



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 21, 2020 – 03:13 PM BST

PDB ID : 6VJ7
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 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

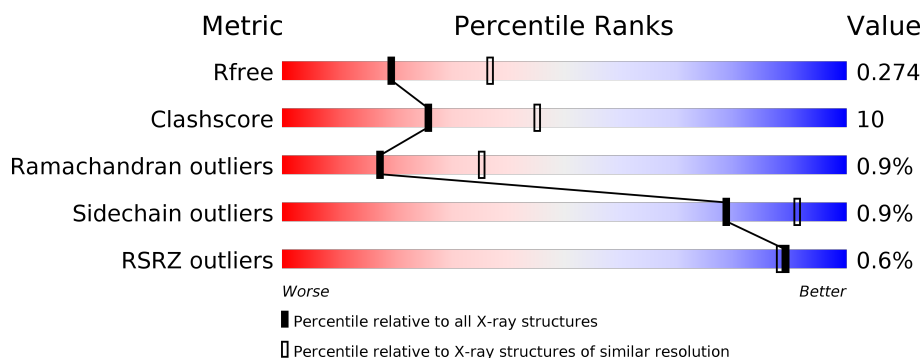
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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.



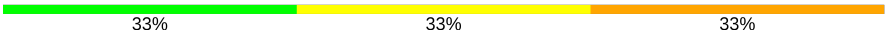

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 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	426	<div> <div>80%</div> <div>19%</div> <div>.</div> </div>
1	B	426	<div> <div>75%</div> <div>24%</div> </div>
1	C	426	<div> <div>81%</div> <div>18%</div> <div>.</div> </div>
1	D	426	<div> <div>%</div> <div>73%</div> <div>26%</div> <div>.</div> </div>
2	E	4	<div> <div>100%</div> </div>
3	F	3	<div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
3	H	3	 33% 67%
4	G	4	 25% 50% 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
11	EDO	A	511	-	-	-	X
12	PGE	D	730	-	-	X	-
4	BMA	G	4	-	-	-	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.

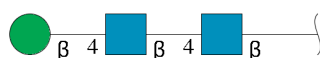
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	424	Total	C	N	O	S	0	2	0
			3506	2250	608	638	10			
1	B	425	Total	C	N	O	S	0	3	0
			3521	2260	611	640	10			
1	C	423	Total	C	N	O	S	0	0	0
			3482	2237	603	632	10			
1	D	426	Total	C	N	O	S	0	5	0
			3546	2275	618	642	11			

- 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.



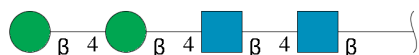
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	3	Total	C	N	O	0	0	0
			39	22	2	15			

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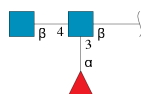
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	H	3	Total	C	N	O	0	0	0
			39	22	2	15			

- 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			

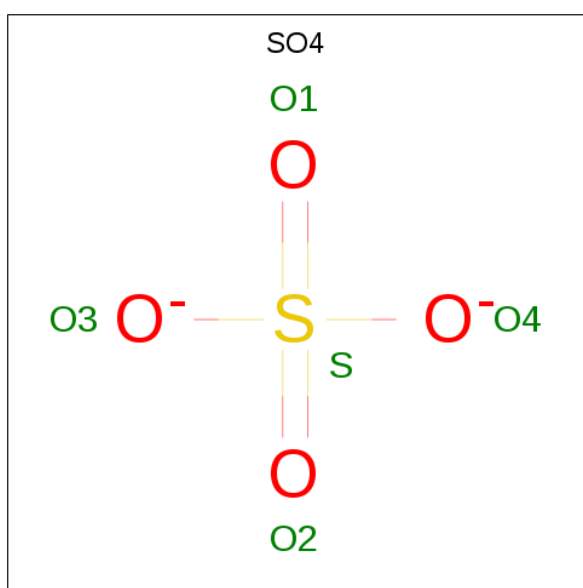
- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 8 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

- Molecule 9 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

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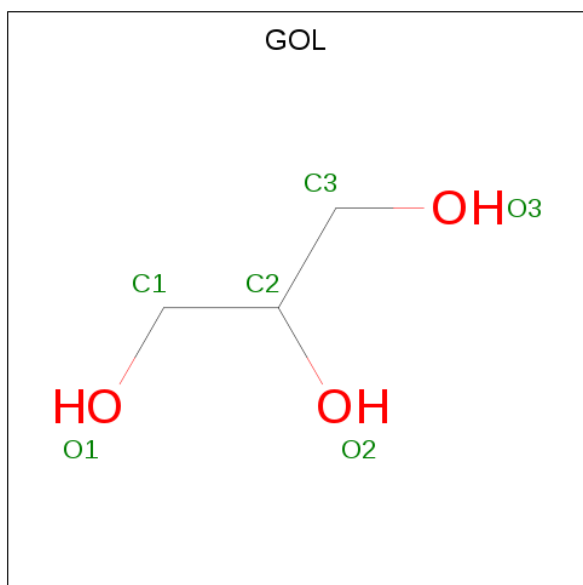
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	O	S	0	0
			5	4	1		
9	A	1	Total	O	S	0	0
			5	4	1		
9	B	1	Total	O	S	0	0
			5	4	1		
9	B	1	Total	O	S	0	0
			5	4	1		
9	B	1	Total	O	S	0	0
			5	4	1		
9	B	1	Total	O	S	0	0
			5	4	1		
9	C	1	Total	O	S	0	0
			5	4	1		
9	C	1	Total	O	S	0	0
			5	4	1		
9	C	1	Total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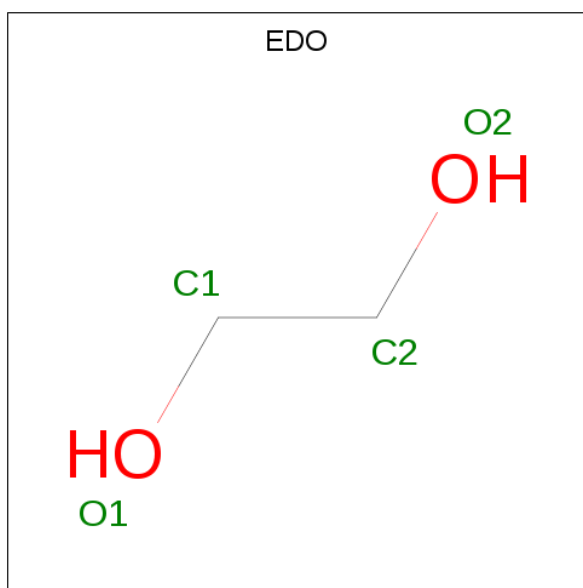
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	D	1	Total	O	S	0	0
			5	4	1		
9	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 10 is GLYCEROL (three-letter code: 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 (three-letter code: EDO) (formula: C₂H₆O₂).



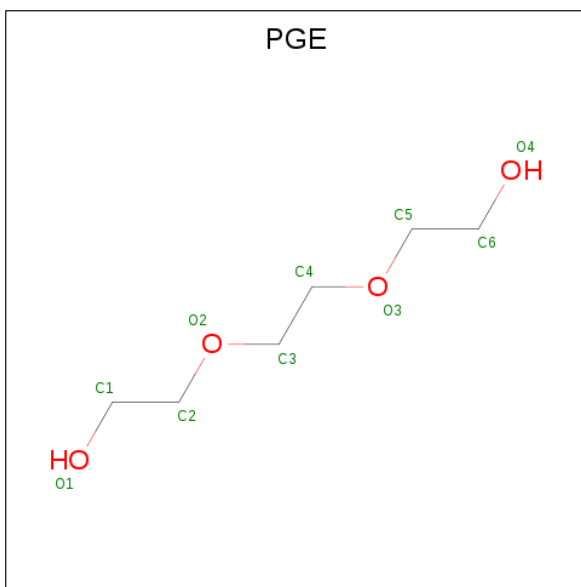
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	O	0	0
			4	2	2		
11	A	1	Total	C	O	0	0
			4	2	2		
11	A	1	Total	C	O	0	0
			4	2	2		
11	A	1	Total	C	O	0	0
			4	2	2		
11	A	1	Total	C	O	0	0
			4	2	2		
11	B	1	Total	C	O	0	0
			4	2	2		
11	B	1	Total	C	O	0	0
			4	2	2		
11	B	1	Total	C	O	0	0
			4	2	2		
11	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 (three-letter code: PGE) (formula: C₆H₁₄O₄).



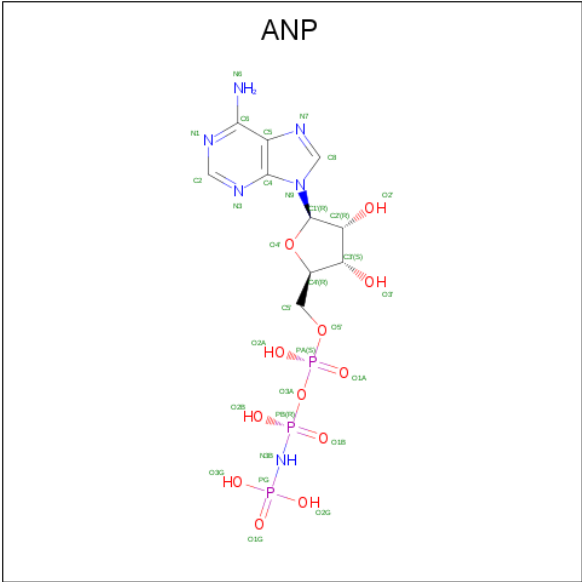
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	C	O	0	0
			7	4	3		
12	B	1	Total	C	O	0	0
			7	4	3		
12	B	1	Total	C	O	0	0
			7	4	3		
12	C	1	Total	C	O	0	0
			10	6	4		
12	C	1	Total	C	O	0	0
			7	4	3		
12	D	1	Total	C	O	0	0
			7	4	3		
12	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 13 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



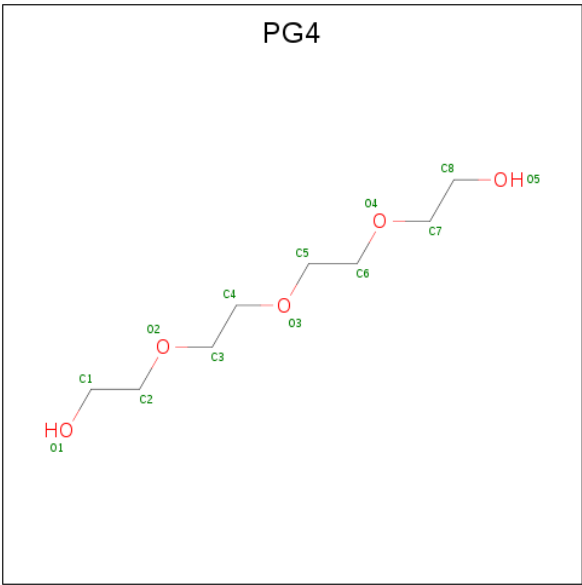
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	A	1	Total	C	N	O	0	0
			14	8	1	5		
13	A	1	Total	C	N	O	0	0
			14	8	1	5		
13	B	1	Total	C	N	O	0	0
			14	8	1	5		
13	C	1	Total	C	N	O	0	0
			14	8	1	5		
13	C	1	Total	C	N	O	0	0
			14	8	1	5		
13	D	1	Total	C	N	O	0	0
			14	8	1	5		
13	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 14 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: 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 (three-letter code: PG4) (formula: C₈H₁₈O₅).



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

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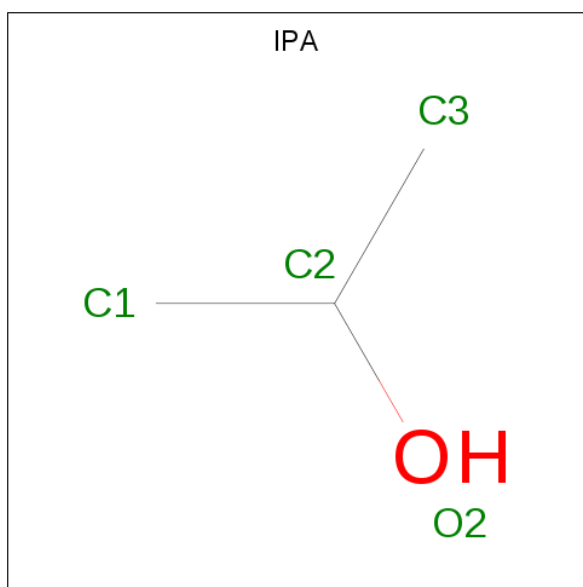
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	D	1	Total	C	O	0	0
			13	8	5		

- Molecule 16 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 17 is ISOPROPYL ALCOHOL (three-letter code: 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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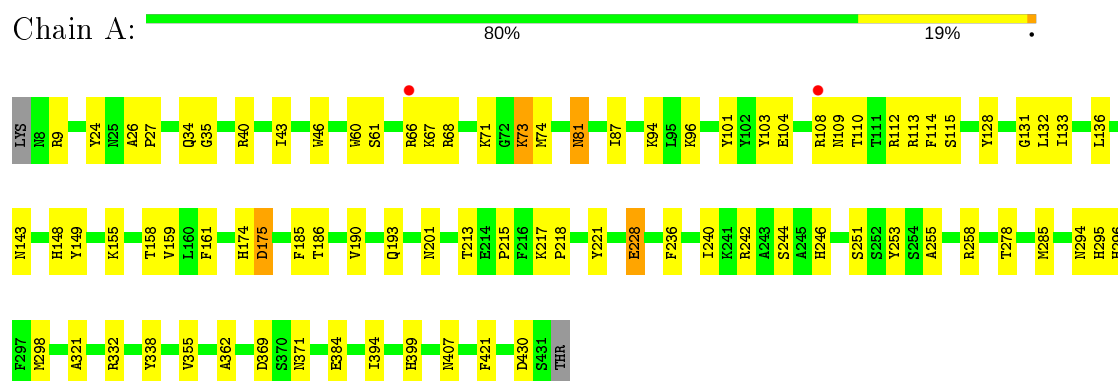
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	C	192	Total 192	O 192	0	0
18	D	192	Total 192	O 192	0	0

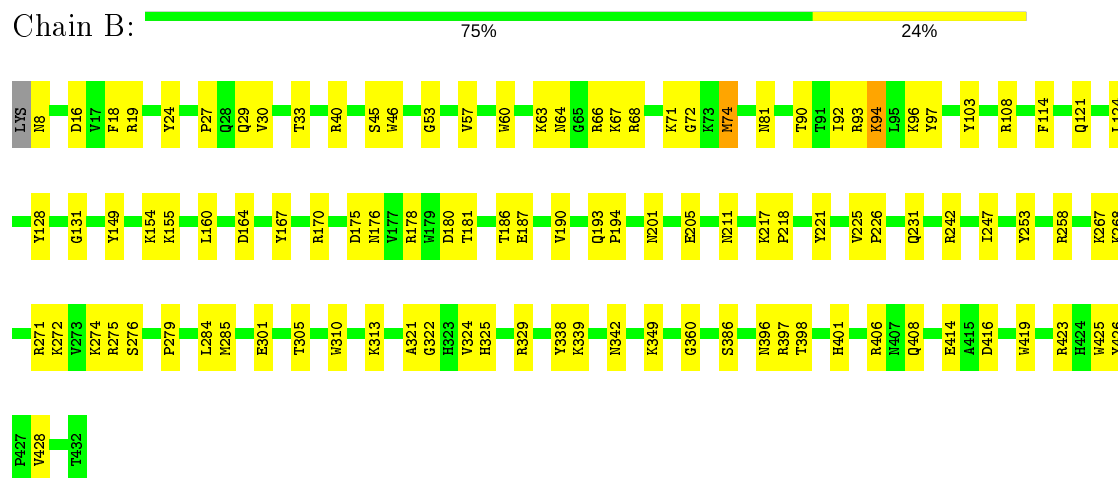
3 Residue-property plots

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.

