



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:17 PM UTC

PDB ID : 3S1C / pdb_00003s1c
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

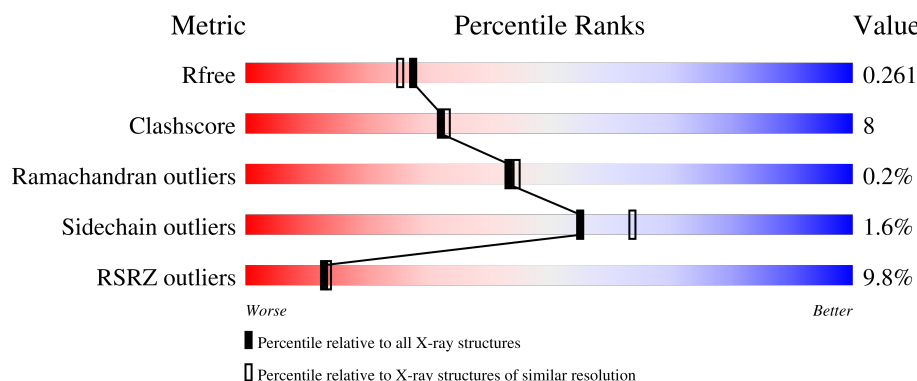
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	516	9% 85% 10% ••
2	B	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
4	ZIR	A	536	-	-	X	-
5	GOL	A	548	-	-	X	-
5	GOL	A	550	-	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:

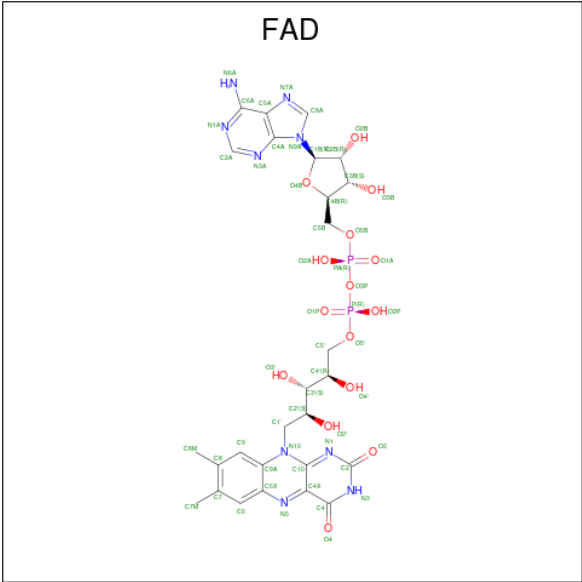
Chain	Residue	Modelled	Actual	Comment	Reference
A	79	ALA	GLY	SEE REMARK 999	UNP Q9T0N8
A	168	THR	ASN	SEE REMARK 999	UNP Q9T0N8
A	254	LEU	PHE	SEE REMARK 999	UNP Q9T0N8

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



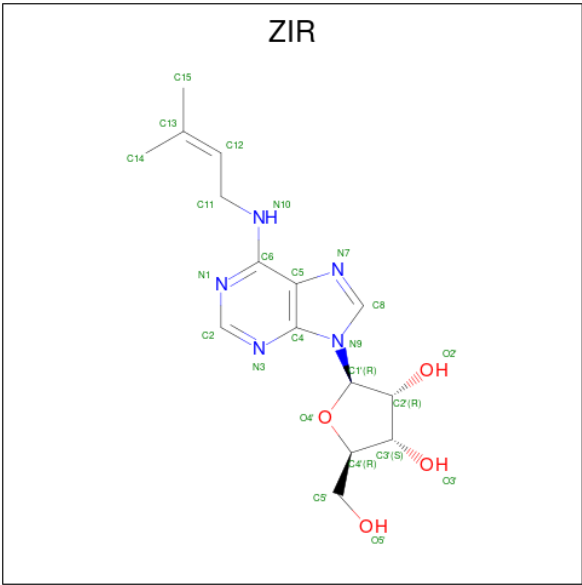
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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 (CCD ID: ZIR) (formula: C₁₅H₂₁N₅O₄).



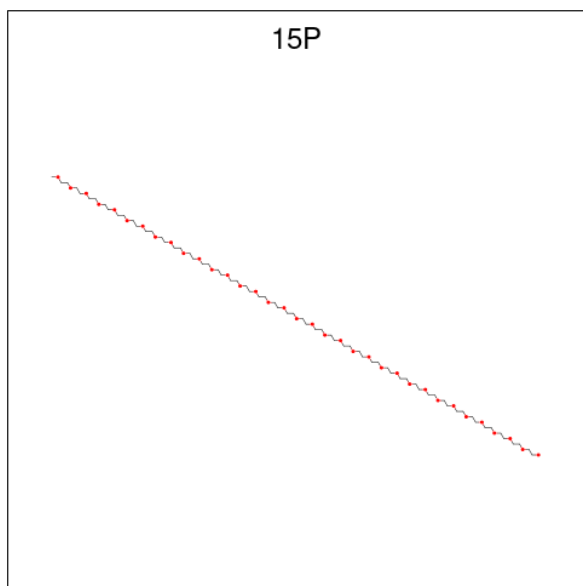
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			24	15	5	4		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



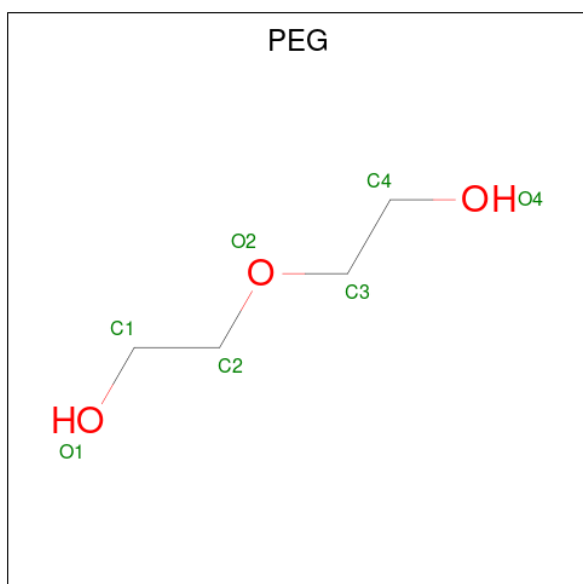
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total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

