



Full wwPDB X-ray Structure Validation Report i

Jun 12, 2024 – 08:17 PM EDT

PDB ID : 2YA7
Title : Crystal structure of Streptococcus pneumoniae NanA (TIGR4) in complex with Zanamivir
Authors : Gut, H.; Xu, G.; Taylor, G.L.; Walsh, M.A.
Deposited on : 2011-02-18
Resolution : 1.89 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 i 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](#) i) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.20.1
EDS : 2.36.2
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) : 2.36.2

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total C N O 23 12 4 7	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0
3	B	1	Total Cl 1 1	0	0
3	C	1	Total Cl 1 1	0	0
3	D	1	Total Cl 1 1	0	0

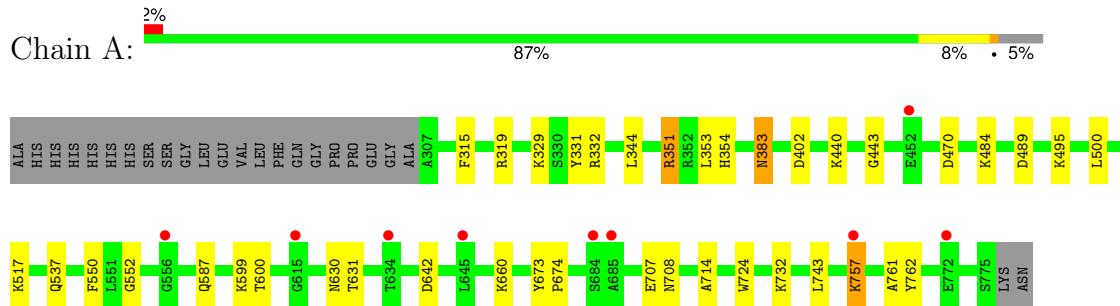
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	347	Total O 349 349	0	2
4	B	297	Total O 297 297	0	0
4	C	343	Total O 344 344	0	1
4	D	307	Total O 307 307	0	0

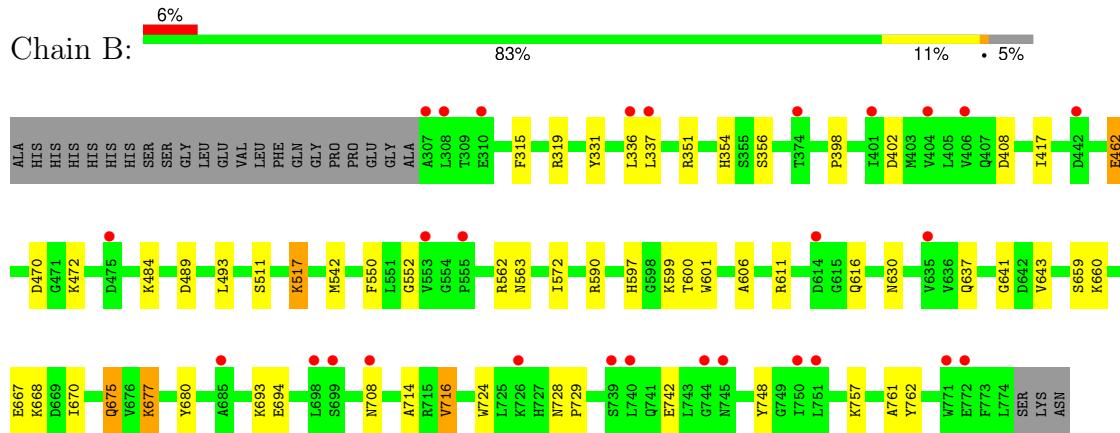
3 Residue-property plots

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.

