



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 20, 2024 – 07:37 pm GMT

PDB ID : 7OJ7
Title : Crystal structure of human coxsackievirus A24v in complex with a pentavalent N-acetylneuraminic acid conjugate
Authors : Zocher, G.; Stehle, T.
Deposited on : 2021-05-14
Resolution : 1.78 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

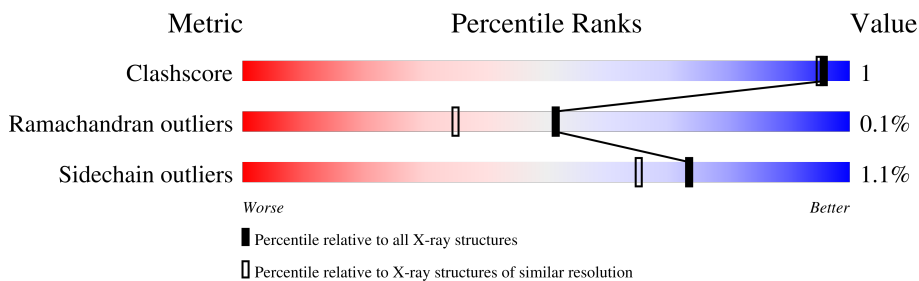
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.78 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	111	305	
2	222	271	
3	333	240	
4	444	69	

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 7478 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 Capsid protein VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	111	281	2267	1442	382	435	8	0	6	0

- Molecule 2 is a protein called Capsid protein VP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	222	264	2068	1318	343	393	14	0	4	0

- Molecule 3 is a protein called Capsid protein VP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	333	234	1855	1193	293	347	22	0	12	0

- Molecule 4 is a protein called Capsid protein VP4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	444	57	438	274	72	91	1	0	2	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	111	3	Total	Ca	0	0
			3	3		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

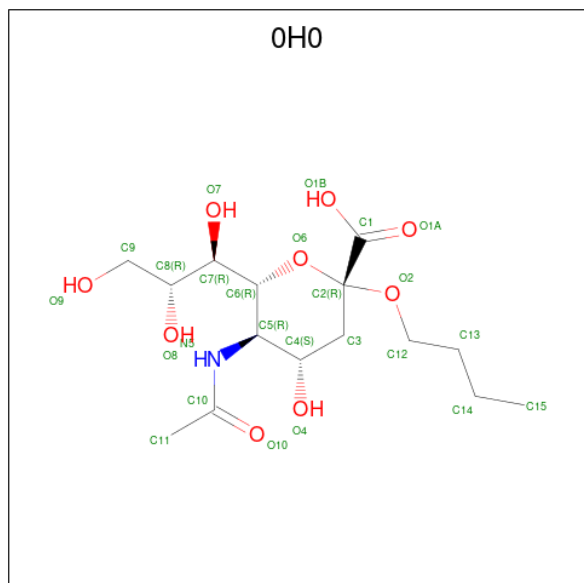
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	111	3	Total	Cl	0	0
			3	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	222	3	Total Cl 3 3	0	0
6	333	1	Total Cl 1 1	0	0

- Molecule 7 is Carbohydrate component from a pentavalent N-acetylneuraminic acid conjugate (three-letter code: 0H0) (formula: C₁₅H₂₇NO₉).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	111	1	Total C N O 24 14 1 9	0	0

- Molecule 8 is water.

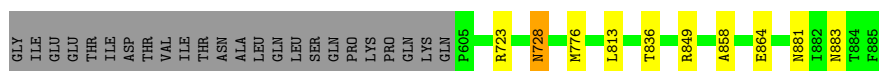
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	111	286	Total O 286 286	0	0
8	222	238	Total O 238 238	0	0
8	333	226	Total O 226 226	0	0
8	444	66	Total O 66 66	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: Capsid protein VP1