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



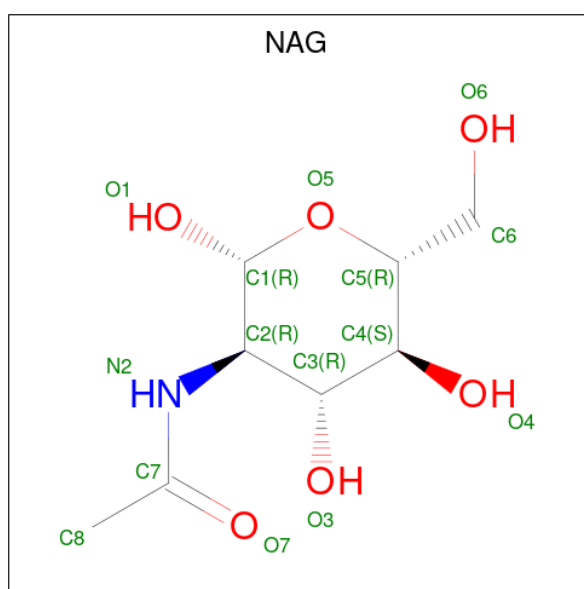
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			11	7	4		
6	A	1	Total	C	O	0	0
			11	7	4		
6	A	1	Total	C	O	0	0
			11	7	4		
6	A	1	Total	C	O	0	0
			11	7	4		

- Molecule 7 is DI(HYDROXYETHYL)ETHER (CCD ID: 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 (CCD ID: 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		

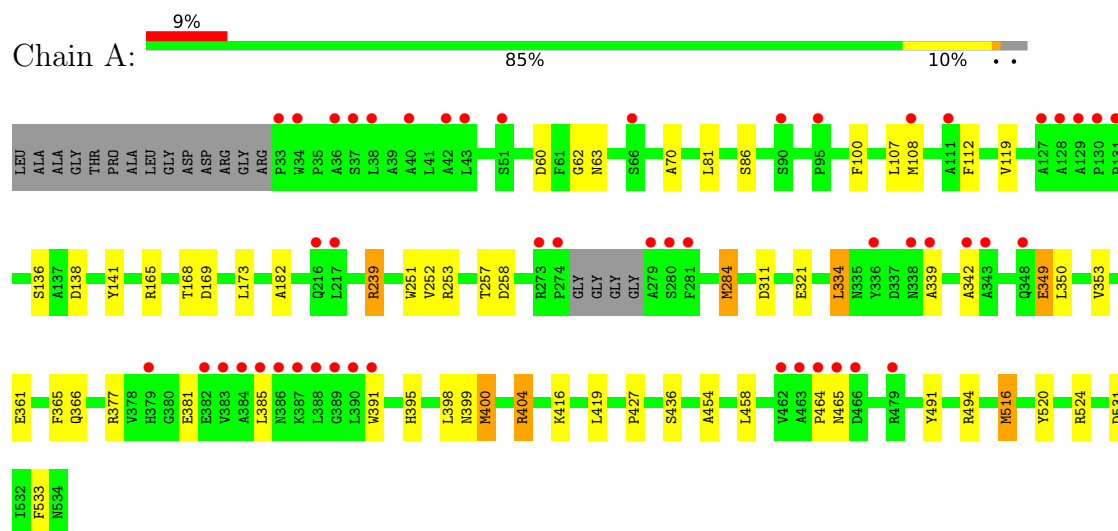
- Molecule 9 is water.

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

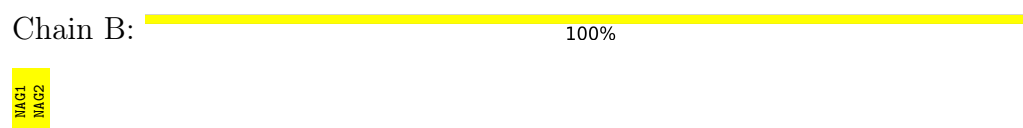
3 Residue-property plots [i](#)

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, α , β , γ	250.95Å 50.62Å 51.40Å 90.00° 93.97° 90.00°	Depositor
Resolution (Å)	32.50 – 2.09 32.50 – 2.09	Depositor EDS
% Data completeness (in resolution range)	(Not available) (32.50-2.09) 91.1 (32.50-2.09)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	27.6	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 67.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4414	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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: ZIR, 15P, FAD, NAG, GOL, PEG

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	0.85	3/3894 (0.1%)	1.29	14/5306 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	400	MET	SD-CE	-8.29	1.58	1.79
1	A	516	MET	SD-CE	-7.28	1.61	1.79
1	A	284	MET	SD-CE	-5.12	1.66	1.79

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	60	ASP	CA-CB-CG	6.81	119.41	112.60
1	A	112	PHE	CA-CB-CG	5.57	119.37	113.80
1	A	531	ASP	CA-CB-CG	5.55	118.15	112.60
1	A	311	ASP	CA-CB-CG	5.48	118.08	112.60
1	A	63	ASN	CA-CB-CG	5.42	118.02	112.60
1	A	138	ASP	CA-CB-CG	5.37	117.97	112.60
1	A	257	THR	N-CA-C	-5.28	106.86	113.72
1	A	465	ASN	CA-C-N	5.20	127.51	120.44
1	A	465	ASN	C-N-CA	5.20	127.51	120.44
1	A	464	PRO	CA-C-N	5.04	127.28	120.38
1	A	464	PRO	C-N-CA	5.04	127.28	120.38
1	A	168	THR	N-CA-C	-5.03	101.90	109.85
1	A	258	ASP	CA-CB-CG	5.03	117.63	112.60
1	A	454	ALA	N-CA-C	-5.02	101.58	109.25

There are no chirality outliers.

There are no planarity outliers.

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	3801	0	3724	45	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	65	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 (65) 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:H17	6:A:551:15P:C2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:284:MET:HE3	1:A:353:VAL:HG11	1.92	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
1:A:377:ARG:NE	6:A:552:15P:H17	2.14	0.50
4:A:536:ZIR:H5'A	6:A:552:15P:C6	2.41	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
4:A:536:ZIR:C5'	6:A:552:15P:O3	2.65	0.45
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:HE1	1:A:520:TYR:HE2	1.83	0.43
1:A:377:ARG:HD2	6:A:552:15P:H16	2.01	0.43
3:A:535:FAD:N5	4:A:536:ZIR:H11A	2.34	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:165:ARG:HH22	5:A:549:GOL:H12	1.84	0.42
1:A:381:GLU:HG2	5:A:548:GOL:H12	2.01	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
1:A:398:LEU:HG	1:A:400:MET:HE2	2.02	0.41
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:552:15P:H26	6:A:552:15P:O1	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
1:A:516:MET:HE3	1:A:520:TYR:HE2	1.86	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%)	43 44

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%)	382 (98%)	6 (2%)	57 65

All (6) 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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	ASN
1	A	181	ASN
1	A	218	ASN
1	A	395	HIS