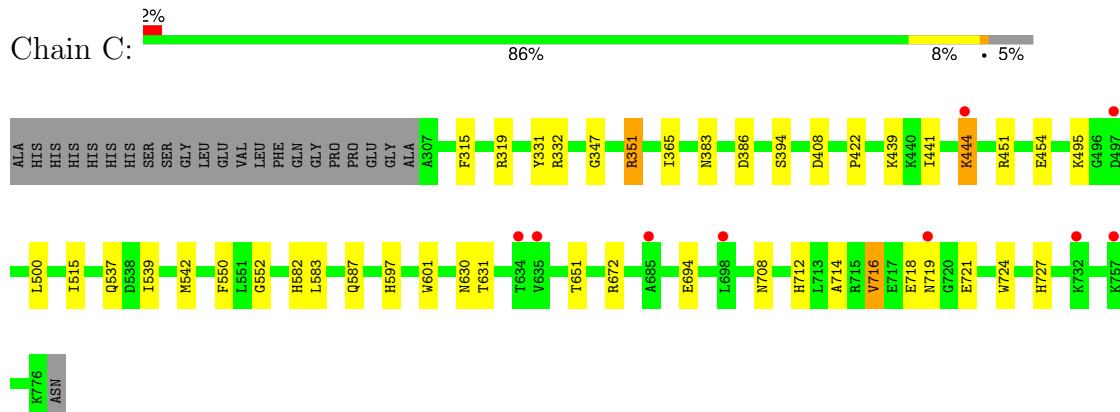
- Molecule 1: NEURAMINIDASE A



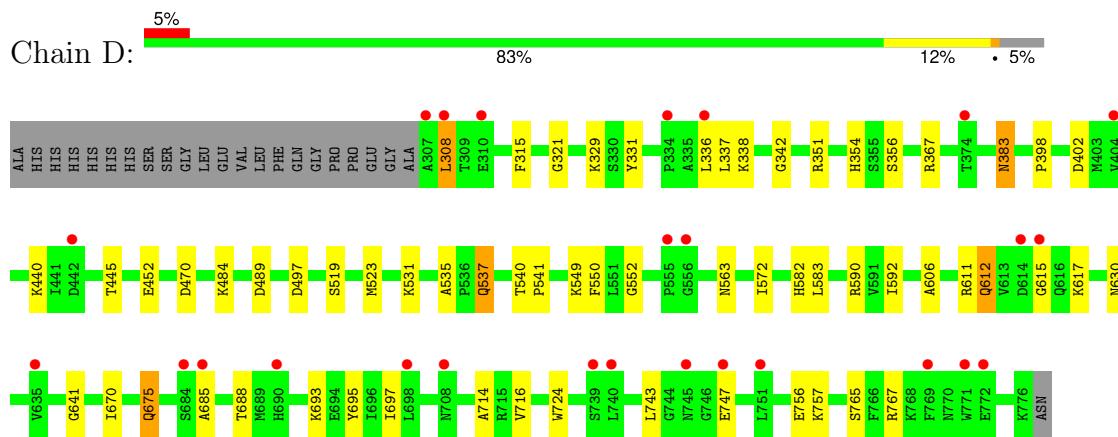
- Molecule 1: NEURAMINIDASE A



- Molecule 1: NEURAMINIDASE A



- Molecule 1: NEURAMINIDASE A



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	49.86 Å 87.16 Å 126.41 Å 104.06° 91.04° 106.68°	Depositor
Resolution (Å)	27.81 – 1.89 27.81 – 1.89	Depositor EDS
% Data completeness (in resolution range)	100.0 (27.81-1.89) 94.7 (27.81-1.89)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle^1$	2.02 (at 1.89 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R , R_{free}	0.208 , 0.257 0.206 , 0.255	Depositor DCC
R_{free} test set	3718 reflections (2.50%)	wwPDB-VP
Wilson B-factor (Å ²)	29.1	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.107 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16385	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.80% 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.

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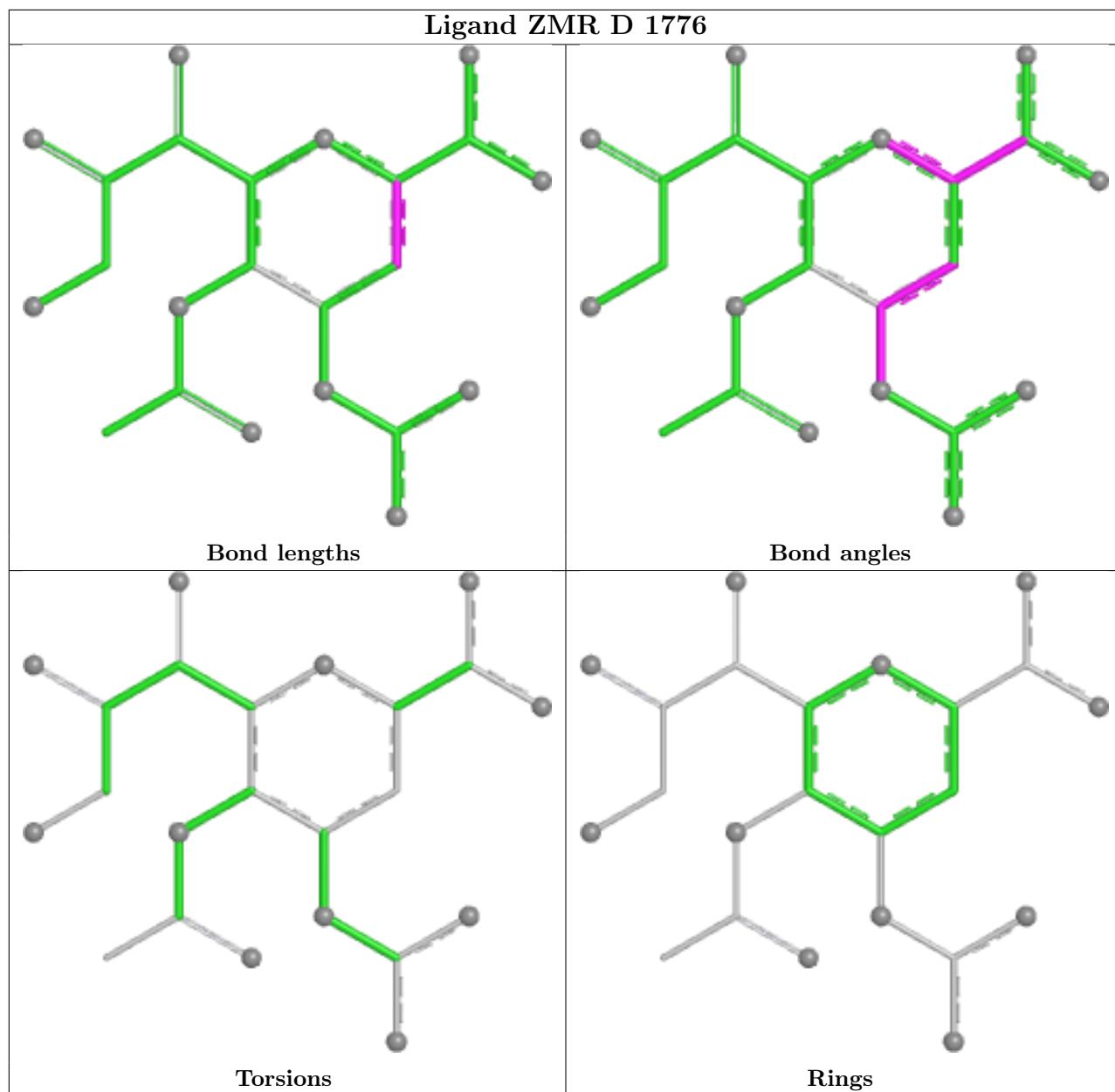
Mol	Chain	Res	Type
1	C	537[B]	GLN
1	C	630	ASN
1	C	716	VAL
1	C	718	GLU
1	D	308	LEU
1	D	336	LEU
1	D	337	LEU
1	D	351	ARG
1	D	383	ASN
1	D	470	ASP
1	D	519	SER
1	D	537	GLN
1	D	612	GLN
1	D	630	ASN
1	D	675	GLN
1	D	693	LYS
1	D	716	VAL

