WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 21, 2025 – 11:59 PM EDT

PDB ID	:	7LSK / pdb_00007lsk
Title	:	Structure of HIV-1 Reverse Transcriptase in complex with DNA, L-dTTP, and CA(2+) ion
Authors	:	Hoang, A.; Ruiz, F.X.; Arnold, E.
Deposited on	:	2021-02-18
Resolution	:	2.70 Å(reported)

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

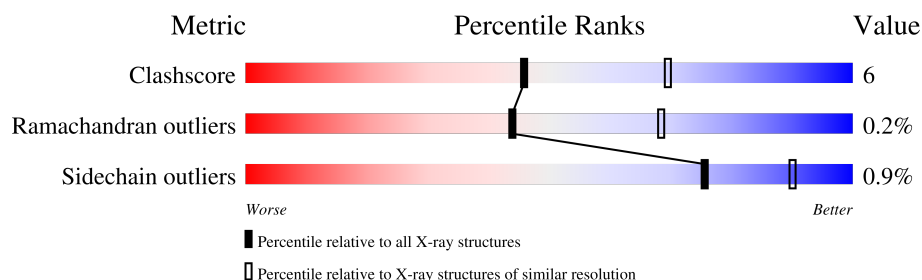|		
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

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 2.70 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	Percentile Ranks	Value
Clashscore		6
Ramachandran outliers		0.2%
Sidechain outliers		0.9%

Worse   *Better*

▌Percentile relative to all X-ray structures

▯Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	180529	3684 (2.70-2.70)
Ramachandran outliers	177936	3633 (2.70-2.70)
Sidechain outliers	177891	3633 (2.70-2.70)

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 <=5%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	555	84% 16%
1	C	555	84% 15%
2	B	429	80% 16% •
2	D	429	84% 12% •
3	E	38	58% 29% 5% 8%
3	F	38	63% 26% • 8%
4	N	2	100%
4	O	2	100%

WORLDWIDE PDB
PROTEIN DATA BANK

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	GLC	O	1	-	-	X	-
4	FRU	O	2	-	-	X	-

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 17642 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 Reverse transcriptase p66.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	554	Total 4509	C 2919	N 751	O 832	S 7	0	0	0
1	C	554	Total 4509	C 2919	N 751	O 832	S 7	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	280	SER	CYS	engineered mutation	UNP P03366
A	498	ASN	ASP	engineered mutation	UNP P03366
C	280	SER	CYS	engineered mutation	UNP P03366
C	498	ASN	ASP	engineered mutation	UNP P03366

- Molecule 2 is a protein called Reverse transcriptase p51.

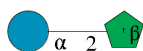| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	412	Total 3400	C 2212	N 563	O 619	S 6	0	0	0
2	D	412	Total 3400	C 2212	N 563	O 619	S 6	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLY	-	expression tag	UNP P03366
B	280	SER	CYS	engineered mutation	UNP P03366
D	0	GLY	-	expression tag	UNP P03366
D	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 3 is a DNA chain called DNA/RNA (38-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	35	Total 720	C 340	N 130	O 215	P 35	0	0	0
3	E	35	Total 720	C 340	N 130	O 215	P 35	0	0	0

- Molecule 4 is an oligosaccharide called beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	N	2	Total 23	C 12	O 11	0	0	0
4	O	2	Total 23	C 12	O 11	0	0	0

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	Ca 1	0	0
5	C	1	Total 1	Ca 1	0	0

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O_4S).
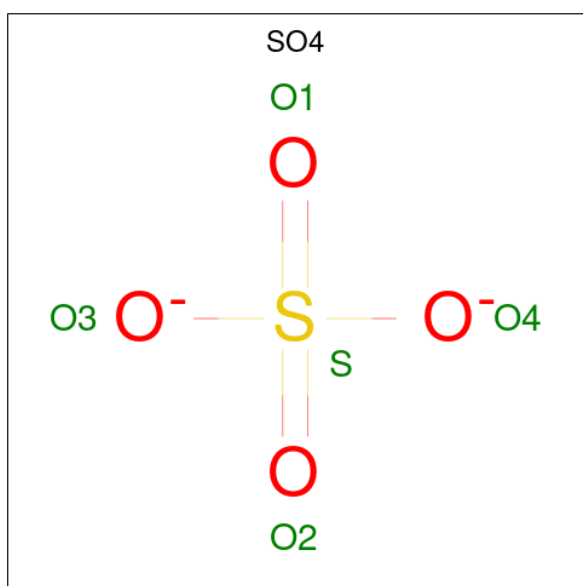
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 5	O 4	S 1	0	0
6	C	1	Total 5	O 4	S 1	0	0

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).