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 ⓘ

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	1.74	7 (50%)	17,19,21	2.11	6 (35%)
2	NAG	B	2	2	14,14,15	1.71	3 (21%)	17,19,21	1.98	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 (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	NAG	C1-C2	3.84	1.57	1.52
2	B	1	NAG	O5-C5	2.68	1.48	1.43
2	B	1	NAG	C3-C2	2.67	1.58	1.52
2	B	1	NAG	C2-N2	2.37	1.50	1.46
2	B	2	NAG	O5-C5	2.29	1.47	1.43
2	B	1	NAG	C4-C5	2.17	1.57	1.53
2	B	1	NAG	C7-N2	2.13	1.41	1.34
2	B	2	NAG	C3-C2	2.13	1.57	1.52
2	B	1	NAG	C4-C3	2.03	1.57	1.52
2	B	1	NAG	C1-C2	2.01	1.55	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	NAG	C1-O5-C5	5.74	119.88	112.19
2	B	2	NAG	O5-C1-C2	4.15	117.71	111.29
2	B	1	NAG	C1-C2-N2	4.07	116.84	110.43
2	B	1	NAG	C3-C4-C5	4.00	117.49	110.23
2	B	1	NAG	C2-N2-C7	3.61	127.74	122.90
2	B	1	NAG	C1-O5-C5	2.26	115.21	112.19
2	B	1	NAG	O7-C7-N2	2.09	125.68	121.98
2	B	1	NAG	C4-C3-C2	2.07	114.05	111.02

There are no chirality outliers.

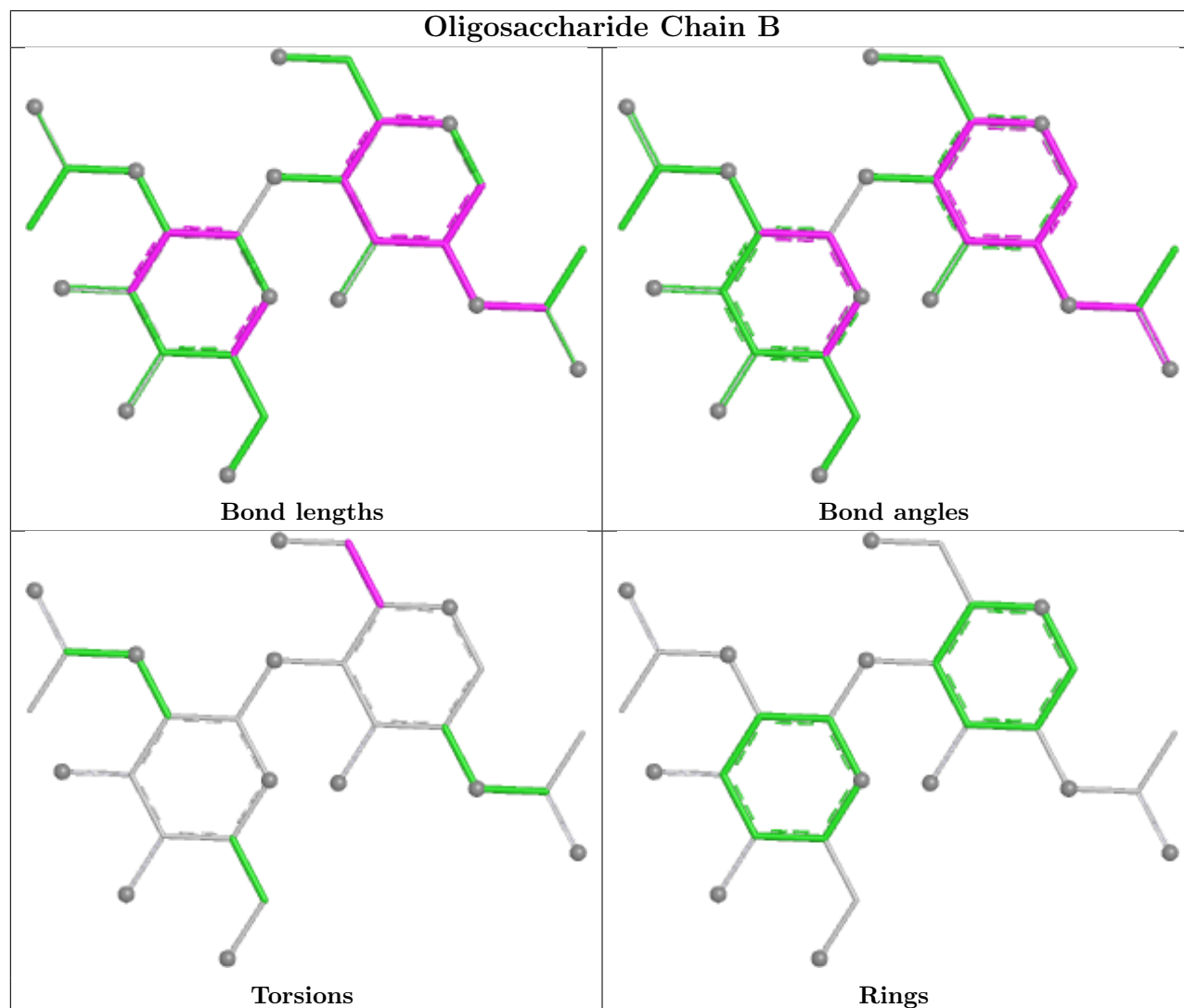
All (2) torsion outliers are listed below:

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
5	GOL	A	541	-	5,5,5	0.31	0	5,5,5	0.79	0
5	GOL	A	546	-	5,5,5	0.50	0	5,5,5	0.50	0
5	GOL	A	550	-	5,5,5	1.28	1 (20%)	5,5,5	1.42	1 (20%)
6	15P	A	553	-	10,10,103	1.03	0	9,9,102	0.73	0
6	15P	A	552	-	10,10,103	0.63	0	9,9,102	0.92	0
7	PEG	A	558	-	6,6,6	0.35	0	5,5,5	0.51	0
5	GOL	A	540	-	5,5,5	0.45	0	5,5,5	0.24	0
5	GOL	A	542	-	5,5,5	0.67	0	5,5,5	0.53	0
5	GOL	A	548	-	5,5,5	0.31	0	5,5,5	0.72	0
6	15P	A	551	-	10,10,103	0.57	0	9,9,102	0.91	0
5	GOL	A	547	-	5,5,5	0.42	0	5,5,5	0.27	0
7	PEG	A	557	-	6,6,6	0.16	0	5,5,5	0.23	0
8	NAG	A	604	1	14,14,15	1.89	3 (21%)	17,19,21	1.67	4 (23%)
5	GOL	A	545	-	5,5,5	0.28	0	5,5,5	0.26	0
6	15P	A	554	-	10,10,103	0.72	0	9,9,102	0.55	0
5	GOL	A	549	-	5,5,5	0.29	0	5,5,5	0.72	0
5	GOL	A	537	-	5,5,5	0.81	0	5,5,5	1.07	0
7	PEG	A	556	-	6,6,6	0.15	0	5,5,5	0.19	0
8	NAG	A	601	1	14,14,15	1.67	4 (28%)	17,19,21	1.49	2 (11%)
7	PEG	A	555	-	6,6,6	0.56	0	5,5,5	0.50	0
5	GOL	A	539	-	5,5,5	0.48	0	5,5,5	0.37	0
5	GOL	A	538	-	5,5,5	0.57	0	5,5,5	0.65	0
5	GOL	A	544	-	5,5,5	0.68	0	5,5,5	0.42	0
3	FAD	A	535	1	58,58,58	1.50	7 (12%)	85,89,89	1.19	7 (8%)
4	ZIR	A	536	-	26,26,26	1.82	8 (30%)	36,37,37	2.77	15 (41%)
5	GOL	A	543	-	5,5,5	0.66	0	5,5,5	0.59	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
5	GOL	A	541	-	-	2/4/4/4	-
5	GOL	A	546	-	-	2/4/4/4	-
5	GOL	A	550	-	-	4/4/4/4	-
6	15P	A	553	-	-	2/8/8/101	-
6	15P	A	552	-	-	4/8/8/101	-
7	PEG	A	558	-	-	0/4/4/4	-
5	GOL	A	540	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	542	-	-	3/4/4/4	-
5	GOL	A	548	-	-	3/4/4/4	-
6	15P	A	551	-	-	7/8/8/101	-
5	GOL	A	547	-	-	0/4/4/4	-
7	PEG	A	557	-	-	1/4/4/4	-
8	NAG	A	604	1	-	4/6/23/26	0/1/1/1
5	GOL	A	545	-	-	2/4/4/4	-
6	15P	A	554	-	-	3/8/8/101	-
5	GOL	A	549	-	-	0/4/4/4	-
5	GOL	A	537	-	-	2/4/4/4	-
7	PEG	A	556	-	-	2/4/4/4	-
8	NAG	A	601	1	-	0/6/23/26	0/1/1/1
7	PEG	A	555	-	-	3/4/4/4	-
5	GOL	A	539	-	-	2/4/4/4	-
5	GOL	A	538	-	-	2/4/4/4	-
5	GOL	A	544	-	-	2/4/4/4	-
3	FAD	A	535	1	-	5/34/50/50	0/6/6/6
4	ZIR	A	536	-	-	4/12/28/28	0/3/3/3
5	GOL	A	543	-	-	0/4/4/4	-

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	535	FAD	PA-O3P	4.55	1.64	1.59
8	A	604	NAG	C1-C2	4.13	1.58	1.52
4	A	536	ZIR	C1'-N9	3.75	1.56	1.46
4	A	536	ZIR	C5-N7	-3.56	1.32	1.39
3	A	535	FAD	C4X-C10	3.43	1.54	1.44
4	A	536	ZIR	C8-N9	-3.42	1.31	1.37
8	A	604	NAG	C3-C2	3.17	1.59	1.52
3	A	535	FAD	C9A-C5X	2.98	1.46	1.41
8	A	601	NAG	C4-C3	2.87	1.59	1.52
4	A	536	ZIR	C6-N10	-2.87	1.30	1.34
8	A	601	NAG	C3-C2	2.87	1.58	1.52
4	A	536	ZIR	C4-N9	-2.86	1.31	1.37
4	A	536	ZIR	C2-N1	-2.76	1.29	1.33
8	A	601	NAG	C4-C5	2.64	1.58	1.53
3	A	535	FAD	C2A-N3A	2.58	1.38	1.33
3	A	535	FAD	C6-C7	2.47	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	601	NAG	O5-C5	2.39	1.48	1.43
3	A	535	FAD	C9-C9A	2.31	1.43	1.39
3	A	535	FAD	C2A-N1A	2.30	1.38	1.33
4	A	536	ZIR	C12-C13	2.13	1.38	1.32
4	A	536	ZIR	C11-C12	-2.11	1.37	1.47
5	A	550	GOL	O2-C2	-2.03	1.37	1.43
8	A	604	NAG	C2-N2	2.02	1.49	1.46

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	536	ZIR	C5-C4-N3	-7.73	116.08	126.72
4	A	536	ZIR	N3-C2-N1	-5.64	120.05	128.58
4	A	536	ZIR	C2-N3-C4	5.44	125.12	111.83
4	A	536	ZIR	N3-C4-N9	4.99	135.65	127.17
8	A	601	NAG	C4-C3-C2	4.17	117.13	111.02
8	A	604	NAG	C1-C2-N2	4.02	116.77	110.43
4	A	536	ZIR	C11-C12-C13	-3.83	120.14	127.01
3	A	535	FAD	O2P-P-O3P	3.78	117.50	107.27
4	A	536	ZIR	C5-C6-N1	3.73	122.15	118.15
4	A	536	ZIR	C5'-C4'-C3'	-3.64	106.50	115.10
4	A	536	ZIR	C2'-C1'-N9	3.62	122.30	113.30
8	A	604	NAG	C3-C4-C5	-3.34	104.17	110.23
4	A	536	ZIR	C4-C5-N7	-3.34	106.77	110.58
3	A	535	FAD	C1'-C2'-C3'	-3.26	100.81	109.66
4	A	536	ZIR	C15-C13-C14	3.17	121.89	114.59
3	A	535	FAD	C4'-C3'-C2'	3.05	118.65	113.57
4	A	536	ZIR	C6-C5-N7	2.76	135.44	132.43
3	A	535	FAD	O4-C4-C4X	-2.72	119.35	126.53
5	A	550	GOL	O3-C3-C2	2.57	121.96	110.38
4	A	536	ZIR	O4'-C1'-C2'	-2.54	101.18	106.62
3	A	535	FAD	O4-C4-N3	2.53	124.86	120.11
4	A	536	ZIR	C5-N7-C8	2.52	107.42	103.45
3	A	535	FAD	O3'-C3'-C4'	2.36	114.28	108.93
8	A	604	NAG	C2-N2-C7	2.31	126.00	122.90
4	A	536	ZIR	C5-C4-N9	2.26	108.27	105.81
3	A	535	FAD	C10-N1-C2	2.18	121.56	116.85
4	A	536	ZIR	C15-C13-C12	-2.15	116.21	122.66
8	A	604	NAG	O4-C4-C5	2.14	114.59	109.32
8	A	601	NAG	C3-C4-C5	2.03	113.92	110.23

There are no chirality outliers.