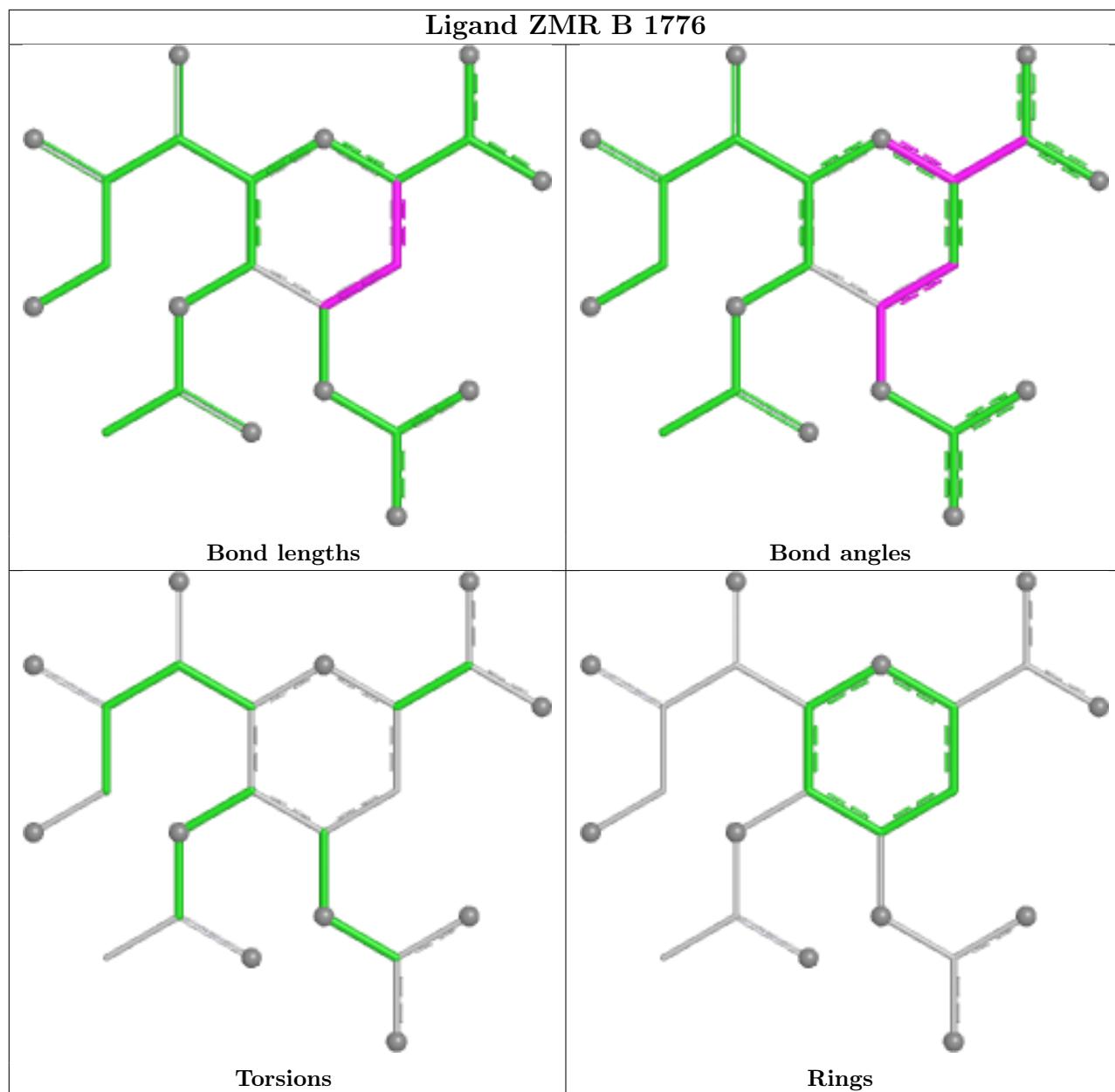
Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

