% 73% 27% .

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Mol	Chain	Length	Quality of chain
2	E	4	 100%
3	F	3	 100%
3	H	3	 33% 67%
4	G	4	 75% 25%
5	I	3	 33% 33% 33%
5	J	3	 33% 67%
6	K	2	 100%
6	L	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
12	PGE	D	730	-	-	X	-

2 Entry composition [i](#)

There are 18 unique types of molecules in this entry. The entry contains 15691 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 Fe(3+)-Zn(2+) purple acid phosphatase.

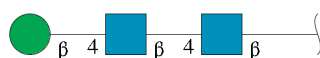
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	424	Total	C	N	O	S	0	2	0
			3506	2250	608	638	10			
1	B	425	Total	C	N	O	S	0	3	0
			3521	2260	611	640	10			
1	C	423	Total	C	N	O	S	0	0	0
			3482	2237	603	632	10			
1	D	426	Total	C	N	O	S	0	5	0
			3546	2275	618	642	11			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	4	Total	C	N	O	0	0	0
			50	28	2	20			

- 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.



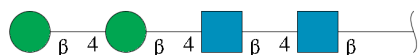
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	3	Total	C	N	O	0	0	0
			39	22	2	15			

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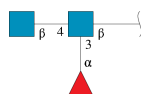
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	H	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-4)-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
4	G	4	Total	C	N	O	0	0	0
			50	28	2	20			

- 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	I	3	Total	C	N	O	0	0	0
			38	22	2	14			
5	J	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	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	L	2	Total	C	N	O	0	0	0
			28	16	2	10			

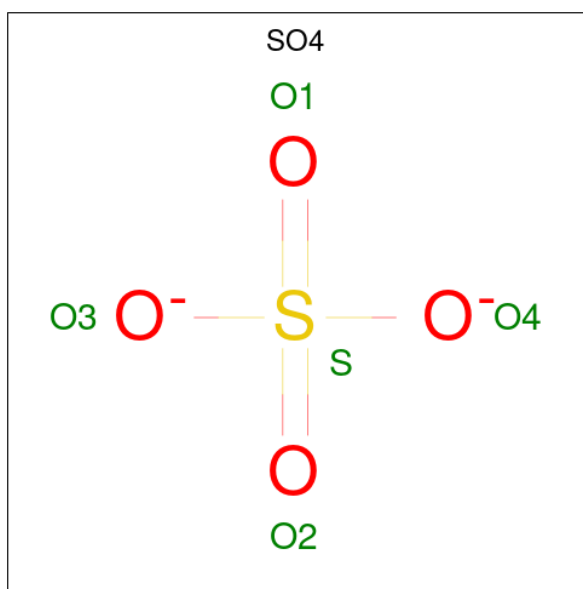
- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Zn	0	0
			1	1		
7	B	1	Total	Zn	0	0
			1	1		
7	C	1	Total	Zn	0	0
			1	1		
7	D	1	Total	Zn	0	0
			1	1		

- Molecule 8 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Fe	0	0
			1	1		
8	B	1	Total	Fe	0	0
			1	1		
8	C	1	Total	Fe	0	0
			1	1		
8	D	1	Total	Fe	0	0
			1	1		

- Molecule 9 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	O	S	0	0
			5	4	1		

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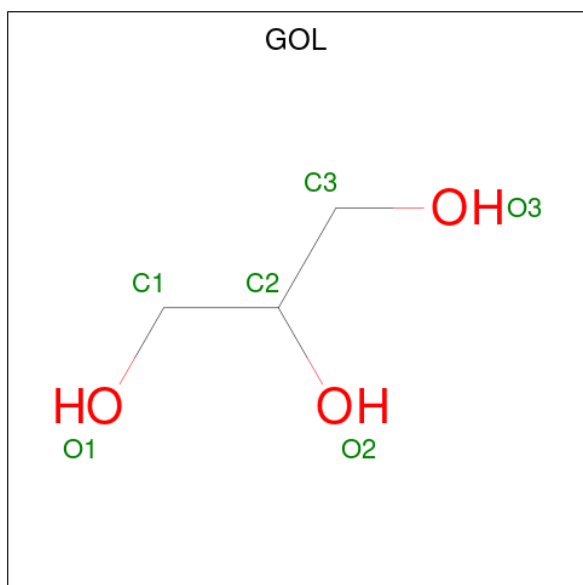
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	O	S	0	0
			5	4	1		
9	A	1	Total	O	S	0	0
			5	4	1		
9	B	1	Total	O	S	0	0
			5	4	1		
9	B	1	Total	O	S	0	0
			5	4	1		
9	B	1	Total	O	S	0	0
			5	4	1		
9	B	1	Total	O	S	0	0
			5	4	1		
9	C	1	Total	O	S	0	0
			5	4	1		
9	C	1	Total	O	S	0	0
			5	4	1		
9	C	1	Total	O	S	0	0
			5	4	1		
9	C	1	Total	O	S	0	0
			5	4	1		
9	C	1	Total	O	S	0	0
			5	4	1		
9	C	1	Total	O	S	0	0
			5	4	1		
9	C	1	Total	O	S	0	0
			5	4	1		
9	D	1	Total	O	S	0	0
			5	4	1		
9	D	1	Total	O	S	0	0
			5	4	1		
9	D	1	Total	O	S	0	0
			5	4	1		
9	D	1	Total	O	S	0	0
			5	4	1		
9	D	1	Total	O	S	0	0
			5	4	1		
9	D	1	Total	O	S	0	0
			5	4	1		

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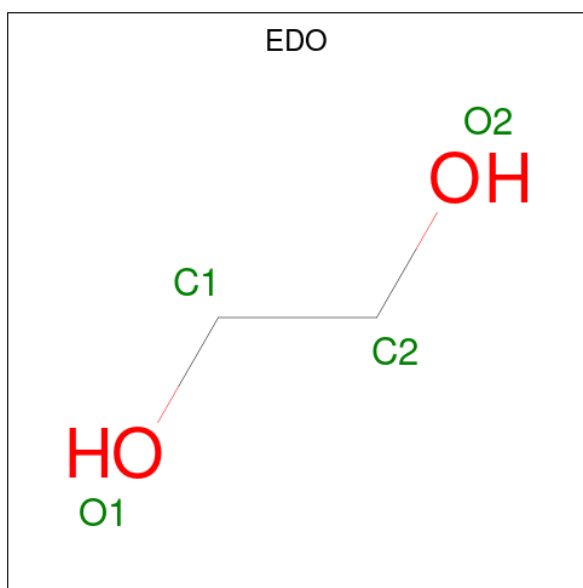
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	D	1	Total	O	S	0	0
			5	4	1		
9	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 10 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			6	3	3		
10	A	1	Total	C	O	0	1
			12	6	6		
10	A	1	Total	C	O	0	0
			6	3	3		
10	A	1	Total	C	O	0	0
			6	3	3		
10	C	1	Total	C	O	0	0
			6	3	3		
10	D	1	Total	C	O	0	0
			6	3	3		
10	D	1	Total	C	O	0	0
			6	3	3		
10	D	1	Total	C	O	0	0
			6	3	3		
10	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 11 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



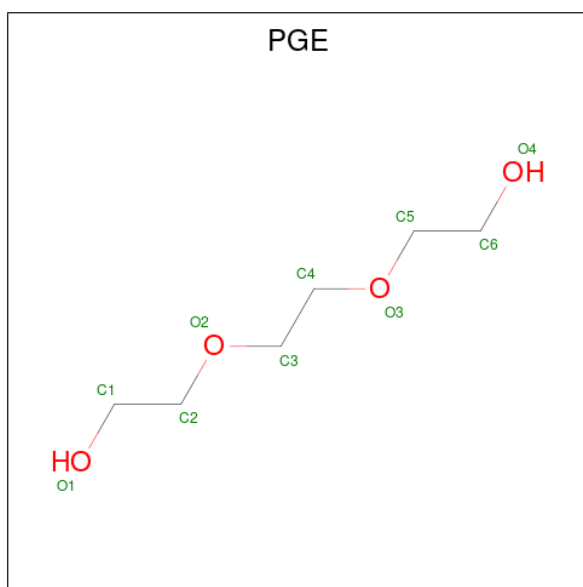
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	O	0	0
			4	2	2		
11	A	1	Total	C	O	0	0
			4	2	2		
11	A	1	Total	C	O	0	0
			4	2	2		
11	A	1	Total	C	O	0	0
			4	2	2		
11	A	1	Total	C	O	0	0
			4	2	2		
11	B	1	Total	C	O	0	0
			4	2	2		
11	B	1	Total	C	O	0	0
			4	2	2		
11	B	1	Total	C	O	0	0
			4	2	2		
11	B	1	Total	C	O	0	0
			4	2	2		
11	B	1	Total	C	O	0	0
			4	2	2		
11	C	1	Total	C	O	0	0
			4	2	2		
11	C	1	Total	C	O	0	0
			4	2	2		

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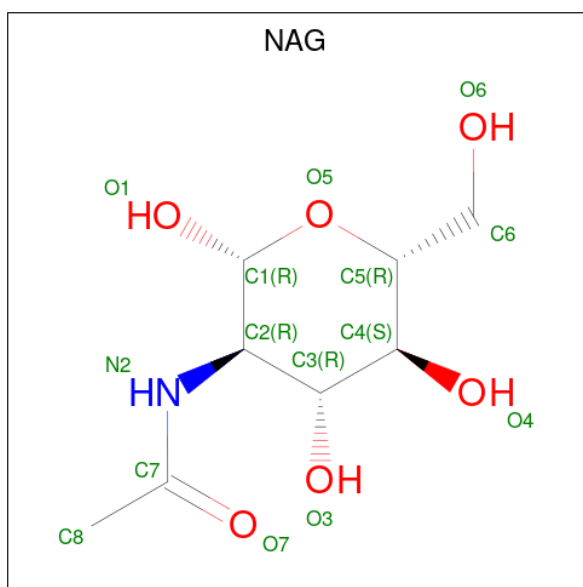
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	C	1	Total	C	O	0	0
			4	2	2		
11	C	1	Total	C	O	0	0
			4	2	2		
11	C	1	Total	C	O	0	0
			4	2	2		
11	C	1	Total	C	O	0	0
			4	2	2		
11	C	1	Total	C	O	0	0
			4	2	2		
11	D	1	Total	C	O	0	0
			4	2	2		
11	D	1	Total	C	O	0	0
			4	2	2		
11	D	1	Total	C	O	0	0
			4	2	2		
11	D	1	Total	C	O	0	0
			4	2	2		
11	D	1	Total	C	O	0	0
			4	2	2		
11	D	1	Total	C	O	0	0
			4	2	2		
11	D	1	Total	C	O	0	0
			4	2	2		
11	D	1	Total	C	O	0	0
			4	2	2		
11	D	1	Total	C	O	0	0
			4	2	2		
11	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 12 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



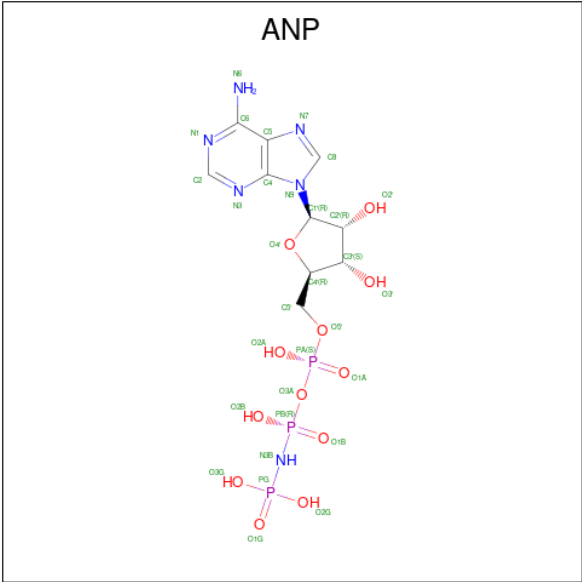
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	C	O	0	0
			7	4	3		
12	B	1	Total	C	O	0	0
			7	4	3		
12	B	1	Total	C	O	0	0
			7	4	3		
12	C	1	Total	C	O	0	0
			10	6	4		
12	C	1	Total	C	O	0	0
			7	4	3		
12	D	1	Total	C	O	0	0
			7	4	3		
12	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 13 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



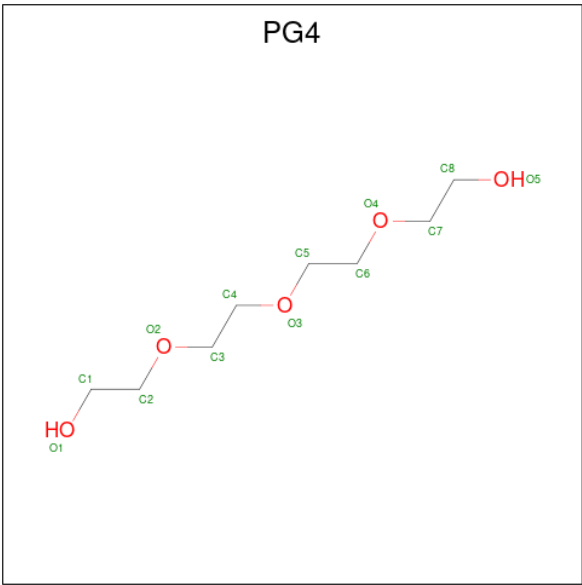
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	A	1	Total	C	N	O	0	0
			14	8	1	5		
13	A	1	Total	C	N	O	0	0
			14	8	1	5		
13	B	1	Total	C	N	O	0	0
			14	8	1	5		
13	C	1	Total	C	N	O	0	0
			14	8	1	5		
13	C	1	Total	C	N	O	0	0
			14	8	1	5		
13	D	1	Total	C	N	O	0	0
			14	8	1	5		
13	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 14 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
14	C	1	Total	C	N	O	P	0	0
			15	2	1	9	3		
14	D	1	Total	C	N	O	P	0	0
			14	1	1	9	3		

- Molecule 15 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	A	1	Total	C	O	0	0
			13	8	5		

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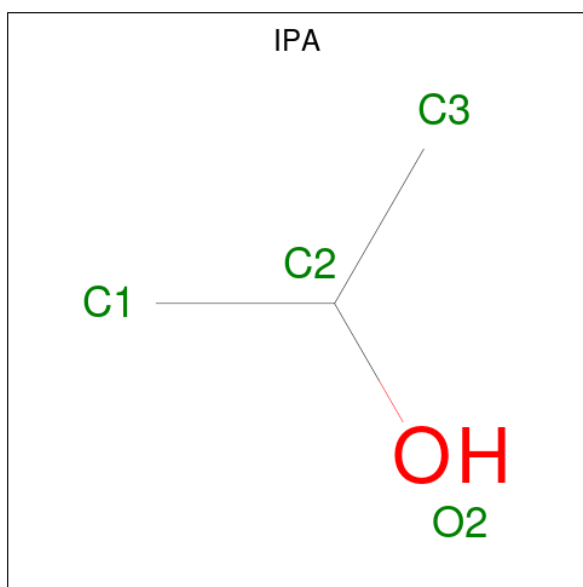
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	D	1	Total	C	O	0	0
			13	8	5		