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

- Molecule 8 is 1-{2-deoxy-5-O-[(S)-hydroxy{[(S)-hydroxy(phosphonooxy)phosphoryl]oxy}phosphoryl]-beta-L-erythro-pentofuranosyl}-5-methylpyrimidine-2,4(1H,3H)-dione (CCD ID: XRF) (formula: $C_{10}H_{17}N_2O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).
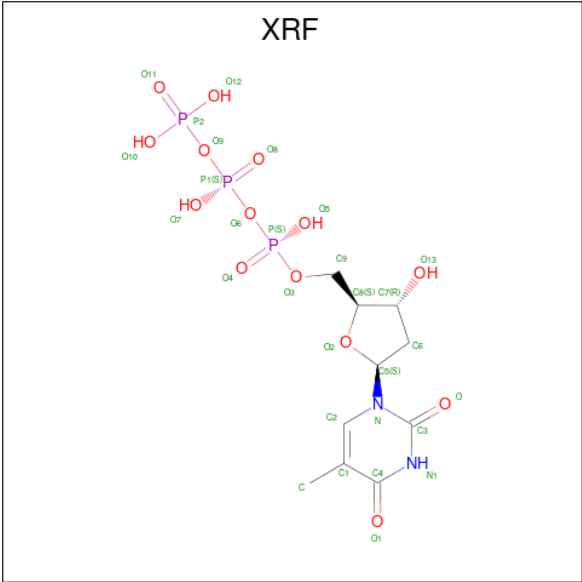
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	N	O	P	0	0
			29	10	2	14	3		
8	C	1	Total	C	N	O	P	0	0
			29	10	2	14	3		

- Molecule 9 is AMMONIUM ION (CCD ID: NH4) (formula: H_4N).
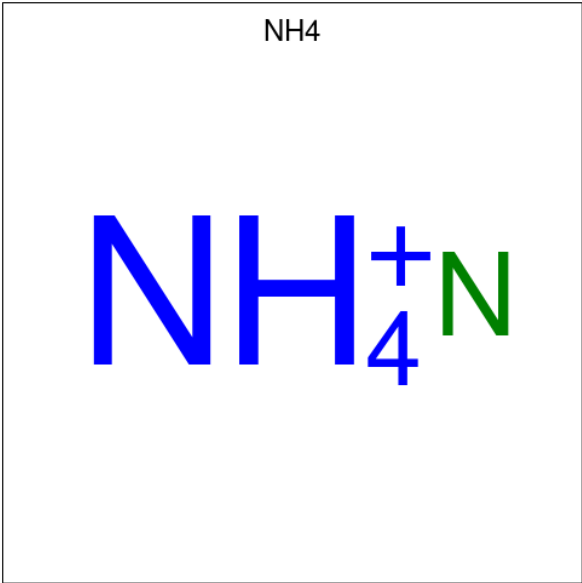
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	N	0	0
			1	1		
9	C	1	Total	N	0	0
			1	1		

- Molecule 10 is water.

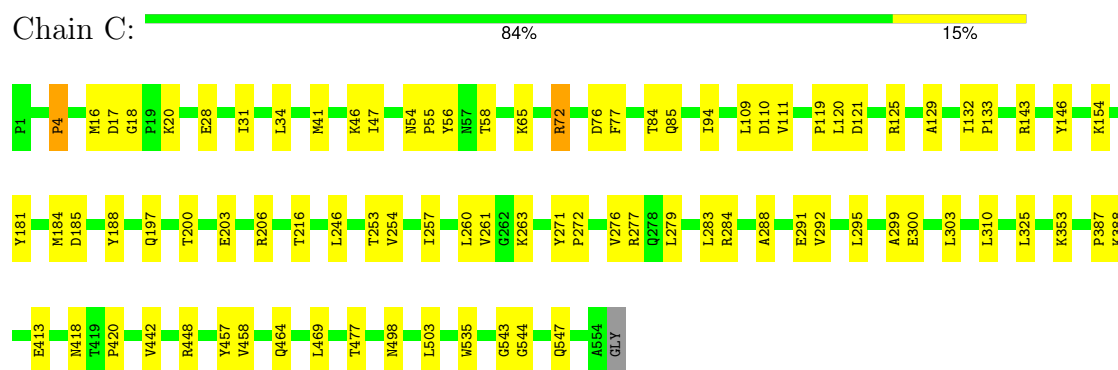| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	49	Total 49	O 49	0	0
10	B	57	Total 57	O 57	0	0
10	C	72	Total 72	O 72	0	0
10	D	51	Total 51	O 51	0	0
10	F	8	Total 8	O 8	0	0
10	E	11	Total 11	O 11	0	0