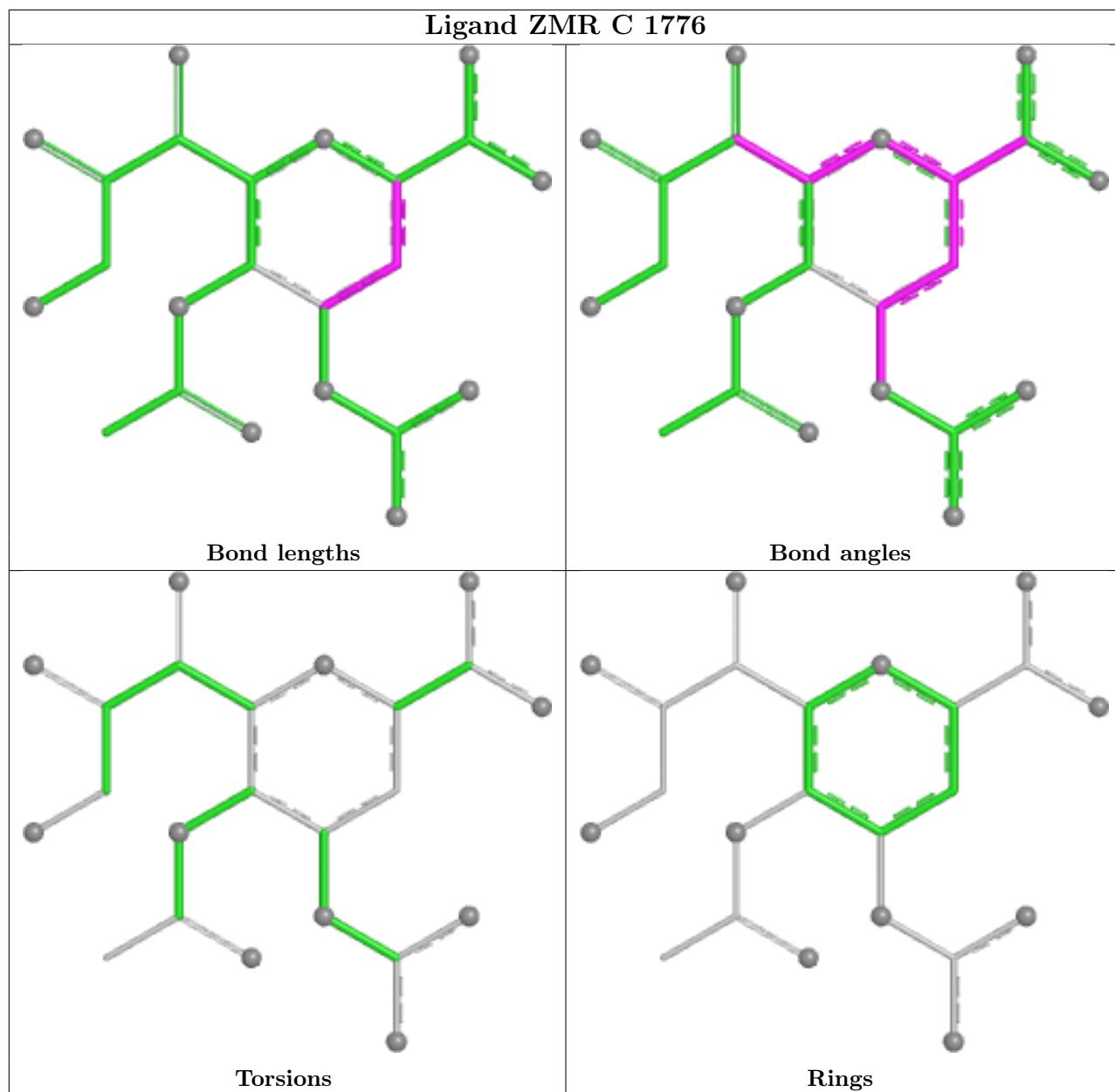
Mol	Chain	Res	Type
1	A	383	ASN
1	B	322	ASN
1	B	371	ASN
1	B	579	ASN
1	B	587	GLN
1	B	597	HIS
1	B	616	GLN
1	B	637	GLN
1	B	690	HIS
1	C	597	HIS
1	C	712	HIS
1	C	727	HIS
1	D	322	ASN
1	D	383	ASN
1	D	579	ASN
1	D	655	GLN

