



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 05:36 PM BST

PDB ID : 3S1C  
Title : Maize cytokinin oxidase/dehydrogenase complexed with N6-isopentenyladenosine  
Authors : Kopečný, D.; Briozzo, P.; Morera, S.  
Deposited on : 2011-05-15  
Resolution : 2.09 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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

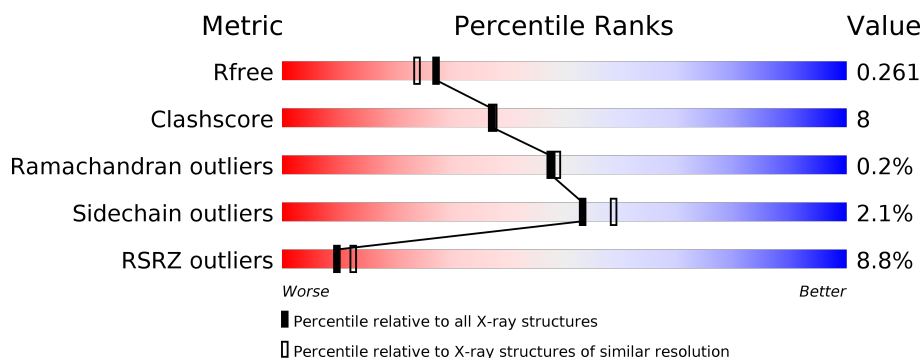
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.09 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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  $\geq 3$ , 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	516	<div> <div>9%</div> <div>88%</div> <div>8%</div> <div>••</div> </div>
2	B	2	<div> <div>100%</div> </div>

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
4	ZIR	A	536	-	-	X	-
5	GOL	A	548	-	-	X	-

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 4414 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 Cytokinin dehydrogenase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	498	Total	C	N	O	S	0	1	0
			3801	2414	667	708	12			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	79	ALA	GLY	SEE REMARK 999	UNP Q9T0N8
A	168	THR	ASN	SEE REMARK 999	UNP Q9T0N8
A	254	LEU	PHE	SEE REMARK 999	UNP Q9T0N8

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



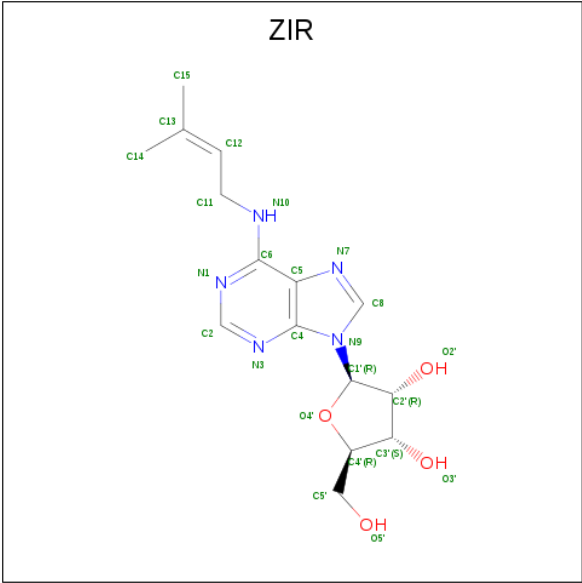
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C<sub>27</sub>H<sub>33</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 4 is N-(3-methylbut-2-en-1-yl)adenosine (three-letter code: ZIR) (formula: C<sub>15</sub>H<sub>21</sub>N<sub>5</sub>O<sub>4</sub>).



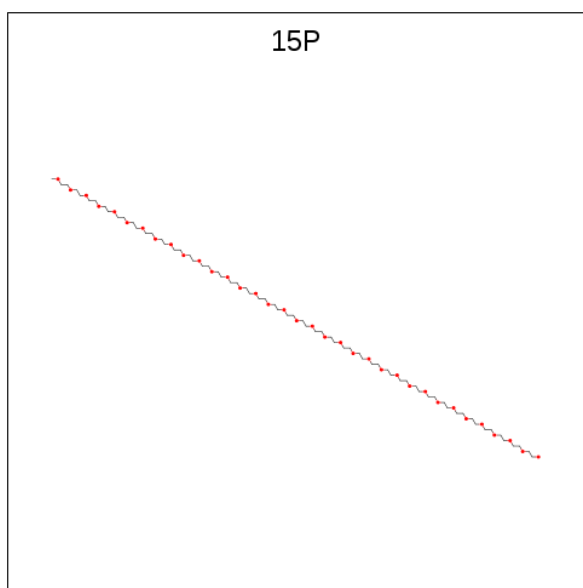
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			24	15	5	4		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



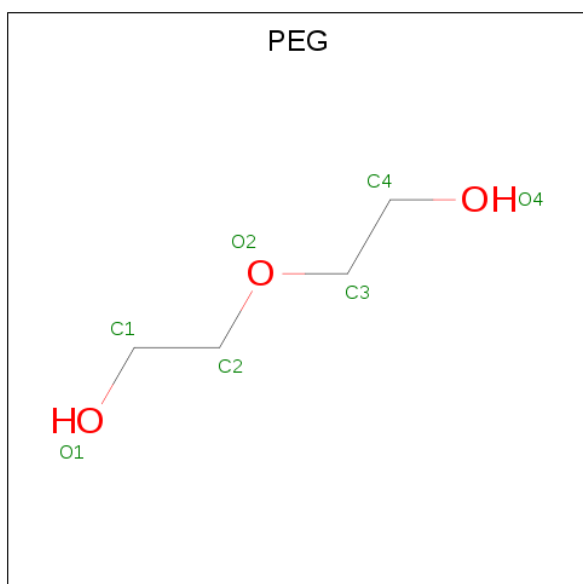
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is POLYETHYLENE GLYCOL (N=34) (three-letter code: 15P) (formula:  $C_{69}H_{140}O_{35}$ ).



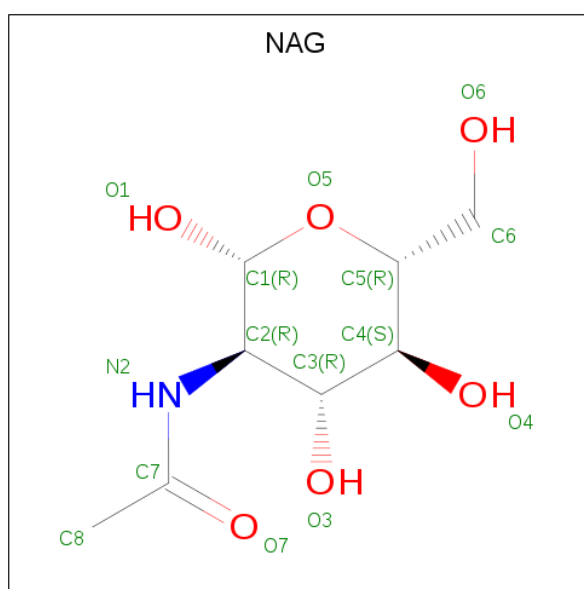
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			11	7	4		
6	A	1	Total	C	O	0	0
			11	7	4		
6	A	1	Total	C	O	0	0
			11	7	4		
6	A	1	Total	C	O	0	0
			11	7	4		

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			7	4	3		
7	A	1	Total	C	O	0	0
			7	4	3		
7	A	1	Total	C	O	0	0
			7	4	3		
7	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 9 is water.