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. 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.

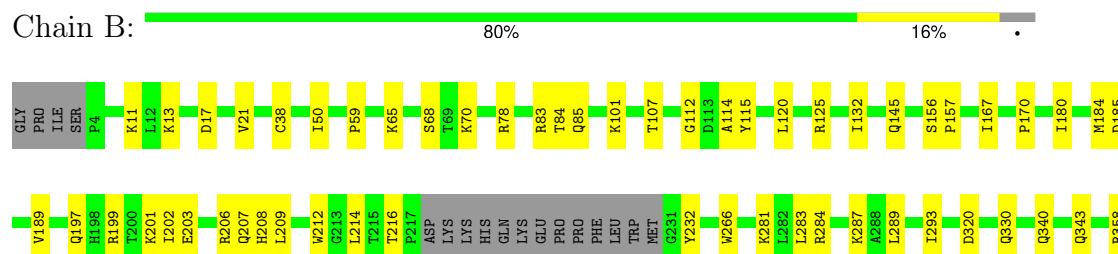Note EDS failed to run properly.

• Molecule 1: Reverse transcriptase p66
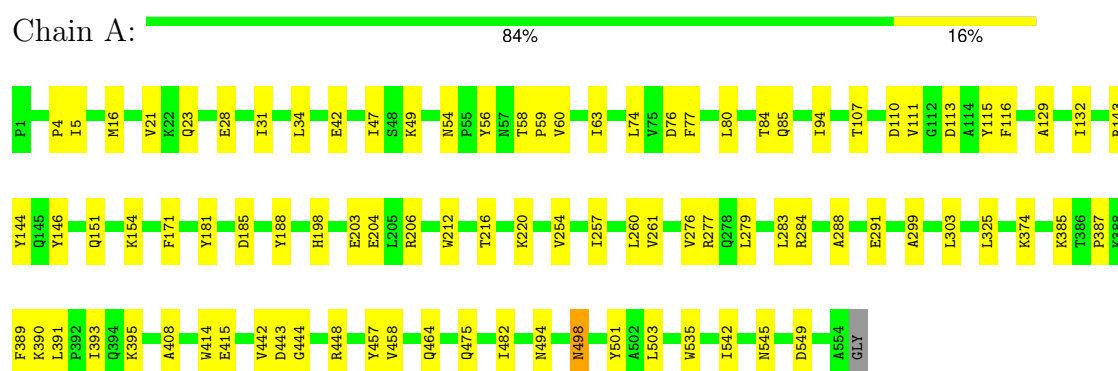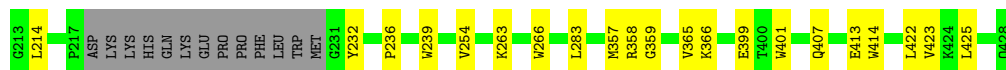
Chain A:

• Molecule 1: Reverse transcriptase p66
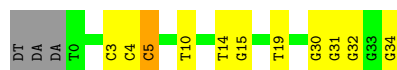
Chain C:

• Molecule 2: Reverse transcriptase p51

Chain B:

D364 V365 L368 I382 K390 W401 Y405 E415 L422 V423 K424 L425 Q428

• Molecule 2: Reverse transcriptase p51

Chain D: 84% 12% •

GLY PRO ILE SER P4 K11 D17 V21 P59 K65 K66 D67 S68 T69 K70 R83 T84 T107 V108 A114 Y115 L120 R125 T128 S156 P157 I167 P170 I180 M184 D185 V189 R199 I202 E203 Q207 H208 L209 W212