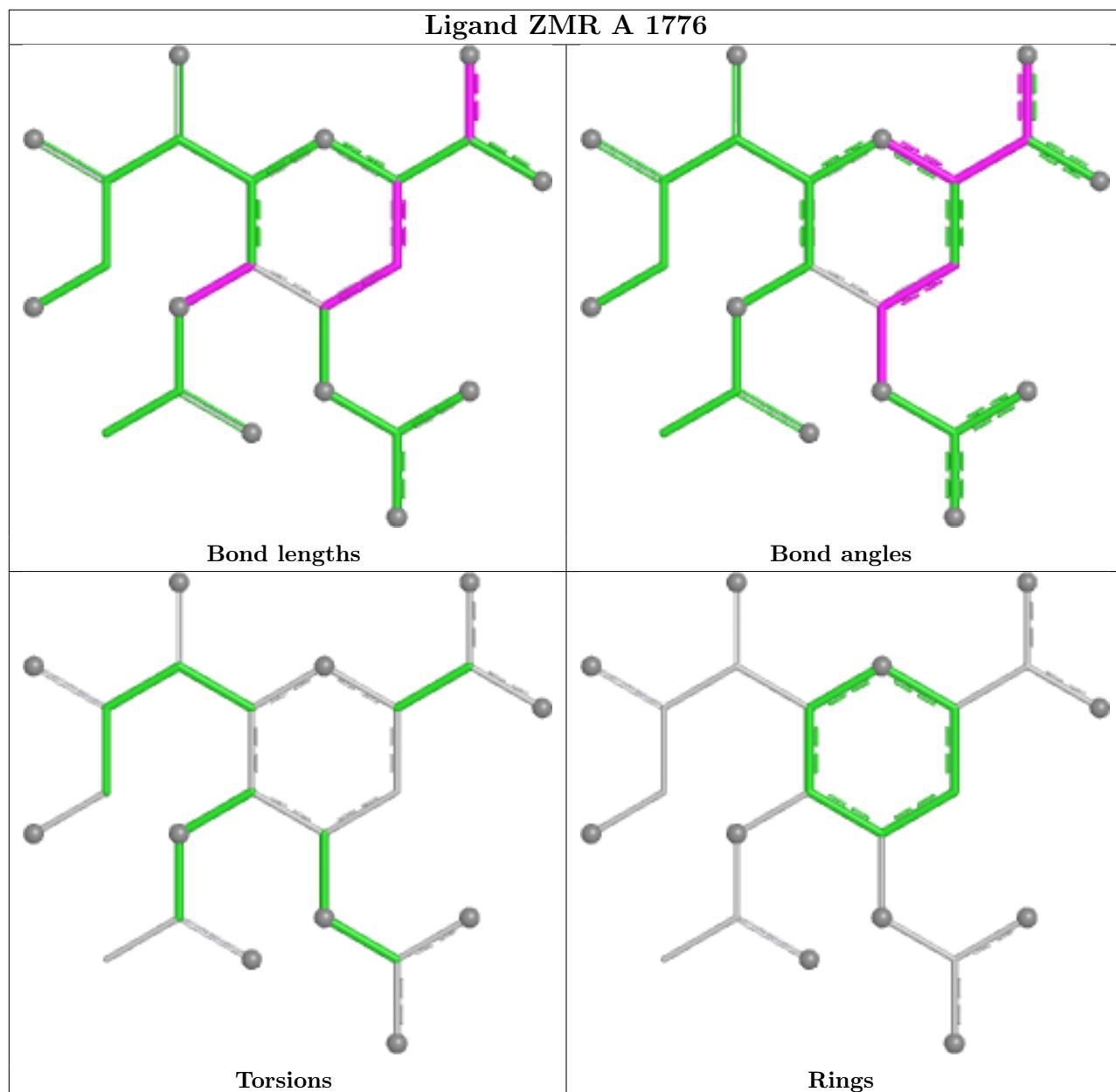
5.3.3 RNA [\(i\)](#)

There are no RNA molecules in this entry.