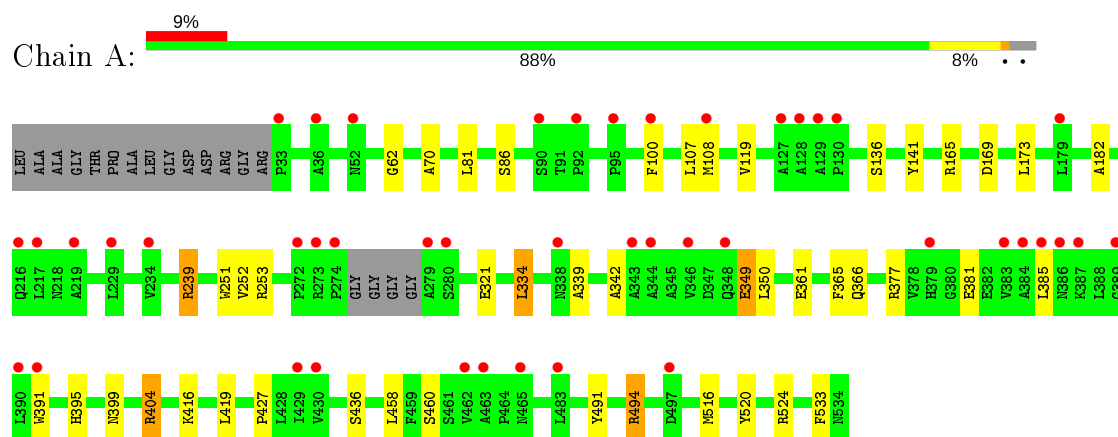
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	324	Total	O	0	0
			324	324		



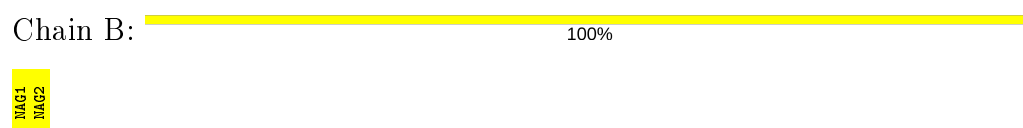
### 3 Residue-property plots [i](#)

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: Cytokinin dehydrogenase 1



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	250.95Å 50.62Å 51.40Å 90.00° 93.97° 90.00°	Depositor
Resolution (Å)	32.50 – 2.09 31.32 – 2.09	Depositor EDS
% Data completeness (in resolution range)	(Not available) (32.50-2.09) 91.2 (31.32-2.09)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.23 (at 2.10Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, $R_{free}$	0.213 , 0.252 0.217 , 0.261	Depositor DCC
$R_{free}$ test set	1765 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.6	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 58.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	4414	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.33% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZIR, NAG, 15P, PEG, FAD

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	0.49	0/3894	0.66	0/5306

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3801	0	3724	43	0
2	B	28	0	25	0	0
3	A	53	0	29	3	0
4	A	24	0	21	17	0
5	A	84	0	112	12	0
6	A	44	0	48	27	0
7	A	28	0	40	2	0
8	A	28	0	26	0	0
9	A	324	0	0	2	0
All	All	4414	0	4025	63	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 8.

All (63) 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:377:ARG:HE	6:A:552:15P:H17	1.33	0.90
4:A:536:ZIR:H8	6:A:552:15P:H28	1.56	0.87
4:A:536:ZIR:H5'A	6:A:552:15P:H15	1.56	0.87
4:A:536:ZIR:H1'	5:A:548:GOL:C1	2.14	0.77
6:A:551:15P:C2	6:A:551:15P:H17	2.16	0.76
1:A:366:GLN:H	6:A:554:15P:H26	1.59	0.67
4:A:536:ZIR:H5'A	6:A:552:15P:C5	2.23	0.66
4:A:536:ZIR:H1'	5:A:548:GOL:O1	1.97	0.65
1:A:81:LEU:HD21	1:A:119:VAL:HG11	1.77	0.64
1:A:108[B]:MET:HG3	1:A:494:ARG:HG3	1.80	0.63
1:A:377:ARG:HE	6:A:552:15P:C7	2.10	0.62
1:A:252:VAL:HG12	1:A:366:GLN:HG2	1.80	0.62
1:A:361:GLU:HB3	6:A:551:15P:H27	1.83	0.61
4:A:536:ZIR:H14B	9:A:817:HOH:O	2.05	0.56
1:A:385:LEU:HD11	5:A:548:GOL:H2	1.88	0.56
4:A:536:ZIR:H8	6:A:552:15P:C8	2.33	0.55
1:A:251:TRP:CZ2	6:A:552:15P:H23	2.43	0.54
6:A:552:15P:C2	6:A:552:15P:H26	2.38	0.53
1:A:516:MET:CE	1:A:520:TYR:HE2	2.22	0.53
1:A:136:SER:HB3	1:A:141:TYR:CE1	2.45	0.52
4:A:536:ZIR:H1'	5:A:548:GOL:H11	1.91	0.51
6:A:552:15P:H18	9:A:740:HOH:O	2.09	0.51
1:A:404:ARG:HH11	7:A:555:PEG:H22	1.76	0.51
4:A:536:ZIR:H5'A	6:A:552:15P:C6	2.41	0.50
1:A:377:ARG:NE	6:A:552:15P:H17	2.14	0.50
1:A:381:GLU:HG2	5:A:548:GOL:C1	2.42	0.50
1:A:427:PRO:HD3	5:A:548:GOL:H32	1.94	0.49
1:A:169:ASP:HB2	4:A:536:ZIR:HN10	1.77	0.49
1:A:252:VAL:HG11	1:A:350:LEU:HD21	1.93	0.49
1:A:365:PHE:HB3	6:A:554:15P:H17	1.93	0.49
1:A:141:TYR:CE1	1:A:239:ARG:HD2	2.47	0.49
1:A:334:LEU:HD11	1:A:349:GLU:HG2	1.94	0.49
1:A:427:PRO:HD2	1:A:458:LEU:HB2	1.96	0.48
4:A:536:ZIR:H5'A	6:A:552:15P:O3	2.14	0.47
1:A:524:ARG:HG2	1:A:533:PHE:HB3	1.97	0.47
1:A:416:LYS:HB3	6:A:553:15P:H26	1.97	0.46
1:A:253:ARG:HE	6:A:552:15P:C2	2.29	0.45
1:A:436:SER:O	5:A:541:GOL:H11	2.16	0.45
1:A:516:MET:HE3	1:A:520:TYR:HE2	1.81	0.45
4:A:536:ZIR:C5'	6:A:552:15P:O3	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:GLN:HG3	6:A:554:15P:H23	1.99	0.45
1:A:366:GLN:N	6:A:554:15P:H26	2.29	0.45
4:A:536:ZIR:C8	6:A:552:15P:H28	2.39	0.44
4:A:536:ZIR:H2'	6:A:552:15P:C5	2.47	0.44
1:A:516:MET:HE3	1:A:520:TYR:CE2	2.53	0.43
3:A:535:FAD:N5	4:A:536:ZIR:H11A	2.34	0.43
1:A:377:ARG:HD2	6:A:552:15P:H16	2.01	0.43
1:A:391:TRP:O	1:A:395:HIS:HE1	2.00	0.43
1:A:427:PRO:HG2	1:A:458:LEU:HD12	2.01	0.43
1:A:70:ALA:HB1	7:A:557:PEG:H11	2.01	0.42
1:A:100:PHE:O	3:A:535:FAD:H2B	2.19	0.42
1:A:381:GLU:HG2	5:A:548:GOL:H12	2.01	0.42
1:A:165:ARG:HH22	5:A:549:GOL:H12	1.84	0.42
1:A:399:ASN:HB2	1:A:491:TYR:O	2.20	0.42
1:A:385:LEU:CD1	5:A:548:GOL:H2	2.49	0.42
1:A:321:GLU:HG3	5:A:543:GOL:H2	2.02	0.42
4:A:536:ZIR:H3'	6:A:552:15P:H15	2.01	0.41
4:A:536:ZIR:N3	5:A:548:GOL:C1	2.83	0.41
6:A:552:15P:O1	6:A:552:15P:H26	2.20	0.41
1:A:173:LEU:HD13	3:A:535:FAD:H2'	2.01	0.41
1:A:361:GLU:HB3	6:A:551:15P:H15	2.03	0.41
1:A:339:ALA:HB3	1:A:342:ALA:HB2	2.03	0.40
1:A:62:GLY:HA3	1:A:107:LEU:O	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	495/516 (96%)	481 (97%)	13 (3%)	1 (0%)	47 49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	182	ALA