Chain 111:  89% 8%



- Molecule 2: Capsid protein VP2

Chain 222:  94%




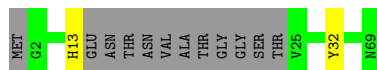
- Molecule 3: Capsid protein VP3

Chain 333:  93%



- Molecule 4: Capsid protein VP4

Chain 444:  80% 17%



4 Data and refinement statistics i

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	305.52Å 365.55Å 366.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.96 – 1.78 49.96 – 1.78	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.96-1.78) 99.9 (49.96-1.78)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 1.78Å)	Xtrriage
Refinement program	REFMAC 5.8.0232 2018/13/08	Depositor
R, R_{free}	0.158 , (Not available) 0.408 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	21.2	Xtrriage
Anisotropy	0.101	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 62.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.017 for -h,-l,-k	Xtrriage
F_o, F_c correlation	0.75	EDS
Total number of atoms	7478	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.25% 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: OH0, CA, CL

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	111	0.60	0/2348	0.76	0/3207
2	222	0.59	0/2136	0.78	0/2917
3	333	0.60	0/1939	0.74	0/2640
4	444	0.64	0/451	0.71	0/608
All	All	0.60	0/6874	0.76	0/9372

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
2	222	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	222	151	LEU	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	111	2267	0	2198	5	0
2	222	2068	0	1994	4	0
3	333	1855	0	1856	8	0
4	444	438	0	428	1	0
5	111	3	0	0	0	0
6	111	3	0	0	0	0
6	222	3	0	0	0	0
6	333	1	0	0	0	0
7	111	24	0	0	0	0
8	111	286	0	0	2	0
8	222	238	0	0	0	0
8	333	226	0	0	0	0
8	444	66	0	0	0	0
All	All	7478	0	6476	15	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 1.

All (15) 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)
3:333:360:GLN:HE22	4:444:32:TYR:H	1.31	0.79
1:111:836[B]:THR:HG22	8:111:1116:HOH:O	2.05	0.55
1:111:858:ALA:HA	3:333:569[A]:HIS:CE1	2.43	0.53
1:111:728:ASN:HD22	1:111:728:ASN:H	1.60	0.50
3:333:472[A]:SER:OG	3:333:530[A]:THR:OG1	2.29	0.49
1:111:881[B]:ASN:HD22	1:111:883:ASN:H	1.63	0.46
3:333:495:TRP:CD1	3:333:503:CYS:HB2	2.51	0.46
2:222:248:LEU:HA	2:222:253:VAL:O	2.17	0.45
1:111:849:ARG:NH1	8:111:1010:HOH:O	2.51	0.43
2:222:201[B]:MET:HB2	2:222:242:PHE:CD1	2.54	0.42
2:222:168:HIS:CG	2:222:328:PHE:HB3	2.55	0.42
2:222:106:GLU:CD	3:333:375:HIS:HE2	2.23	0.41
3:333:457:PHE:O	3:333:502:SER:HA	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	111	285/305 (93%)	274 (96%)	11 (4%)	0	100	100
2	222	266/271 (98%)	251 (94%)	14 (5%)	1 (0%)	34	19
3	333	243/240 (101%)	232 (96%)	11 (4%)	0	100	100
4	444	55/69 (80%)	53 (96%)	2 (4%)	0	100	100
All	All	849/885 (96%)	810 (95%)	38 (4%)	1 (0%)	51	35

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	222	117	ASN

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	111	252/268 (94%)	247 (98%)	5 (2%)	55	40
2	222	223/225 (99%)	222 (100%)	1 (0%)	91	88
3	333	218/212 (103%)	217 (100%)	1 (0%)	88	86
4	444	49/57 (86%)	48 (98%)	1 (2%)	55	40
All	All	742/762 (97%)	734 (99%)	8 (1%)	73	65

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

Mol	Chain	Res	Type
1	111	723	ARG
1	111	728	ASN
1	111	776	MET
1	111	813	LEU
1	111	864	GLU
2	222	332	ARG
3	333	488	MET
4	444	13	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 10 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	OH0	111	907	-	23,24,25	2.11	6 (26%)	29,34,35	0.89	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
7	OH0	111	907	-	-	5/25/43/44	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	111	907	OH0	O6-C2	5.12	1.49	1.42
7	111	907	OH0	C4-C5	-4.07	1.49	1.53
7	111	907	OH0	C10-N5	3.47	1.46	1.34
7	111	907	OH0	C5-N5	3.33	1.51	1.45
7	111	907	OH0	C11-C10	2.87	1.56	1.50
7	111	907	OH0	O6-C6	2.86	1.48	1.44

There are no bond angle outliers.