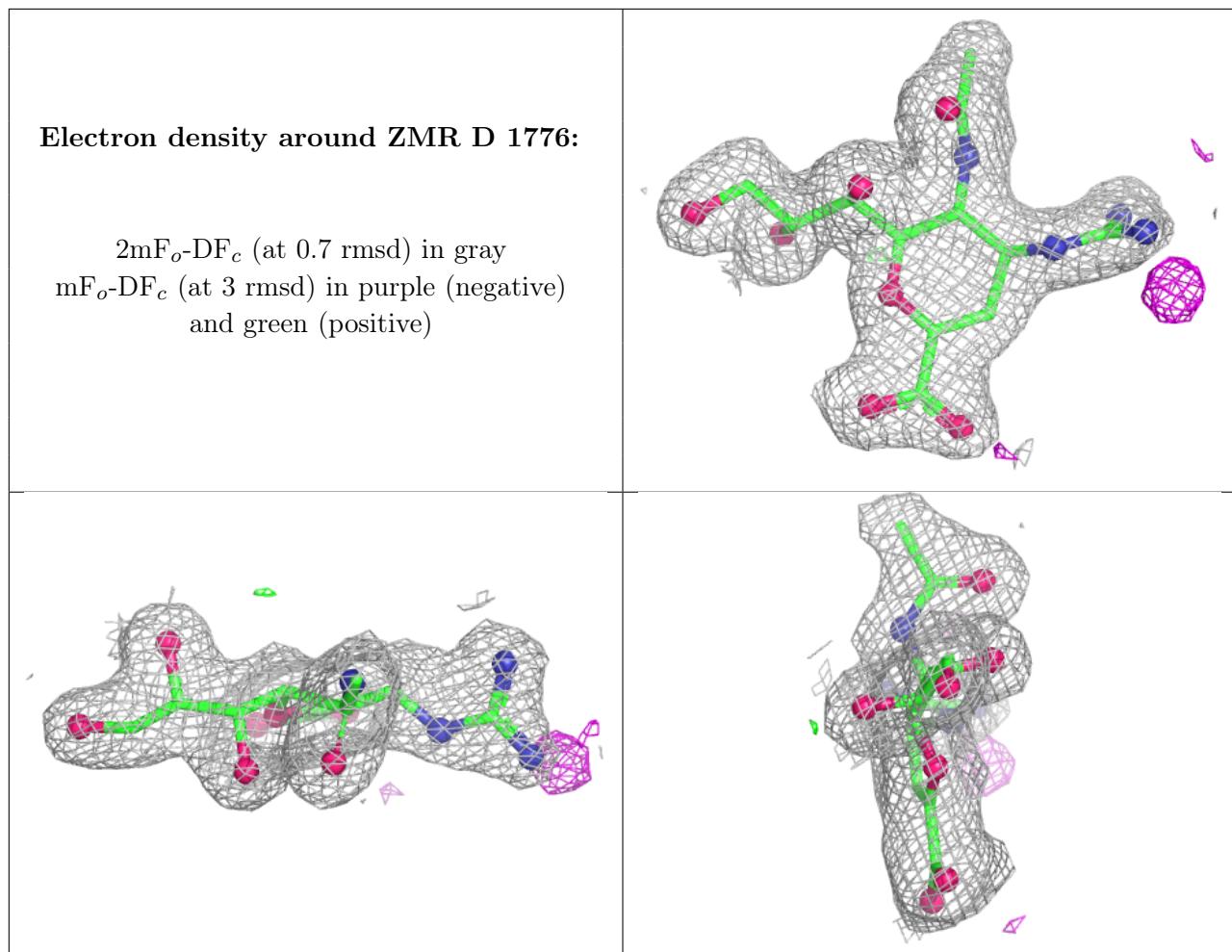


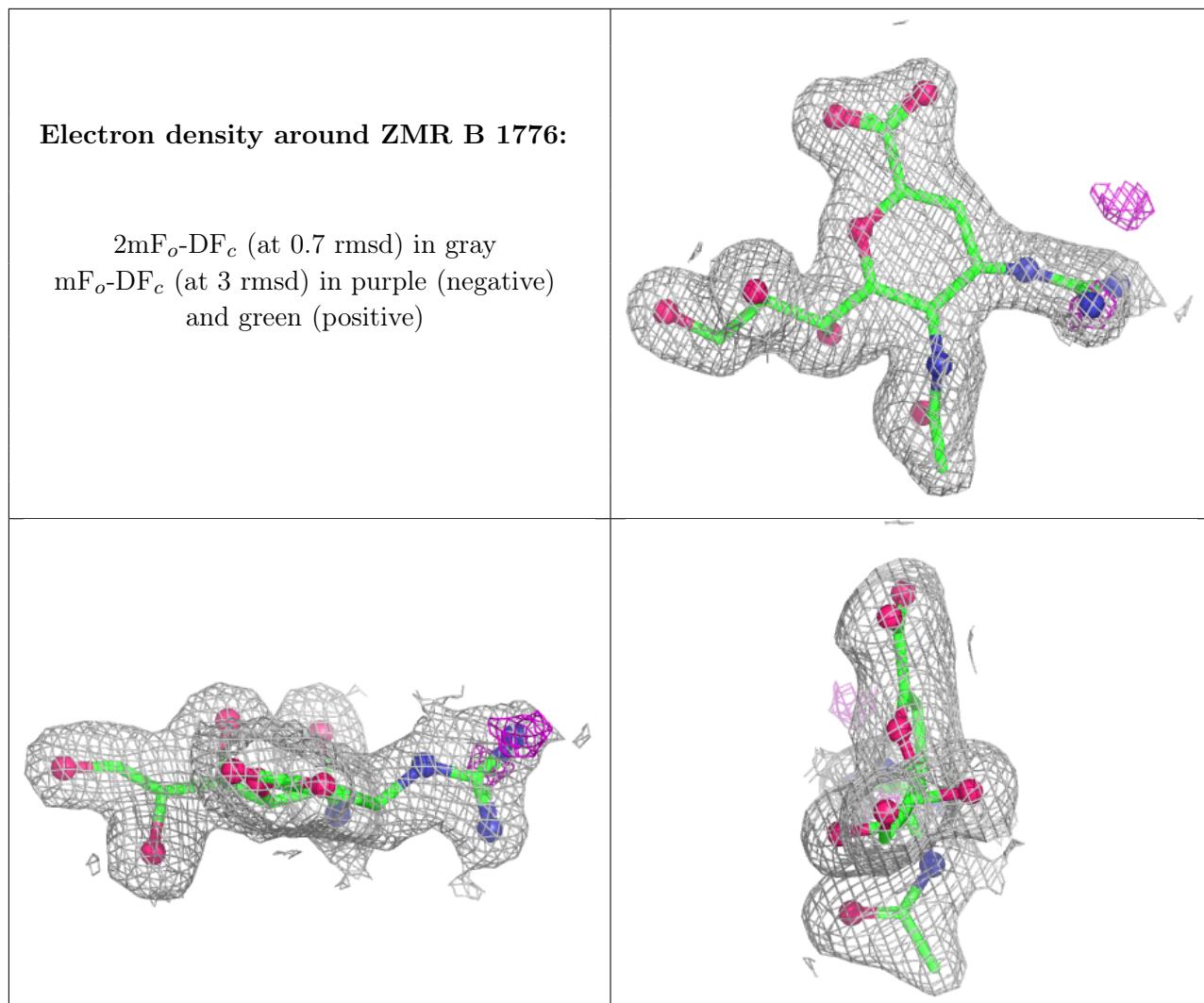
5.7 Other polymers [\(i\)](#)

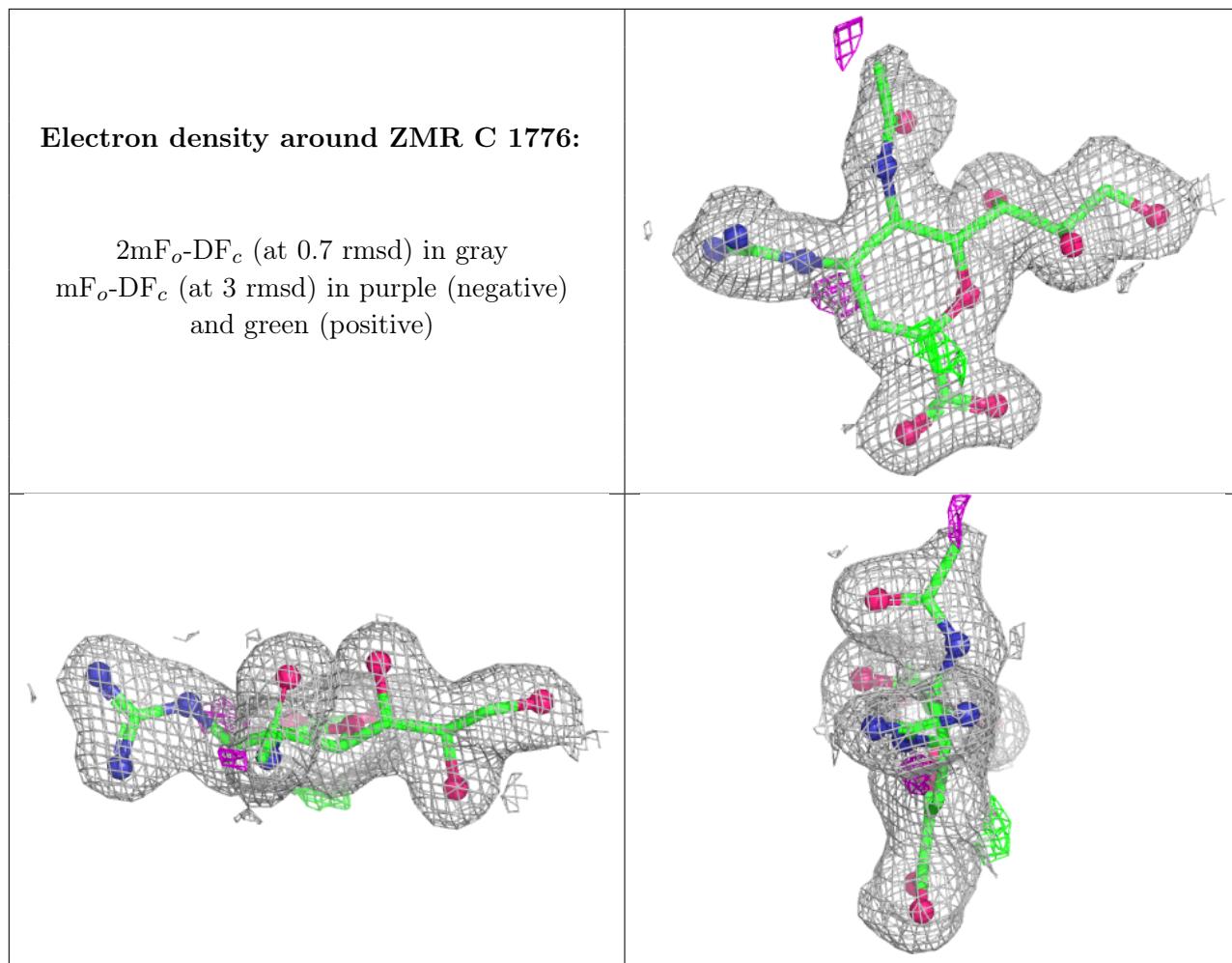
There are no such residues in this entry.