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	388/395 (98%)	380 (98%)	8 (2%)	53 59

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	SER
1	A	239	ARG
1	A	334	LEU
1	A	349	GLU
1	A	404	ARG
1	A	419	LEU
1	A	460	SER
1	A	494	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	395	HIS
1	A	495	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

2 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	B	1	1,2	14,14,15	1.70	6 (42%)	17,19,21	2.06	7 (41%)
2	NAG	B	2	2	14,14,15	1.65	3 (21%)	17,19,21	1.96	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	NAG	C1-C2	3.51	1.57	1.52
2	B	1	NAG	C3-C2	2.64	1.58	1.52
2	B	1	NAG	O5-C5	2.57	1.48	1.43
2	B	1	NAG	C2-N2	2.27	1.50	1.46
2	B	2	NAG	O5-C5	2.20	1.47	1.43
2	B	1	NAG	C4-C5	2.19	1.57	1.53
2	B	2	NAG	C3-C2	2.10	1.57	1.52
2	B	1	NAG	C4-C3	2.07	1.57	1.52
2	B	1	NAG	C7-N2	2.00	1.41	1.34

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	NAG	C1-O5-C5	5.67	119.88	112.19
2	B	2	NAG	O5-C1-C2	4.07	117.71	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	NAG	C3-C4-C5	4.06	117.49	110.24
2	B	1	NAG	C1-C2-N2	3.72	116.84	110.49
2	B	1	NAG	C2-N2-C7	3.39	127.74	122.90
2	B	1	NAG	C1-O5-C5	2.23	115.21	112.19
2	B	1	NAG	C4-C3-C2	2.07	114.05	111.02
2	B	1	NAG	C6-C5-C4	-2.03	108.25	113.00
2	B	1	NAG	O7-C7-N2	2.03	125.68	121.95

There are no chirality outliers.

All (2) torsion outliers are listed below:

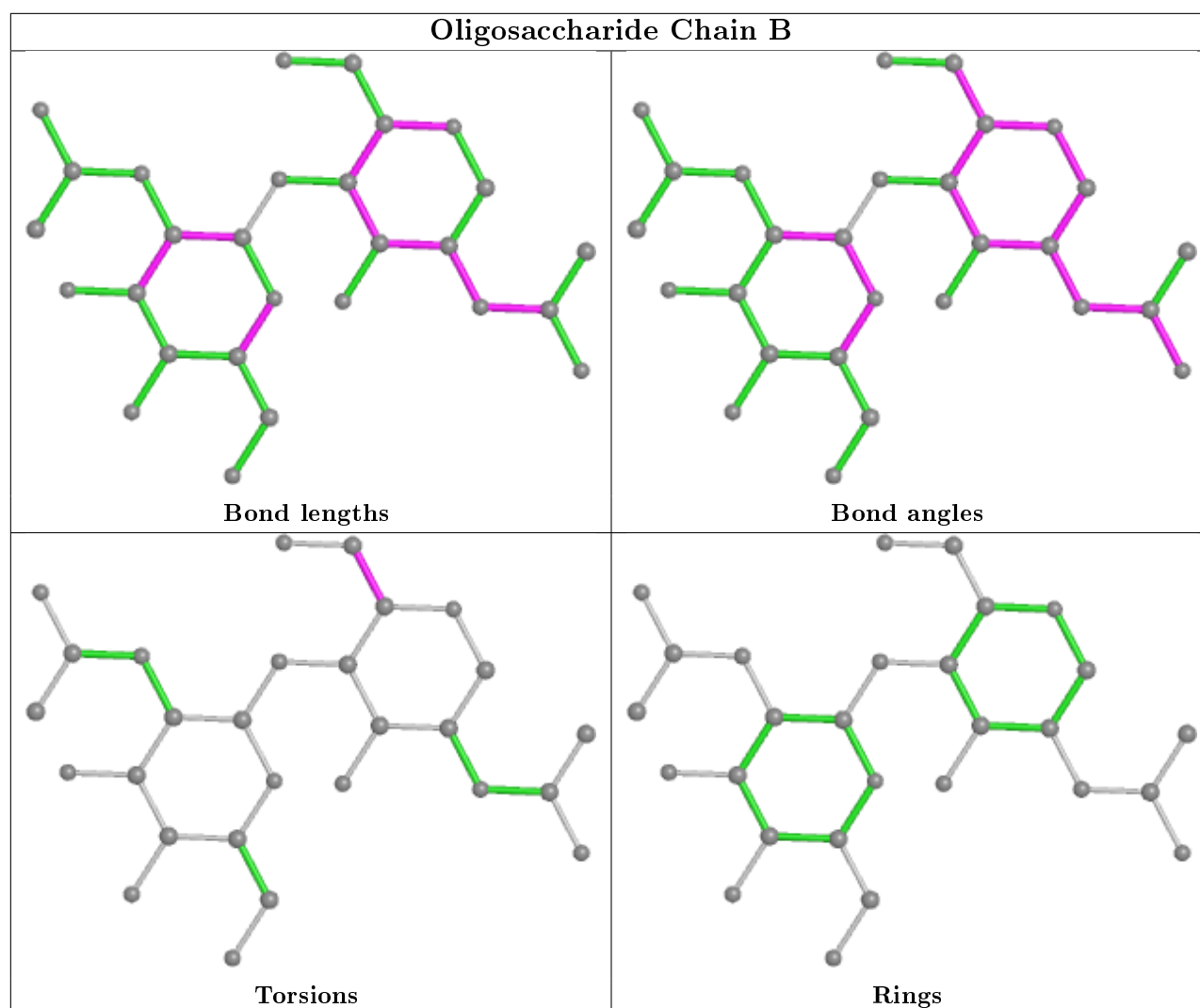
Mol	Chain	Res	Type	Atoms
2	B	1	NAG	C4-C5-C6-O6
2	B	1	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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