- Molecule 16 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	A	1	Total	Na		0	0
			1	1			
16	B	1	Total	Na		0	0
			1	1			
16	C	1	Total	Na		0	0
			1	1			

- Molecule 17 is ISOPROPYL ALCOHOL (CCD ID: IPA) (formula: C₃H₈O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
17	C	1	Total	C	O	0	0
			4	3	1		

- Molecule 18 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	A	208	Total	O		0	0
			208	208			
18	B	179	Total	O		0	0
			179	179			

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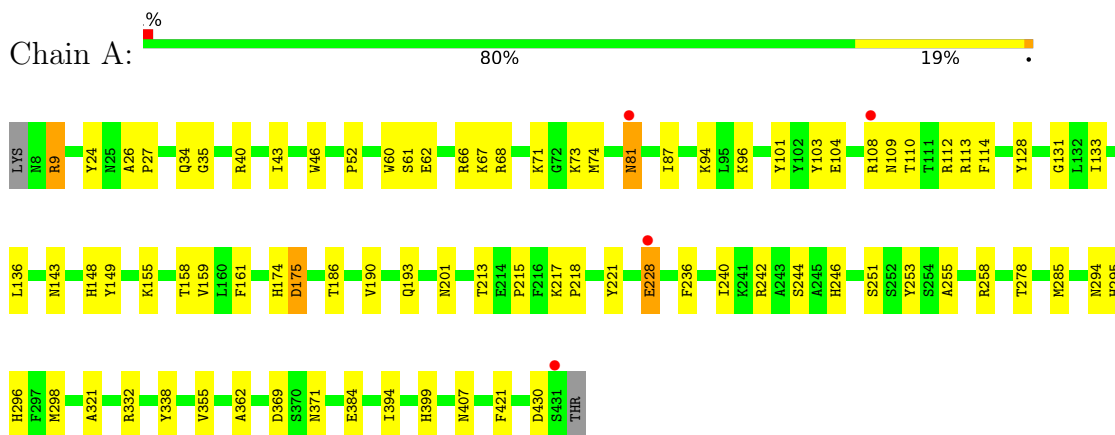
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	C	192	Total 192	O 192	0	0
18	D	192	Total 192	O 192	0	0

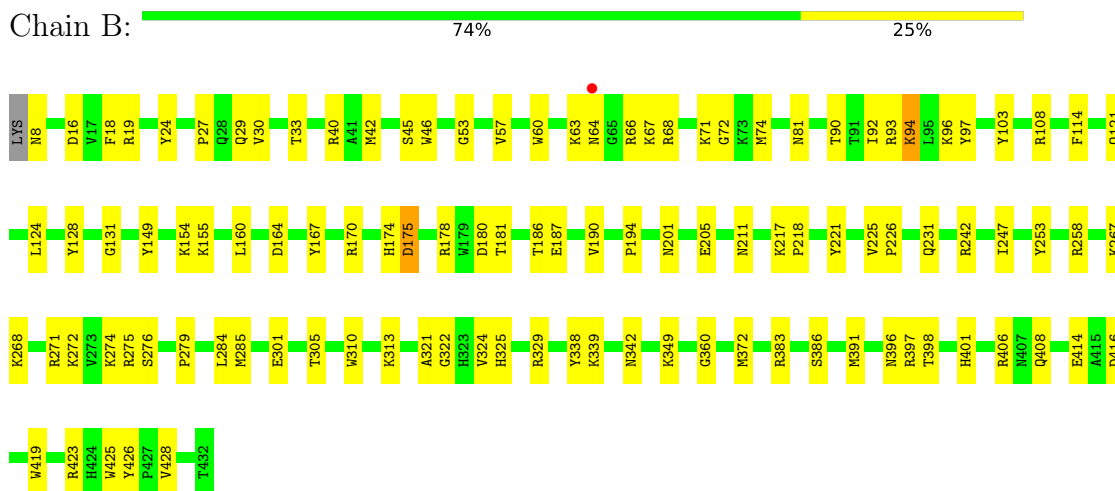
3 Residue-property plots [i](#)

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.

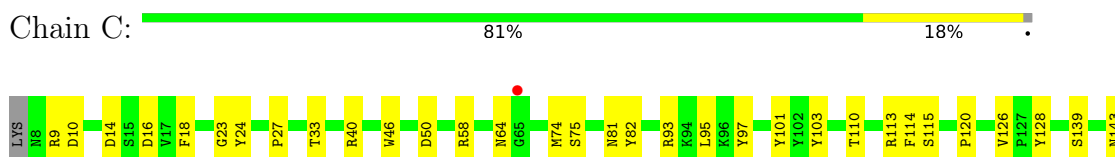
- Molecule 1: Fe(3+)-Zn(2+) purple acid phosphatase

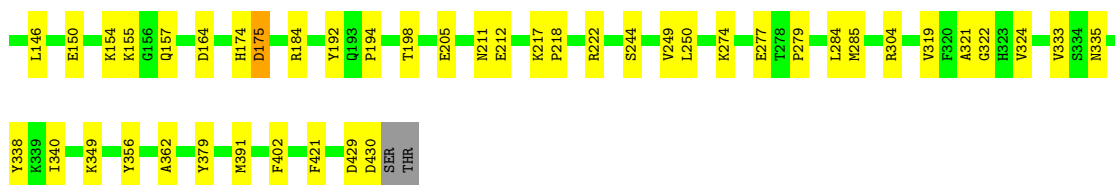


- Molecule 1: Fe(3+)-Zn(2+) purple acid phosphatase

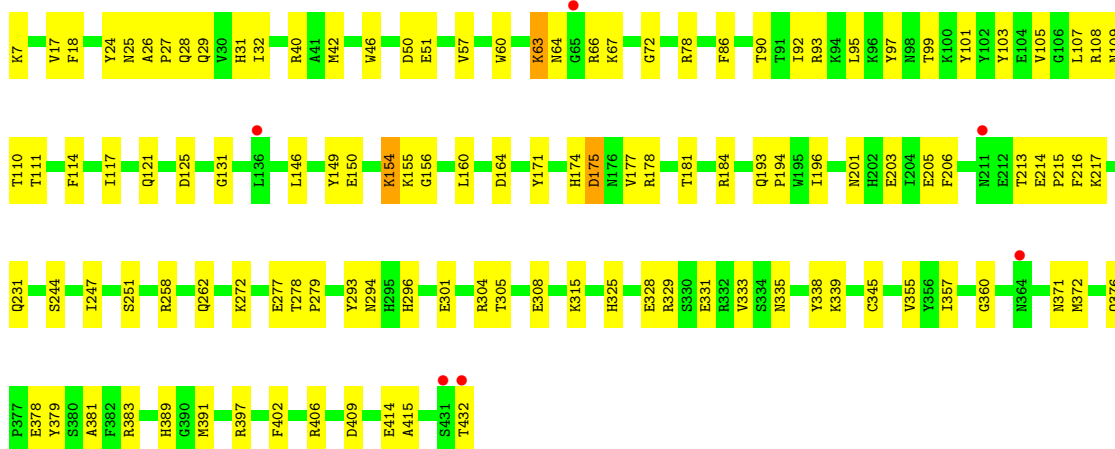


- Molecule 1: Fe(3+)-Zn(2+) purple acid phosphatase

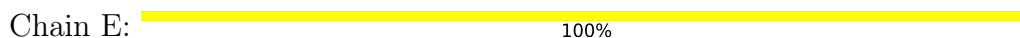




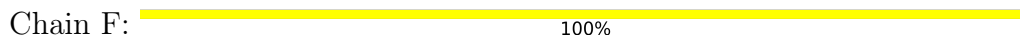
- Molecule 1: Fe(3+)-Zn(2+) purple acid phosphatase



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



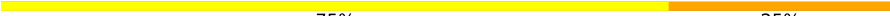
- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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

Chain G:  75% 25%

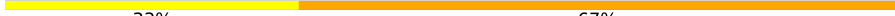
MAG1
MAG2
BMA3
BMA4

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

Chain I:  33% 33% 33%

MAG1
FUC2
MAG3

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

Chain J:  33% 67%

MAG1
FUC2
MAG3

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

Chain K:  100%

MAG1
MAG2

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

Chain L:  100%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	125.70Å 125.70Å 298.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.76 – 2.60 40.76 – 2.60	Depositor EDS
% Data completeness (in resolution range)	74.9 (40.76-2.60) 74.8 (40.76-2.60)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.213 , 0.274 0.215 , 0.274	Depositor DCC
R_{free} test set	3263 reflections (3.85%)	wwPDB-VP
Wilson B-factor (Å ²)	36.2	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	15691	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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: GOL, NA, PGE, IPA, ANP, FUC, SO4, NAG, BMA, FE, EDO, ZN, PG4

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	0.34	2/3628 (0.1%)	0.47	2/4933 (0.0%)
1	B	0.24	0/3643	0.44	0/4954
1	C	0.24	0/3601	0.44	0/4898
1	D	0.25	0/3674	0.47	0/4992
All	All	0.27	2/14546 (0.0%)	0.46	2/19777 (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	D	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	81	ASN	CA-CB	7.92	1.65	1.53
1	A	228	GLU	CG-CD	5.75	1.66	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	81	ASN	CB-CA-C	5.86	120.72	110.64
1	A	9	ARG	N-CA-C	5.02	121.49	110.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	154	LYS	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3506	0	3319	67	0
1	B	3521	0	3337	82	0
1	C	3482	0	3291	56	0
1	D	3546	0	3371	100	0
2	E	50	0	43	2	0
3	F	39	0	34	0	0
3	H	39	0	34	0	0
4	G	50	0	43	1	0
5	I	38	0	34	2	0
5	J	38	0	34	3	0
6	K	28	0	25	3	0
6	L	28	0	25	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	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	15	0	0	1	0
9	B	20	0	0	0	0
9	C	40	0	0	3	0
9	D	45	0	0	1	0
10	A	30	0	40	3	0
10	C	6	0	8	0	0
10	D	24	0	32	6	0
11	A	20	0	30	1	0
11	B	24	0	36	3	0
11	C	32	0	48	4	0
11	D	48	0	71	7	0
12	A	7	0	9	1	0
12	B	14	0	18	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	C	17	0	23	1	0
12	D	14	0	18	7	0
13	A	28	0	26	7	0
13	B	14	0	13	1	0
13	C	28	0	26	4	0
13	D	28	0	26	0	0
14	A	31	0	13	5	0
14	C	15	0	3	1	0
14	D	14	0	1	4	0
15	A	13	0	18	1	0
15	D	13	0	18	1	0
16	A	1	0	0	0	0
16	B	1	0	0	0	0
16	C	1	0	0	0	0
17	C	4	0	8	1	0
18	A	208	0	0	10	0
18	B	179	0	0	10	0
18	C	192	0	0	8	0
18	D	192	0	0	12	0
All	All	15691	0	14075	317	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 11.

The worst 5 of 317 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:A:81:ASN:ND2	13:A:521:NAG:C1	1.98	1.27
1:A:81:ASN:HD22	13:A:521:NAG:C1	1.48	1.25
1:A:81:ASN:HD21	13:A:521:NAG:H2	1.01	1.16
1:A:81:ASN:HD21	13:A:521:NAG:C2	1.69	1.04
1:A:81:ASN:ND2	13:A:521:NAG:C2	2.24	1.00

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	424/426 (100%)	399 (94%)	22 (5%)	3 (1%)	18	38
1	B	426/426 (100%)	396 (93%)	24 (6%)	6 (1%)	9	19
1	C	421/426 (99%)	397 (94%)	20 (5%)	4 (1%)	12	28
1	D	429/426 (101%)	394 (92%)	32 (8%)	3 (1%)	18	38
All	All	1700/1704 (100%)	1586 (93%)	98 (6%)	16 (1%)	14	30

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	175	ASP
1	B	155	LYS
1	B	175	ASP
1	C	64	ASN
1	C	175	ASP

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	375/375 (100%)	373 (100%)	2 (0%)	81	92
1	B	377/375 (100%)	376 (100%)	1 (0%)	86	94
1	C	371/375 (99%)	371 (100%)	0	100	100
1	D	380/375 (101%)	380 (100%)	0	100	100
All	All	1503/1500 (100%)	1500 (100%)	3 (0%)	88	95

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62[A]	GLU
1	A	62[B]	GLU
1	B	396	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	109	ASN
1	D	294	ASN
1	D	389	HIS
1	D	335	ASN
1	B	193	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 ⓘ

24 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	2,1	14,14,15	0.38	0	17,19,21	0.70	0
2	NAG	E	2	2	14,14,15	0.49	0	17,19,21	0.53	0
2	BMA	E	3	2	11,11,12	1.07	1 (9%)	15,15,17	2.41	2 (13%)
2	BMA	E	4	2	11,11,12	0.59	0	15,15,17	0.82	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	F	1	3,1	14,14,15	0.46	0	17,19,21	1.15	1 (5%)
3	NAG	F	2	3	14,14,15	1.43	1 (7%)	17,19,21	1.70	1 (5%)
3	BMA	F	3	3	11,11,12	1.54	3 (27%)	15,15,17	1.41	3 (20%)
4	NAG	G	1	4,1	14,14,15	0.42	0	17,19,21	0.86	1 (5%)
4	NAG	G	2	4	14,14,15	0.30	0	17,19,21	0.72	1 (5%)
4	BMA	G	3	4	11,11,12	1.08	1 (9%)	15,15,17	0.98	1 (6%)
4	BMA	G	4	4	11,11,12	1.38	2 (18%)	15,15,17	2.32	5 (33%)
3	NAG	H	1	3,1	14,14,15	0.65	1 (7%)	17,19,21	0.54	0
3	NAG	H	2	3	14,14,15	0.36	0	17,19,21	0.72	0
3	BMA	H	3	3	11,11,12	1.57	2 (18%)	15,15,17	1.74	3 (20%)
5	NAG	I	1	5,1	14,14,15	0.46	0	17,19,21	1.56	2 (11%)
5	FUC	I	2	5	10,10,11	1.04	1 (10%)	14,14,16	1.46	2 (14%)
5	NAG	I	3	5	14,14,15	0.46	0	17,19,21	0.46	0
5	NAG	J	1	5,1	14,14,15	0.53	0	17,19,21	1.28	4 (23%)
5	FUC	J	2	5	10,10,11	1.13	1 (10%)	14,14,16	1.78	5 (35%)
5	NAG	J	3	5	14,14,15	0.29	0	17,19,21	1.31	2 (11%)
6	NAG	K	1	6,1	14,14,15	0.93	1 (7%)	17,19,21	0.92	1 (5%)
6	NAG	K	2	6	14,14,15	0.58	0	17,19,21	1.54	2 (11%)
6	NAG	L	1	6,1	14,14,15	0.50	0	17,19,21	0.55	0
6	NAG	L	2	6	14,14,15	0.42	0	17,19,21	0.37	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	NAG	E	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	BMA	E	3	2	-	1/2/19/22	0/1/1/1
2	BMA	E	4	2	-	0/2/19/22	1/1/1/1
3	NAG	F	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	BMA	F	3	3	-	2/2/19/22	0/1/1/1
4	NAG	G	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	BMA	G	3	4	-	1/2/19/22	1/1/1/1

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

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	2	NAG	O5-C1	5.22	1.52	1.43
3	H	3	BMA	C1-C2	3.45	1.60	1.52
3	F	3	BMA	C2-C3	3.25	1.57	1.52
5	J	2	FUC	C1-C2	2.86	1.59	1.52
3	H	3	BMA	C2-C3	2.74	1.56	1.52

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	3	BMA	C1-O5-C5	8.37	123.41	112.19
4	G	4	BMA	C1-O5-C5	6.72	121.20	112.19
3	F	2	NAG	C1-O5-C5	6.53	120.93	112.19
6	K	2	NAG	C2-N2-C7	4.93	129.51	122.90
5	I	1	NAG	C1-O5-C5	4.64	118.41	112.19

There are no chirality outliers.