All (61) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
6	A	552	15P	C5-C6-O3-C7
7	A	555	PEG	C1-C2-O2-C3
7	A	556	PEG	C4-C3-O2-C2
3	A	535	FAD	C2'-C3'-C4'-C5'
3	A	535	FAD	PA-O3P-P-O1P
6	A	551	15P	C3-C4-O2-C5
5	A	540	GOL	O1-C1-C2-O2
5	A	542	GOL	O2-C2-C3-O3
6	A	552	15P	C4-C3-O1-C2
6	A	551	15P	C5-C6-O3-C7
7	A	557	PEG	C1-C2-O2-C3
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	C6-C5-O2-C4
6	A	551	15P	C8-C7-O3-C6
6	A	554	15P	C5-C6-O3-C7
6	A	552	15P	O2-C5-C6-O3
6	A	554	15P	O2-C5-C6-O3

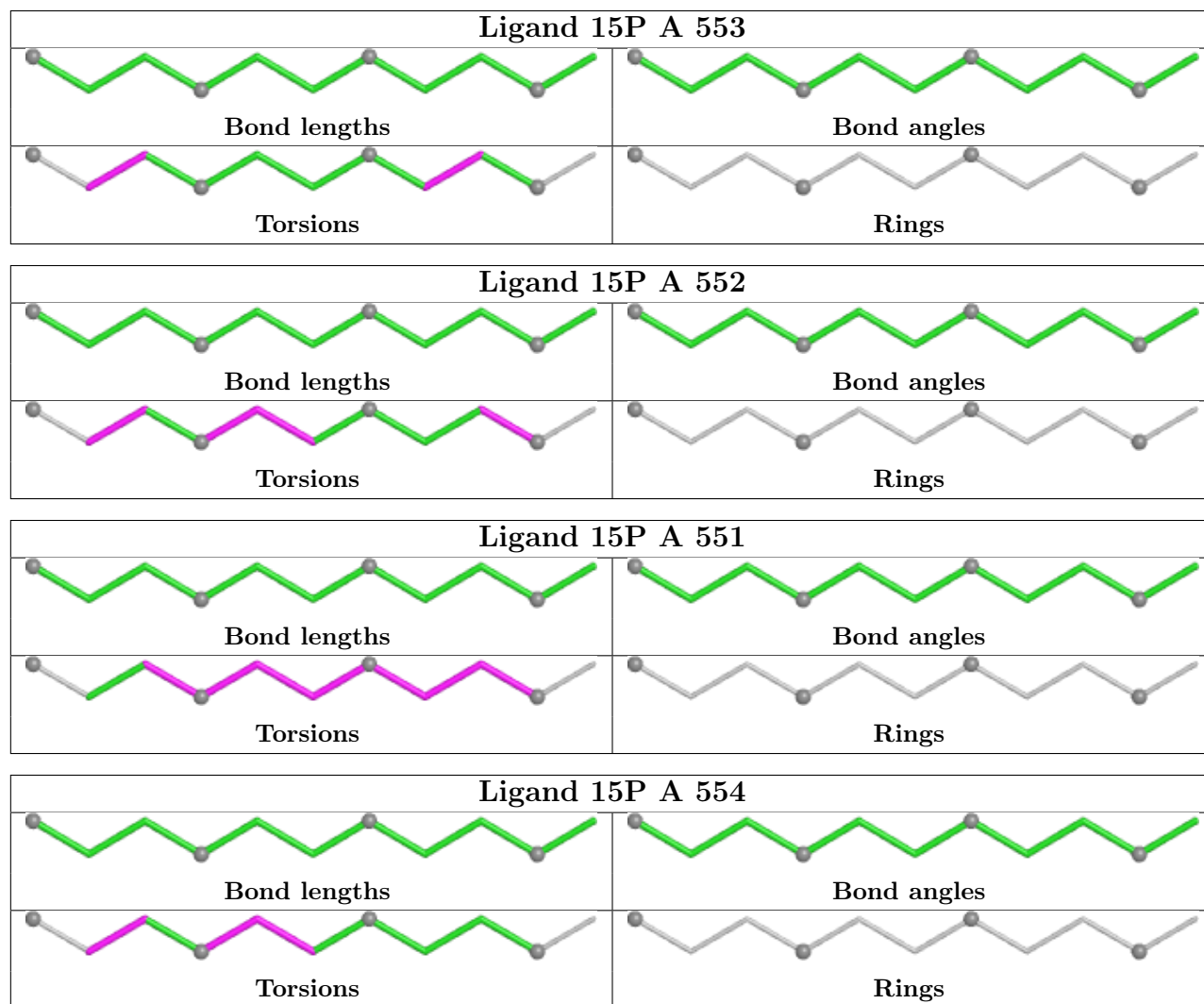
There are no ring outliers.

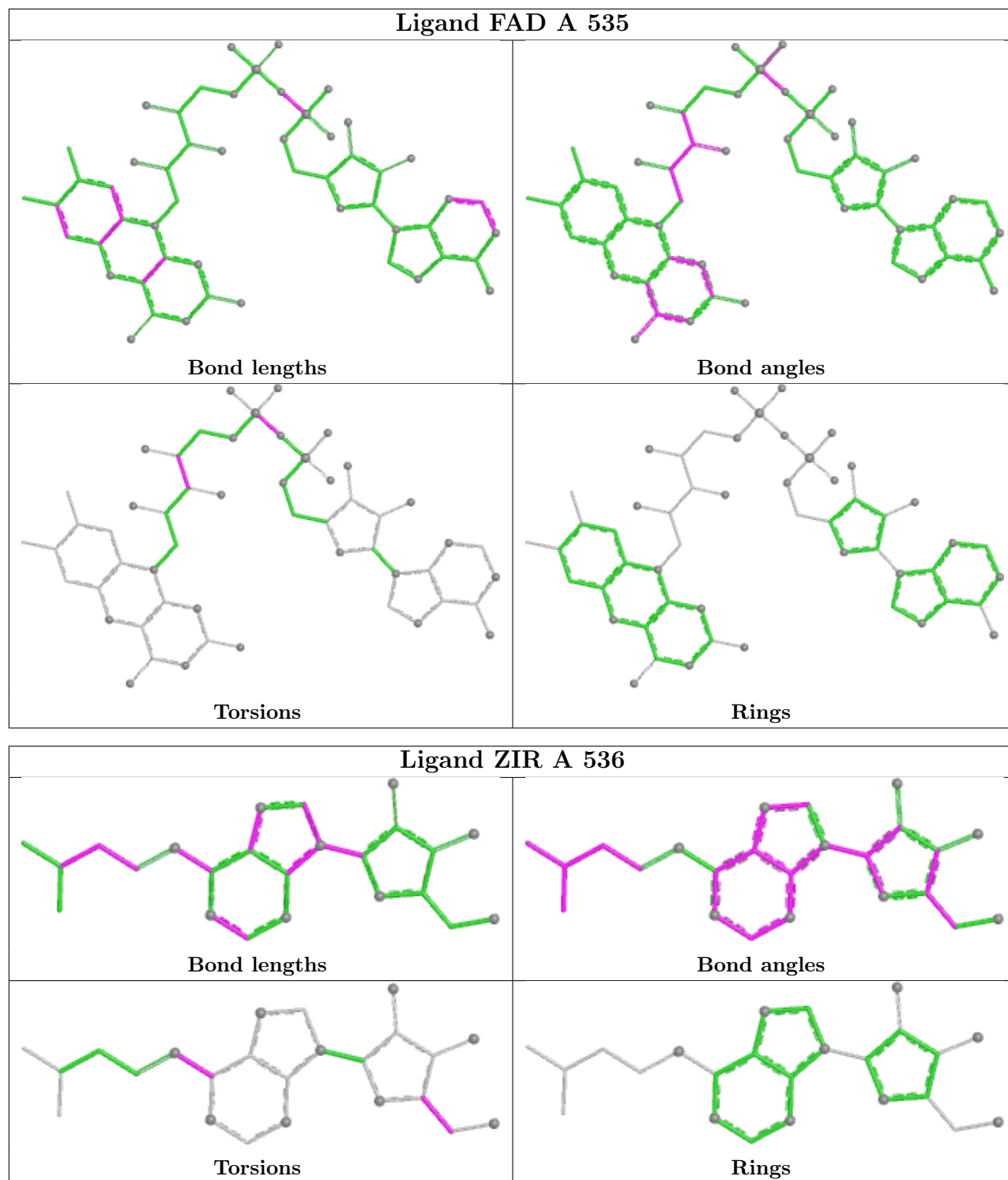
12 monomers are involved in 46 short contacts:

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

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, 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	498/516 (96%)	0.66	49 (9%) 13 13	12, 26, 52, 72	1 (0%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	463	ALA	5.9
1	A	462	VAL	5.7
1	A	274	PRO	5.4
1	A	390	LEU	5.4
1	A	383	VAL	5.1
1	A	129	ALA	5.0
1	A	391	TRP	5.0
1	A	279	ALA	4.9
1	A	465	ASN	4.7
1	A	464	PRO	4.5
1	A	385	LEU	4.4
1	A	388	LEU	4.2
1	A	389	GLY	4.0
1	A	33	PRO	3.8
1	A	280	SER	3.7
1	A	51	SER	3.6
1	A	273	ARG	3.4
1	A	127	ALA	3.3
1	A	384	ALA	3.1
1	A	379	HIS	3.1
1	A	387	LYS	3.0
1	A	128	ALA	3.0
1	A	95	PRO	2.9
1	A	36	ALA	2.7
1	A	342	ALA	2.6
1	A	348	GLN	2.6
1	A	40	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	38	LEU	2.5
1	A	90	SER	2.4
1	A	281	PHE	2.4
1	A	108[A]	MET	2.4
1	A	42	ALA	2.3
1	A	339	ALA	2.3
1	A	216	GLN	2.3
1	A	386	ASN	2.3
1	A	43	LEU	2.3
1	A	130	PRO	2.3
1	A	34	TRP	2.3
1	A	131	PRO	2.2
1	A	338	ASN	2.2
1	A	111	ALA	2.1
1	A	66	SER	2.1
1	A	37	SER	2.1
1	A	382	GLU	2.1
1	A	343	ALA	2.1
1	A	479	ARG	2.0
1	A	336	TYR	2.0
1	A	217	LEU	2.0
1	A	466	ASP	2.0

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

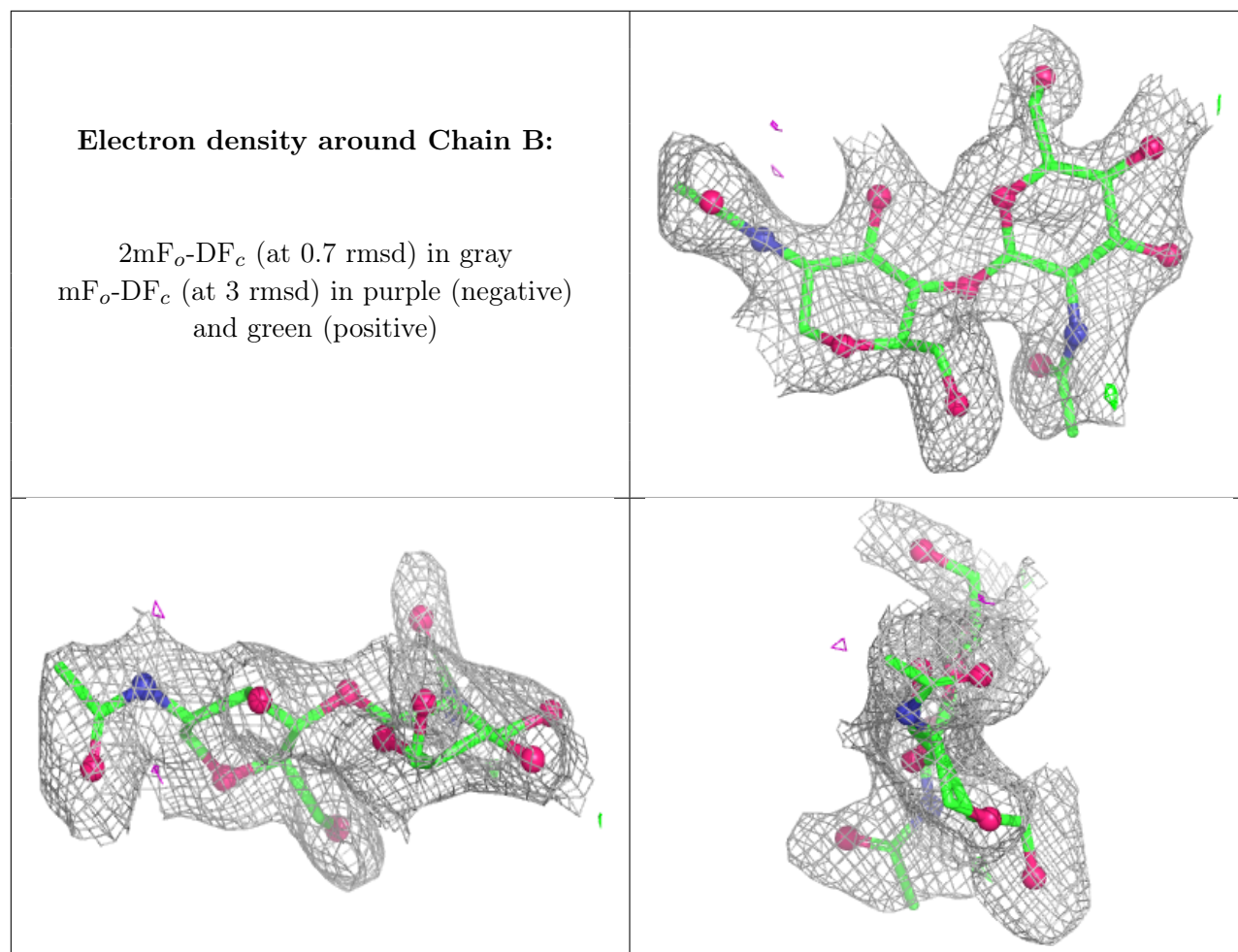
There are no non-standard protein/DNA/RNA residues in this entry.