## 5.6 Ligand geometry [i](#)

26 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
6	15P	A	552	-	10,10,103	0.63	0	9,9,102	0.93	0
6	15P	A	553	-	10,10,103	1.02	0	9,9,102	0.73	0
5	GOL	A	550	-	5,5,5	1.24	0	5,5,5	1.35	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	ZIR	A	536	-	22,26,26	1.64	6 (27%)	22,37,37	2.31	9 (40%)
5	GOL	A	539	-	5,5,5	0.46	0	5,5,5	0.35	0
6	15P	A	551	-	10,10,103	0.57	0	9,9,102	0.92	0
5	GOL	A	540	-	5,5,5	0.43	0	5,5,5	0.23	0
8	NAG	A	601	1	14,14,15	1.66	4 (28%)	17,19,21	1.50	2 (11%)
3	FAD	A	535	1	51,58,58	2.78	11 (21%)	60,89,89	2.45	9 (15%)
5	GOL	A	542	-	5,5,5	0.65	0	5,5,5	0.52	0
5	GOL	A	546	-	5,5,5	0.48	0	5,5,5	0.48	0
8	NAG	A	604	1	14,14,15	1.82	3 (21%)	17,19,21	1.66	5 (29%)
7	PEG	A	555	-	6,6,6	0.57	0	5,5,5	0.51	0
7	PEG	A	556	-	6,6,6	0.15	0	5,5,5	0.19	0
5	GOL	A	538	-	5,5,5	0.56	0	5,5,5	0.59	0
5	GOL	A	541	-	5,5,5	0.30	0	5,5,5	0.74	0
5	GOL	A	548	-	5,5,5	0.31	0	5,5,5	0.68	0
5	GOL	A	545	-	5,5,5	0.26	0	5,5,5	0.23	0
5	GOL	A	543	-	5,5,5	0.63	0	5,5,5	0.58	0
5	GOL	A	547	-	5,5,5	0.41	0	5,5,5	0.26	0
5	GOL	A	549	-	5,5,5	0.28	0	5,5,5	0.67	0
7	PEG	A	557	-	6,6,6	0.16	0	5,5,5	0.23	0
6	15P	A	554	-	10,10,103	0.71	0	9,9,102	0.55	0
7	PEG	A	558	-	6,6,6	0.34	0	5,5,5	0.52	0
5	GOL	A	537	-	5,5,5	0.77	0	5,5,5	1.02	0
5	GOL	A	544	-	5,5,5	0.65	0	5,5,5	0.41	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
6	15P	A	552	-	-	4/8/8/101	-
6	15P	A	553	-	-	2/8/8/101	-
5	GOL	A	550	-	-	4/4/4/4	-
4	ZIR	A	536	-	-	4/8/28/28	0/3/3/3
5	GOL	A	539	-	-	2/4/4/4	-
6	15P	A	551	-	-	8/8/8/101	-
5	GOL	A	540	-	-	3/4/4/4	-
8	NAG	A	601	1	-	0/6/23/26	0/1/1/1
3	FAD	A	535	1	-	5/30/50/50	0/6/6/6
5	GOL	A	542	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	546	-	-	2/4/4/4	-
8	NAG	A	604	1	-	4/6/23/26	0/1/1/1
7	PEG	A	555	-	-	3/4/4/4	-
7	PEG	A	556	-	-	2/4/4/4	-
5	GOL	A	538	-	-	2/4/4/4	-
5	GOL	A	541	-	-	2/4/4/4	-
5	GOL	A	548	-	-	3/4/4/4	-
5	GOL	A	545	-	-	2/4/4/4	-
5	GOL	A	543	-	-	0/4/4/4	-
5	GOL	A	547	-	-	1/4/4/4	-
5	GOL	A	549	-	-	0/4/4/4	-
7	PEG	A	557	-	-	1/4/4/4	-
6	15P	A	554	-	-	4/8/8/101	-
7	PEG	A	558	-	-	0/4/4/4	-
5	GOL	A	537	-	-	2/4/4/4	-
5	GOL	A	544	-	-	2/4/4/4	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	535	FAD	C4X-C10	15.45	1.54	1.38
3	A	535	FAD	C4-C4X	5.81	1.51	1.41
3	A	535	FAD	C9A-N10	4.13	1.44	1.38
3	A	535	FAD	C2A-N3A	3.98	1.38	1.32
3	A	535	FAD	C1'-N10	-3.96	1.44	1.48
8	A	604	NAG	C1-C2	3.77	1.58	1.52
3	A	535	FAD	C5X-N5	3.59	1.41	1.35
4	A	536	ZIR	O4'-C1'	3.44	1.45	1.41
3	A	535	FAD	O4B-C1B	3.25	1.45	1.41
8	A	604	NAG	C3-C2	3.13	1.59	1.52
4	A	536	ZIR	C8-N7	-3.11	1.29	1.34
8	A	601	NAG	C4-C3	2.93	1.59	1.52
8	A	601	NAG	C3-C2	2.83	1.58	1.52
8	A	601	NAG	C4-C5	2.66	1.58	1.53
4	A	536	ZIR	C2-N1	-2.62	1.29	1.33
4	A	536	ZIR	C11-C12	-2.44	1.37	1.48
4	A	536	ZIR	C6-N10	-2.30	1.30	1.34
8	A	601	NAG	O5-C5	2.29	1.48	1.43
4	A	536	ZIR	C12-C13	2.26	1.38	1.32
3	A	535	FAD	C2A-N1A	2.21	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	535	FAD	C8A-N7A	-2.12	1.30	1.34
3	A	535	FAD	C4-N3	2.11	1.36	1.33
3	A	535	FAD	C6-C7	2.07	1.43	1.37
8	A	604	NAG	C4-C3	2.01	1.57	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	535	FAD	C4-N3-C2	13.37	126.43	115.14
3	A	535	FAD	C4-C4X-C10	-6.04	115.95	119.95
3	A	535	FAD	C4X-C4-N3	-5.59	115.78	123.43
4	A	536	ZIR	N3-C2-N1	-5.52	120.05	128.68
3	A	535	FAD	C1'-N10-C9A	4.26	121.64	118.29
8	A	601	NAG	C4-C3-C2	4.17	117.13	111.02
4	A	536	ZIR	O4'-C1'-C2'	-3.93	101.18	106.93
3	A	535	FAD	C4X-C10-N10	-3.88	116.31	120.30
8	A	604	NAG	C1-C2-N2	3.68	116.77	110.49
4	A	536	ZIR	C11-C12-C13	-3.60	120.14	127.14
4	A	536	ZIR	C5'-C4'-C3'	-3.56	106.50	115.09
8	A	604	NAG	C3-C4-C5	-3.40	104.17	110.24
4	A	536	ZIR	C15-C13-C14	3.30	121.89	114.60
3	A	535	FAD	C1'-C2'-C3'	-3.21	100.81	109.79
3	A	535	FAD	C10-C4X-N5	3.18	123.46	121.26
4	A	536	ZIR	C3'-C2'-C1'	2.74	105.11	100.98
4	A	536	ZIR	C2-N1-C6	2.56	118.78	116.59
3	A	535	FAD	C4'-C3'-C2'	2.54	118.65	113.36
4	A	536	ZIR	C4-C5-N7	-2.53	106.77	109.40
5	A	550	GOL	O3-C3-C2	2.45	121.96	110.20
3	A	535	FAD	O3'-C3'-C4'	2.27	114.28	108.81
4	A	536	ZIR	C15-C13-C12	-2.23	116.21	122.65
8	A	604	NAG	C2-N2-C7	2.18	126.00	122.90
8	A	604	NAG	O4-C4-C5	2.13	114.59	109.30
8	A	601	NAG	C3-C4-C5	2.06	113.92	110.24
8	A	604	NAG	O5-C5-C6	2.02	110.36	107.20

There are no chirality outliers.