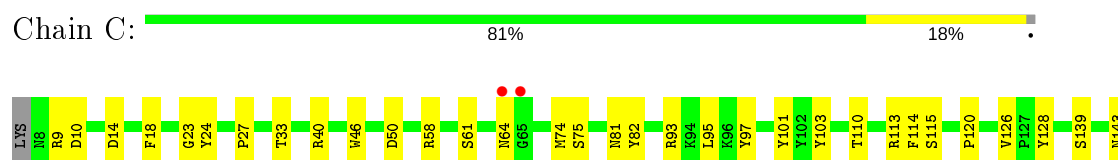
- Molecule 1: Fe(3+)-Zn(2+) purple acid phosphatase

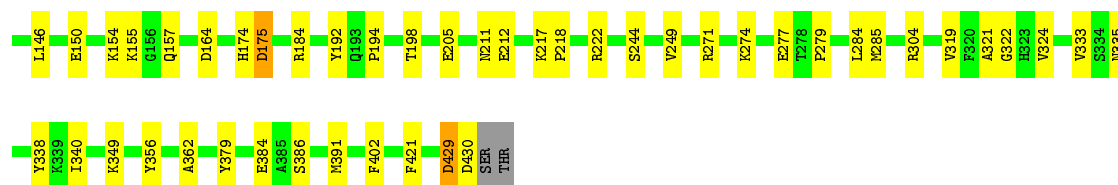


- Molecule 1: Fe(3+)-Zn(2+) purple acid phosphatase

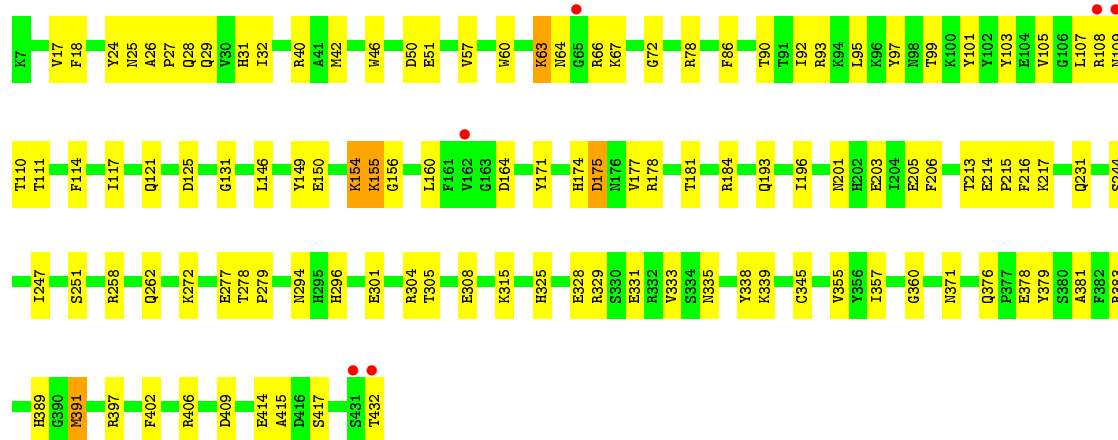


- Molecule 1: Fe(3+)-Zn(2+) purple acid phosphatase





- 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

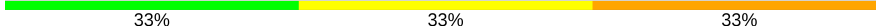


- Molecule 4: beta-D-mannopyranose-(1-4)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  25% 50% 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 I:  33% 33% 33%



- 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%



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

Chain K:  100%



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

Chain L:  100%



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) 74.9 (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	3261 reflections (5.14%)	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)	0.32 , 40.2	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, ZN, BMA, NAG, NA, SO4, EDO, PGE, PG4, IPA, ANP, FUC, FE

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	0.42	3/3628 (0.1%)	0.53	1/4933 (0.0%)
1	B	0.33	0/3643	0.50	0/4954
1	C	0.33	0/3601	0.50	0/4898
1	D	0.33	0/3674	0.52	0/4992
All	All	0.36	3/14546 (0.0%)	0.51	1/19777 (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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	228	GLU	CG-CD	9.64	1.66	1.51
1	A	81	ASN	CB-CG	5.83	1.64	1.51
1	A	228	GLU	CD-OE1	-5.67	1.19	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	81	ASN	CB-CA-C	5.16	120.72	110.40

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	65	0
1	B	3521	0	3337	77	0
1	C	3482	0	3291	55	0
1	D	3546	0	3371	95	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	6	0
13	A	28	0	26	7	0
13	B	14	0	13	1	0
13	C	28	0	26	3	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	9	0
18	C	192	0	0	8	0
18	D	192	0	0	11	0
All	All	15691	0	14075	304	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 10.

The worst 5 of 304 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%)	22	43
1	B	426/426 (100%)	396 (93%)	24 (6%)	6 (1%)	11	22
1	C	421/426 (99%)	397 (94%)	20 (5%)	4 (1%)	15	32
1	D	429/426 (101%)	394 (92%)	32 (8%)	3 (1%)	22	43
All	All	1700/1704 (100%)	1586 (93%)	98 (6%)	16 (1%)	17	35

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%)	371 (99%)	4 (1%)	73	88
1	B	377/375 (100%)	373 (99%)	4 (1%)	73	88
1	C	371/375 (99%)	368 (99%)	3 (1%)	81	92
1	D	380/375 (101%)	377 (99%)	3 (1%)	81	92
All	All	1503/1500 (100%)	1489 (99%)	14 (1%)	78	91

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	193	GLN
1	B	396	ASN
1	D	155	LYS
1	B	176	ASN
1	C	429	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	211	ASN
1	B	364	ASN
1	D	262	GLN
1	A	399	HIS
1	D	176	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

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	1,2	14,14,15	0.39	0	17,19,21	0.69	0
2	NAG	E	2	2	14,14,15	0.48	0	17,19,21	0.51	0
2	BMA	E	3	2	11,11,12	1.07	1 (9%)	15,15,17	2.50	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BMA	E	4	2	11,11,12	0.60	0	15,15,17	0.86	1 (6%)
3	NAG	F	1	1,3	14,14,15	0.44	0	17,19,21	1.14	1 (5%)
3	NAG	F	2	3	14,14,15	1.50	1 (7%)	17,19,21	1.68	1 (5%)
3	BMA	F	3	3	11,11,12	1.59	3 (27%)	15,15,17	1.49	3 (20%)
4	NAG	G	1	1,4	14,14,15	0.42	0	17,19,21	0.85	0
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	1.11	1 (9%)	15,15,17	1.08	1 (6%)
4	BMA	G	4	4	11,11,12	1.40	2 (18%)	15,15,17	2.49	6 (40%)
3	NAG	H	1	1,3	14,14,15	0.60	1 (7%)	17,19,21	0.53	0
3	NAG	H	2	3	14,14,15	0.37	0	17,19,21	0.73	0
3	BMA	H	3	3	11,11,12	1.62	3 (27%)	15,15,17	1.88	4 (26%)
5	NAG	I	1	1,5	14,14,15	0.47	0	17,19,21	1.56	2 (11%)
5	FUC	I	2	5	10,10,11	1.02	1 (10%)	14,14,16	1.64	3 (21%)
5	NAG	I	3	5	14,14,15	0.46	0	17,19,21	0.44	0
5	NAG	J	1	1,5	14,14,15	0.55	0	17,19,21	1.29	4 (23%)
5	FUC	J	2	5	10,10,11	1.17	1 (10%)	14,14,16	2.12	4 (28%)
5	NAG	J	3	5	14,14,15	0.28	0	17,19,21	1.23	2 (11%)
6	NAG	K	1	1,6	14,14,15	0.90	1 (7%)	17,19,21	0.92	1 (5%)
6	NAG	K	2	6	14,14,15	0.56	0	17,19,21	1.45	2 (11%)
6	NAG	L	1	1,6	14,14,15	0.49	0	17,19,21	0.54	0
6	NAG	L	2	6	14,14,15	0.40	0	17,19,21	0.36	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	1,2	-	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	1,3	-	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	1,4	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BMA	G	3	4	-	1/2/19/22	1/1/1/1
4	BMA	G	4	4	-	1/2/19/22	1/1/1/1
3	NAG	H	1	1,3	-	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	1,5	-	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	1,5	-	2/6/23/26	0/1/1/1
5	FUC	J	2	5	-	-	0/1/1/1
5	NAG	J	3	5	-	5/6/23/26	0/1/1/1
6	NAG	K	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	K	2	6	-	5/6/23/26	0/1/1/1
6	NAG	L	1	1,6	-	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 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	2	NAG	O5-C1	5.48	1.52	1.43
3	H	3	BMA	C1-C2	3.62	1.60	1.52
3	F	3	BMA	C2-C3	3.37	1.57	1.52
5	J	2	FUC	C1-C2	3.00	1.59	1.52
3	H	3	BMA	C2-C3	2.83	1.56	1.52

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	3	BMA	C1-O5-C5	8.28	123.41	112.19
4	G	4	BMA	C1-O5-C5	6.65	121.20	112.19
3	F	2	NAG	C1-O5-C5	6.45	120.93	112.19
6	K	2	NAG	C2-N2-C7	4.64	129.51	122.90
5	I	1	NAG	C1-O5-C5	4.59	118.41	112.19

There are no chirality outliers.

5 of 45 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

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Mol	Chain	Res	Type	Atoms
6	K	2	NAG	O5-C5-C6-O6
6	K	1	NAG	C4-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6

All (3) ring outliers are listed below:

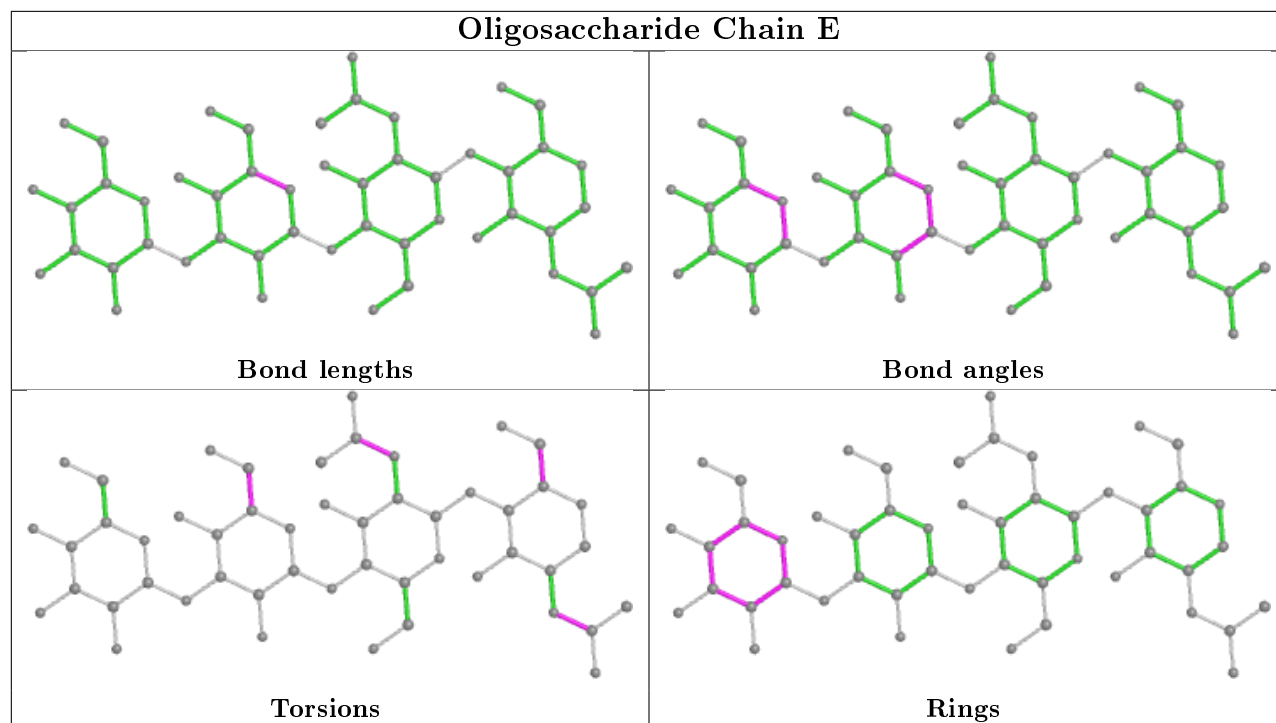
Mol	Chain	Res	Type	Atoms
4	G	4	BMA	C1-C2-C3-C4-C5-O5
4	G	3	BMA	C1-C2-C3-C4-C5-O5
2	E	4	BMA	C1-C2-C3-C4-C5-O5