There are no chirality outliers.

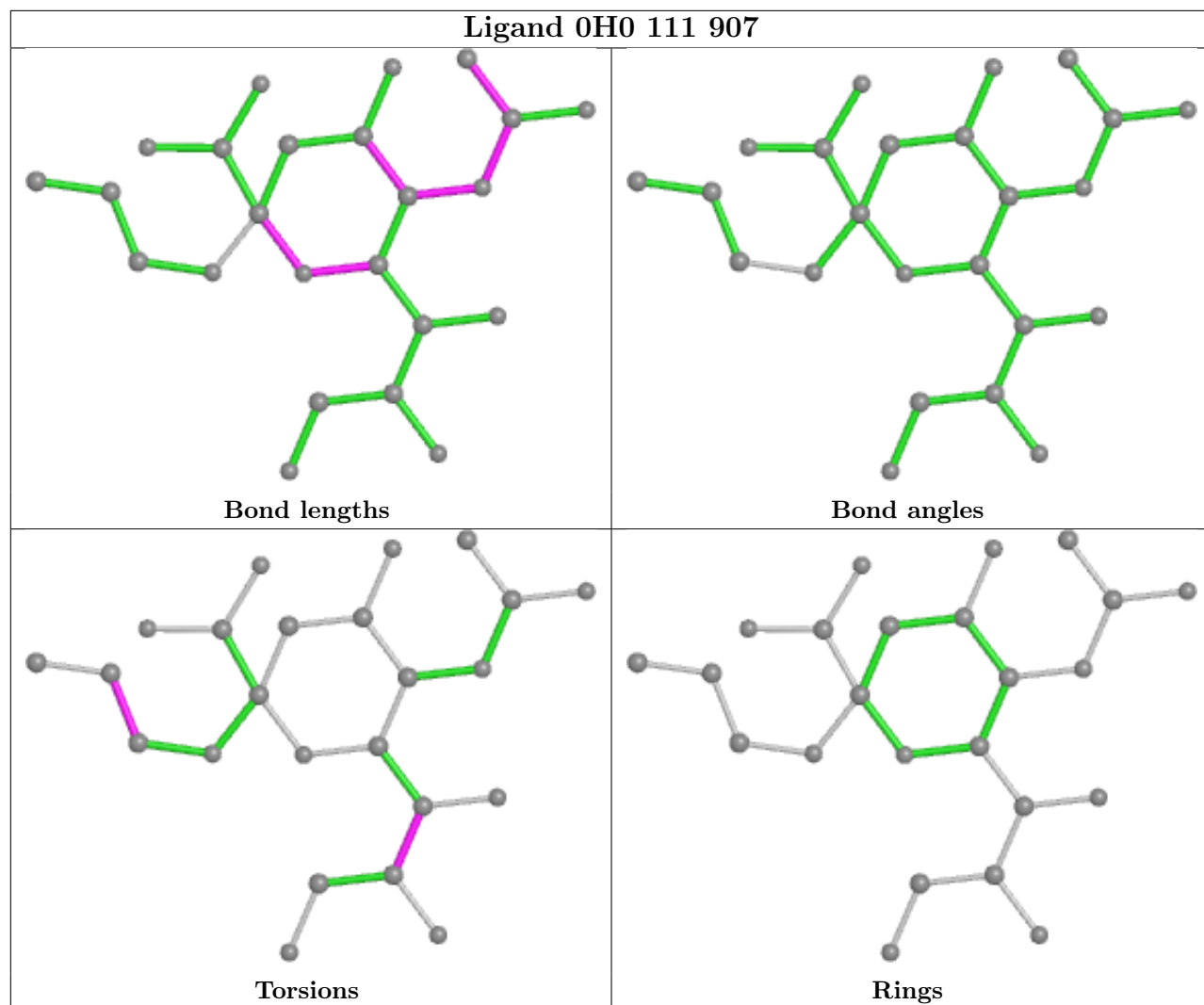
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	111	907	OH0	O2-C12-C13-C14
7	111	907	OH0	O7-C7-C8-C9
7	111	907	OH0	C6-C7-C8-C9
7	111	907	OH0	O7-C7-C8-O8
7	111	907	OH0	C6-C7-C8-O8