G213 L214 P217 ASP LYS LYS HIS GLN LYS GLU PRO PRO PHE LEU TRP MET G231 Y232 P236 W239 V254 K263 W266 L283 M357 R358 G359 V365 K366 E399 T400 W401 Q407 E413 W414 L422 V423 K424 L425 Q428

• Molecule 3: DNA/RNA (38-MER)

Chain F: 63% 26% • 8%

DT DA DA T0 C3 C4 C5 T10 T14 G15 T19 G30 G31 G32 G33 G34

• Molecule 3: DNA/RNA (38-MER)

Chain E: 58% 29% 5% 8%

DT DA DA T0 A1 C2 C3 C4 C5 T10 C11 G12 T19 C24 G25 G30 G31 G32 G33 G34
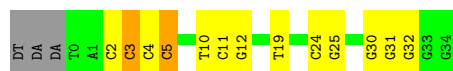
• Molecule 4: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain N: 100%

GLC1 FRU2

• Molecule 4: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain O: 100%

GLC1 FRU2

4 Data and refinement statistics ⓘ

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	89.94Å 132.47Å 139.34Å 90.00° 97.60° 90.00°	Depositor
Resolution (Å)	70.76 – 2.70	Depositor
% Data completeness (in resolution range)	100.0 (70.76-2.70)	Depositor
R_{merge}	0.34	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.56 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.215 , 0.253	Depositor
Wilson B-factor (Å^2)	63.6	Xtriage
Anisotropy	0.302	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	17642	wwPDB-VP
Average B, all atoms (Å^2)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \|L\| >$, $< L^2 >$ 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: SO4, CA, NH4, GOL, GLC, FRU, XRF, OMC

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	0.25	0/4627	0.42	0/6286
1	C	0.25	0/4627	0.42	0/6286
2	B	0.24	0/3497	0.41	0/4751
2	D	0.24	0/3497	0.42	0/4751
3	E	0.48	0/759	0.90	0/1170
3	F	0.50	0/759	0.89	0/1170
All	All	0.28	0/17766	0.49	0/24414

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 ⓘ

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	4509	0	4572	53	0
1	C	4509	0	4572	49	0
2	B	3400	0	3433	40	0
2	D	3400	0	3433	36	0
3	E	720	0	397	9	0
3	F	720	0	397	10	0
4	N	23	0	21	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	O	23	0	21	12	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	A	5	0	0	0	0
6	C	5	0	0	0	0
7	A	12	0	16	0	0
7	D	6	0	8	0	0
8	A	29	0	0	0	0
8	C	29	0	0	0	0
9	A	1	0	0	0	0
9	C	1	0	0	0	0
10	A	49	0	0	1	0
10	B	57	0	0	2	0
10	C	72	0	0	0	0
10	D	51	0	0	2	0
10	E	11	0	0	0	0
10	F	8	0	0	0	0
All	All	17642	0	16870	195	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 6.

The worst 5 of 195 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:110:ASP:HB3	1:A:220:LYS:HB3	1.48	0.95
4:O:1:GLC:O5	4:O:2:FRU:H61	1.73	0.88
2:D:399:GLU:OE2	4:N:2:FRU:H12	1.78	0.83
4:O:1:GLC:C5	4:O:2:FRU:H61	2.13	0.79
2:D:413:GLU:OE1	4:N:1:GLC:H3	1.83	0.78

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	552/555 (100%)	533 (97%)	18 (3%)	1 (0%)	44	68
1	C	552/555 (100%)	534 (97%)	16 (3%)	2 (0%)	30	55
2	B	408/429 (95%)	391 (96%)	17 (4%)	0	100	100
2	D	408/429 (95%)	390 (96%)	18 (4%)	0	100	100
All	All	1920/1968 (98%)	1848 (96%)	69 (4%)	3 (0%)	44	68

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	PRO
1	C	4	PRO
1	C	55	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	495/495 (100%)	490 (99%)	5 (1%)	73	89
1	C	495/495 (100%)	488 (99%)	7 (1%)	62	84
2	B	374/390 (96%)	372 (100%)	2 (0%)	86	95
2	D	374/390 (96%)	372 (100%)	2 (0%)	86	95
All	All	1738/1770 (98%)	1722 (99%)	16 (1%)	75	90