8 monomers are involved in 11 short contacts:

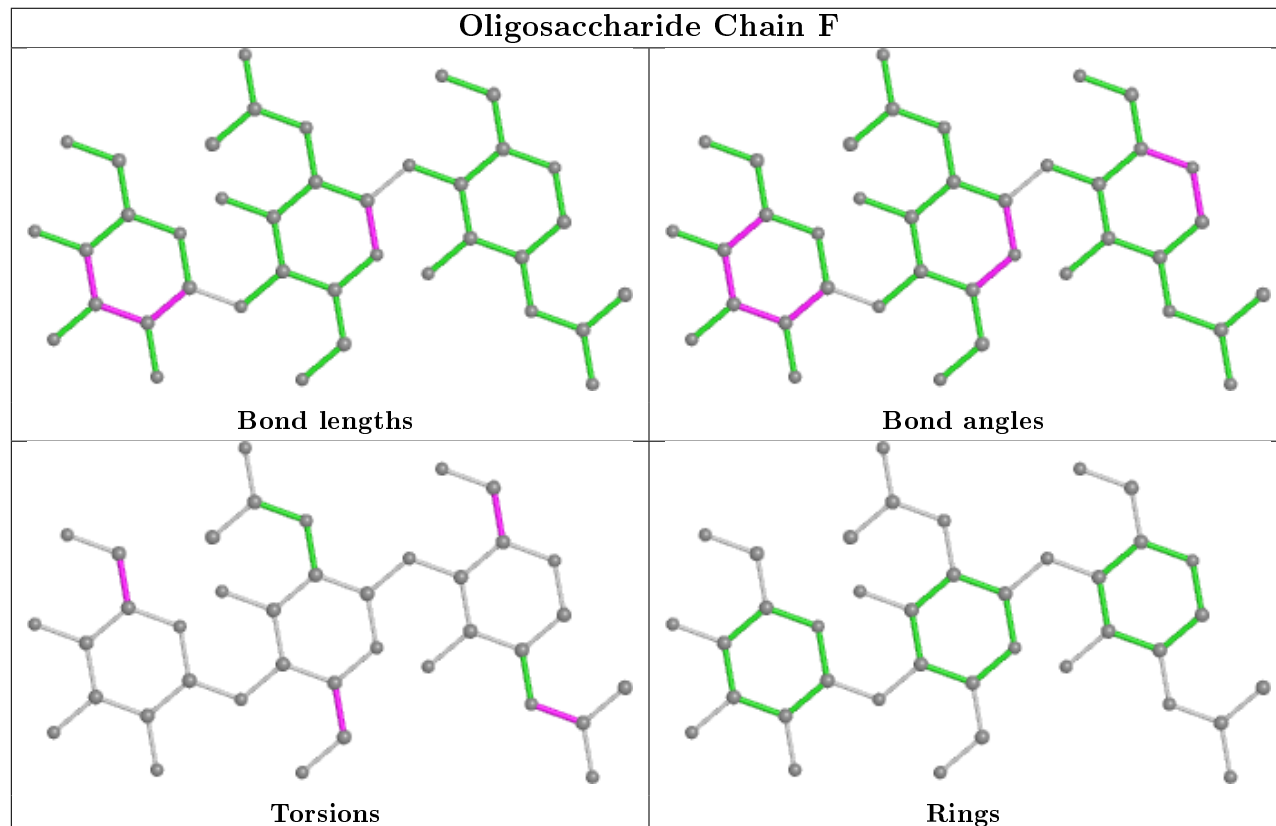
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	K	1	NAG	2	0
2	E	1	NAG	1	0
4	G	3	BMA	1	0
6	K	2	NAG	1	0
2	E	2	NAG	1	0
5	J	1	NAG	2	0
5	I	1	NAG	2	0
5	J	3	NAG	3	0

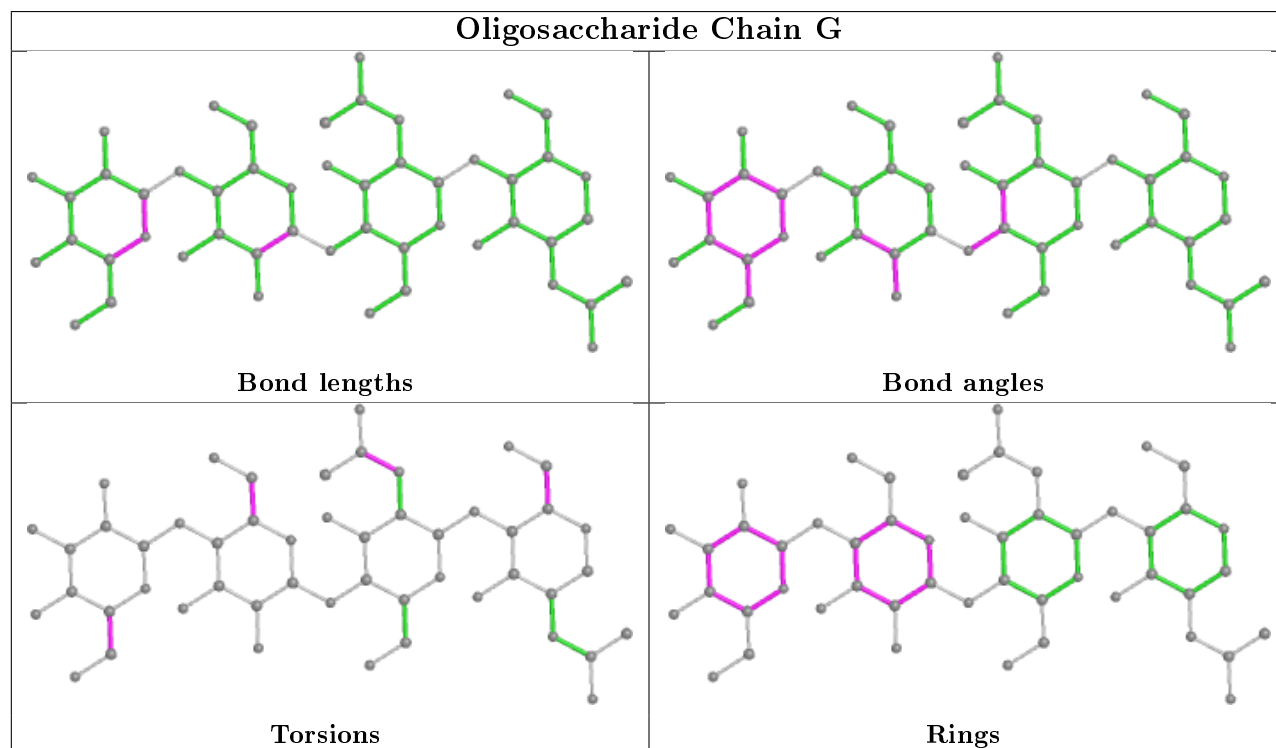
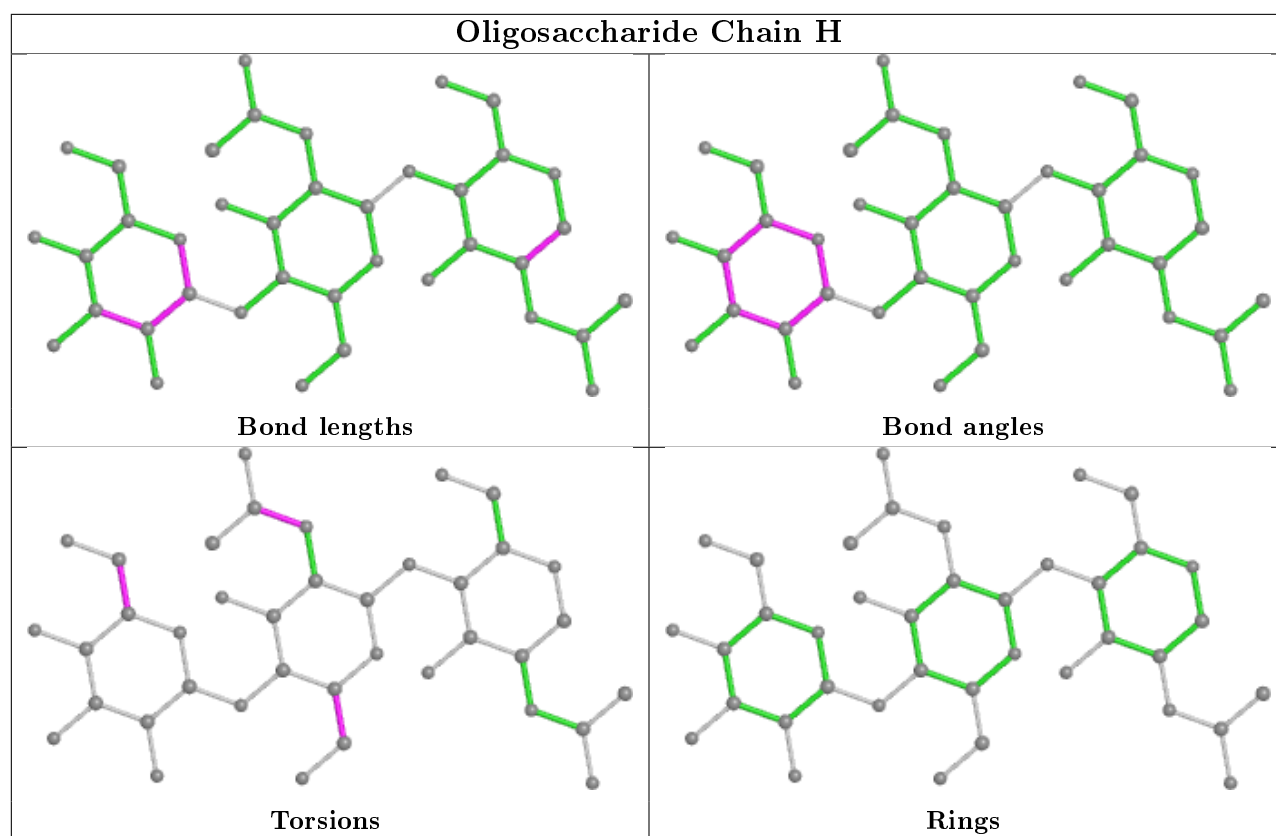
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