5 of 47 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	1	NAG	O5-C5-C6-O6
6	K	1	NAG	O5-C5-C6-O6
6	K	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	F	1	NAG	C4-C5-C6-O6
6	K	1	NAG	C4-C5-C6-O6

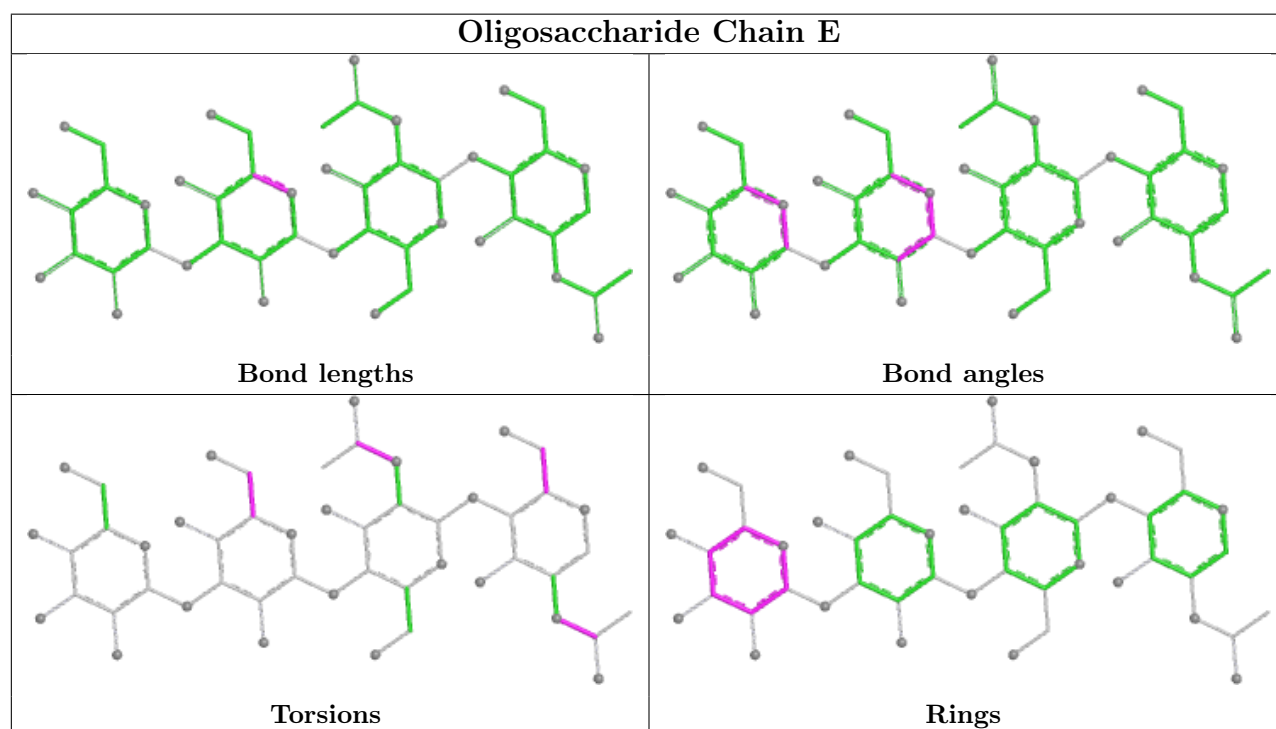
All (3) ring outliers are listed below:

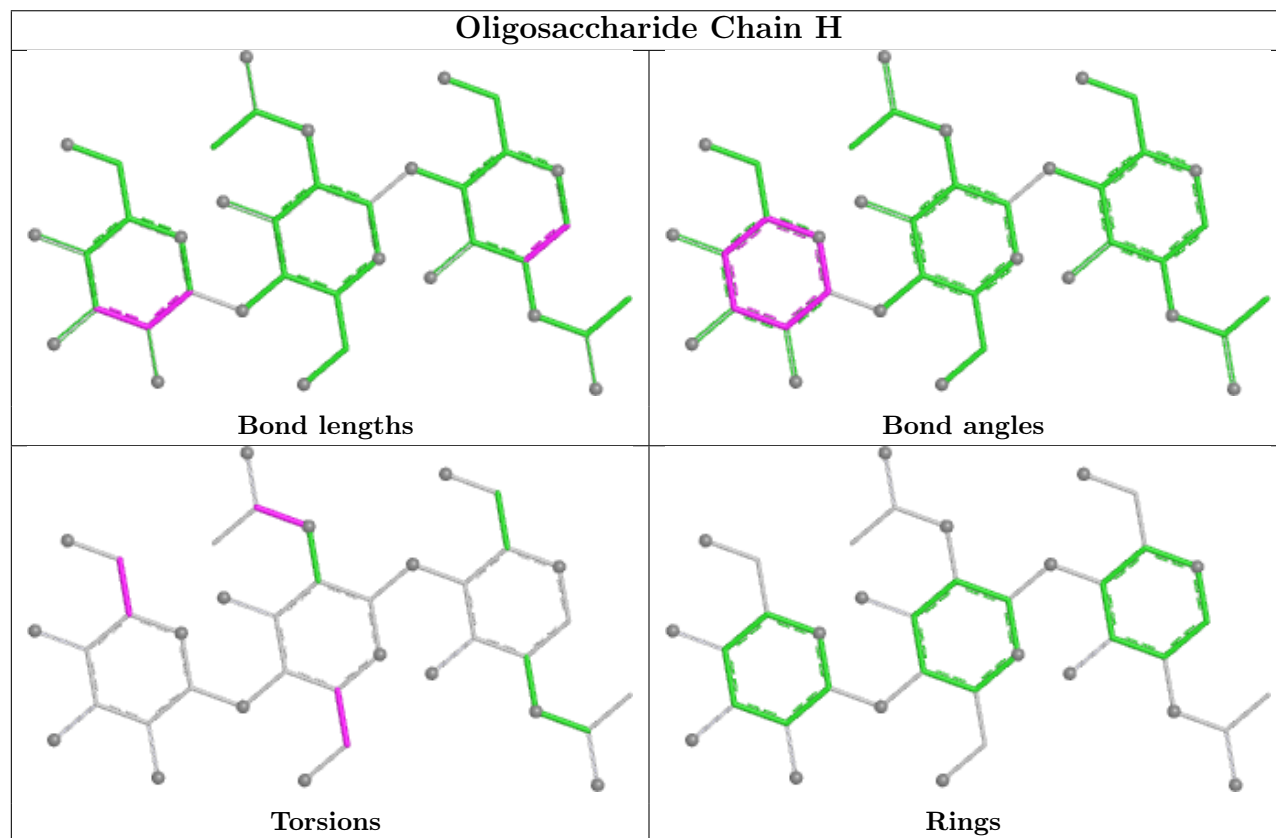
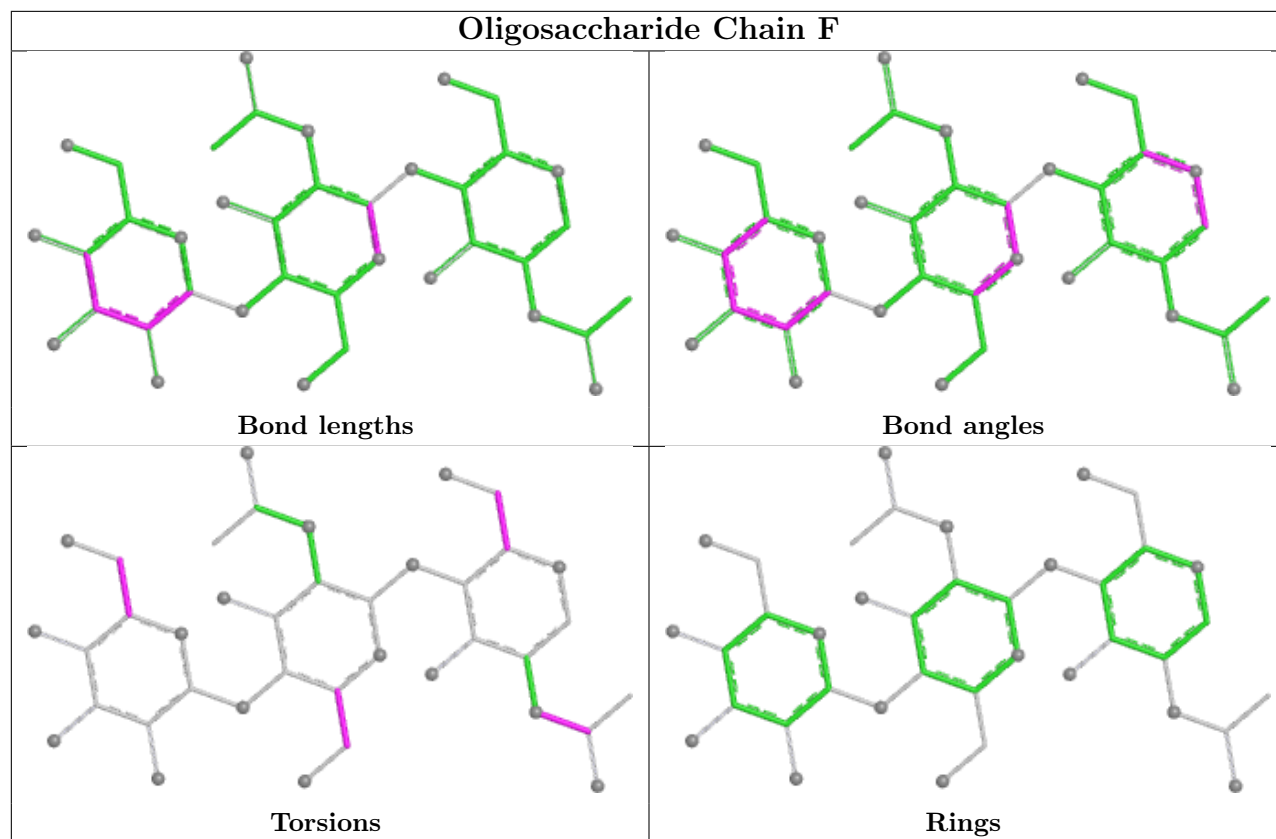
Mol	Chain	Res	Type	Atoms
4	G	4	BMA	C1-C2-C3-C4-C5-O5
4	G	3	BMA	C1-C2-C3-C4-C5-O5
2	E	4	BMA	C1-C2-C3-C4-C5-O5

8 monomers are involved in 11 short contacts:

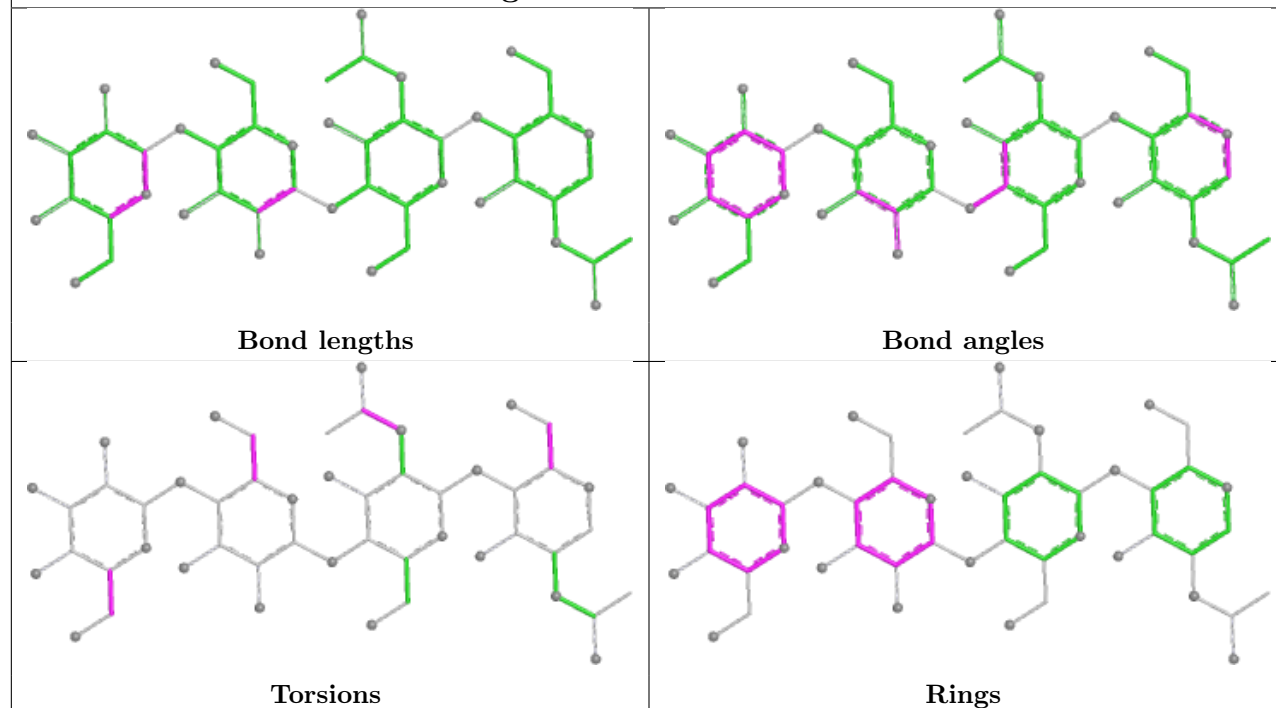
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	K	2	NAG	1	0
2	E	2	NAG	1	0
4	G	3	BMA	1	0
5	J	1	NAG	2	0
2	E	1	NAG	1	0
5	J	3	NAG	3	0
6	K	1	NAG	2	0
5	I	1	NAG	2	0