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	11	LYS
1	C	498	ASN
1	C	72	ARG
1	C	277	ARG
1	C	16	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	373	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\#|Z| > 2$
3	OMC	F	3	3	19,22,23	3.06	7 (36%)	25,31,34	0.77	0
3	OMC	E	5	3	19,22,23	3.09	7 (36%)	25,31,34	0.74	0
3	OMC	F	5	3	19,22,23	3.07	7 (36%)	25,31,34	0.72	0
3	OMC	E	3	3	19,22,23	3.06	7 (36%)	25,31,34	0.73	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
3	OMC	F	3	3	-	0/9/27/28	0/2/2/2
3	OMC	E	5	3	-	0/9/27/28	0/2/2/2
3	OMC	F	5	3	-	0/9/27/28	0/2/2/2
3	OMC	E	3	3	-	0/9/27/28	0/2/2/2

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	5	OMC	C2-N3	6.62	1.49	1.36
3	E	5	OMC	C2-N3	6.59	1.49	1.36
3	E	3	OMC	C2-N3	6.50	1.49	1.36
3	E	5	OMC	C6-C5	6.49	1.50	1.35
3	F	3	OMC	C2-N3	6.49	1.49	1.36

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	5	OMC	1	0
3	F	5	OMC	2	0
3	E	3	OMC	1	0

5.5 Carbohydrates ⓘ

4 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	$\#|Z| > 2$
4	GLC	N	1	4	11,11,12	0.38	0	15,15,17	0.82	0
4	FRU	N	2	4	11,12,12	0.67	0	10,18,18	1.04	0
4	GLC	O	1	4	11,11,12	1.08	2 (18%)	15,15,17	2.15	4 (26%)
4	FRU	O	2	4	11,12,12	0.69	0	10,18,18	2.32	4 (40%)

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
4	GLC	N	1	4	-	0/2/19/22	0/1/1/1
4	FRU	N	2	4	-	1/5/24/24	0/1/1/1
4	GLC	O	1	4	-	1/2/19/22	0/1/1/1
4	FRU	O	2	4	-	5/5/24/24	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	O	1	GLC	C2-C3	-2.40	1.48	1.52
4	O	1	GLC	O5-C1	-2.40	1.39	1.43

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	O	1	GLC	O3-C3-C2	-5.16	99.52	110.05
4	O	1	GLC	C2-C3-C4	-4.05	103.75	110.86
4	O	2	FRU	O6-C6-C5	3.70	123.93	111.33
4	O	1	GLC	C1-O5-C5	-3.49	107.50	112.19
4	O	2	FRU	O1-C1-C2	3.38	119.16	111.67

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	O	2	FRU	O1-C1-C2-O2
4	O	2	FRU	O5-C5-C6-O6
4	O	2	FRU	C4-C5-C6-O6
4	O	2	FRU	O1-C1-C2-C3
4	O	1	GLC	O5-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	O	2	FRU	12	0
4	O	1	GLC	8	0
4	N	2	FRU	3	0
4	N	1	GLC	5	0