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
2	NAG	B	2	14/15	0.72	0.18	54,58,60,61	0
2	NAG	B	1	14/15	0.85	0.12	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, 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
6	15P	A	553	11/104	0.63	0.21	49,51,53,54	0
6	15P	A	552	11/104	0.70	0.19	40,41,44,44	0
5	GOL	A	542	6/6	0.72	0.20	52,53,53,54	0
7	PEG	A	558	7/7	0.73	0.20	59,60,62,64	0
6	15P	A	551	11/104	0.74	0.18	40,41,44,45	0
5	GOL	A	546	6/6	0.75	0.17	65,66,67,67	0
6	15P	A	554	11/104	0.75	0.20	55,57,59,60	0
5	GOL	A	549	6/6	0.75	0.20	69,70,70,71	0
5	GOL	A	544	6/6	0.78	0.20	62,63,63,64	0
5	GOL	A	540	6/6	0.78	0.18	62,63,63,63	0
5	GOL	A	548	6/6	0.78	0.21	66,67,67,69	0

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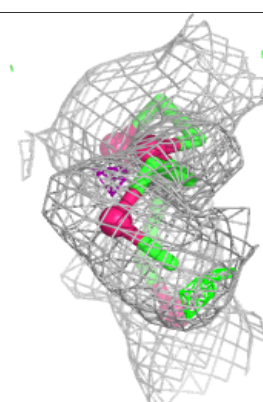
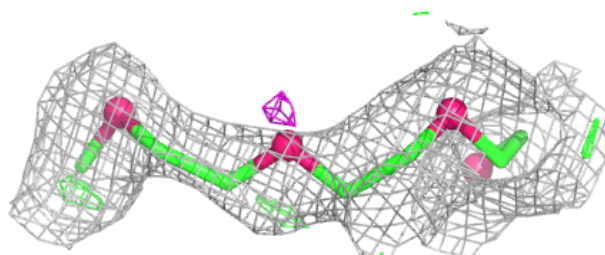
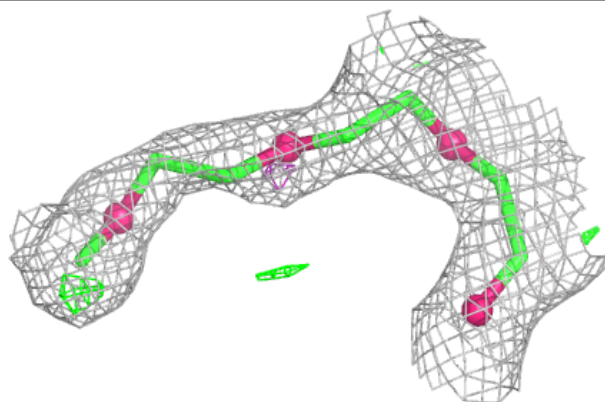
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	PEG	A	556	7/7	0.79	0.22	73,74,77,78	0
5	GOL	A	543	6/6	0.79	0.19	43,43,44,45	0
5	GOL	A	545	6/6	0.80	0.16	53,55,55,56	0
4	ZIR	A	536	24/24	0.80	0.13	29,34,47,52	0
5	GOL	A	547	6/6	0.82	0.17	52,53,54,54	0
7	PEG	A	555	7/7	0.82	0.20	30,33,34,43	0
5	GOL	A	538	6/6	0.83	0.16	29,32,33,34	0
5	GOL	A	537	6/6	0.83	0.14	44,45,46,46	0
7	PEG	A	557	7/7	0.83	0.11	53,54,57,58	0
5	GOL	A	541	6/6	0.83	0.18	57,58,58,59	0
8	NAG	A	604	14/15	0.83	0.14	40,44,47,47	0
8	NAG	A	601	14/15	0.85	0.12	38,42,45,45	0
5	GOL	A	550	6/6	0.88	0.20	28,31,31,32	0
5	GOL	A	539	6/6	0.91	0.12	39,40,40,41	0
3	FAD	A	535	53/53	0.96	0.07	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.

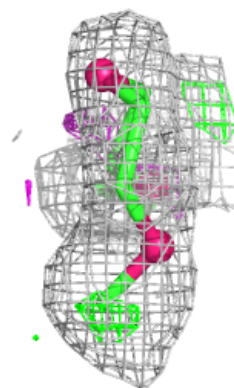
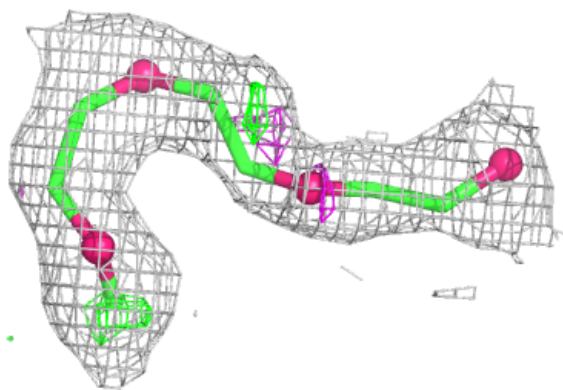
Electron density around 15P A 553:

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



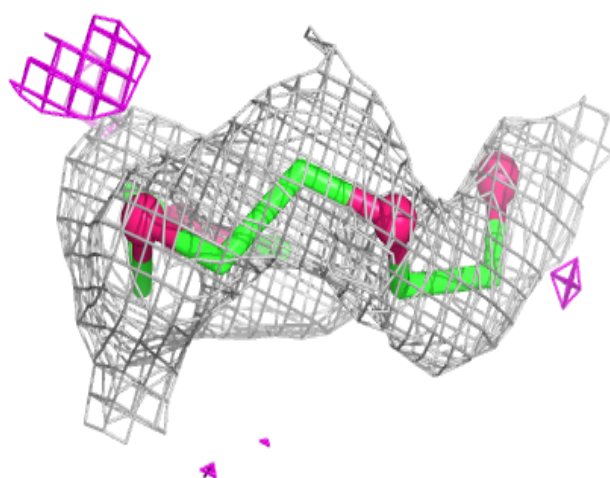
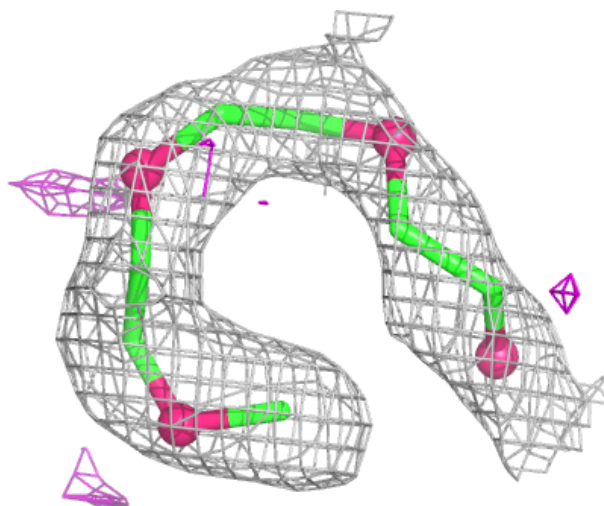
Electron density around 15P A 552:

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



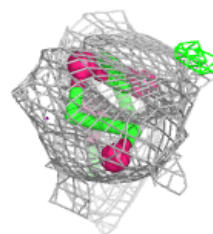
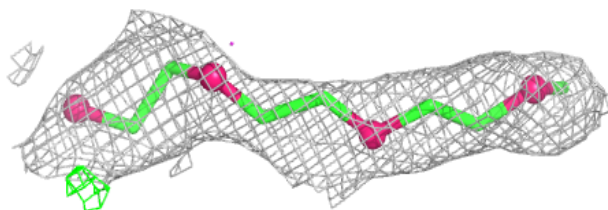
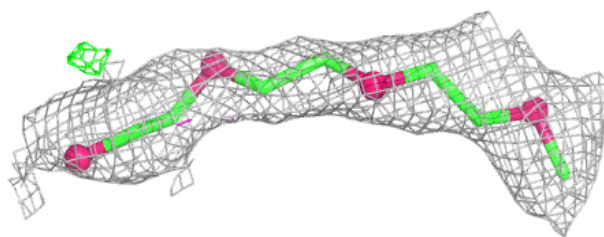
Electron density around 15P A 551:

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

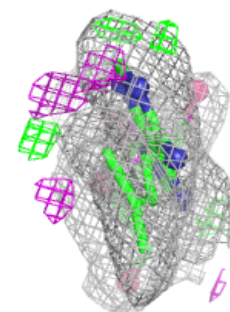
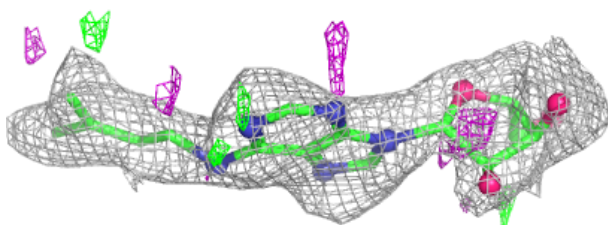
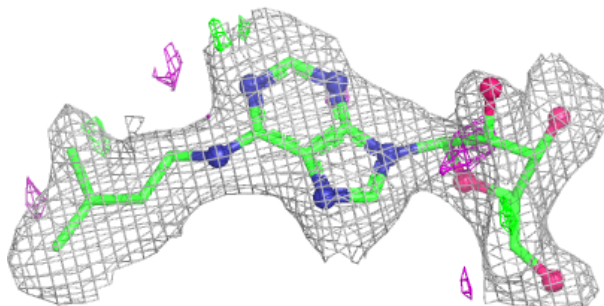


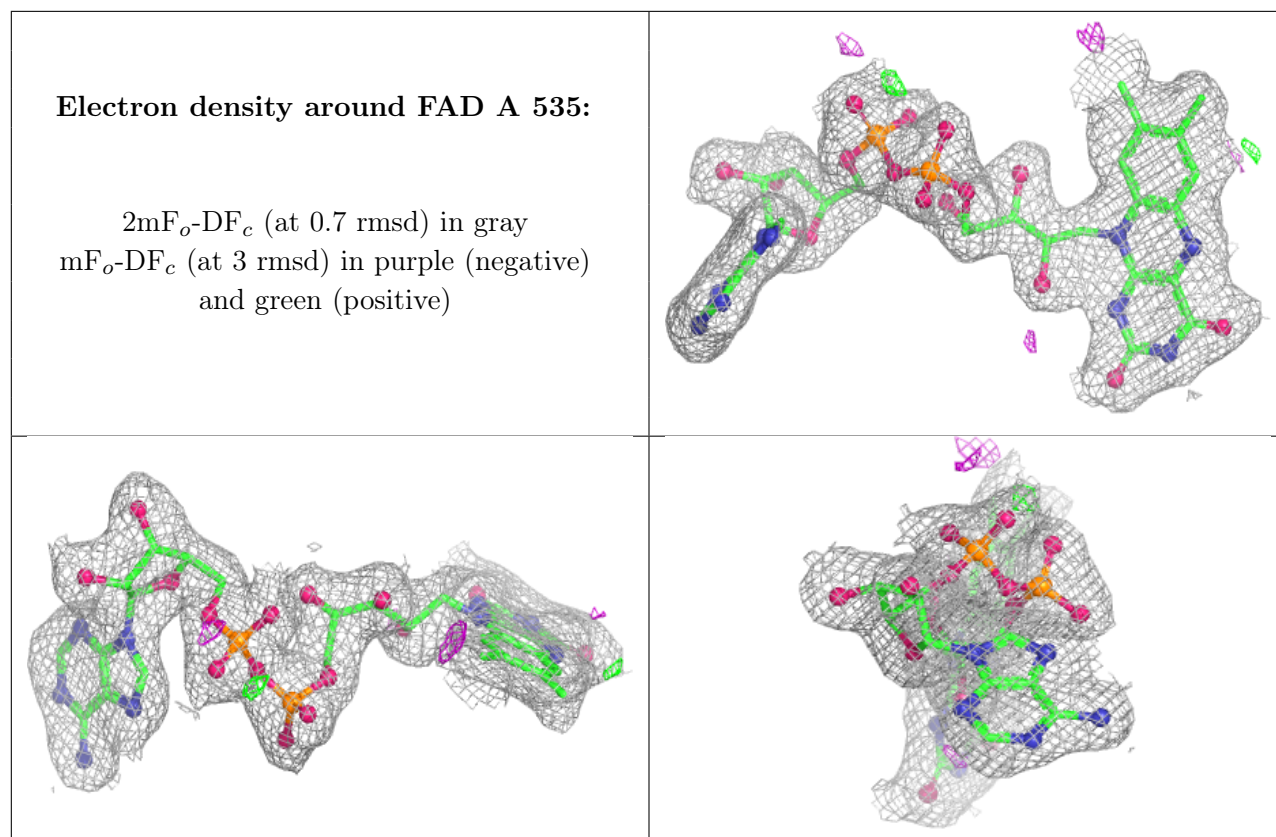
Electron density around 15P A 554:

$2mF_o-DF_c$ (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)





6.5 Other polymers [i](#)

There are no such residues in this entry.