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 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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

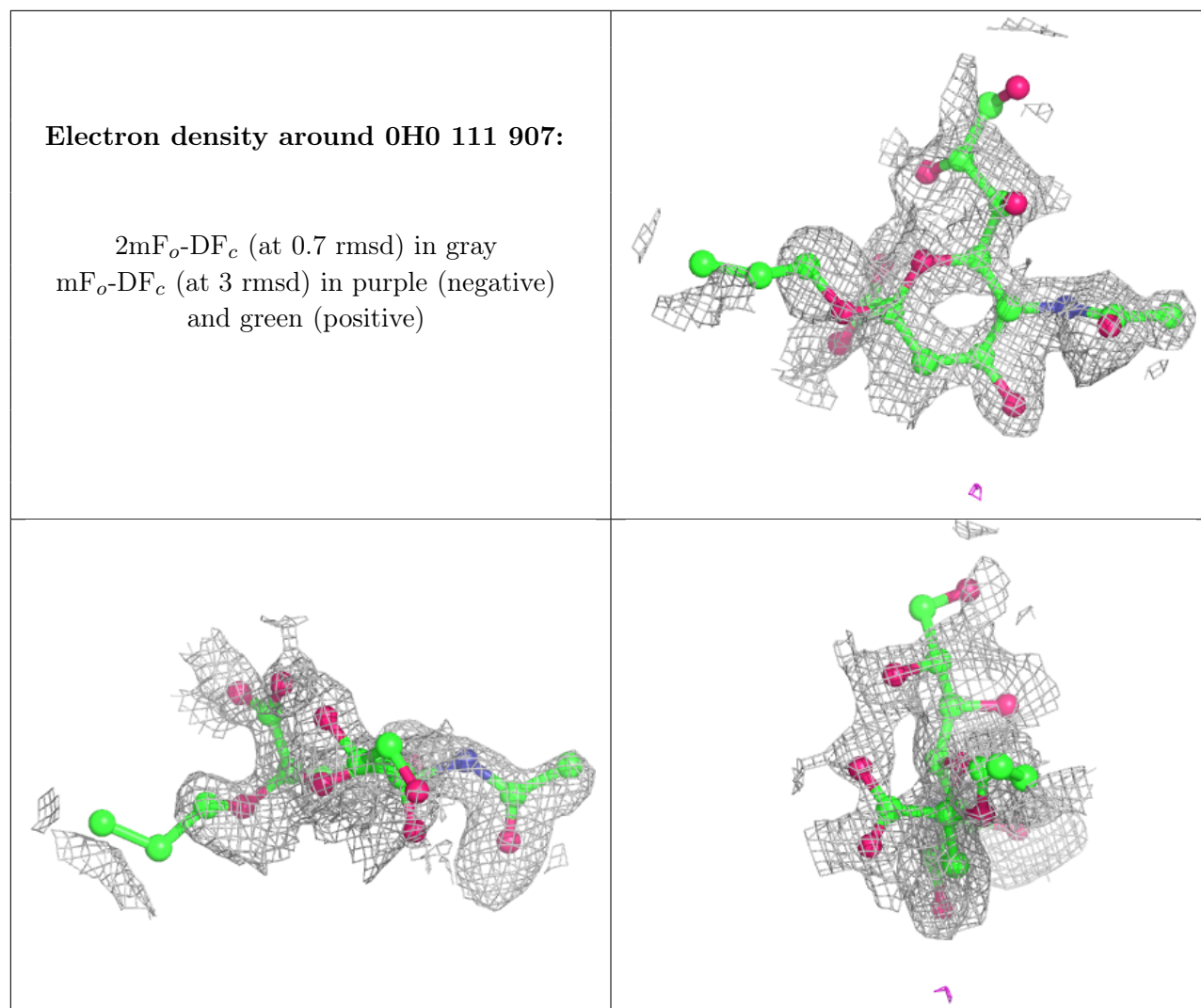
6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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.



6.5 Other polymers [i](#)

Unable to reproduce the depositor's R factor - this section is therefore empty.