All (65) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	550	GOL	C1-C2-C3-O3
4	A	536	ZIR	C5-C6-N10-C11
5	A	539	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
5	A	540	GOL	O1-C1-C2-C3
5	A	538	GOL	O1-C1-C2-O2
5	A	541	GOL	C1-C2-C3-O3
5	A	548	GOL	C1-C2-C3-O3
5	A	548	GOL	O2-C2-C3-O3
5	A	545	GOL	O1-C1-C2-C3
5	A	544	GOL	O1-C1-C2-O2
5	A	544	GOL	O1-C1-C2-C3
5	A	537	GOL	C1-C2-C3-O3
4	A	536	ZIR	O4'-C4'-C5'-O5'
4	A	536	ZIR	C3'-C4'-C5'-O5'
6	A	551	15P	O2-C5-C6-O3
8	A	604	NAG	C8-C7-N2-C2
8	A	604	NAG	O7-C7-N2-C2
5	A	550	GOL	O2-C2-C3-O3
5	A	539	GOL	O1-C1-C2-O2
6	A	553	15P	O1-C3-C4-O2
6	A	551	15P	O1-C3-C4-O2
3	A	535	FAD	O3'-C3'-C4'-C5'
8	A	604	NAG	C4-C5-C6-O6
7	A	555	PEG	O1-C1-C2-O2
7	A	555	PEG	O2-C3-C4-O4
8	A	604	NAG	O5-C5-C6-O6
5	A	550	GOL	O1-C1-C2-C3
5	A	542	GOL	O1-C1-C2-C3
5	A	546	GOL	O1-C1-C2-C3
5	A	538	GOL	O1-C1-C2-C3
4	A	536	ZIR	N1-C6-N10-C11
5	A	550	GOL	O1-C1-C2-O2
5	A	541	GOL	O2-C2-C3-O3
6	A	552	15P	O3-C7-C8-O4
6	A	554	15P	O3-C7-C8-O4
5	A	542	GOL	O1-C1-C2-O2
5	A	537	GOL	O2-C2-C3-O3
3	A	535	FAD	O3'-C3'-C4'-O4'
5	A	546	GOL	O1-C1-C2-O2
5	A	548	GOL	O1-C1-C2-O2
5	A	545	GOL	O1-C1-C2-O2
6	A	551	15P	C4-C3-O1-C2
6	A	552	15P	C5-C6-O3-C7
7	A	555	PEG	C1-C2-O2-C3
7	A	556	PEG	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
6	A	551	15P	C3-C4-O2-C5
6	A	551	15P	C5-C6-O3-C7
3	A	535	FAD	PA-O3P-P-O1P
3	A	535	FAD	C2'-C3'-C4'-C5'
6	A	552	15P	C4-C3-O1-C2
7	A	557	PEG	C1-C2-O2-C3
5	A	540	GOL	O1-C1-C2-O2
5	A	542	GOL	O2-C2-C3-O3
6	A	553	15P	O3-C7-C8-O4
3	A	535	FAD	PA-O3P-P-O2P
7	A	556	PEG	C1-C2-O2-C3
6	A	551	15P	C8-C7-O3-C6
6	A	551	15P	C6-C5-O2-C4
6	A	554	15P	C5-C6-O3-C7
6	A	552	15P	O2-C5-C6-O3
5	A	540	GOL	C1-C2-C3-O3
5	A	547	GOL	O1-C1-C2-C3
6	A	554	15P	O2-C5-C6-O3
6	A	554	15P	O1-C3-C4-O2
6	A	551	15P	O3-C7-C8-O4

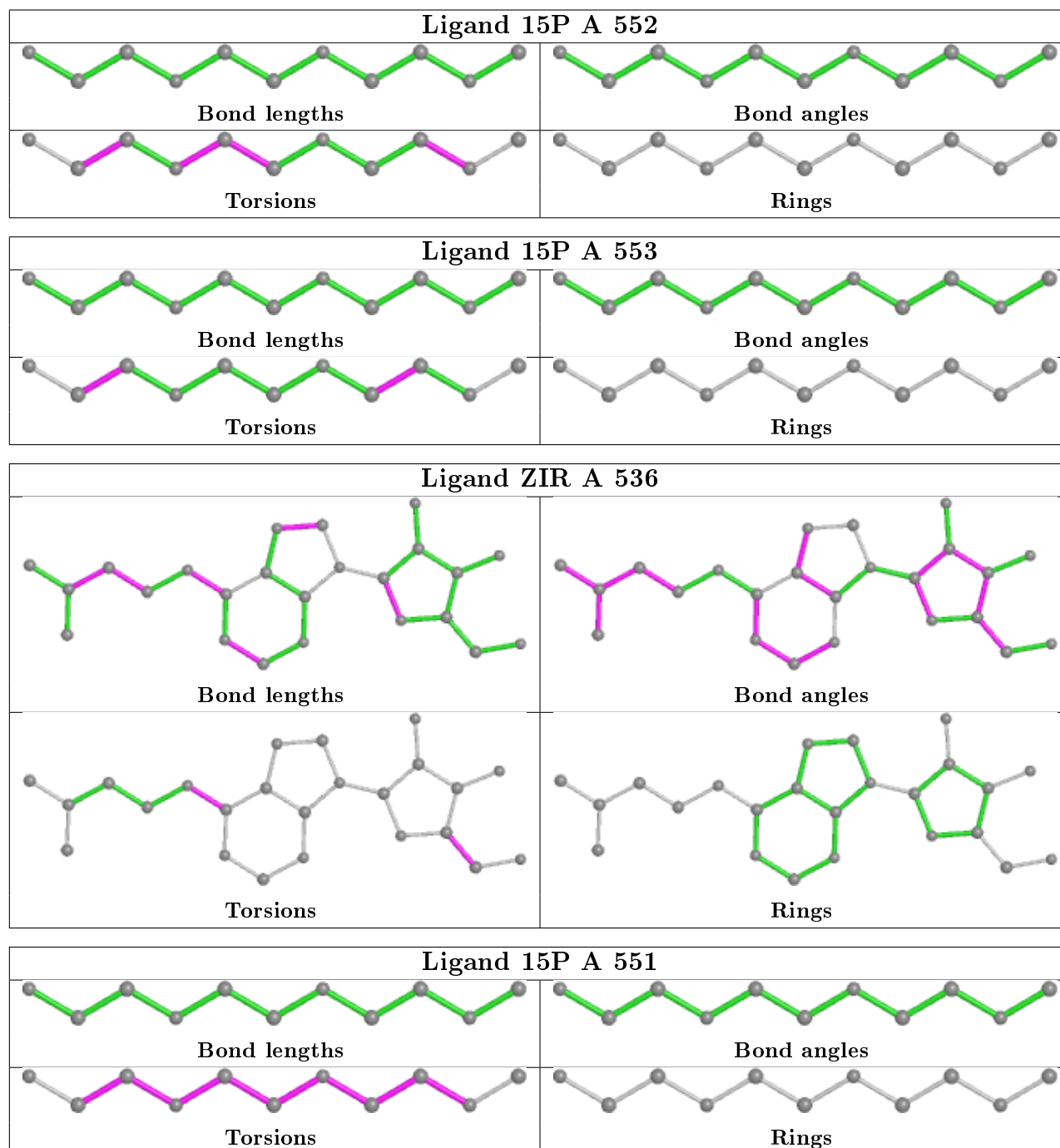
There are no ring outliers.