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

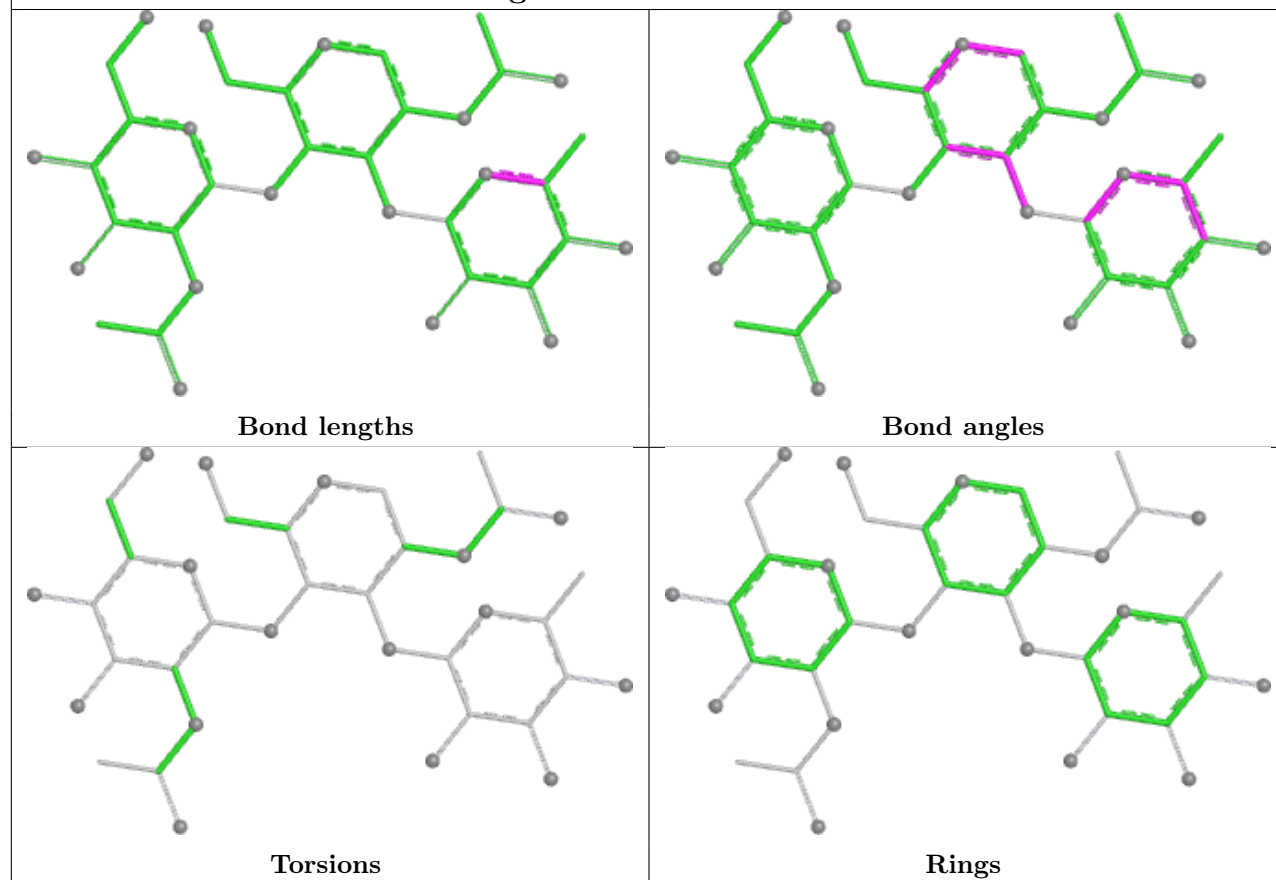


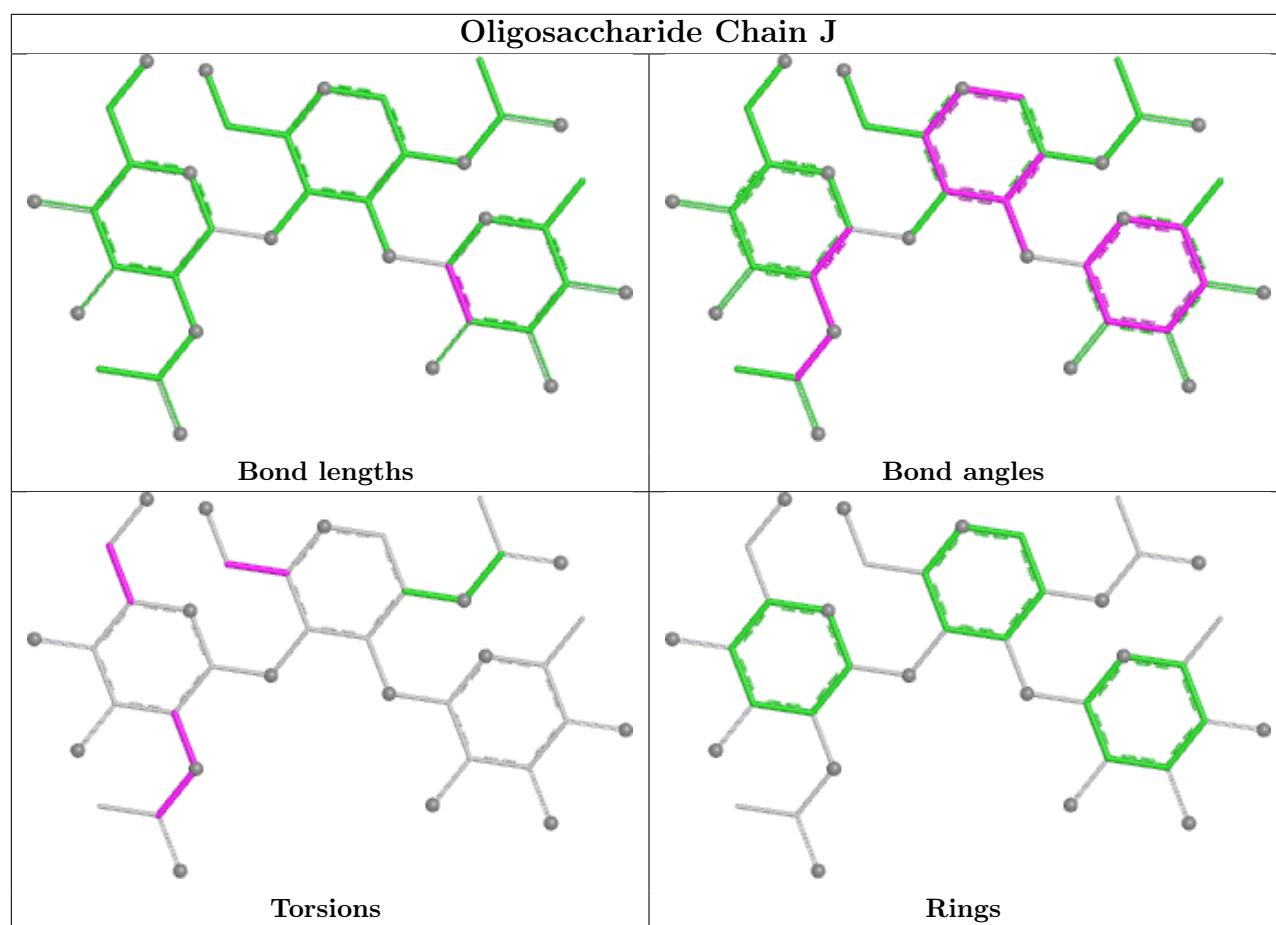


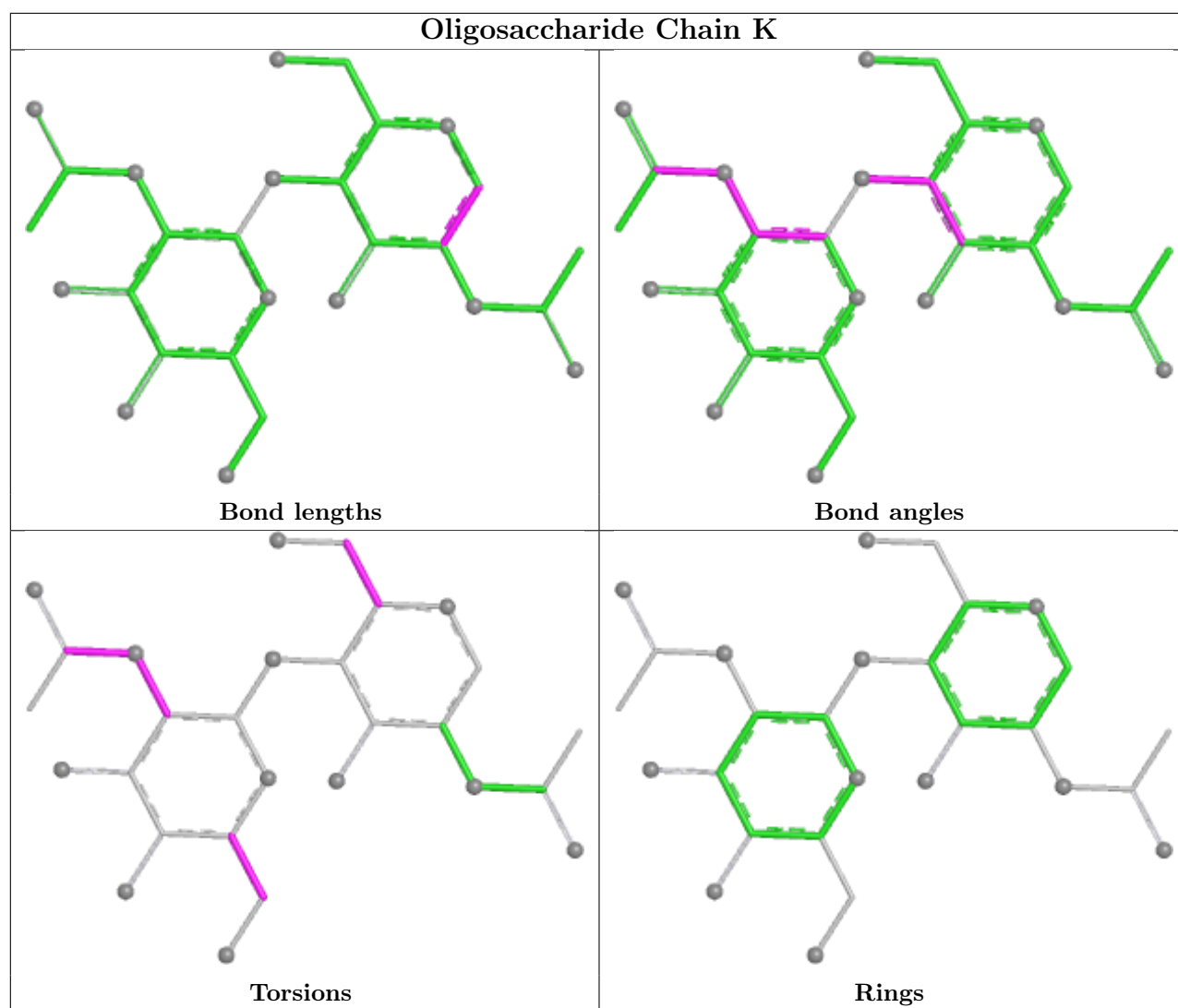
Oligosaccharide Chain G

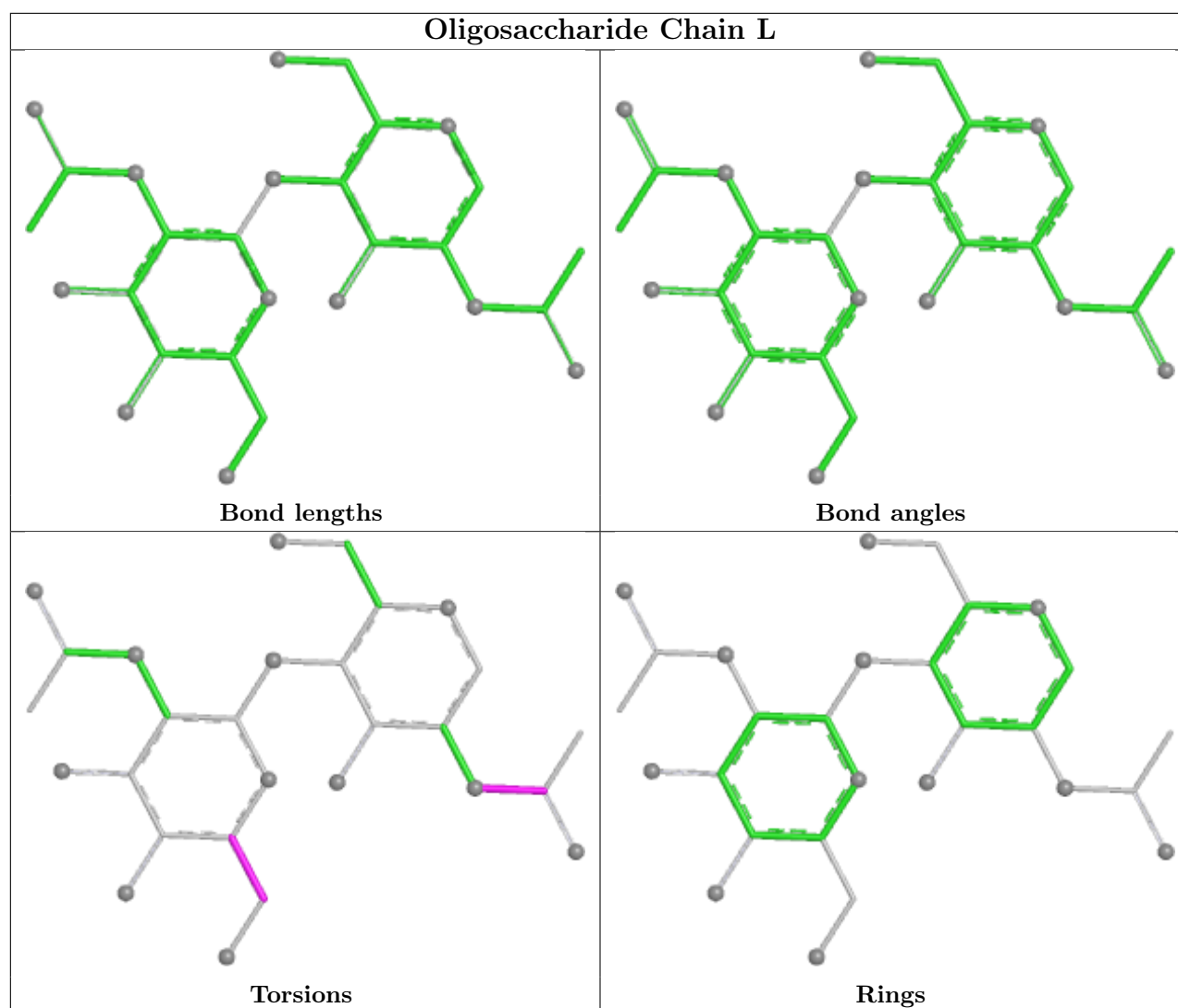


Oligosaccharide Chain I









5.6 Ligand geometry [i](#)

Of 96 ligands modelled in this entry, 11 are monoatomic - leaving 85 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	$\# Z > 2$
9	SO4	C	505	-	4,4,4	0.25	0	6,6,6	0.06	0
14	ANP	C	530	8,7	14,14,33	2.79	5 (35%)	15,22,52	1.27	2 (13%)
10	GOL	A	506	-	5,5,5	1.05	0	5,5,5	0.96	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	EDO	C	516	-	3,3,3	0.42	0	2,2,2	0.39	0
17	IPA	C	529	-	3,3,3	0.55	0	3,3,3	0.23	0
11	EDO	D	727	-	3,3,3	0.51	0	2,2,2	0.82	0
13	NAG	C	502	1	14,14,15	2.12	2 (14%)	17,19,21	2.33	1 (5%)
14	ANP	A	525	8,7	33,33,33	2.00	5 (15%)	45,52,52	1.92	10 (22%)
15	PG4	D	701	-	12,12,12	0.47	0	11,11,11	0.37	0
9	SO4	D	708	-	4,4,4	0.20	0	6,6,6	0.13	0
11	EDO	D	724	-	3,3,3	0.69	0	2,2,2	0.13	0
11	EDO	B	511	-	3,3,3	0.50	0	2,2,2	0.18	0
9	SO4	A	504	-	4,4,4	0.26	0	6,6,6	0.13	0
10	GOL	A	507[B]	-	5,5,5	0.89	0	5,5,5	1.13	0
11	EDO	D	726	-	3,3,3	0.66	0	2,2,2	0.44	0
9	SO4	A	505	-	4,4,4	0.55	0	6,6,6	0.40	0
11	EDO	A	513	-	3,3,3	0.60	0	2,2,2	0.51	0
10	GOL	A	509	-	5,5,5	1.20	0	5,5,5	1.01	0
13	NAG	C	526	1	14,14,15	0.32	0	17,19,21	0.67	1 (5%)
9	SO4	D	707	-	4,4,4	0.26	0	6,6,6	0.27	0
9	SO4	C	509	-	4,4,4	0.26	0	6,6,6	0.15	0
12	PGE	C	522	-	6,6,9	0.32	0	5,5,8	0.26	0
11	EDO	D	720	-	3,3,3	0.49	0	2,2,2	0.31	0
9	SO4	B	506	-	4,4,4	0.23	0	6,6,6	0.09	0
10	GOL	D	713	-	5,5,5	0.97	0	5,5,5	0.83	0
11	EDO	D	725	-	3,3,3	0.64	0	2,2,2	0.32	0
10	GOL	D	716	-	5,5,5	0.93	0	5,5,5	1.08	0
10	GOL	A	507[A]	-	5,5,5	1.01	0	5,5,5	1.05	0
9	SO4	B	505	-	4,4,4	0.25	0	6,6,6	0.19	0
9	SO4	D	710	-	4,4,4	0.22	0	6,6,6	0.22	0
11	EDO	A	512	-	3,3,3	0.67	0	2,2,2	0.33	0
9	SO4	C	508	-	4,4,4	0.25	0	6,6,6	0.11	0
11	EDO	D	717	-	3,3,3	0.48	0	2,2,2	0.34	0
12	PGE	B	514	-	6,6,9	0.45	0	5,5,8	0.44	0
9	SO4	D	709	-	4,4,4	0.26	0	6,6,6	0.11	0
10	GOL	C	512	-	5,5,5	0.88	0	5,5,5	1.10	0
11	EDO	C	518	-	3,3,3	0.65	0	2,2,2	0.59	0
9	SO4	D	706	-	4,4,4	0.23	0	6,6,6	0.19	0
14	ANP	D	735	8,7	13,13,33	3.07	5 (38%)	14,21,52	1.21	2 (14%)
11	EDO	D	722	-	3,3,3	0.39	0	2,2,2	0.36	0
9	SO4	C	511	-	4,4,4	0.24	0	6,6,6	0.16	0
11	EDO	A	511	-	3,3,3	0.51	0	2,2,2	0.32	0
13	NAG	A	521	-	14,14,15	1.68	3 (21%)	17,19,21	1.38	3 (17%)
10	GOL	D	714	-	5,5,5	0.85	0	5,5,5	1.10	1 (20%)
12	PGE	D	730	-	6,6,9	0.56	0	5,5,8	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	SO4	D	711	-	4,4,4	0.25	0	6,6,6	0.06	0
9	SO4	C	506	-	4,4,4	0.27	0	6,6,6	0.13	0
11	EDO	D	721	-	3,3,3	0.51	0	2,2,2	0.53	0
10	GOL	A	508	-	5,5,5	1.40	1 (20%)	5,5,5	0.94	0
12	PGE	D	729	-	6,6,9	0.27	0	5,5,8	0.70	0
13	NAG	D	733	1	14,14,15	0.99	1 (7%)	17,19,21	1.95	5 (29%)
11	EDO	A	514	-	3,3,3	0.67	0	2,2,2	0.37	0
9	SO4	B	504	-	4,4,4	0.22	0	6,6,6	0.09	0
9	SO4	C	501	16	4,4,4	0.30	0	6,6,6	0.29	0
11	EDO	A	510	-	3,3,3	0.49	0	2,2,2	0.27	0
11	EDO	B	508	-	3,3,3	0.55	0	2,2,2	0.19	0
9	SO4	D	704	-	4,4,4	0.25	0	6,6,6	0.08	0
11	EDO	B	509	-	3,3,3	0.47	0	2,2,2	0.21	0
11	EDO	C	519	-	3,3,3	0.63	0	2,2,2	0.32	0
11	EDO	D	719	-	3,3,3	0.42	0	2,2,2	0.56	0
9	SO4	C	510	-	4,4,4	0.20	0	6,6,6	0.11	0
13	NAG	A	520	1	14,14,15	0.39	0	17,19,21	0.58	0
13	NAG	D	734	1	14,14,15	0.45	0	17,19,21	0.76	1 (5%)
13	NAG	B	522	1	14,14,15	0.25	0	17,19,21	0.37	0
15	PG4	A	526	-	12,12,12	0.45	0	11,11,11	0.38	0