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

Oligosaccharide Chain N

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain O

Bond lengths

Bond angles

Torsions

Rings
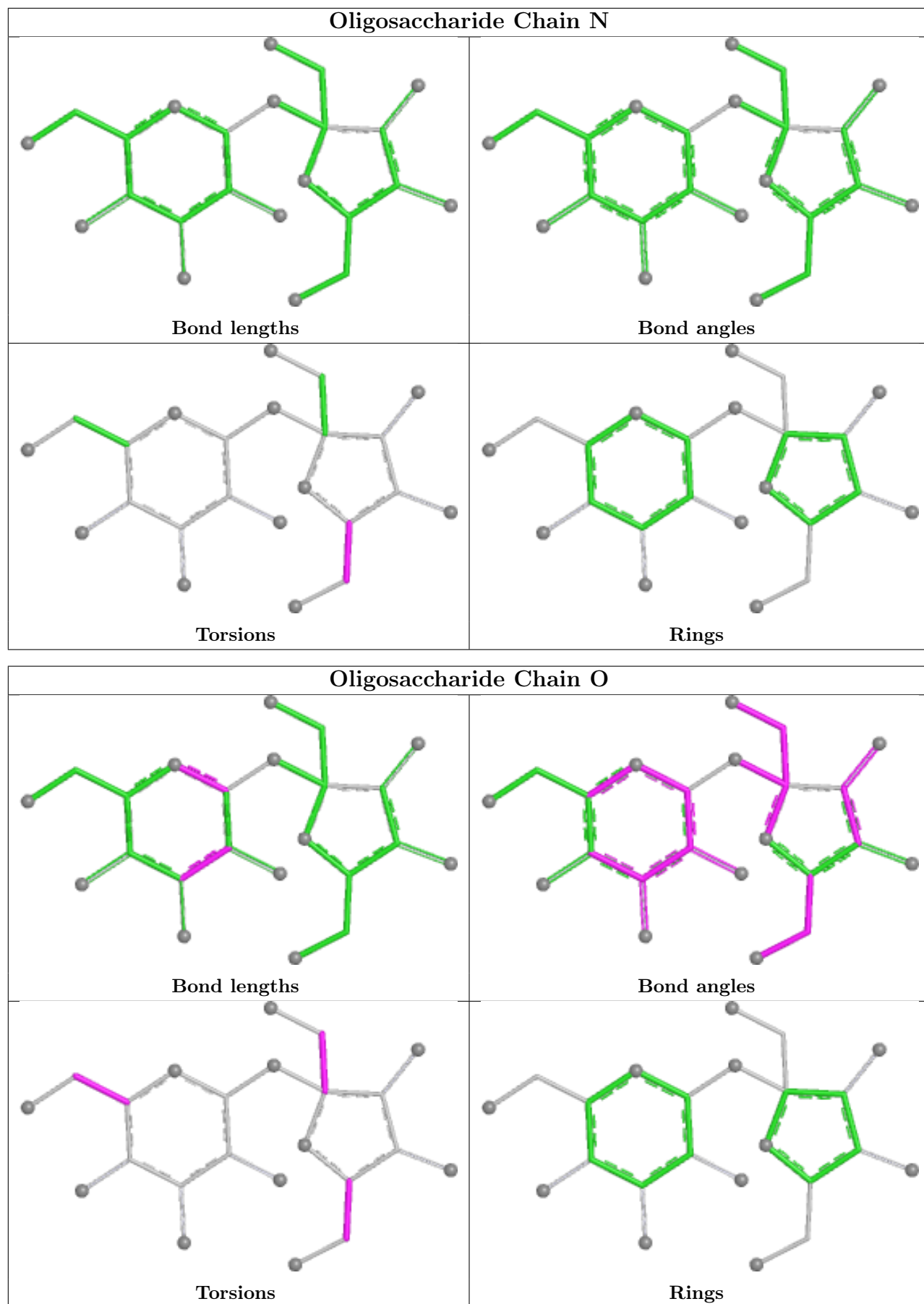
5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 2 are monoatomic and 2 are modelled with single atom - leaving 7 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	GOL	D	501	-	5,5,5	0.94	0	5,5,5	1.07	0
7	GOL	A	604	-	5,5,5	0.95	0	5,5,5	1.08	0
6	SO4	A	602	-	4,4,4	0.24	0	6,6,6	0.08	0
6	SO4	C	602	-	4,4,4	0.24	0	6,6,6	0.08	0
8	XRF	A	605	5	29,30,30	1.03	1 (3%)	43,47,47	0.97	4 (9%)
7	GOL	A	603	-	5,5,5	0.97	0	5,5,5	1.02	0
8	XRF	C	603	5	29,30,30	0.50	0	43,47,47	0.73	1 (2%)

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	GOL	D	501	-	-	0/4/4/4	-
7	GOL	A	604	-	-	0/4/4/4	-
8	XRF	A	605	5	-	9/22/34/34	0/2/2/2
7	GOL	A	603	-	-	1/4/4/4	-
8	XRF	C	603	5	-	4/22/34/34	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	605	XRF	P2-O10	-3.74	1.40	1.54

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	605	XRF	O10-P2-O9	2.95	114.52	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	605	XRF	O7-P1-O9	2.37	113.67	107.27
8	C	603	XRF	O10-P2-O9	2.14	111.80	104.64
8	A	605	XRF	O3-P-O4	2.12	117.35	108.94
8	A	605	XRF	O7-P1-O6	2.12	113.00	107.27

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	605	XRF	C9-O3-P-O4
8	A	605	XRF	C9-O3-P-O6
8	C	603	XRF	C9-O3-P-O6
8	A	605	XRF	C6-C5-N-C2
8	A	605	XRF	C6-C5-N-C3

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 then 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.