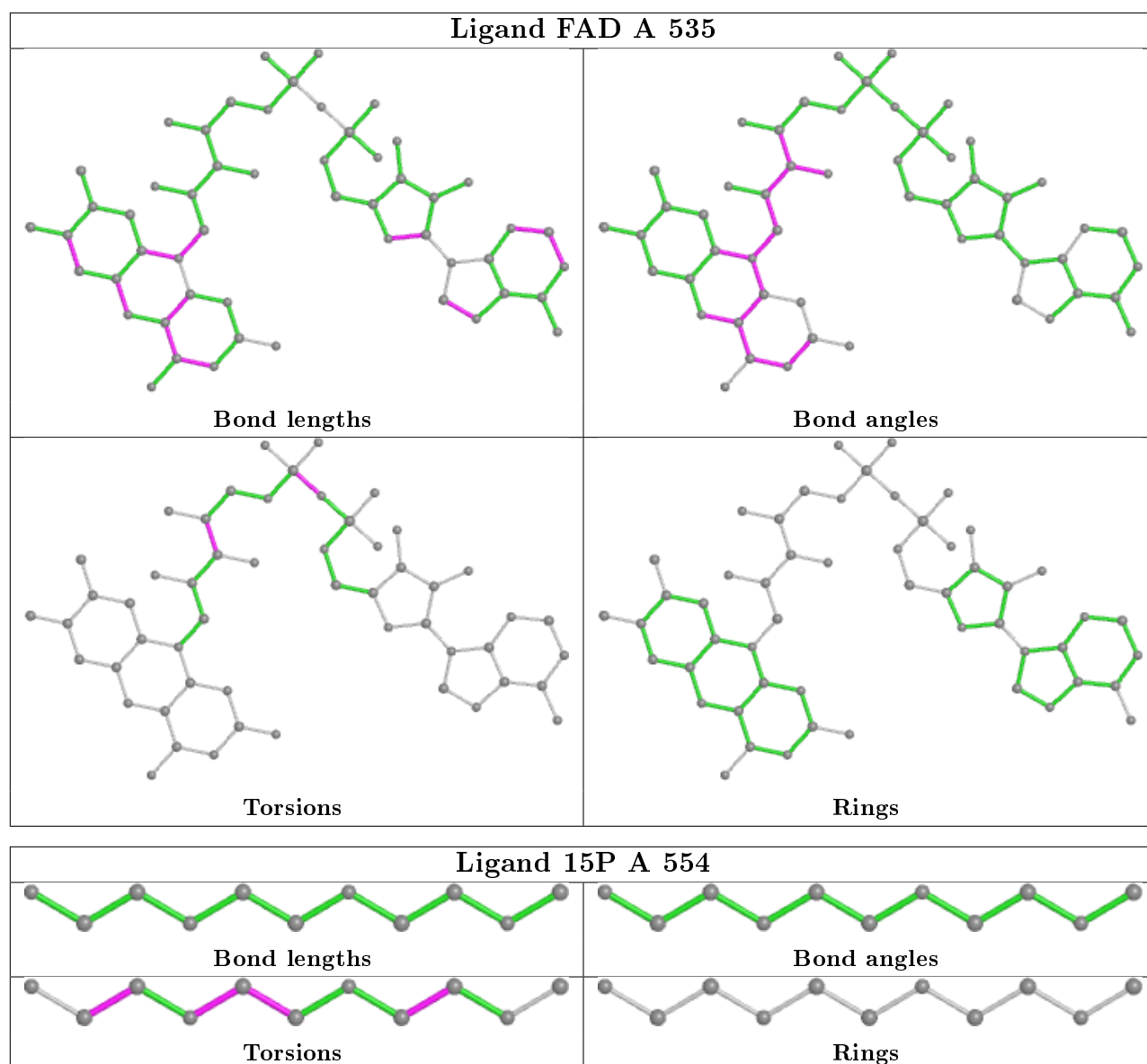
12 monomers are involved in 46 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	552	15P	19	0
6	A	553	15P	1	0
4	A	536	ZIR	17	0
6	A	551	15P	3	0
3	A	535	FAD	3	0
7	A	555	PEG	1	0
5	A	541	GOL	1	0
5	A	548	GOL	9	0
5	A	543	GOL	1	0
5	A	549	GOL	1	0
7	A	557	PEG	1	0
6	A	554	15P	4	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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	498/516 (96%)	0.54	44 (8%) 10 12	14, 26, 52, 72	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	129	ALA	10.3
1	A	462	VAL	7.2
1	A	128	ALA	7.0
1	A	390	LEU	6.9
1	A	274	PRO	6.7
1	A	279	ALA	6.3
1	A	127	ALA	5.9
1	A	389	GLY	5.1
1	A	391	TRP	4.2
1	A	92	PRO	4.0
1	A	465	ASN	3.9
1	A	273	ARG	3.5
1	A	463	ALA	3.4
1	A	385	LEU	3.3
1	A	386	ASN	3.3
1	A	383	VAL	3.3
1	A	387	LYS	3.2
1	A	216	GLN	3.1
1	A	343	ALA	3.0
1	A	217	LEU	3.0
1	A	130	PRO	2.9
1	A	280	SER	2.9
1	A	348	GLN	2.8
1	A	346	VAL	2.8
1	A	379	HIS	2.7
1	A	229	LEU	2.7
1	A	33	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	344	ALA	2.7
1	A	100	PHE	2.6
1	A	384	ALA	2.5
1	A	497	ASP	2.4
1	A	52	ASN	2.4
1	A	179	LEU	2.2
1	A	219	ALA	2.2
1	A	36	ALA	2.2
1	A	483	LEU	2.1
1	A	90	SER	2.1
1	A	95	PRO	2.1
1	A	234	VAL	2.1
1	A	338	ASN	2.1
1	A	430	VAL	2.1
1	A	272	PRO	2.0
1	A	429	ILE	2.0
1	A	108[A]	MET	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

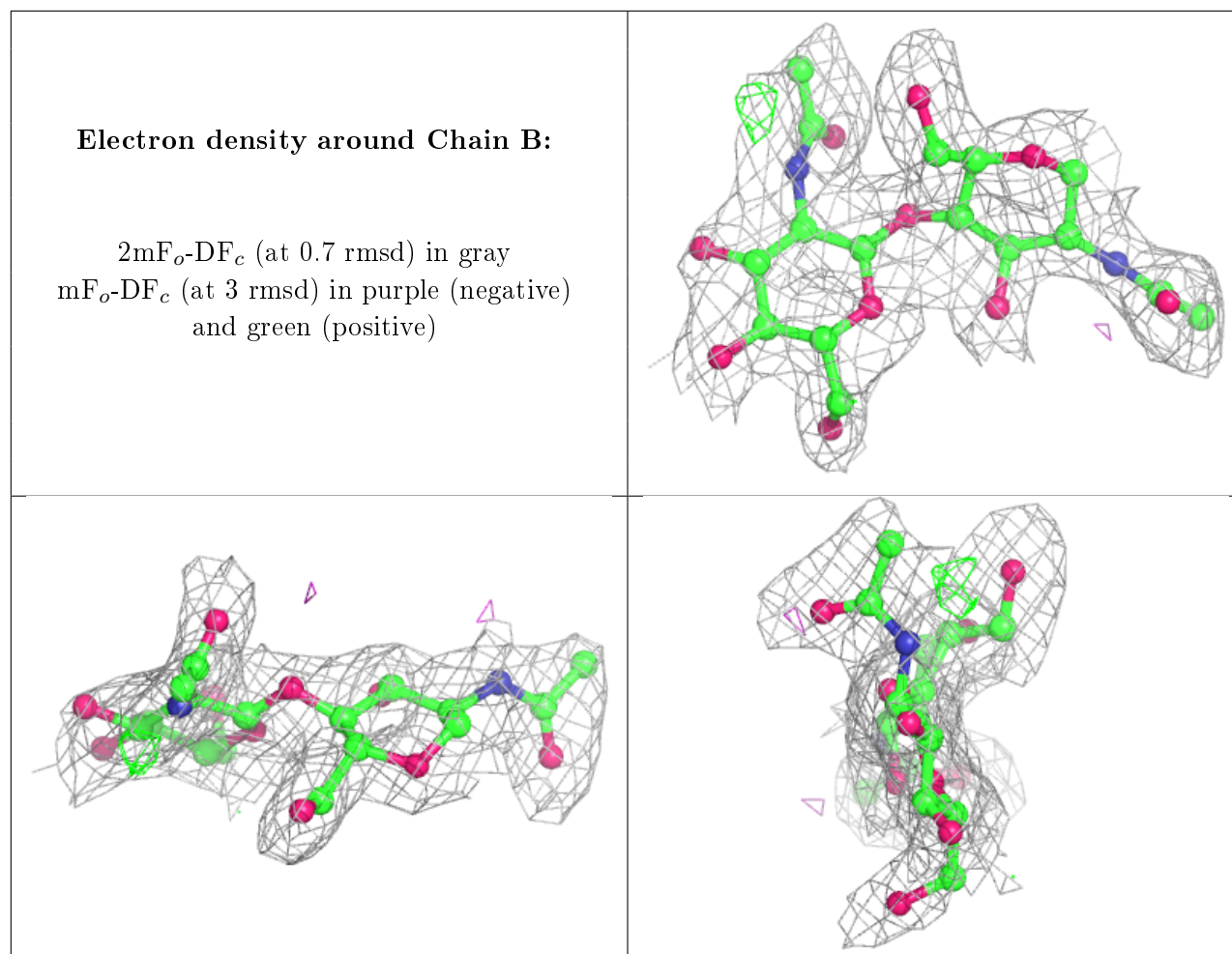
There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	B	2	14/15	0.72	0.28	54,58,60,61	0
2	NAG	B	1	14/15	0.81	0.17	39,43,46,46	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.



## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
5	GOL	A	544	6/6	0.49	0.38	62,63,63,64	0
6	15P	A	553	11/104	0.56	0.30	49,51,53,54	0
5	GOL	A	543	6/6	0.64	0.28	43,43,44,45	0
5	GOL	A	540	6/6	0.68	0.22	62,63,63,63	0
7	PEG	A	556	7/7	0.72	0.29	73,74,77,78	0
6	15P	A	552	11/104	0.72	0.31	40,41,44,44	0
6	15P	A	554	11/104	0.72	0.24	55,57,59,60	0
5	GOL	A	542	6/6	0.72	0.29	52,53,53,54	0
5	GOL	A	546	6/6	0.74	0.21	65,66,67,67	0
4	ZIR	A	536	24/24	0.75	0.21	29,34,47,52	0

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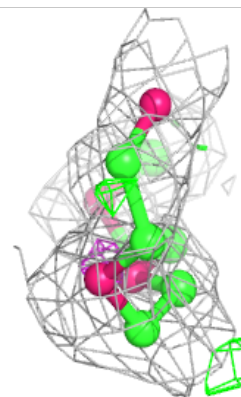
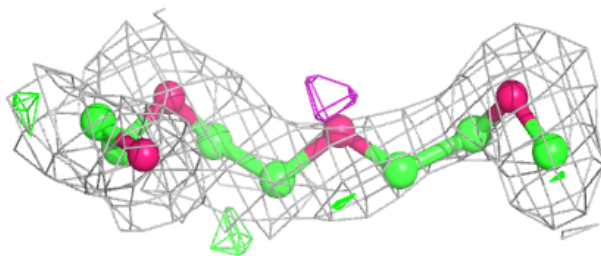
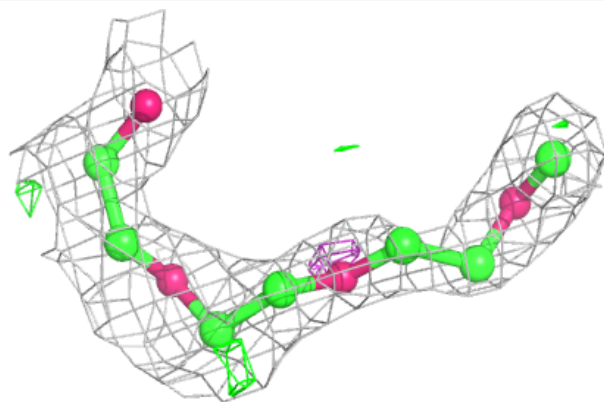
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	GOL	A	537	6/6	0.76	0.15	44,45,46,46	0
6	15P	A	551	11/104	0.79	0.30	40,41,44,45	0
7	PEG	A	558	7/7	0.80	0.20	59,60,62,64	0
8	NAG	A	601	14/15	0.80	0.24	38,42,45,45	0
5	GOL	A	548	6/6	0.84	0.28	66,67,67,69	0
5	GOL	A	547	6/6	0.85	0.21	52,53,54,54	0
5	GOL	A	545	6/6	0.86	0.29	53,55,55,56	0
7	PEG	A	555	7/7	0.86	0.28	30,33,34,43	0
5	GOL	A	549	6/6	0.87	0.19	69,70,70,71	0
8	NAG	A	604	14/15	0.87	0.20	40,44,47,47	0
5	GOL	A	538	6/6	0.88	0.19	29,32,33,34	0
7	PEG	A	557	7/7	0.89	0.12	53,54,57,58	0
5	GOL	A	541	6/6	0.89	0.24	57,58,58,59	0
5	GOL	A	550	6/6	0.89	0.18	28,31,31,32	0
5	GOL	A	539	6/6	0.89	0.24	39,40,40,41	0
3	FAD	A	535	53/53	0.95	0.16	19,20,21,22	0

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

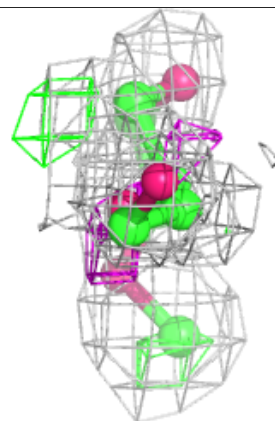
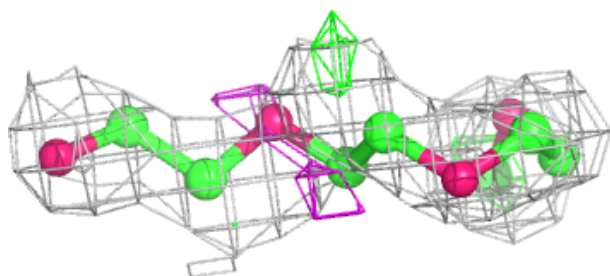
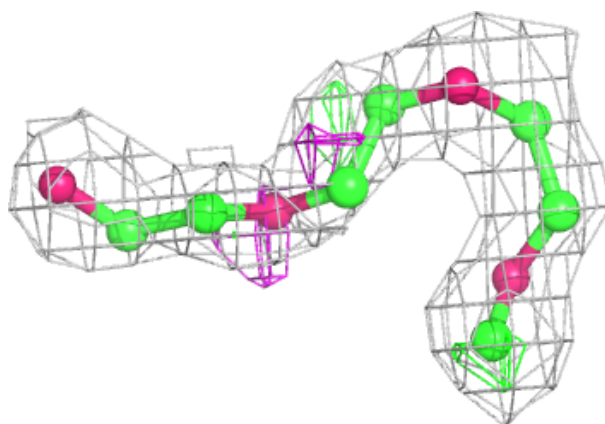
**Electron density around 15P A 553:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

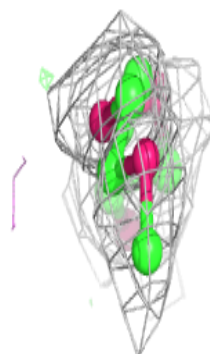
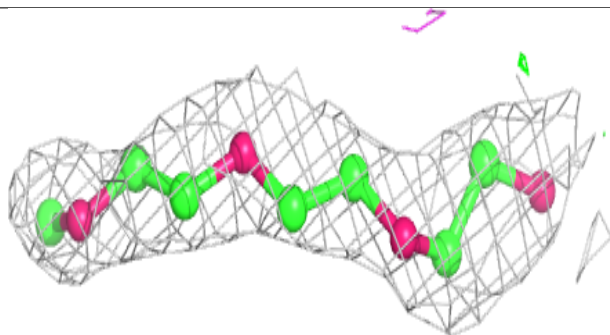
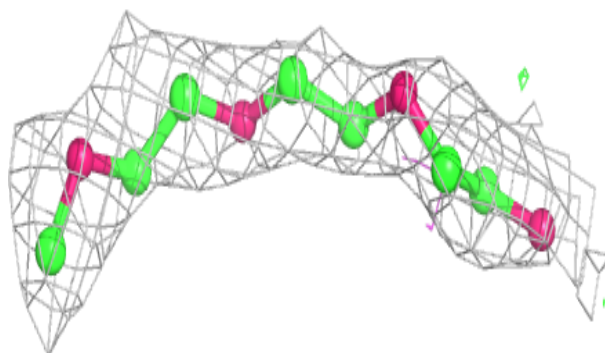