11	EDO	D	718	-	3,3,3	0.47	0	2,2,2	0.23	0
11	EDO	B	507	-	3,3,3	0.45	0	2,2,2	0.46	0
11	EDO	C	514	-	3,3,3	0.45	0	2,2,2	0.46	0
9	SO4	A	503	-	4,4,4	0.23	0	6,6,6	0.14	0
11	EDO	D	723	-	3,3,3	0.69	0	2,2,2	0.56	0
9	SO4	D	705	-	4,4,4	0.26	0	6,6,6	0.19	0
11	EDO	C	520	-	3,3,3	0.67	0	2,2,2	0.10	0
12	PGE	C	521	-	9,9,9	0.35	0	8,8,8	0.23	0
11	EDO	C	513	-	3,3,3	0.51	0	2,2,2	0.32	0
9	SO4	D	712	-	4,4,4	0.25	0	6,6,6	0.10	0
9	SO4	C	507	-	4,4,4	0.26	0	6,6,6	0.11	0
10	GOL	D	715	-	5,5,5	0.95	0	5,5,5	1.11	0
11	EDO	B	510	-	3,3,3	0.46	0	2,2,2	0.32	0
12	PGE	B	513	-	6,6,9	0.31	0	5,5,8	0.43	0
12	PGE	A	515	-	6,6,9	0.30	0	5,5,8	0.30	0
9	SO4	B	503	-	4,4,4	0.24	0	6,6,6	0.20	0
11	EDO	C	517	-	3,3,3	0.63	0	2,2,2	0.38	0
11	EDO	D	728	-	3,3,3	0.54	0	2,2,2	0.41	0
11	EDO	B	512	-	3,3,3	0.51	0	2,2,2	0.36	0
11	EDO	C	515	-	3,3,3	0.50	0	2,2,2	0.33	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
12	PGE	D	730	-	-	1/4/4/7	-
14	ANP	C	530	8,7	-	1/12/16/38	-
11	EDO	D	718	-	-	0/1/1/1	-
10	GOL	A	506	-	-	0/4/4/4	-
11	EDO	B	507	-	-	1/1/1/1	-
11	EDO	C	516	-	-	0/1/1/1	-
11	EDO	D	721	-	-	0/1/1/1	-
10	GOL	A	508	-	-	3/4/4/4	-
11	EDO	C	514	-	-	0/1/1/1	-
11	EDO	D	727	-	-	1/1/1/1	-
13	NAG	C	502	1	-	2/6/23/26	0/1/1/1
11	EDO	D	723	-	-	0/1/1/1	-
14	ANP	A	525	8,7	-	5/18/38/38	0/3/3/3
11	EDO	C	520	-	-	0/1/1/1	-
11	EDO	A	512	-	-	1/1/1/1	-
12	PGE	D	729	-	-	1/4/4/7	-
13	NAG	D	733	1	-	4/6/23/26	0/1/1/1
13	NAG	D	734	1	-	2/6/23/26	0/1/1/1
12	PGE	B	514	-	-	2/4/4/7	-
11	EDO	D	717	-	-	0/1/1/1	-
12	PGE	C	521	-	-	4/7/7/7	-
15	PG4	D	701	-	-	5/10/10/10	-
11	EDO	A	514	-	-	1/1/1/1	-
11	EDO	D	724	-	-	1/1/1/1	-
11	EDO	B	511	-	-	1/1/1/1	-
11	EDO	C	513	-	-	0/1/1/1	-
10	GOL	C	512	-	-	3/4/4/4	-
10	GOL	A	507[B]	-	-	2/4/4/4	-
11	EDO	C	518	-	-	0/1/1/1	-
11	EDO	D	726	-	-	0/1/1/1	-
11	EDO	A	513	-	-	1/1/1/1	-
10	GOL	A	509	-	-	1/4/4/4	-
10	GOL	D	715	-	-	2/4/4/4	-
13	NAG	C	526	1	-	2/6/23/26	0/1/1/1
14	ANP	D	735	8,7	-	1/11/15/38	-
12	PGE	C	522	-	-	1/4/4/7	-
11	EDO	A	510	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	EDO	B	510	-	-	0/1/1/1	-
11	EDO	B	508	-	-	0/1/1/1	-
11	EDO	D	720	-	-	0/1/1/1	-
11	EDO	D	722	-	-	1/1/1/1	-
12	PGE	B	513	-	-	2/4/4/7	-
15	PG4	A	526	-	-	3/10/10/10	-
12	PGE	A	515	-	-	3/4/4/7	-
10	GOL	D	713	-	-	2/4/4/4	-
11	EDO	B	509	-	-	0/1/1/1	-
11	EDO	C	519	-	-	1/1/1/1	-
11	EDO	D	719	-	-	1/1/1/1	-
11	EDO	A	511	-	-	0/1/1/1	-
11	EDO	C	517	-	-	1/1/1/1	-
11	EDO	D	725	-	-	1/1/1/1	-
13	NAG	A	521	-	-	2/6/23/26	0/1/1/1
11	EDO	D	728	-	-	1/1/1/1	-
10	GOL	D	716	-	-	1/4/4/4	-
10	GOL	D	714	-	-	2/4/4/4	-
13	NAG	A	520	1	-	2/6/23/26	0/1/1/1
11	EDO	B	512	-	-	0/1/1/1	-
11	EDO	C	515	-	-	1/1/1/1	-
10	GOL	A	507[A]	-	-	2/4/4/4	-
13	NAG	B	522	1	-	2/6/23/26	0/1/1/1

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	D	735	ANP	PG-O1G	7.30	1.57	1.46
13	C	502	NAG	O5-C1	7.12	1.55	1.43
14	A	525	ANP	PG-O1G	6.87	1.56	1.46
14	C	530	ANP	PG-O1G	6.47	1.56	1.46
14	C	530	ANP	PB-O1B	6.24	1.55	1.46

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	C	502	NAG	C1-O5-C5	8.83	124.02	112.19
14	A	525	ANP	C5-C4-N3	-5.79	118.75	126.72
13	D	733	NAG	C1-O5-C5	5.31	119.30	112.19
14	A	525	ANP	N3-C4-N9	4.93	135.56	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	525	ANP	N3-C2-N1	-3.80	122.83	128.58

There are no chirality outliers.

5 of 77 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	507[A]	GOL	O1-C1-C2-O2
10	A	507[A]	GOL	O1-C1-C2-C3
10	A	508	GOL	O1-C1-C2-C3
10	A	509	GOL	C1-C2-C3-O3
10	C	512	GOL	O1-C1-C2-C3

There are no ring outliers.