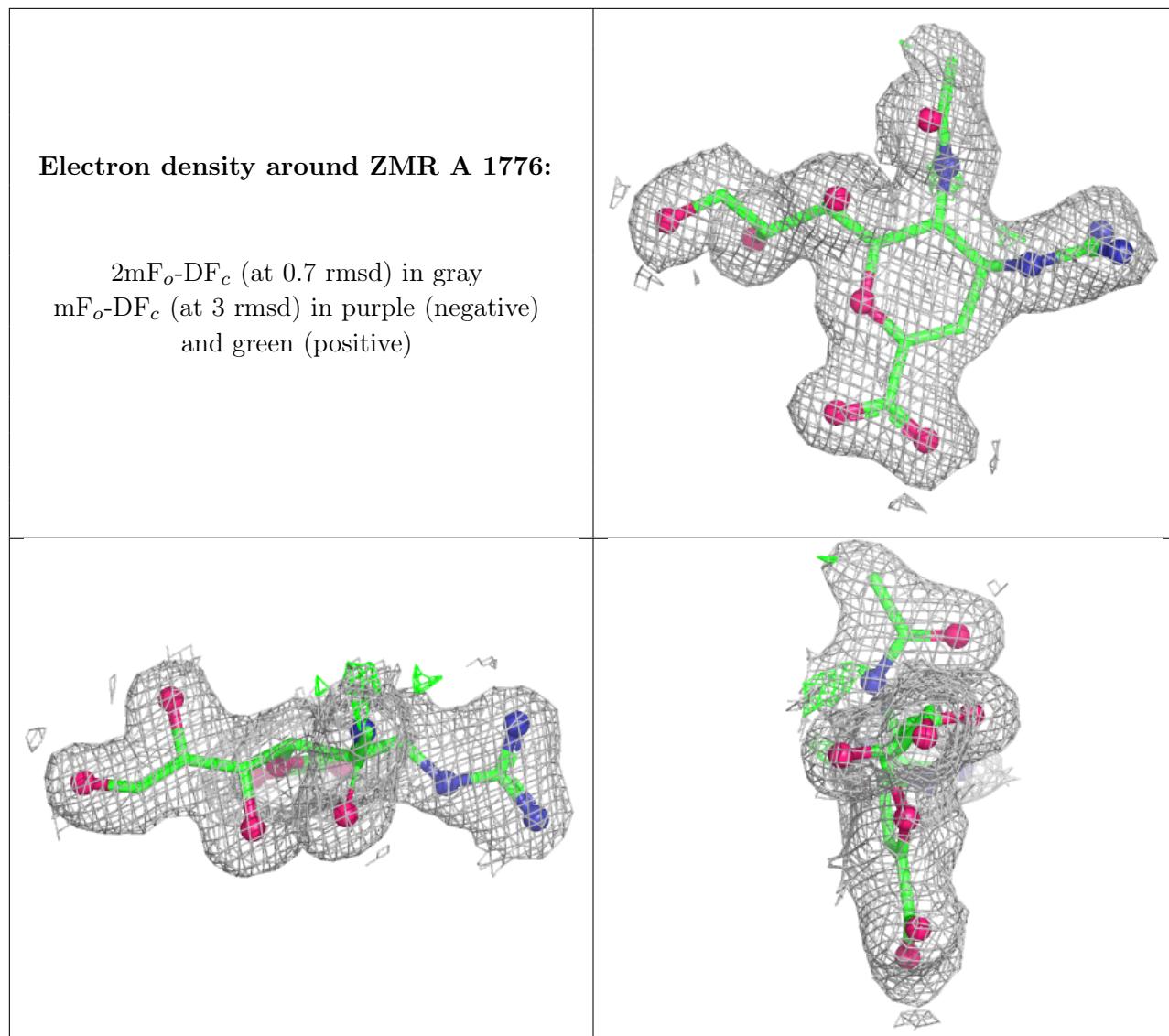
5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.









6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.