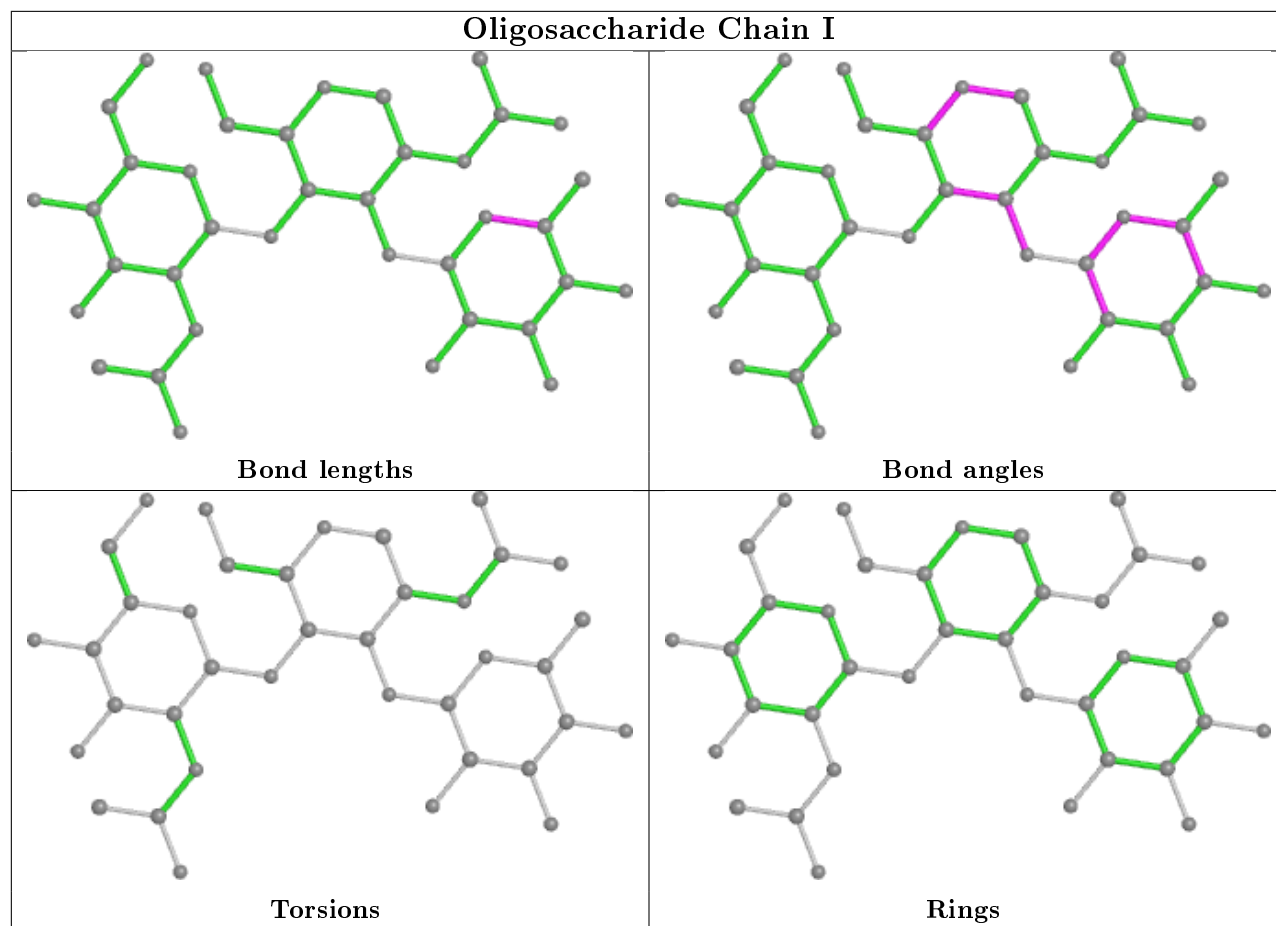
Oligosaccharide Chain E

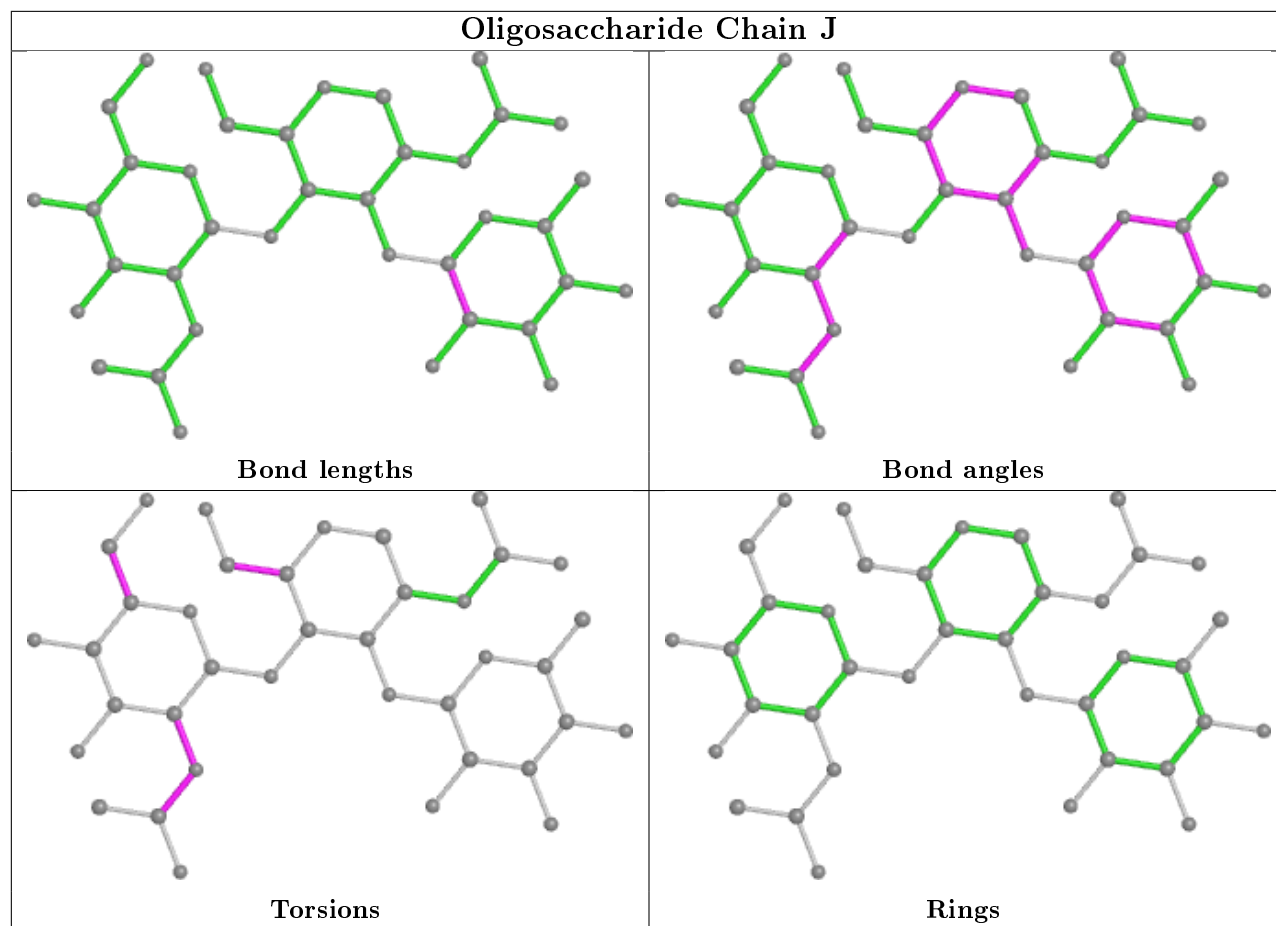


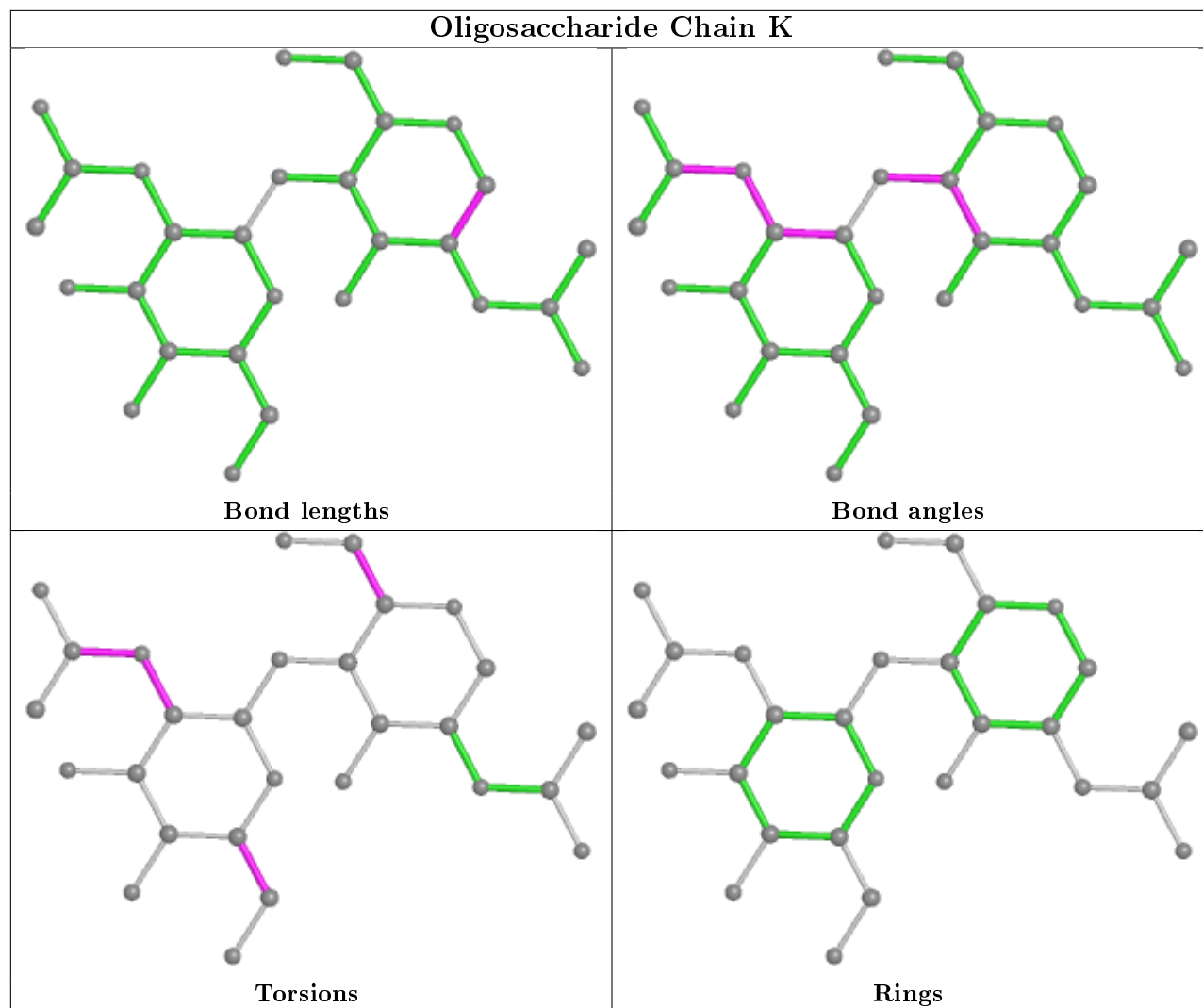
Oligosaccharide Chain F

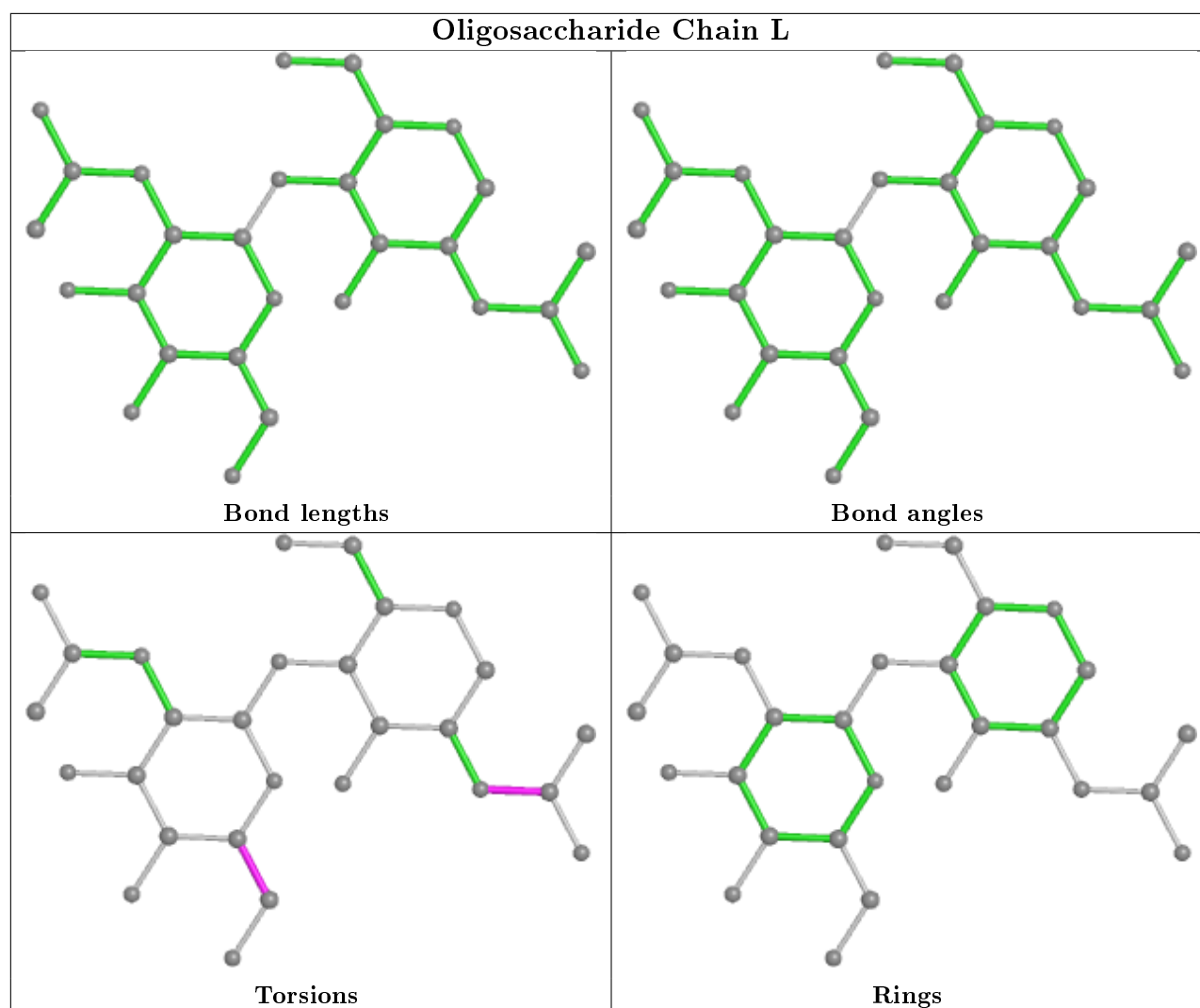












5.6 Ligand geometry [i](#)

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	$\# Z > 2$
11	EDO	A	513	-	3,3,3	0.63	0	2,2,2	0.47	0
9	SO4	A	505	-	4,4,4	0.47	0	6,6,6	0.42	0
11	EDO	D	717	-	3,3,3	0.51	0	2,2,2	0.29	0
15	PG4	A	526	-	12,12,12	0.44	0	11,11,11	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	SO4	D	704	-	4,4,4	0.15	0	6,6,6	0.07	0
11	EDO	A	512	-	3,3,3	0.70	0	2,2,2	0.28	0
9	SO4	D	710	-	4,4,4	0.12	0	6,6,6	0.20	0
9	SO4	D	708	-	4,4,4	0.10	0	6,6,6	0.12	0
11	EDO	B	509	-	3,3,3	0.51	0	2,2,2	0.16	0
10	GOL	C	512	-	5,5,5	0.86	0	5,5,5	1.02	0
11	EDO	C	515	-	3,3,3	0.53	0	2,2,2	0.29	0
11	EDO	A	511	-	3,3,3	0.54	0	2,2,2	0.27	0
11	EDO	B	512	-	3,3,3	0.53	0	2,2,2	0.34	0
11	EDO	D	724	-	3,3,3	0.72	0	2,2,2	0.20	0
11	EDO	D	725	-	3,3,3	0.68	0	2,2,2	0.28	0
11	EDO	A	510	-	3,3,3	0.53	0	2,2,2	0.22	0
9	SO4	C	510	-	4,4,4	0.12	0	6,6,6	0.10	0
11	EDO	A	514	-	3,3,3	0.70	0	2,2,2	0.33	0
13	NAG	D	733	1	14,14,15	0.96	1 (7%)	17,19,21	1.91	5 (29%)
10	GOL	A	508	-	5,5,5	1.31	1 (20%)	5,5,5	0.88	0
11	EDO	C	517	-	3,3,3	0.66	0	2,2,2	0.33	0
9	SO4	B	506	-	4,4,4	0.13	0	6,6,6	0.08	0
13	NAG	B	522	1	14,14,15	0.25	0	17,19,21	0.36	0
9	SO4	C	506	-	4,4,4	0.16	0	6,6,6	0.10	0
9	SO4	C	511	-	4,4,4	0.13	0	6,6,6	0.12	0
11	EDO	D	722	-	3,3,3	0.42	0	2,2,2	0.32	0
9	SO4	D	712	-	4,4,4	0.15	0	6,6,6	0.09	0
12	PGE	B	513	-	6,6,9	0.30	0	5,5,8	0.43	0
11	EDO	C	516	-	3,3,3	0.45	0	2,2,2	0.35	0
12	PGE	B	514	-	6,6,9	0.44	0	5,5,8	0.44	0
11	EDO	D	720	-	3,3,3	0.53	0	2,2,2	0.26	0
14	ANP	C	530	8,7	13,14,33	2.68	4 (30%)	14,22,52	2.06	3 (21%)
9	SO4	A	503	-	4,4,4	0.14	0	6,6,6	0.15	0
9	SO4	D	706	-	4,4,4	0.12	0	6,6,6	0.19	0
11	EDO	C	519	-	3,3,3	0.66	0	2,2,2	0.28	0
11	EDO	D	728	-	3,3,3	0.58	0	2,2,2	0.37	0
11	EDO	C	520	-	3,3,3	0.71	0	2,2,2	0.04	0
10	GOL	D	713	-	5,5,5	0.92	0	5,5,5	0.78	0
9	SO4	B	505	-	4,4,4	0.14	0	6,6,6	0.16	0
11	EDO	D	726	-	3,3,3	0.69	0	2,2,2	0.40	0
14	ANP	A	525	8,7	29,33,33	2.03	6 (20%)	31,52,52	1.70	5 (16%)
9	SO4	C	505	-	4,4,4	0.15	0	6,6,6	0.07	0
10	GOL	A	509	-	5,5,5	1.13	0	5,5,5	0.94	0
11	EDO	D	727	-	3,3,3	0.54	0	2,2,2	0.81	0
13	NAG	D	734	1	14,14,15	0.45	0	17,19,21	0.74	1 (5%)
11	EDO	D	718	-	3,3,3	0.50	0	2,2,2	0.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	SO4	B	504	-	4,4,4	0.13	0	6,6,6	0.16	0
10	GOL	D	715	-	5,5,5	0.92	0	5,5,5	1.03	0
12	PGE	D	729	-	6,6,9	0.26	0	5,5,8	0.70	0
10	GOL	D	716	-	5,5,5	0.89	0	5,5,5	1.00	0
12	PGE	C	522	-	6,6,9	0.31	0	5,5,8	0.26	0
12	PGE	D	730	-	6,6,9	0.56	0	5,5,8	0.56	0
11	EDO	D	719	-	3,3,3	0.45	0	2,2,2	0.53	0
9	SO4	D	707	-	4,4,4	0.15	0	6,6,6	0.24	0
17	IPA	C	529	-	3,3,3	0.56	0	3,3,3	0.23	0
11	EDO	C	514	-	3,3,3	0.48	0	2,2,2	0.43	0
14	ANP	D	735	8,7	12,13,33	2.94	4 (33%)	14,21,52	1.83	4 (28%)
9	SO4	C	507	-	4,4,4	0.16	0	6,6,6	0.12	0
13	NAG	C	502	1	14,14,15	2.18	2 (14%)	17,19,21	2.31	1 (5%)
11	EDO	B	508	-	3,3,3	0.59	0	2,2,2	0.15	0
13	NAG	C	526	1	14,14,15	0.30	0	17,19,21	0.65	1 (5%)
10	GOL	D	714	-	5,5,5	0.82	0	5,5,5	1.02	0
10	GOL	A	507[B]	-	5,5,5	0.85	0	5,5,5	1.05	0
9	SO4	D	705	-	4,4,4	0.16	0	6,6,6	0.16	0
9	SO4	D	711	-	4,4,4	0.14	0	6,6,6	0.07	0
10	GOL	A	507[A]	-	5,5,5	0.97	0	5,5,5	0.98	0
9	SO4	C	501	16	4,4,4	0.22	0	6,6,6	0.34	0
9	SO4	D	709	-	4,4,4	0.16	0	6,6,6	0.08	0
9	SO4	C	509	-	4,4,4	0.15	0	6,6,6	0.12	0
11	EDO	B	507	-	3,3,3	0.48	0	2,2,2	0.42	0
11	EDO	B	511	-	3,3,3	0.53	0	2,2,2	0.17	0
9	SO4	C	508	-	4,4,4	0.15	0	6,6,6	0.10	0
12	PGE	C	521	-	9,9,9	0.34	0	8,8,8	0.23	0
13	NAG	A	521	-	14,14,15	1.69	3 (21%)	17,19,21	1.36	3 (17%)
11	EDO	B	510	-	3,3,3	0.49	0	2,2,2	0.28	0