35 monomers are involved in 59 short contacts:

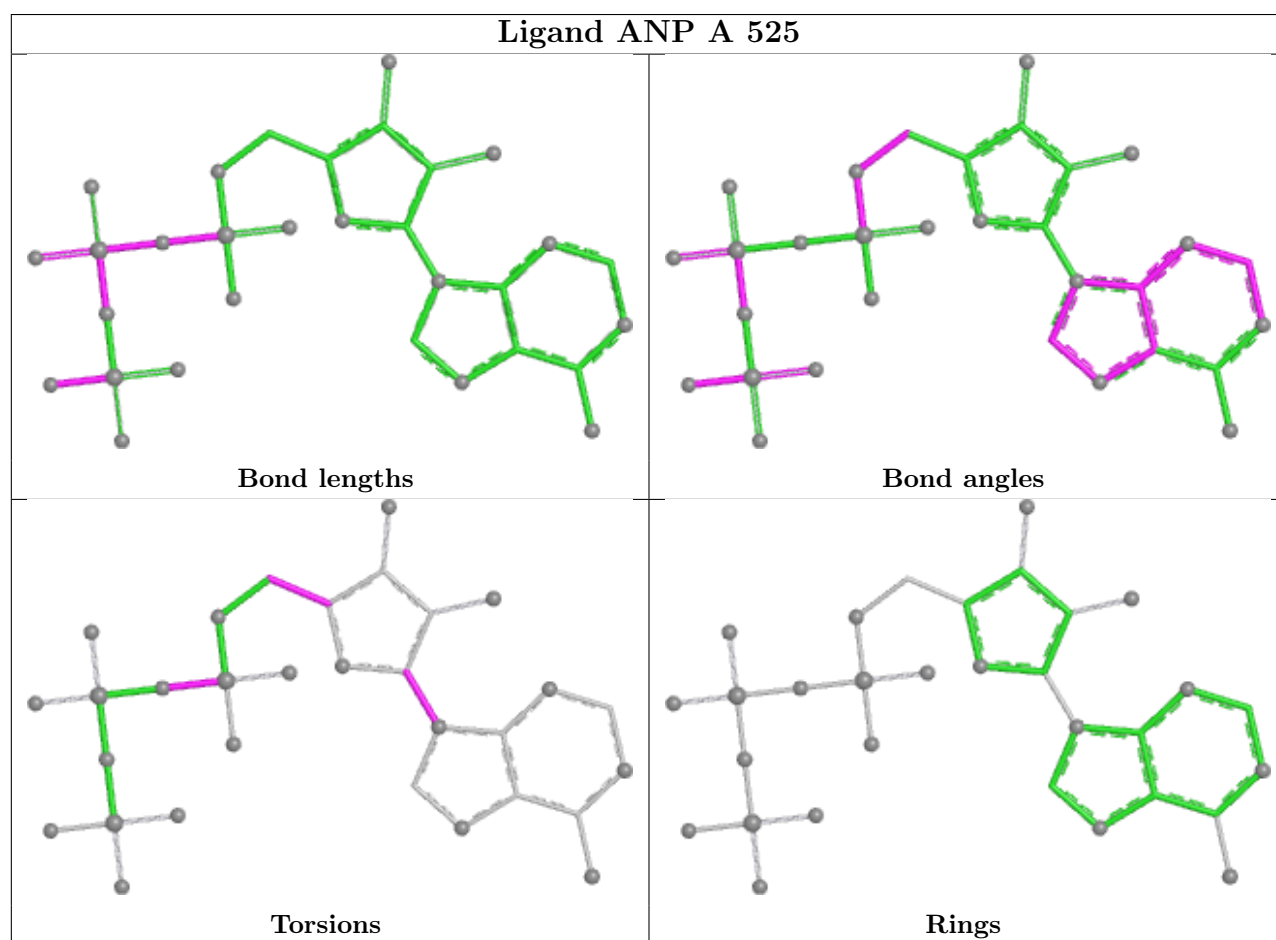
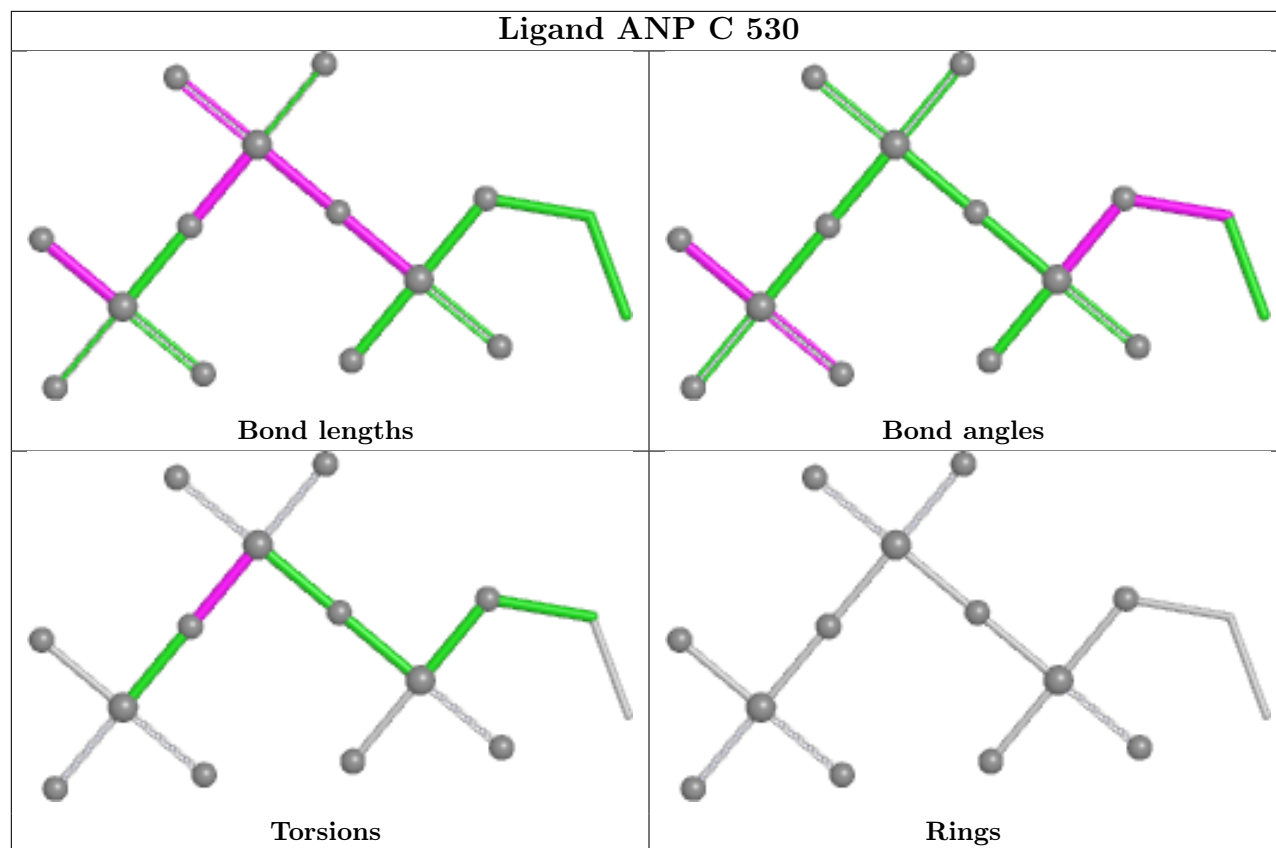
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	C	530	ANP	1	0
17	C	529	IPA	1	0
11	D	727	EDO	2	0
13	C	502	NAG	2	0
14	A	525	ANP	5	0
15	D	701	PG4	1	0
11	D	724	EDO	3	0
11	B	511	EDO	1	0
10	A	507[B]	GOL	1	0
9	A	505	SO4	1	0
10	A	509	GOL	1	0
13	C	526	NAG	2	0
10	D	713	GOL	3	0
12	B	514	PGE	1	0
9	D	709	SO4	1	0
14	D	735	ANP	4	0
11	D	722	EDO	1	0
13	A	521	NAG	6	0
10	D	714	GOL	1	0
12	D	730	PGE	7	0
11	D	721	EDO	1	0
10	A	508	GOL	1	0
9	C	501	SO4	1	0
11	A	510	EDO	1	0
9	C	510	SO4	1	0

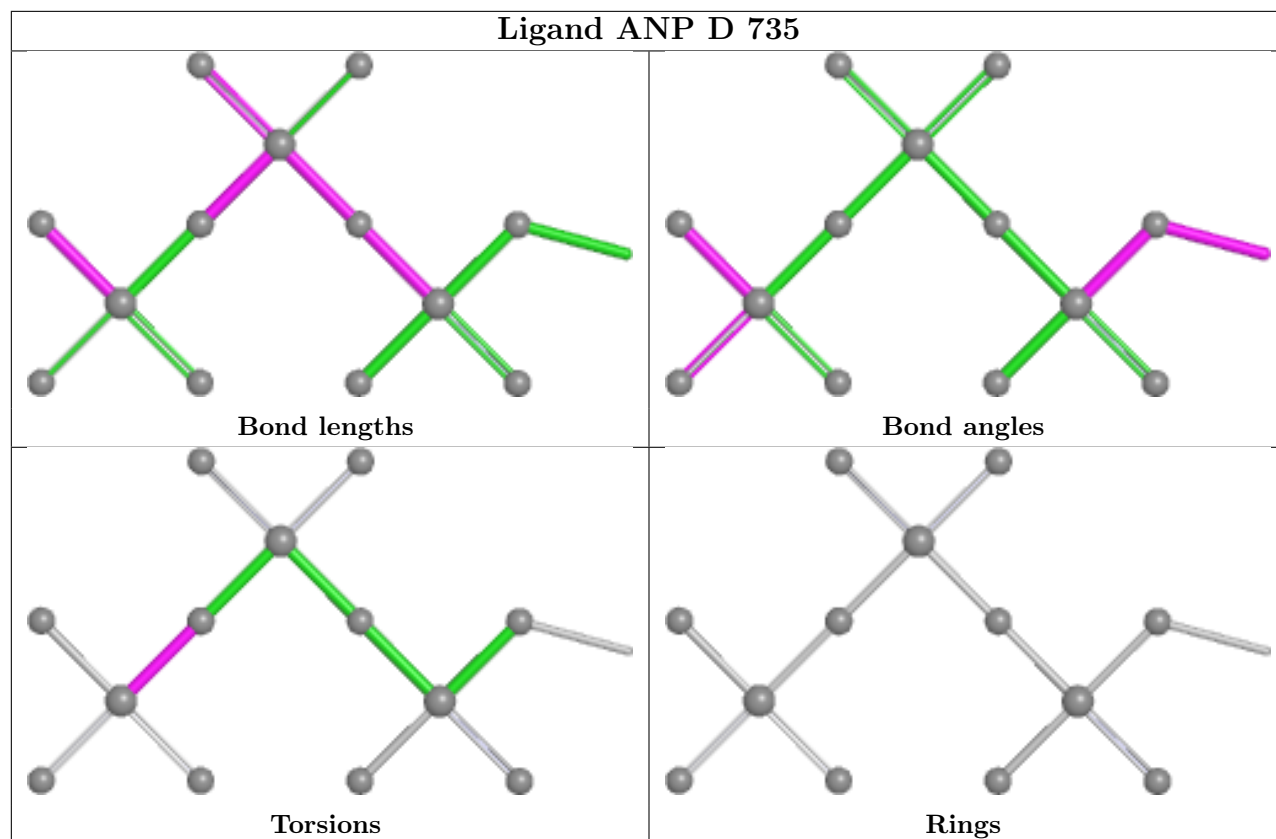
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	A	520	NAG	1	0
13	B	522	NAG	1	0
15	A	526	PG4	1	0
11	C	520	EDO	2	0
12	C	521	PGE	1	0
9	C	507	SO4	1	0
10	D	715	GOL	2	0
12	A	515	PGE	1	0
11	C	517	EDO	2	0
11	B	512	EDO	2	0

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	424/426 (99%)	0.00	4 (0%) 81 78	16, 33, 44, 73	2 (0%)
1	B	425/426 (99%)	0.06	1 (0%) 91 90	16, 36, 47, 68	3 (0%)
1	C	423/426 (99%)	0.06	1 (0%) 91 90	25, 35, 45, 69	0
1	D	426/426 (100%)	0.12	6 (1%) 73 69	16, 35, 46, 70	5 (1%)
All	All	1698/1704 (99%)	0.06	12 (0%) 84 82	16, 35, 46, 73	10 (0%)

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	431	SER	6.6
1	D	432	THR	5.0
1	A	108	ARG	3.9
1	D	65	GLY	2.6
1	A	228	GLU	2.5

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	H	3	11/12	0.54	0.19	76,83,85,89	0
5	FUC	I	2	10/11	0.62	0.19	61,68,82,82	0

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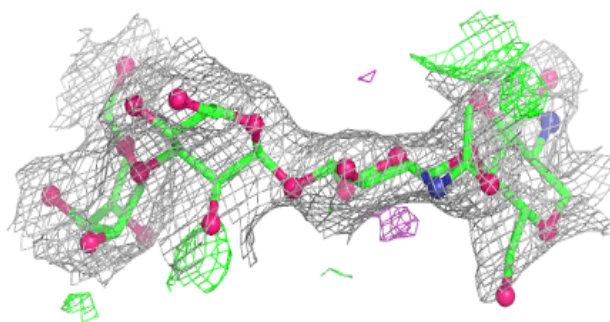
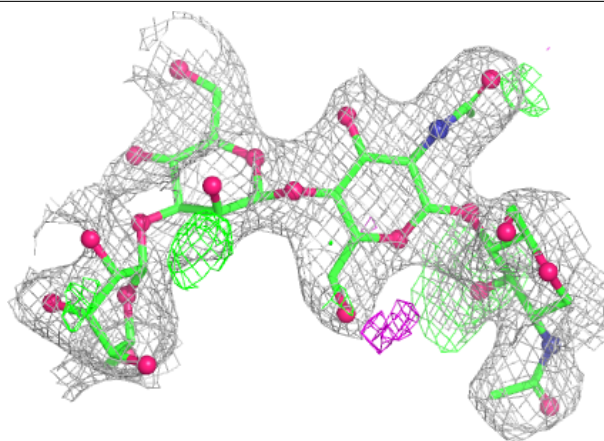
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	BMA	G	4	11/12	0.67	0.17	73,85,90,93	0
3	BMA	F	3	11/12	0.67	0.16	67,80,82,82	0
3	NAG	H	2	14/15	0.68	0.19	61,70,79,82	0
2	BMA	E	4	11/12	0.68	0.14	56,65,72,73	0
4	BMA	G	3	11/12	0.71	0.18	64,68,77,85	0
6	NAG	K	2	14/15	0.71	0.18	60,63,70,70	0
5	NAG	J	3	14/15	0.74	0.17	50,54,61,65	0
3	NAG	F	2	14/15	0.77	0.14	59,63,74,80	0
3	NAG	H	1	14/15	0.78	0.17	49,57,62,68	0
2	BMA	E	3	11/12	0.78	0.13	52,57,64,69	0
4	NAG	G	1	14/15	0.79	0.19	35,43,48,50	0
5	FUC	J	2	10/11	0.80	0.15	57,62,70,70	0
2	NAG	E	1	14/15	0.81	0.16	34,36,41,42	0
6	NAG	K	1	14/15	0.82	0.16	51,59,66,67	0
3	NAG	F	1	14/15	0.82	0.12	28,48,57,65	0
5	NAG	I	3	14/15	0.83	0.15	47,59,65,67	0
6	NAG	L	1	14/15	0.83	0.16	41,43,51,52	0
6	NAG	L	2	14/15	0.86	0.11	43,54,59,63	0
2	NAG	E	2	14/15	0.87	0.13	36,40,47,51	0
4	NAG	G	2	14/15	0.87	0.13	43,51,53,60	0
5	NAG	I	1	14/15	0.89	0.10	45,50,59,63	0
5	NAG	J	1	14/15	0.90	0.13	42,47,55,58	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.