Ligand XRF A 605

Bond lengths

Bond angles

Torsions

Rings

Ligand XRF C 603

Bond lengths

Bond angles

Torsions

Rings
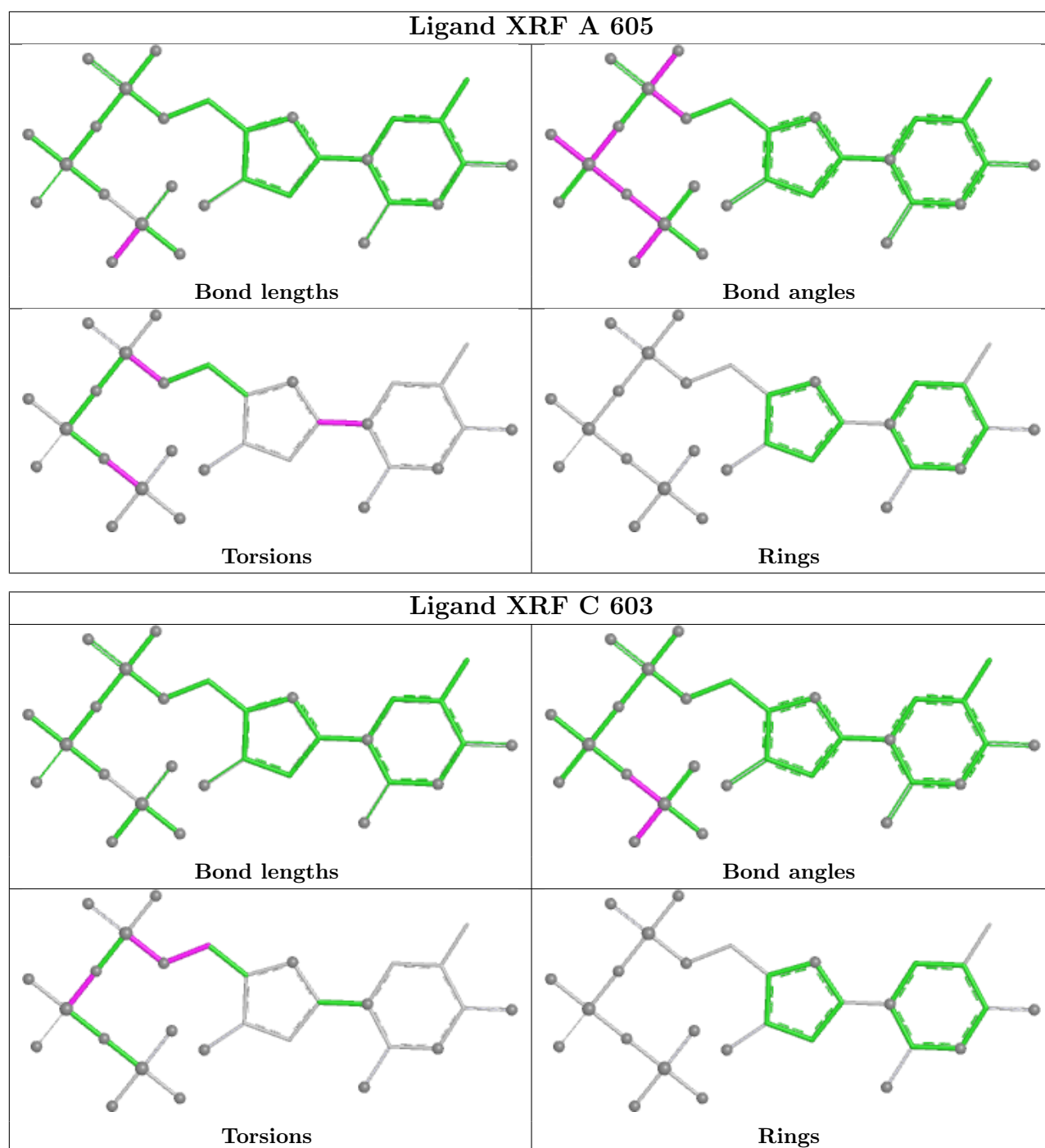