13	NAG	A	520	1	14,14,15	0.38	0	17,19,21	0.56	0
11	EDO	D	723	-	3,3,3	0.72	0	2,2,2	0.53	0
9	SO4	A	504	-	4,4,4	0.16	0	6,6,6	0.12	0
9	SO4	B	503	-	4,4,4	0.14	0	6,6,6	0.17	0
10	GOL	A	506	-	5,5,5	1.01	0	5,5,5	0.89	0
11	EDO	C	518	-	3,3,3	0.68	0	2,2,2	0.56	0
12	PGE	A	515	-	6,6,9	0.29	0	5,5,8	0.30	0
15	PG4	D	701	-	12,12,12	0.47	0	11,11,11	0.38	0
11	EDO	C	513	-	3,3,3	0.54	0	2,2,2	0.28	0
11	EDO	D	721	-	3,3,3	0.54	0	2,2,2	0.53	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
11	EDO	A	513	-	-	1/1/1/1	-
12	PGE	B	513	-	-	2/4/4/7	-
11	EDO	D	717	-	-	0/1/1/1	-
15	PG4	A	526	-	-	3/10/10/10	-
11	EDO	D	726	-	-	0/1/1/1	-
11	EDO	B	509	-	-	0/1/1/1	-
11	EDO	C	515	-	-	1/1/1/1	-
11	EDO	A	511	-	-	0/1/1/1	-
11	EDO	B	512	-	-	0/1/1/1	-
11	EDO	D	724	-	-	1/1/1/1	-
11	EDO	A	510	-	-	0/1/1/1	-
11	EDO	A	514	-	-	1/1/1/1	-
13	NAG	D	733	1	-	3/6/23/26	0/1/1/1
10	GOL	A	508	-	-	4/4/4/4	-
11	EDO	C	517	-	-	1/1/1/1	-
11	EDO	D	719	-	-	1/1/1/1	-
13	NAG	B	522	1	-	2/6/23/26	0/1/1/1
11	EDO	B	510	-	-	0/1/1/1	-
11	EDO	D	722	-	-	1/1/1/1	-
11	EDO	B	511	-	-	1/1/1/1	-
11	EDO	C	516	-	-	0/1/1/1	-
12	PGE	B	514	-	-	2/4/4/7	-
11	EDO	D	720	-	-	0/1/1/1	-
14	ANP	C	530	8,7	-	1/12/16/38	-
11	EDO	C	519	-	-	1/1/1/1	-
11	EDO	D	728	-	-	1/1/1/1	-
11	EDO	C	520	-	-	0/1/1/1	-
10	GOL	D	713	-	-	2/4/4/4	-
11	EDO	D	723	-	-	0/1/1/1	-
14	ANP	A	525	8,7	-	3/14/38/38	0/3/3/3
10	GOL	A	509	-	-	1/4/4/4	-
13	NAG	D	734	1	-	2/6/23/26	0/1/1/1
11	EDO	D	718	-	-	0/1/1/1	-
10	GOL	D	715	-	-	2/4/4/4	-
11	EDO	D	727	-	-	1/1/1/1	-
10	GOL	D	716	-	-	1/4/4/4	-
12	PGE	C	522	-	-	1/4/4/7	-
12	PGE	D	730	-	-	1/4/4/7	-
11	EDO	A	512	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	EDO	D	725	-	-	1/1/1/1	-
11	EDO	C	514	-	-	0/1/1/1	-
14	ANP	D	735	8,7	-	1/11/15/38	-
13	NAG	C	502	1	-	2/6/23/26	0/1/1/1
11	EDO	B	508	-	-	0/1/1/1	-
13	NAG	C	526	1	-	2/6/23/26	0/1/1/1
10	GOL	D	714	-	-	2/4/4/4	-
10	GOL	A	507[B]	-	-	2/4/4/4	-
12	PGE	D	729	-	-	1/4/4/7	-
10	GOL	A	507[A]	-	-	2/4/4/4	-
11	EDO	B	507	-	-	1/1/1/1	-
12	PGE	C	521	-	-	4/7/7/7	-
13	NAG	A	521	-	-	2/6/23/26	0/1/1/1
12	PGE	A	515	-	-	3/4/4/7	-
13	NAG	A	520	1	-	2/6/23/26	0/1/1/1
10	GOL	C	512	-	-	4/4/4/4	-
10	GOL	A	506	-	-	0/4/4/4	-
11	EDO	C	518	-	-	0/1/1/1	-
15	PG4	D	701	-	-	5/10/10/10	-
11	EDO	C	513	-	-	0/1/1/1	-
11	EDO	D	721	-	-	0/1/1/1	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	502	NAG	O5-C1	7.47	1.55	1.43
14	D	735	ANP	PG-O1G	6.98	1.57	1.46
14	A	525	ANP	PG-O1G	6.57	1.56	1.46
14	C	530	ANP	PG-O1G	6.18	1.56	1.46
14	C	530	ANP	PB-O1B	5.97	1.55	1.46

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	C	502	NAG	C1-O5-C5	8.73	124.02	112.19
14	C	530	ANP	PA-O3A-PB	-6.05	111.30	132.62
13	D	733	NAG	C1-O5-C5	5.25	119.30	112.19
14	D	735	ANP	PA-O3A-PB	-4.80	115.72	132.62
14	A	525	ANP	PA-O3A-PB	-4.63	116.29	132.62

There are no chirality outliers.

5 of 76 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	C	530	ANP	PG-N3B-PB-O1B
10	D	713	GOL	C1-C2-C3-O3
10	D	713	GOL	O2-C2-C3-O3
10	C	512	GOL	O1-C1-C2-C3
14	A	525	ANP	C3'-C4'-C5'-O5'

There are no ring outliers.

35 monomers are involved in 57 short contacts:

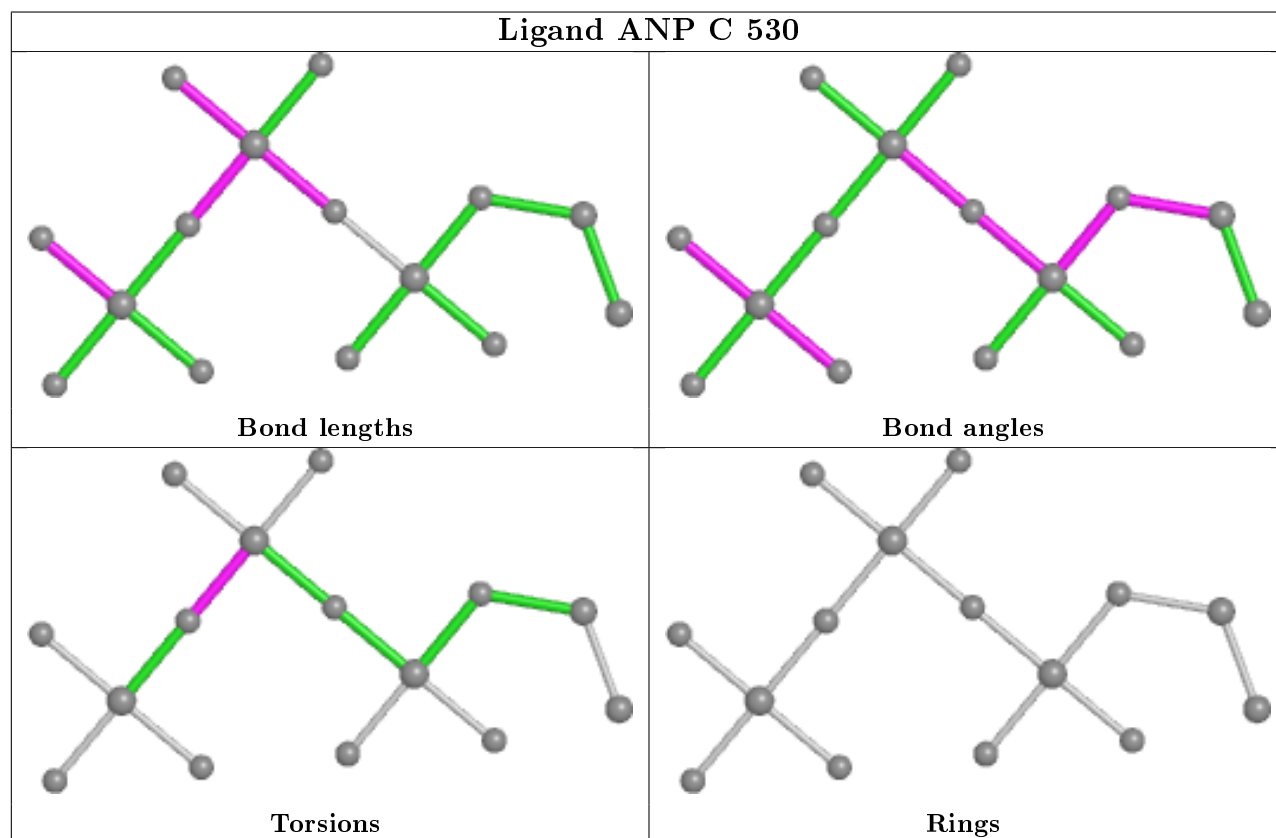
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	505	SO4	1	0
15	A	526	PG4	1	0
11	B	512	EDO	2	0
11	D	724	EDO	3	0
11	A	510	EDO	1	0
9	C	510	SO4	1	0
10	A	508	GOL	1	0
11	C	517	EDO	2	0
13	B	522	NAG	1	0
11	D	722	EDO	1	0
12	B	514	PGE	1	0
14	C	530	ANP	1	0
11	C	520	EDO	2	0
10	D	713	GOL	3	0
14	A	525	ANP	5	0
10	A	509	GOL	1	0
11	D	727	EDO	2	0
10	D	715	GOL	2	0
12	D	730	PGE	6	0
17	C	529	IPA	1	0
14	D	735	ANP	4	0
9	C	507	SO4	1	0
13	C	502	NAG	2	0
13	C	526	NAG	1	0
10	D	714	GOL	1	0
10	A	507[B]	GOL	1	0
9	C	501	SO4	1	0
9	D	709	SO4	1	0
11	B	511	EDO	1	0
12	C	521	PGE	1	0