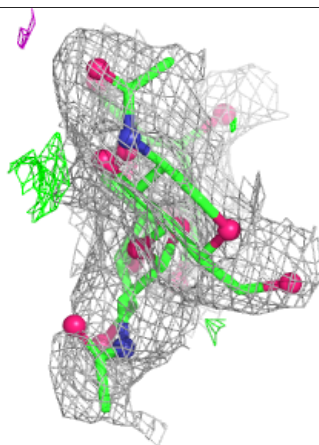
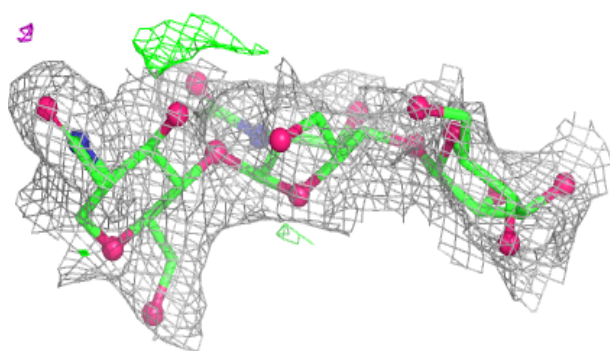
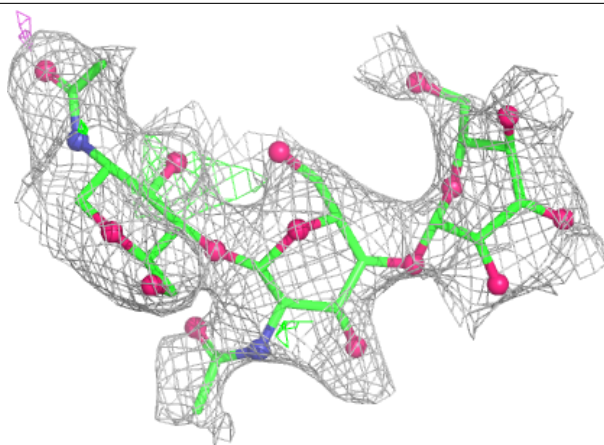
Electron density around Chain E:

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

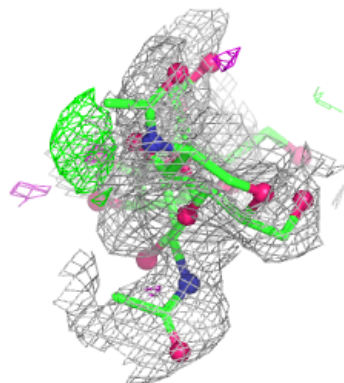
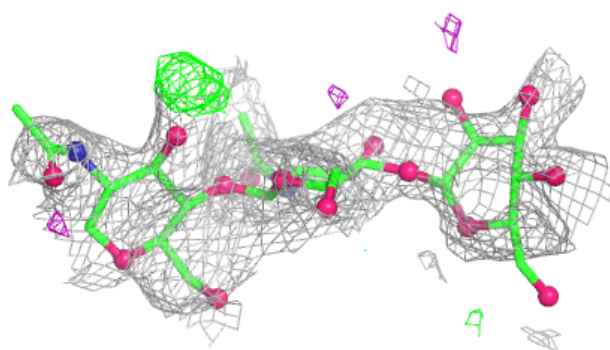
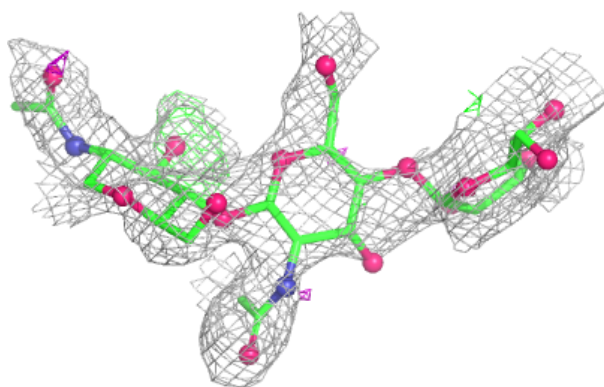


Electron density around Chain F:

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

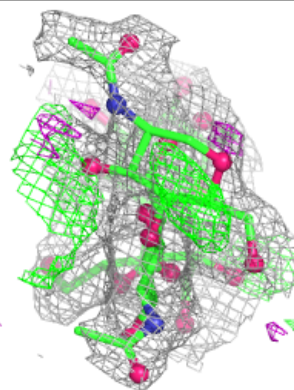
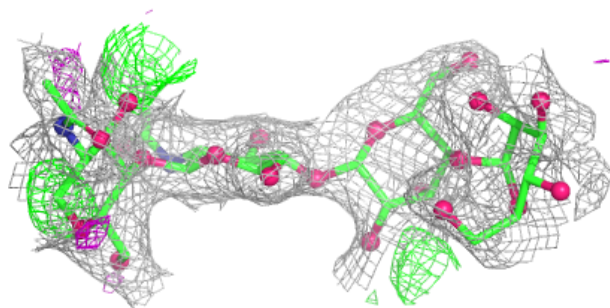
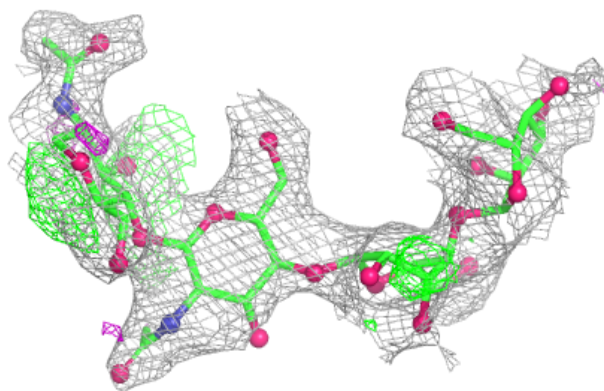
**Electron density around Chain H:**

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



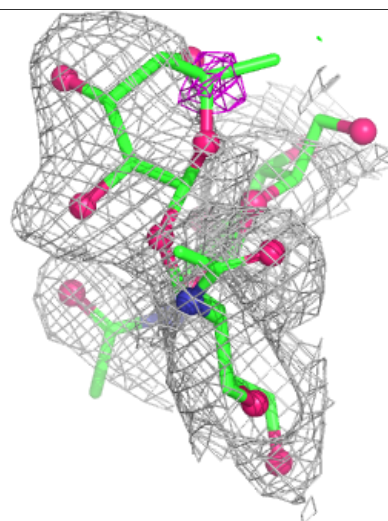
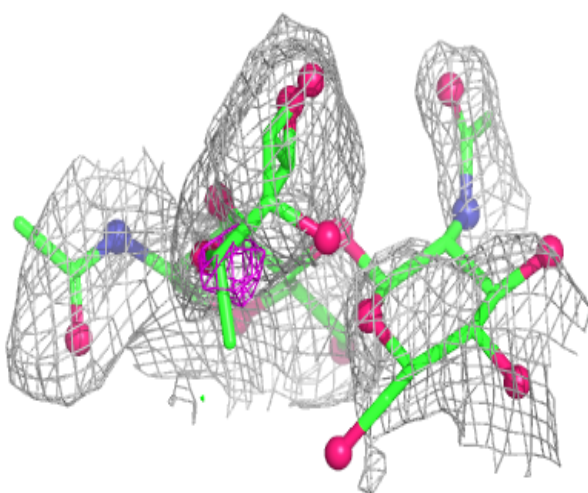
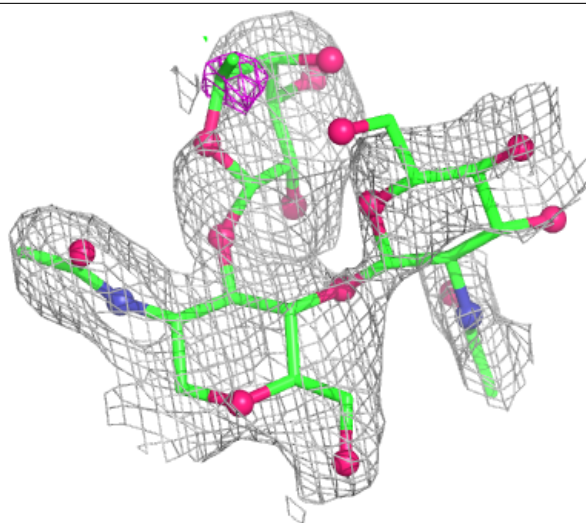
Electron density around Chain G:

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



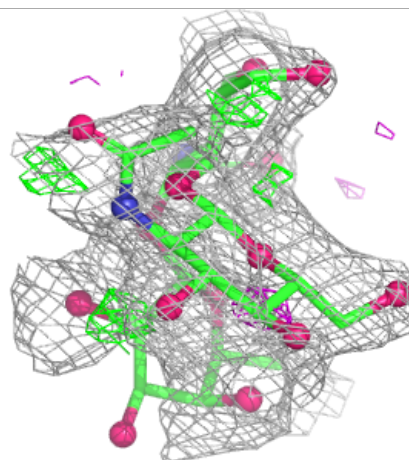
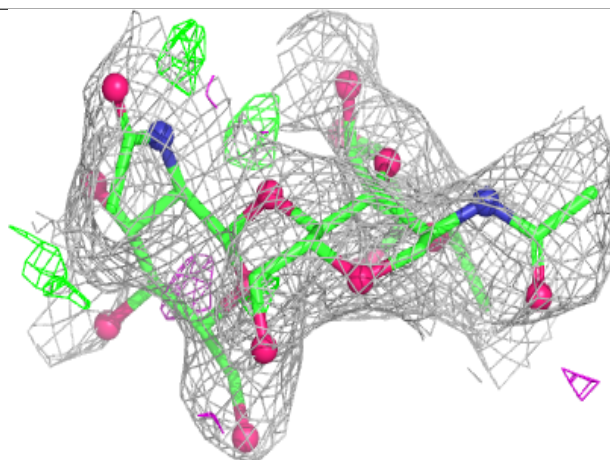
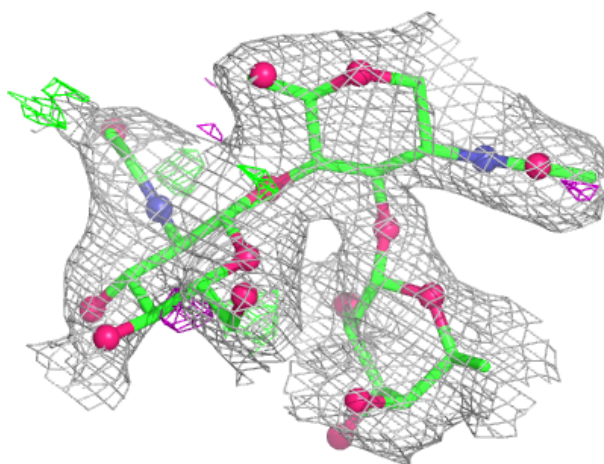
Electron density around Chain I:

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and green (positive)



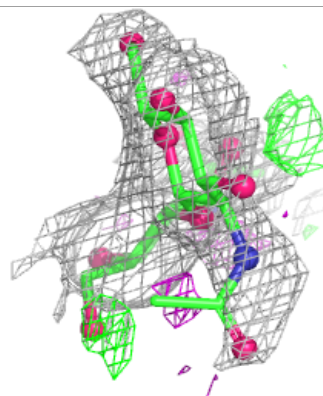
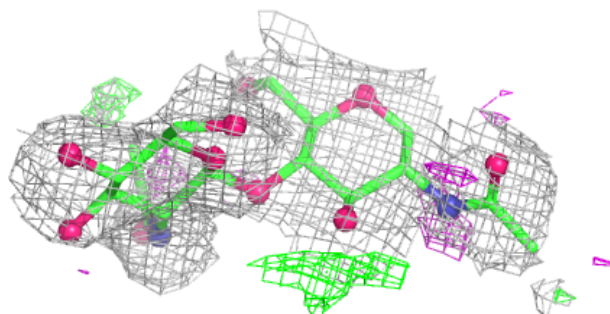
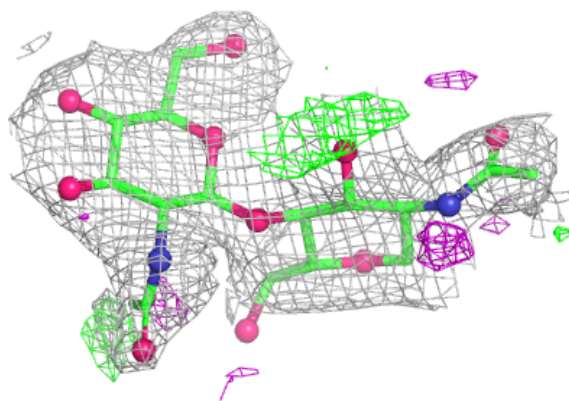
Electron density around Chain J:

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

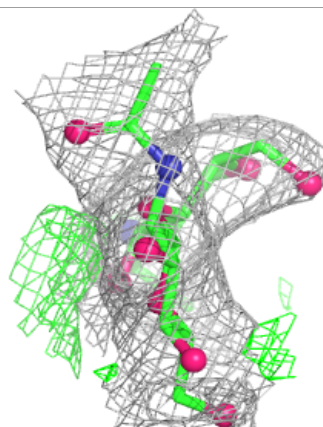
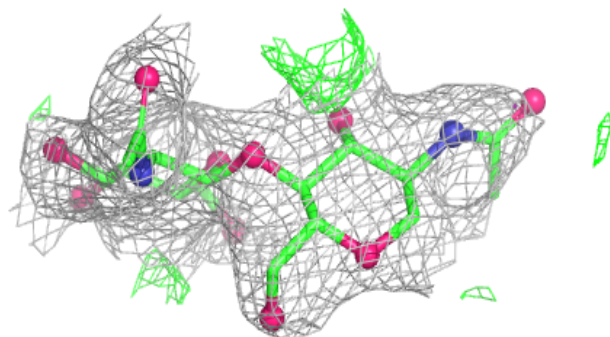
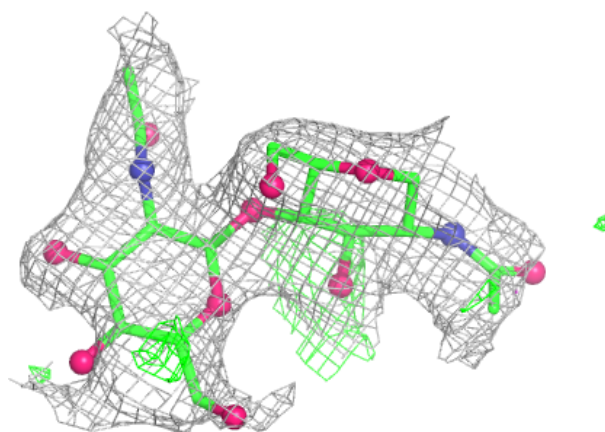