**Electron density around 15P A 552:**

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

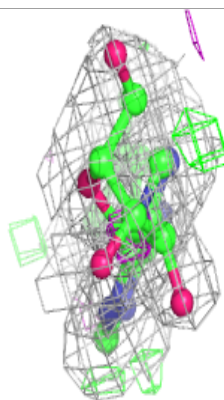
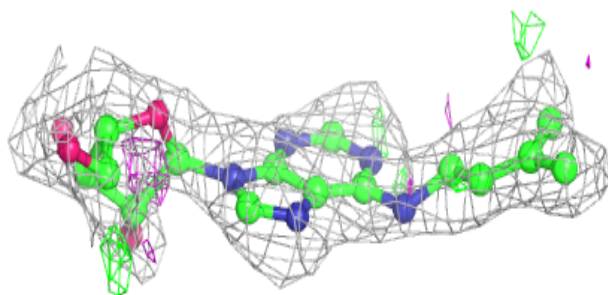
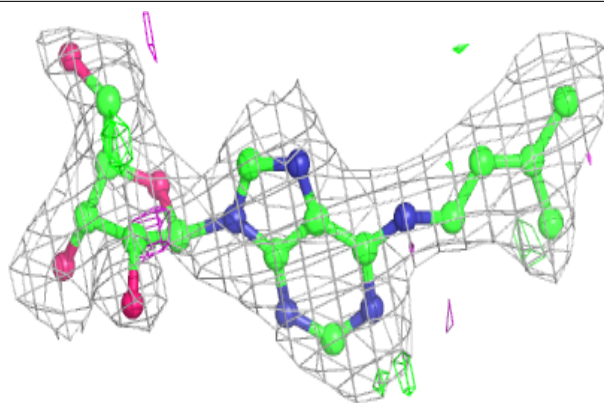
**Electron density around 15P A 554:**

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



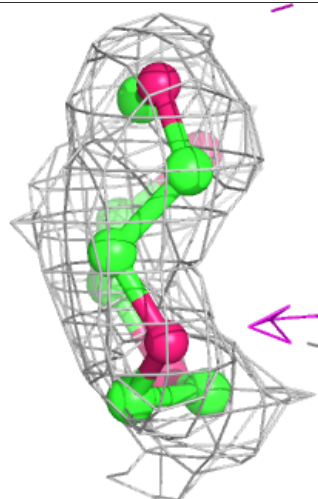
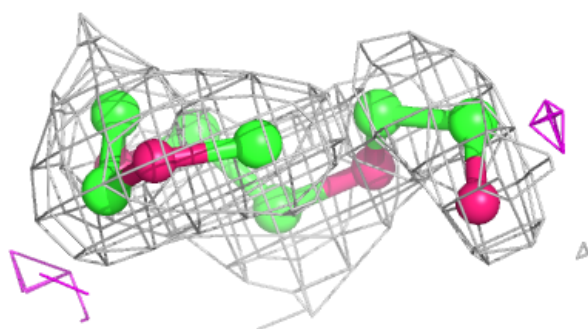
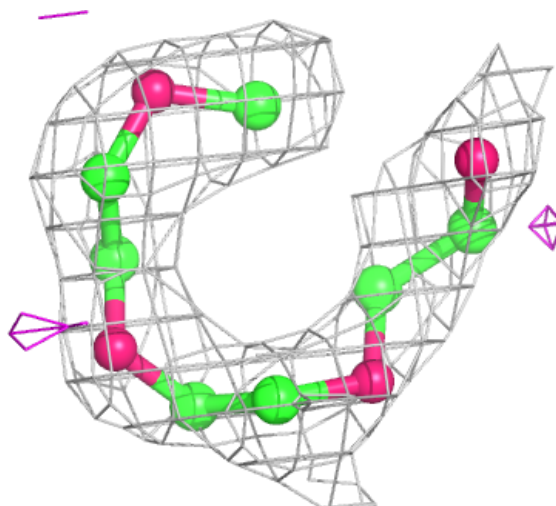
**Electron density around ZIR A 536:**

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

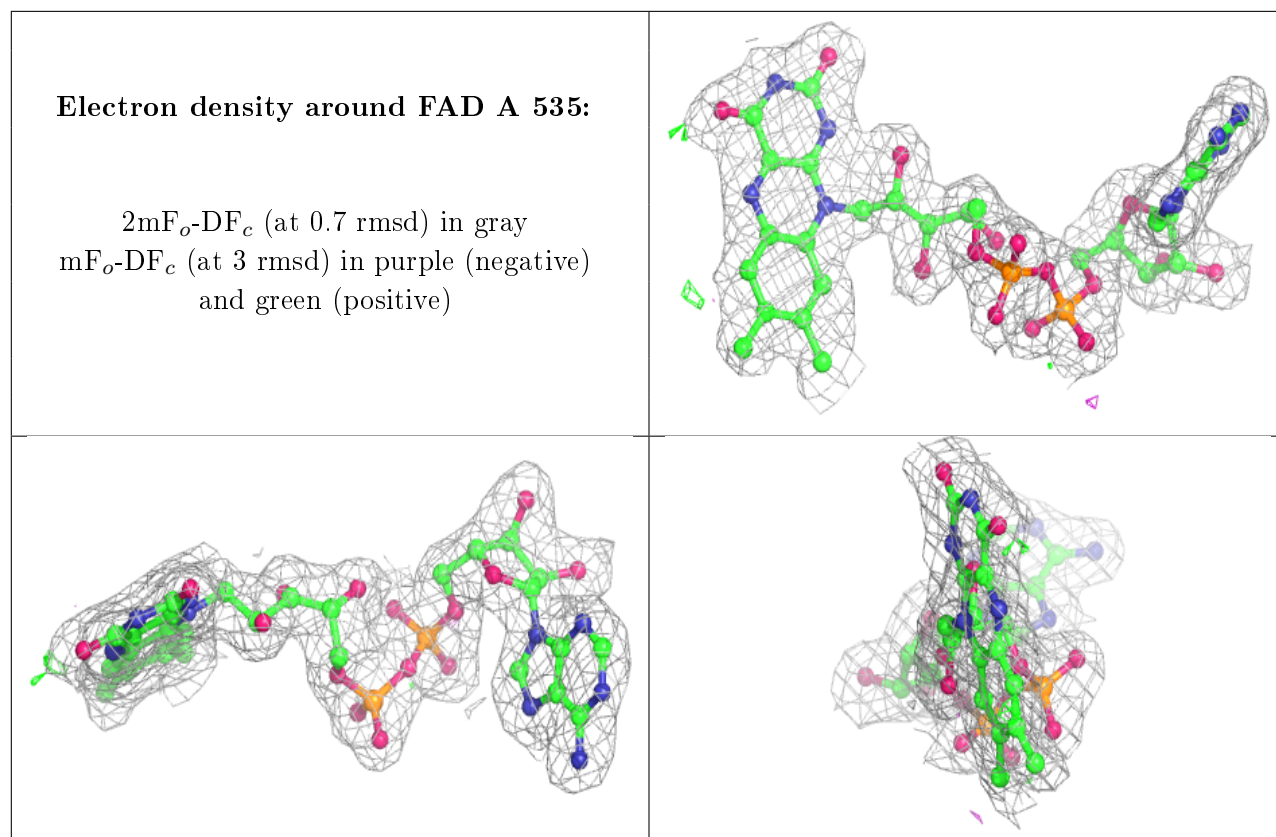


**Electron density around 15P A 551:**

$2mF_o-DF_c$  (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.