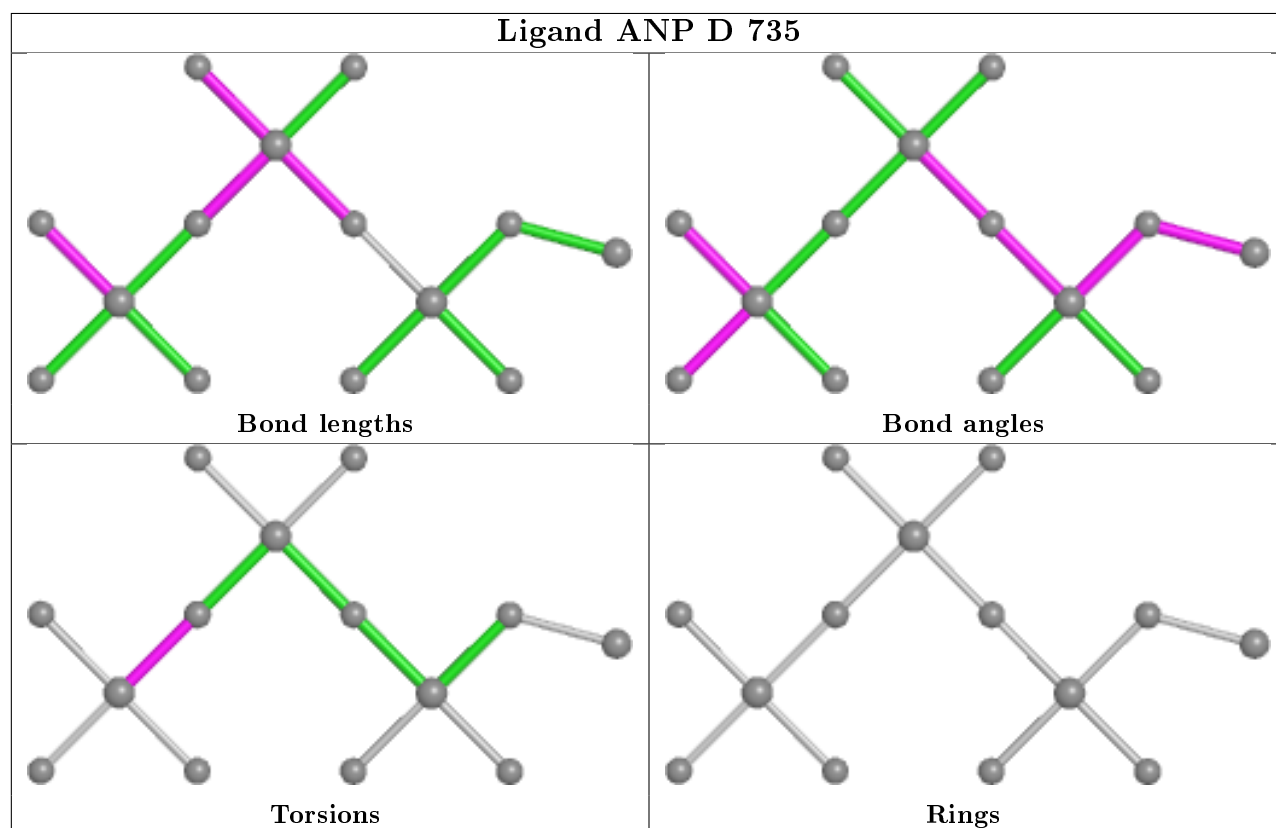
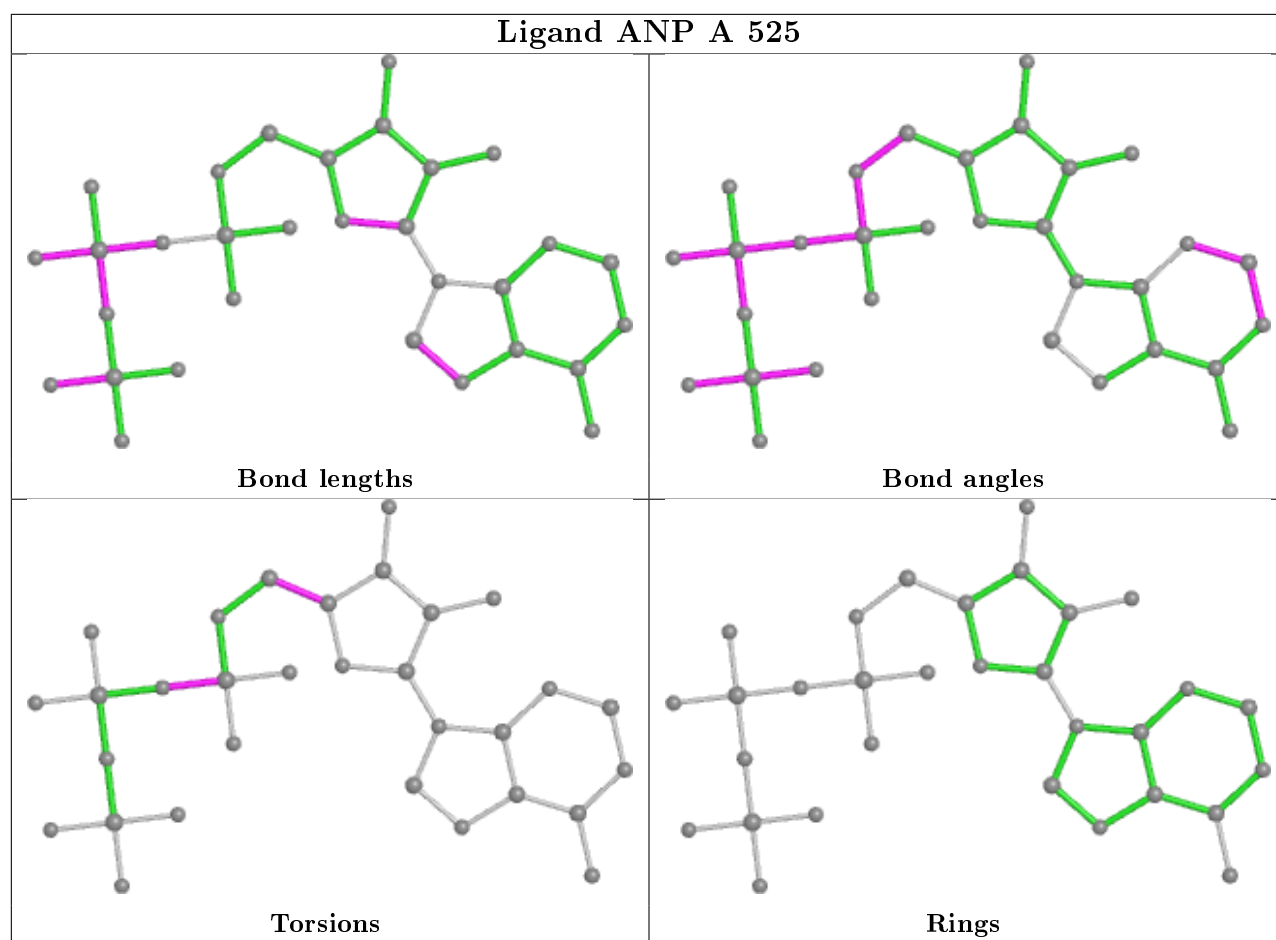
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	A	521	NAG	6	0
13	A	520	NAG	1	0
12	A	515	PGE	1	0
15	D	701	PG4	1	0
11	D	721	EDO	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for 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%)	-0.48	2 (0%) 91 89	25, 33, 44, 73	0
1	B	425/426 (99%)	-0.46	0 100 100	27, 36, 47, 68	0
1	C	423/426 (99%)	-0.38	2 (0%) 91 89	25, 35, 45, 69	0
1	D	426/426 (100%)	-0.34	6 (1%) 75 71	26, 35, 46, 70	0
All	All	1698/1704 (99%)	-0.42	10 (0%) 89 88	25, 35, 46, 73	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	431	SER	4.9
1	D	432	THR	3.2
1	C	64	ASN	3.0
1	A	108	ARG	2.4
1	D	109	ASN	2.2

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	0.75	0.33	76,83,85,89	0
4	BMA	G	4	11/12	0.75	0.40	73,85,90,93	0

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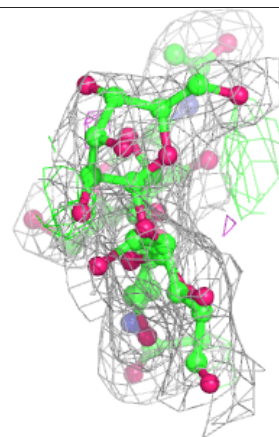
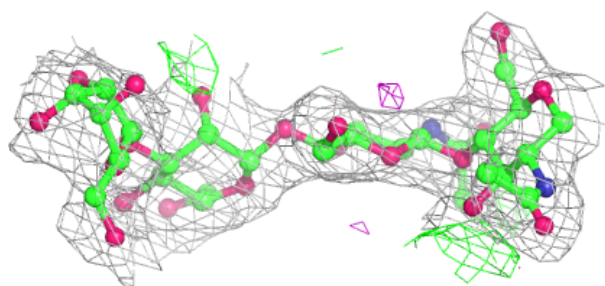
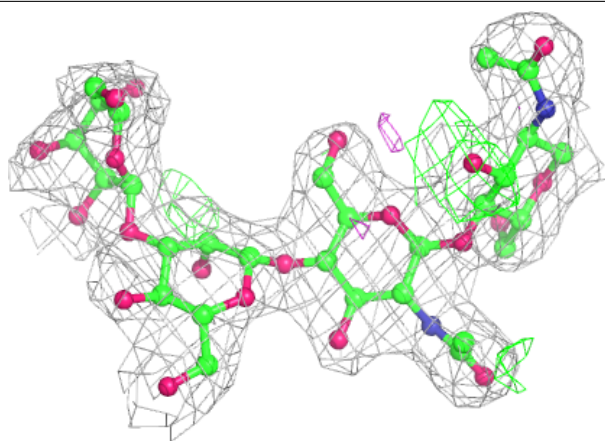
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAG	G	1	14/15	0.76	0.21	35,43,48,50	0
4	BMA	G	3	11/12	0.77	0.28	64,68,77,85	0
3	NAG	H	2	14/15	0.78	0.31	61,70,79,82	0
3	BMA	F	3	11/12	0.80	0.38	67,80,82,82	0
6	NAG	K	1	14/15	0.83	0.27	51,59,66,67	0
6	NAG	K	2	14/15	0.84	0.35	60,63,70,70	0
5	NAG	J	3	14/15	0.84	0.19	50,54,61,65	0
5	FUC	I	2	10/11	0.86	0.39	61,68,82,82	0
3	NAG	F	1	14/15	0.87	0.29	28,48,57,65	0
2	BMA	E	4	11/12	0.87	0.26	56,65,72,73	0
3	NAG	F	2	14/15	0.87	0.31	59,63,74,80	0
2	BMA	E	3	11/12	0.88	0.17	52,57,64,69	0
5	FUC	J	2	10/11	0.89	0.24	57,62,70,70	0
3	NAG	H	1	14/15	0.91	0.34	49,57,62,68	0
4	NAG	G	2	14/15	0.92	0.19	43,51,53,60	0
5	NAG	I	1	14/15	0.92	0.25	45,50,59,63	0
6	NAG	L	2	14/15	0.93	0.22	43,54,59,63	0
5	NAG	J	1	14/15	0.93	0.14	42,47,55,58	0
2	NAG	E	1	14/15	0.93	0.18	34,36,41,42	0
5	NAG	I	3	14/15	0.94	0.33	47,59,65,67	0
6	NAG	L	1	14/15	0.94	0.14	41,43,51,52	0
2	NAG	E	2	14/15	0.94	0.19	36,40,47,51	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.