Electron density around Chain K:

$2mF_o-DF_c$ (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)



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
9	SO4	C	505	5/5	0.60	0.14	60,65,73,79	5
9	SO4	D	710	5/5	0.64	0.21	49,52,58,63	5
12	PGE	B	514	7/10	0.68	0.14	31,49,54,58	0
11	EDO	A	511	4/4	0.69	0.19	43,44,50,50	4
7	ZN	B	501	1/1	0.69	0.14	69,69,69,69	0
11	EDO	C	517	4/4	0.71	0.17	43,53,54,56	0
10	GOL	A	507[B]	6/6	0.73	0.22	39,43,45,46	6
10	GOL	A	507[A]	6/6	0.73	0.22	40,43,44,45	6
11	EDO	D	725	4/4	0.74	0.16	48,53,57,57	0
11	EDO	D	719	4/4	0.74	0.16	44,45,47,53	0
10	GOL	D	716	6/6	0.75	0.17	54,64,72,72	0
11	EDO	D	726	4/4	0.75	0.14	46,46,54,54	0
11	EDO	C	513	4/4	0.75	0.16	42,52,53,57	0
11	EDO	A	512	4/4	0.76	0.16	51,59,62,64	0
11	EDO	C	519	4/4	0.77	0.14	46,47,49,50	0
12	PGE	B	513	7/10	0.78	0.19	53,55,64,68	0
9	SO4	C	511	5/5	0.78	0.14	50,55,62,70	5
10	GOL	D	715	6/6	0.79	0.18	38,43,47,47	6
11	EDO	A	513	4/4	0.79	0.12	47,53,57,65	0
11	EDO	B	509	4/4	0.79	0.13	45,52,52,55	0
11	EDO	B	511	4/4	0.79	0.15	28,39,41,42	0
13	NAG	C	502	14/15	0.79	0.14	42,55,61,65	0
17	IPA	C	529	4/4	0.79	0.16	28,34,41,47	0
11	EDO	C	514	4/4	0.80	0.13	49,50,52,54	0
15	PG4	D	701	13/13	0.80	0.16	47,65,73,77	0
13	NAG	A	521	14/15	0.80	0.17	45,56,60,61	0
14	ANP	C	530	15/31	0.81	0.22	34,46,59,73	15
11	EDO	B	508	4/4	0.81	0.18	35,38,40,42	0
12	PGE	D	729	7/10	0.81	0.20	36,38,44,45	7
10	GOL	D	713	6/6	0.82	0.20	42,44,51,54	0
13	NAG	D	733	14/15	0.83	0.15	33,40,50,52	0
13	NAG	D	734	14/15	0.83	0.12	34,42,44,51	0
9	SO4	D	711	5/5	0.83	0.13	54,56,68,69	5
15	PG4	A	526	13/13	0.83	0.18	29,44,54,57	13
9	SO4	A	505	5/5	0.83	0.29	66,72,76,105	0
9	SO4	C	506	5/5	0.83	0.15	33,37,46,49	5
12	PGE	C	521	10/10	0.84	0.14	45,47,50,54	10

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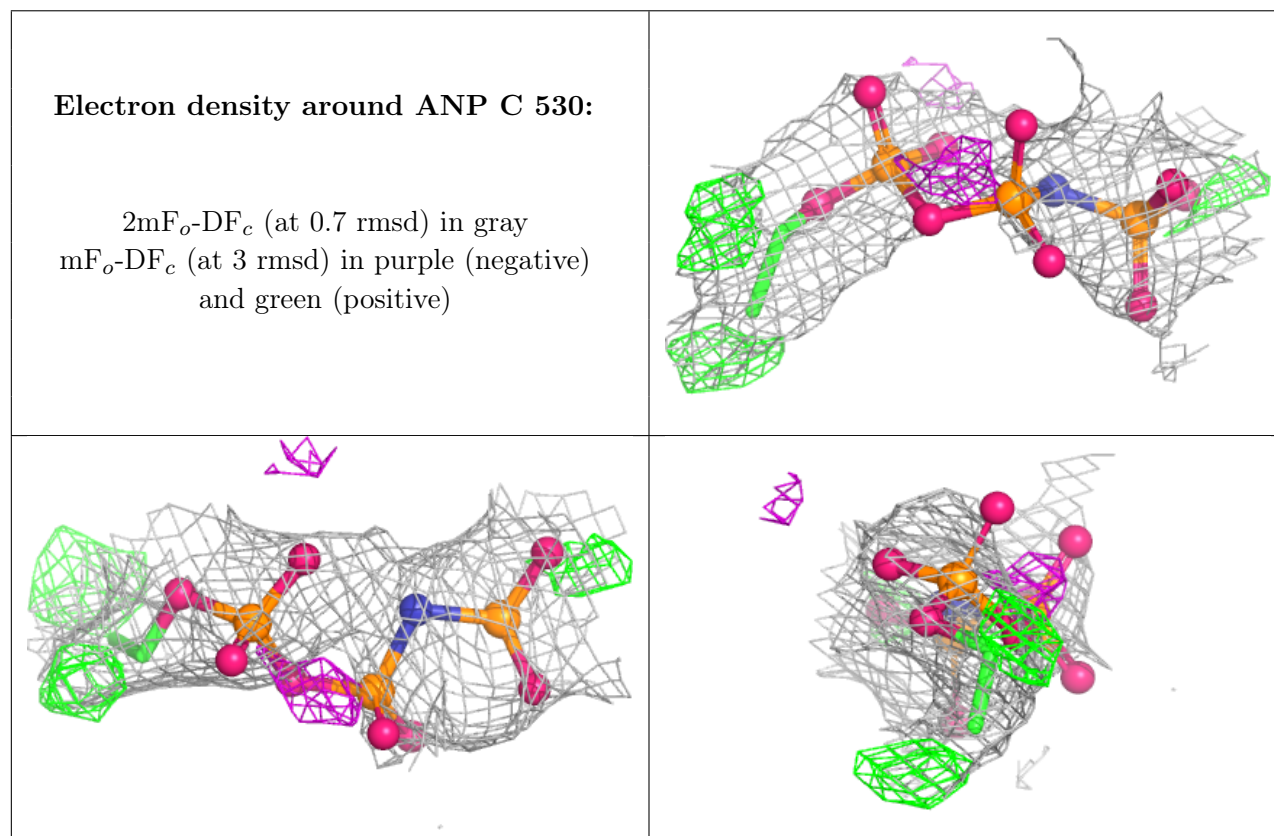
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
13	NAG	C	526	14/15	0.84	0.12	31,37,44,47	0
9	SO4	C	509	5/5	0.84	0.15	48,48,51,56	5
11	EDO	D	720	4/4	0.84	0.17	50,51,53,54	0
11	EDO	C	515	4/4	0.85	0.18	43,49,49,52	0
9	SO4	B	503	5/5	0.85	0.12	35,38,40,42	5
9	SO4	C	507	5/5	0.85	0.10	41,44,46,48	5
9	SO4	D	704	5/5	0.85	0.12	46,53,57,62	5
11	EDO	D	724	4/4	0.86	0.20	37,49,49,54	0
11	EDO	C	518	4/4	0.86	0.11	41,47,54,56	0
12	PGE	D	730	7/10	0.87	0.17	37,41,45,46	0
11	EDO	D	727	4/4	0.87	0.20	43,45,46,56	0
11	EDO	D	728	4/4	0.88	0.09	45,46,46,48	0
11	EDO	B	507	4/4	0.88	0.10	31,34,35,41	0
9	SO4	D	712	5/5	0.88	0.11	48,50,55,60	5
10	GOL	A	509	6/6	0.88	0.14	42,51,57,57	0
11	EDO	D	721	4/4	0.88	0.12	23,33,35,35	0
12	PGE	A	515	7/10	0.89	0.18	59,66,69,73	7
11	EDO	D	723	4/4	0.89	0.11	47,49,57,63	0
11	EDO	D	717	4/4	0.89	0.10	39,43,45,51	0
11	EDO	D	718	4/4	0.89	0.19	40,49,51,54	4
14	ANP	A	525	31/31	0.89	0.16	30,53,59,71	31
9	SO4	D	707	5/5	0.89	0.14	35,37,39,41	5
14	ANP	D	735	14/31	0.89	0.17	30,47,56,60	14
11	EDO	A	514	4/4	0.89	0.13	41,51,53,54	0
13	NAG	A	520	14/15	0.89	0.13	32,37,43,49	0
9	SO4	A	504	5/5	0.89	0.13	38,41,45,50	5
10	GOL	A	508	6/6	0.90	0.12	37,46,48,54	0
8	FE	B	502	1/1	0.90	0.08	37,37,37,37	1
9	SO4	C	510	5/5	0.90	0.10	46,53,55,56	5
10	GOL	D	714	6/6	0.90	0.12	34,35,35,37	6
9	SO4	B	504	5/5	0.90	0.16	34,41,46,48	5
9	SO4	C	501	5/5	0.90	0.18	30,31,38,38	5
9	SO4	C	508	5/5	0.90	0.11	45,45,52,53	5
9	SO4	D	706	5/5	0.91	0.12	38,39,43,48	5
9	SO4	B	506	5/5	0.91	0.11	47,51,55,57	5
9	SO4	D	709	5/5	0.91	0.15	40,41,44,44	5
11	EDO	B	510	4/4	0.92	0.14	48,49,51,51	0
13	NAG	B	522	14/15	0.92	0.09	32,40,46,47	0
9	SO4	D	705	5/5	0.92	0.10	40,46,46,49	5
16	NA	B	526	1/1	0.92	0.11	43,43,43,43	0
11	EDO	C	520	4/4	0.92	0.15	41,45,50,52	0
9	SO4	B	505	5/5	0.93	0.09	40,40,50,50	5

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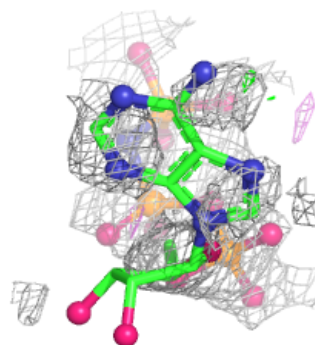
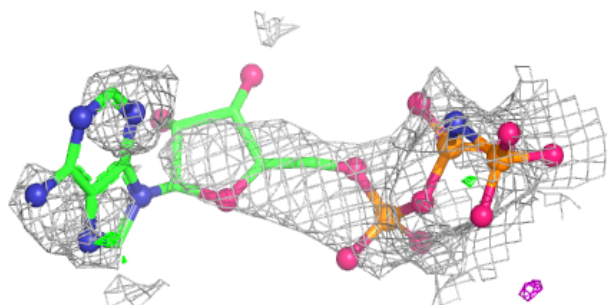
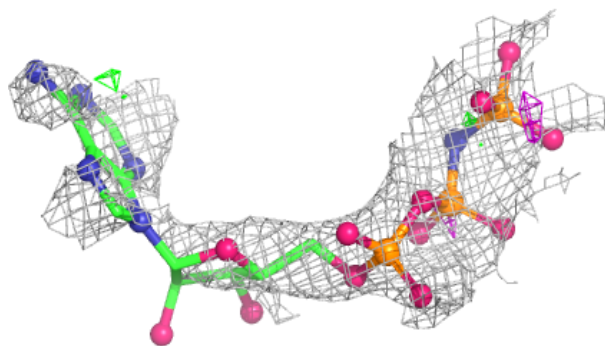
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
11	EDO	A	510	4/4	0.93	0.12	31,39,46,48	4
10	GOL	A	506	6/6	0.93	0.09	26,29,32,32	0
11	EDO	D	722	4/4	0.93	0.16	34,35,37,40	0
10	GOL	C	512	6/6	0.93	0.12	32,34,35,37	0
11	EDO	C	516	4/4	0.94	0.11	41,41,42,43	4
12	PGE	C	522	7/10	0.94	0.11	28,36,39,42	7
16	NA	C	531	1/1	0.94	0.07	29,29,29,29	0
9	SO4	D	708	5/5	0.94	0.10	37,44,47,49	5
16	NA	A	527	1/1	0.95	0.12	46,46,46,46	0
11	EDO	B	512	4/4	0.96	0.18	45,48,54,55	0
9	SO4	A	503	5/5	0.97	0.07	38,44,46,56	0
7	ZN	C	503	1/1	0.98	0.04	35,35,35,35	1
7	ZN	D	702	1/1	0.98	0.04	38,38,38,38	1
7	ZN	A	501	1/1	0.98	0.05	42,42,42,42	1
8	FE	C	504	1/1	0.98	0.06	33,33,33,33	1
8	FE	D	703	1/1	0.99	0.05	35,35,35,35	1
8	FE	A	502	1/1	1.00	0.03	30,30,30,30	1

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.

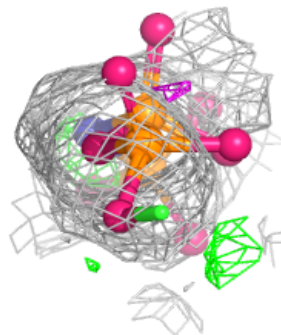
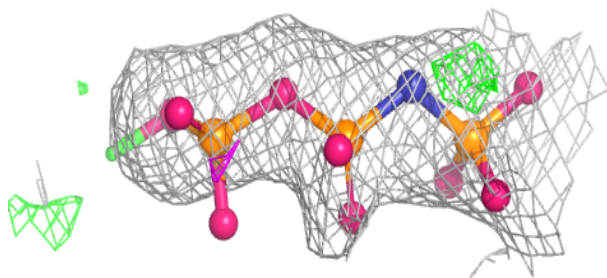
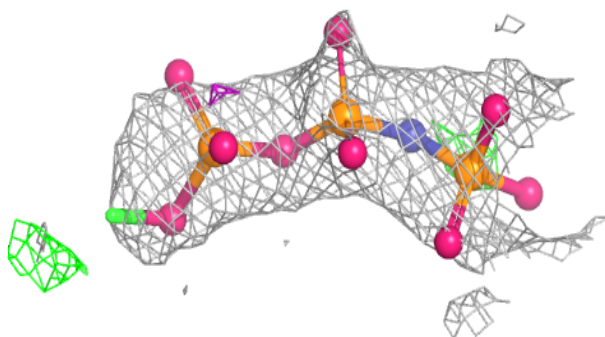


Electron density around ANP A 525:

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

**Electron density around ANP D 735:**

$2mF_o-DF_c$ (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.