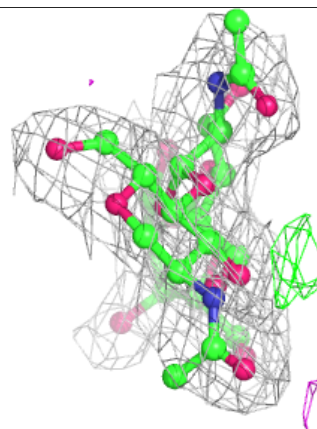
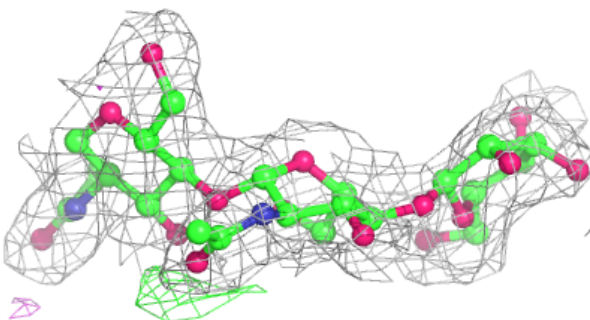
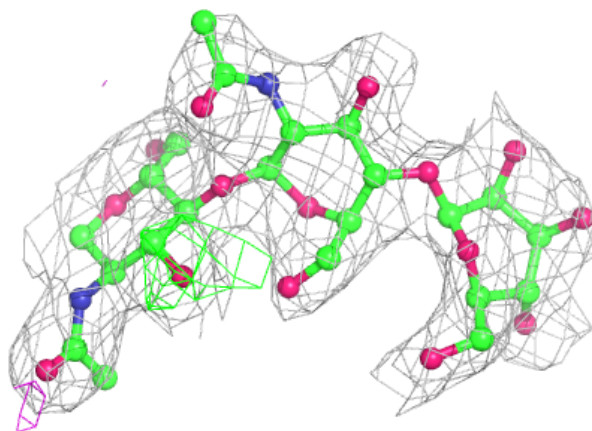
Electron density around Chain E:

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

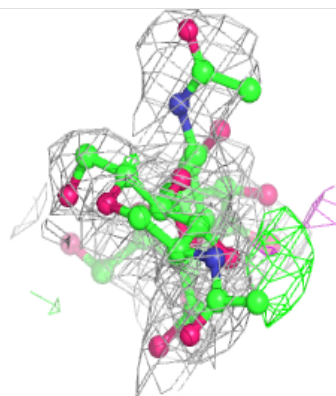
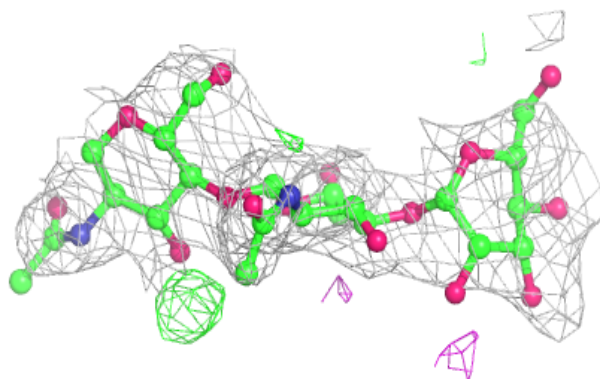
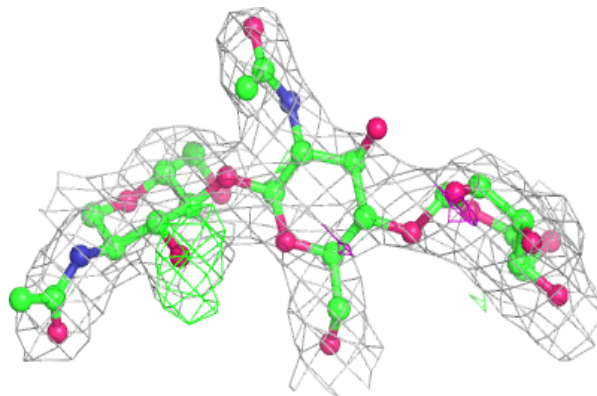


Electron density around Chain F:

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

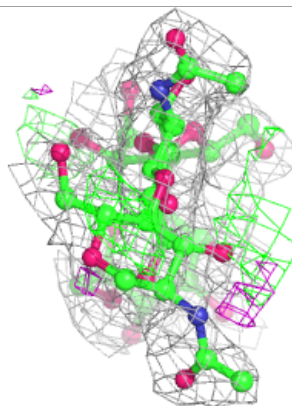
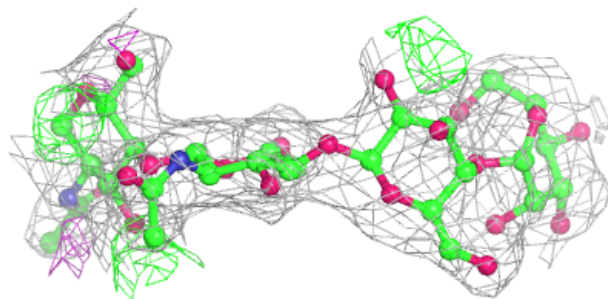
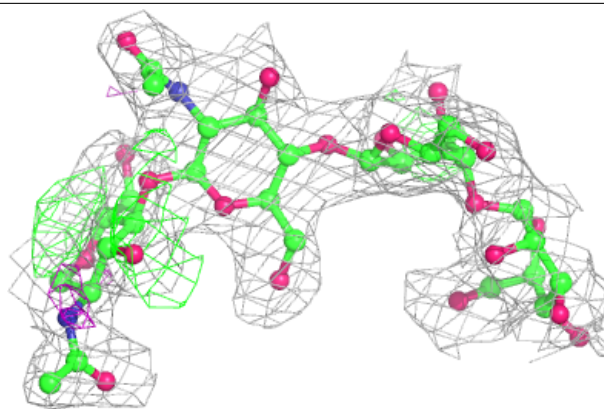
**Electron density around Chain H:**

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



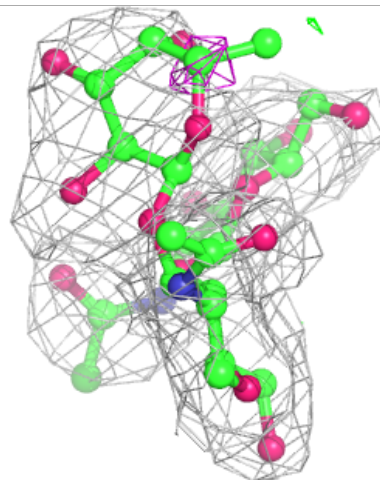
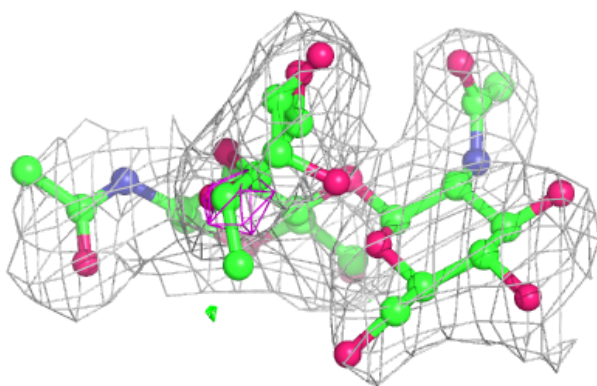
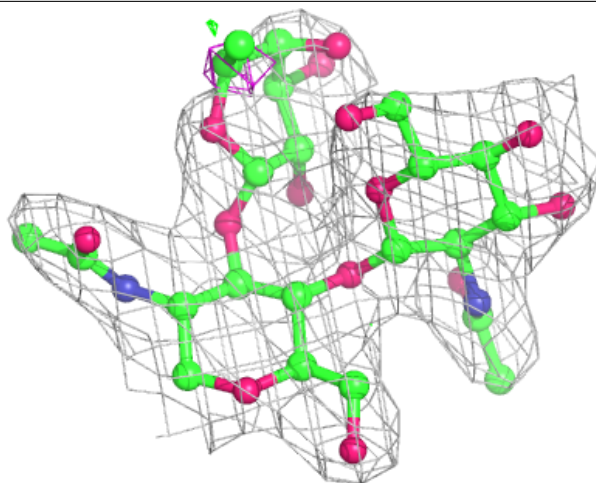
Electron density around Chain G:

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



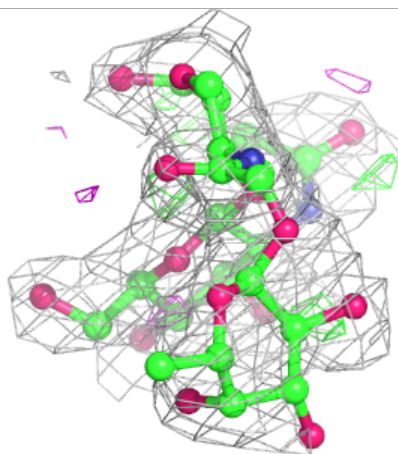
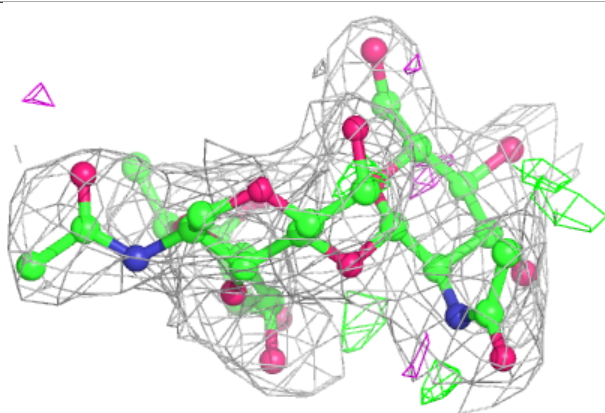
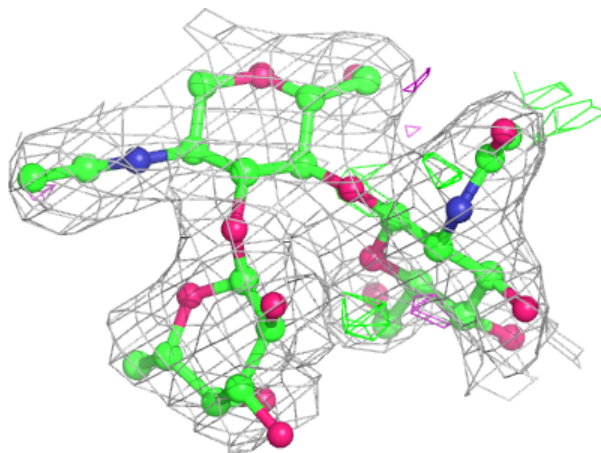
Electron density around Chain I:

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



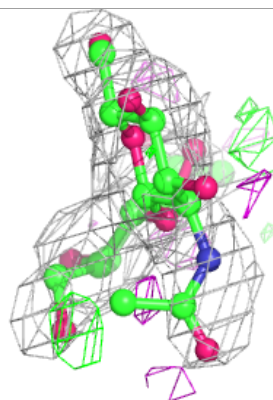
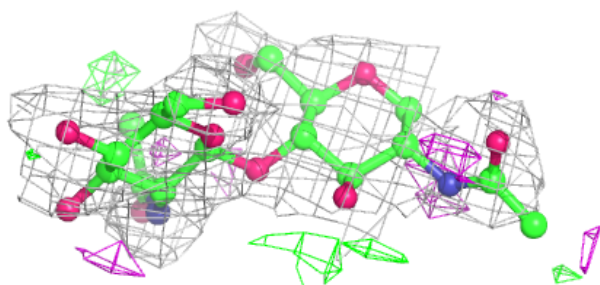
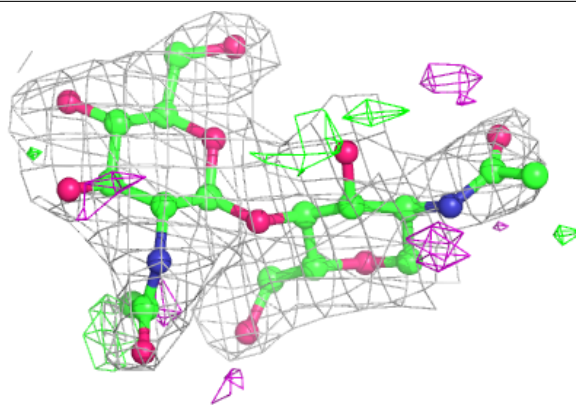
Electron density around Chain J:

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

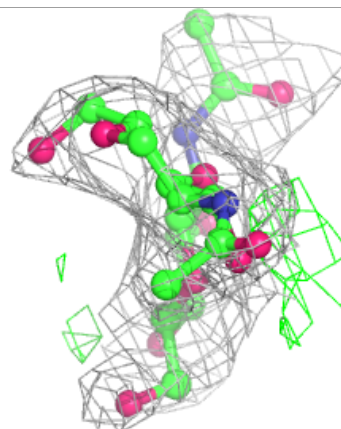
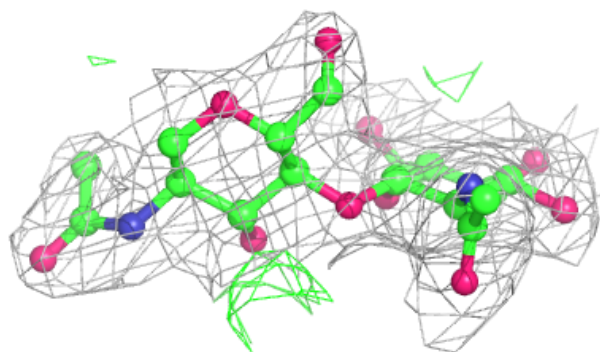
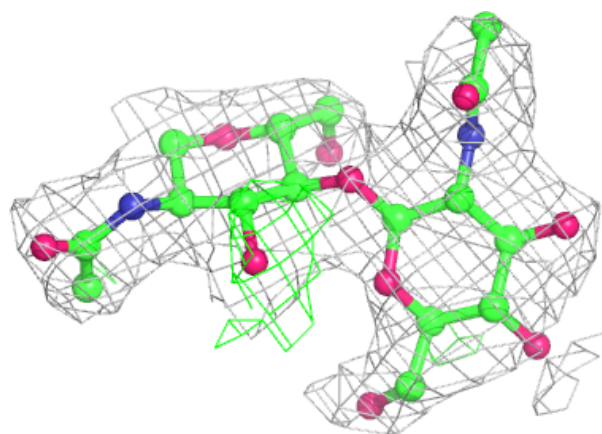


Electron density around Chain K:

$2mF_o-DF_c$ (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
10	GOL	D	716	6/6	0.65	0.36	54,64,72,72	0
11	EDO	A	511	4/4	0.68	0.40	43,44,50,50	4
11	EDO	C	513	4/4	0.75	0.27	42,52,53,57	0
13	NAG	A	521	14/15	0.76	0.30	45,56,60,61	0
12	PGE	A	515	7/10	0.81	0.51	59,66,69,73	7
11	EDO	A	512	4/4	0.82	0.15	51,59,62,64	0
11	EDO	A	510	4/4	0.83	0.29	31,39,46,48	4
13	NAG	C	502	14/15	0.83	0.28	42,55,61,65	0
14	ANP	C	530	15/31	0.83	0.29	34,46,59,73	15
9	SO4	C	505	5/5	0.83	0.33	60,65,73,79	5
7	ZN	B	501	1/1	0.83	0.12	69,69,69,69	0
10	GOL	A	507[A]	6/6	0.84	0.24	40,43,44,45	6
10	GOL	A	507[B]	6/6	0.84	0.24	39,43,45,46	6
9	SO4	D	711	5/5	0.85	0.20	54,56,68,69	5
12	PGE	B	513	7/10	0.85	0.26	53,55,64,68	0
10	GOL	A	509	6/6	0.85	0.31	42,51,57,57	0
11	EDO	A	514	4/4	0.85	0.23	41,51,53,54	0
15	PG4	D	701	13/13	0.86	0.24	47,65,73,77	0
11	EDO	B	508	4/4	0.86	0.19	35,38,40,42	0
11	EDO	C	520	4/4	0.87	0.29	41,45,50,52	0
11	EDO	D	725	4/4	0.87	0.17	48,53,57,57	0
12	PGE	C	521	10/10	0.87	0.22	45,47,50,54	10
11	EDO	D	724	4/4	0.87	0.20	37,49,49,54	0
9	SO4	D	710	5/5	0.87	0.20	49,52,58,63	5
11	EDO	D	718	4/4	0.87	0.47	40,49,51,54	4
12	PGE	D	729	7/10	0.88	0.27	36,38,44,45	7
15	PG4	A	526	13/13	0.88	0.24	29,44,54,57	13
11	EDO	D	717	4/4	0.89	0.18	39,43,45,51	0
10	GOL	A	508	6/6	0.89	0.19	37,46,48,54	0
11	EDO	A	513	4/4	0.89	0.25	47,53,57,65	0
12	PGE	B	514	7/10	0.89	0.15	31,49,54,58	0
11	EDO	B	509	4/4	0.89	0.27	45,52,52,55	0
13	NAG	D	733	14/15	0.89	0.24	33,40,50,52	0
9	SO4	B	503	5/5	0.90	0.20	35,38,40,42	5
9	SO4	D	709	5/5	0.90	0.43	40,41,44,44	5
9	SO4	A	505	5/5	0.90	0.34	66,72,76,105	0
11	EDO	D	720	4/4	0.90	0.13	50,51,53,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
14	ANP	D	735	14/31	0.90	0.21	30,47,56,60	14
11	EDO	D	719	4/4	0.90	0.34	44,45,47,53	0
10	GOL	D	715	6/6	0.90	0.24	38,43,47,47	6
10	GOL	D	713	6/6	0.90	0.22	42,44,51,54	0
14	ANP	A	525	31/31	0.90	0.25	30,53,59,71	31
11	EDO	C	515	4/4	0.90	0.19	43,49,49,52	0
11	EDO	B	511	4/4	0.91	0.10	28,39,41,42	0
11	EDO	C	517	4/4	0.91	0.17	43,53,54,56	0
11	EDO	D	727	4/4	0.91	0.19	43,45,46,56	0
12	PGE	D	730	7/10	0.91	0.20	37,41,45,46	0
9	SO4	C	506	5/5	0.92	0.25	33,37,46,49	5
10	GOL	D	714	6/6	0.92	0.18	34,35,35,37	6
11	EDO	D	721	4/4	0.92	0.17	23,33,35,35	0
9	SO4	C	509	5/5	0.92	0.25	48,48,51,56	5
8	FE	B	502	1/1	0.92	0.07	37,37,37,37	1
11	EDO	C	516	4/4	0.93	0.24	41,41,42,43	4
9	SO4	C	507	5/5	0.93	0.19	41,44,46,48	5
11	EDO	C	519	4/4	0.93	0.18	46,47,49,50	0
16	NA	B	526	1/1	0.93	0.14	43,43,43,43	0
9	SO4	D	704	5/5	0.93	0.27	46,53,57,62	5
9	SO4	D	707	5/5	0.93	0.19	35,37,39,41	5
9	SO4	C	508	5/5	0.93	0.24	45,45,52,53	5
13	NAG	A	520	14/15	0.93	0.14	32,37,43,49	0
9	SO4	D	712	5/5	0.93	0.21	48,50,55,60	5
9	SO4	A	504	5/5	0.93	0.21	38,41,45,50	5
13	NAG	B	522	14/15	0.93	0.12	32,40,46,47	0
9	SO4	B	504	5/5	0.93	0.18	34,41,46,48	5
11	EDO	B	510	4/4	0.94	0.16	48,49,51,51	0
13	NAG	C	526	14/15	0.94	0.16	31,37,44,47	0
16	NA	A	527	1/1	0.94	0.13	46,46,46,46	0
17	IPA	C	529	4/4	0.94	0.18	28,34,41,47	0
11	EDO	C	514	4/4	0.94	0.10	49,50,52,54	0
9	SO4	D	705	5/5	0.94	0.14	40,46,46,49	5
9	SO4	C	511	5/5	0.94	0.20	50,55,62,70	5
11	EDO	D	723	4/4	0.94	0.13	47,49,57,63	0
9	SO4	C	510	5/5	0.95	0.13	46,53,55,56	5
9	SO4	C	501	5/5	0.95	0.20	30,31,38,38	5
11	EDO	D	726	4/4	0.95	0.12	46,46,54,54	0
9	SO4	B	505	5/5	0.95	0.18	40,40,50,50	5
9	SO4	B	506	5/5	0.95	0.18	47,51,55,57	5
13	NAG	D	734	14/15	0.95	0.16	34,42,44,51	0
11	EDO	C	518	4/4	0.95	0.15	41,47,54,56	0

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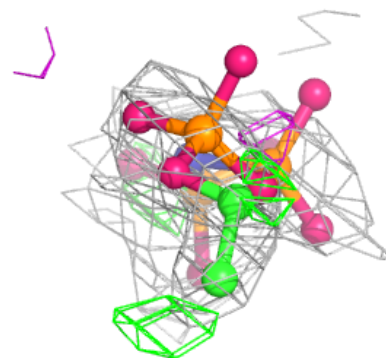
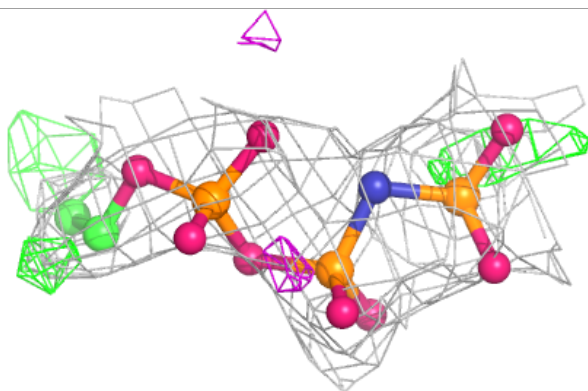
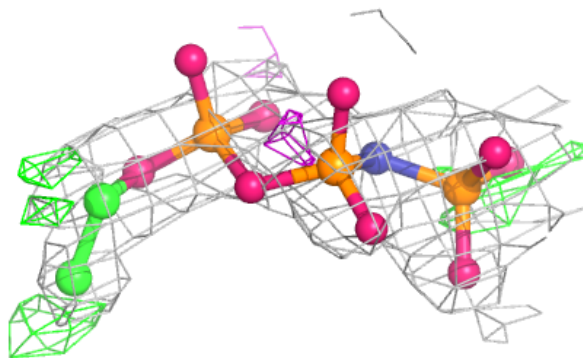
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
9	SO4	D	706	5/5	0.95	0.11	38,39,43,48	5
10	GOL	A	506	6/6	0.95	0.17	26,29,32,32	0
11	EDO	D	722	4/4	0.96	0.20	34,35,37,40	0
11	EDO	D	728	4/4	0.96	0.21	45,46,46,48	0
9	SO4	D	708	5/5	0.97	0.09	37,44,47,49	5
11	EDO	B	512	4/4	0.97	0.40	45,48,54,55	0
12	PGE	C	522	7/10	0.97	0.17	28,36,39,42	7
10	GOL	C	512	6/6	0.97	0.13	32,34,35,37	0
11	EDO	B	507	4/4	0.97	0.14	31,34,35,41	0
16	NA	C	531	1/1	0.97	0.16	29,29,29,29	0
7	ZN	D	702	1/1	0.98	0.05	38,38,38,38	1
7	ZN	A	501	1/1	0.98	0.08	42,42,42,42	1
8	FE	D	703	1/1	0.98	0.10	35,35,35,35	1
8	FE	A	502	1/1	0.98	0.09	30,30,30,30	1
7	ZN	C	503	1/1	0.98	0.09	35,35,35,35	1
9	SO4	A	503	5/5	0.99	0.09	38,44,46,56	0
8	FE	C	504	1/1	0.99	0.12	33,33,33,33	1

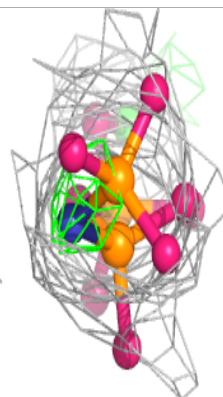
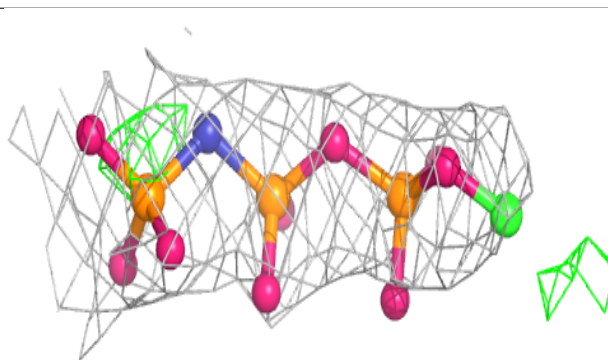
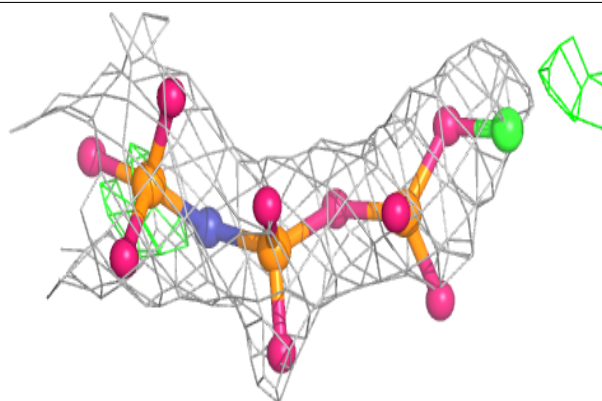
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

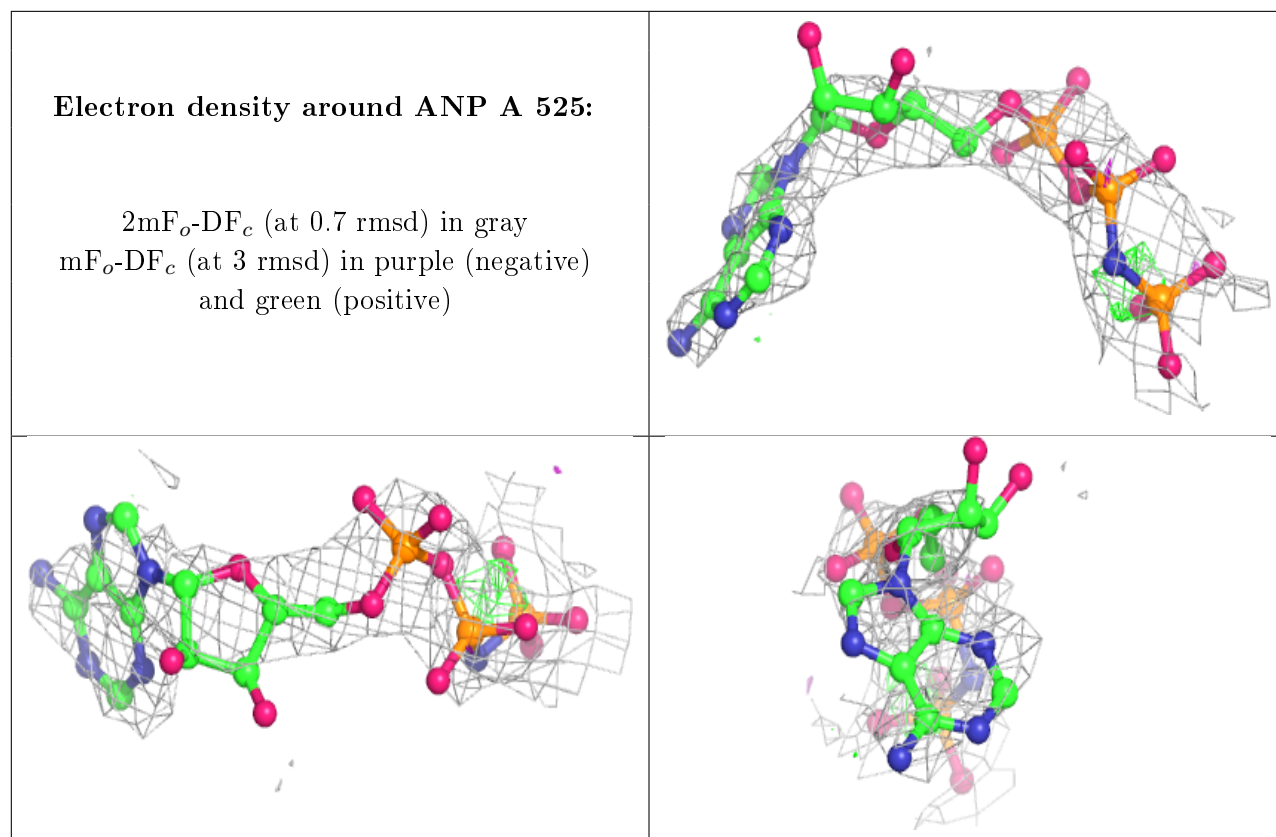
Electron density around ANP C 530:

$2mF_o-DF_c$ (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.