5.7 Other polymers ⓘ

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 ⓘ

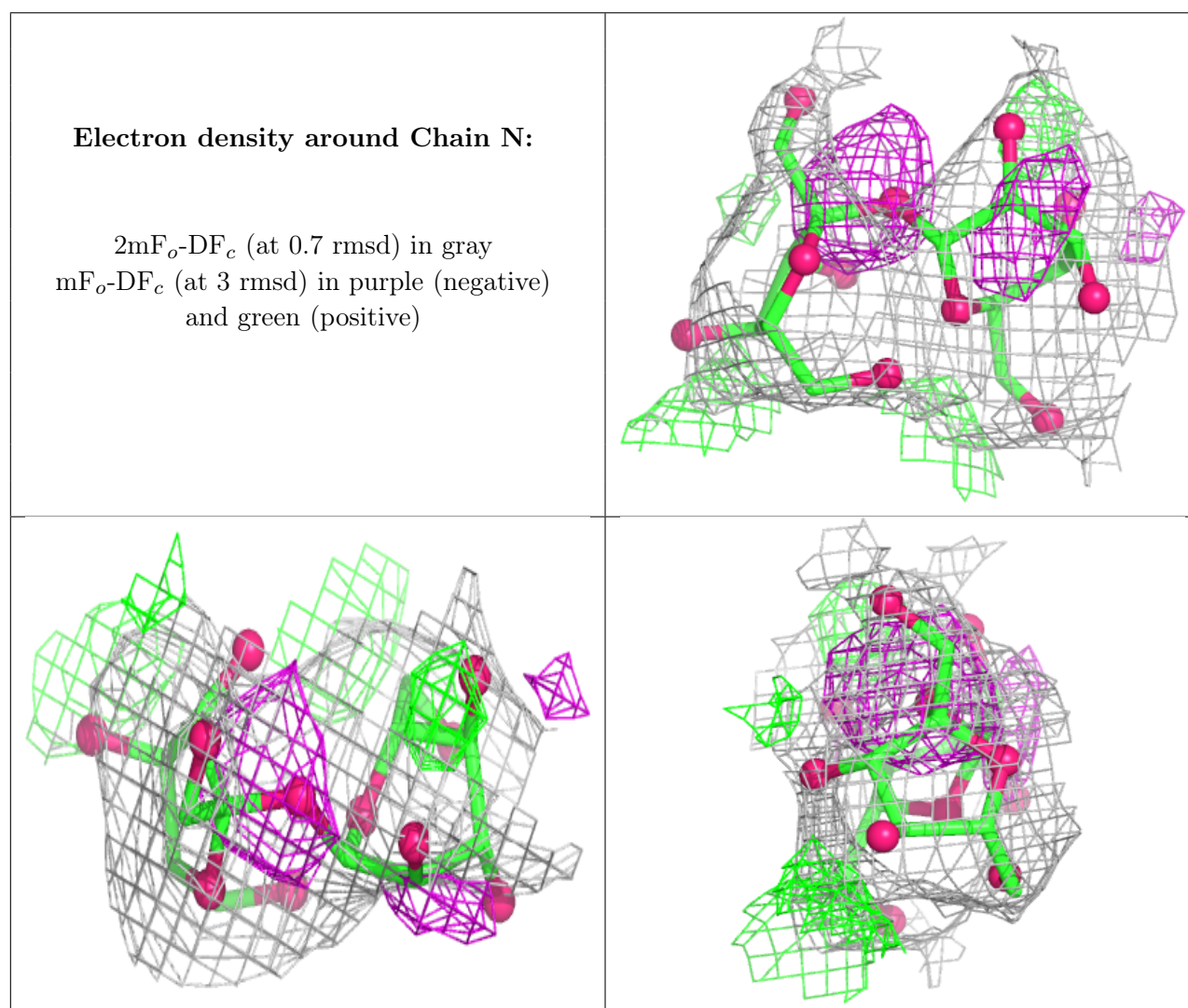EDS failed to run properly - this section is therefore empty.
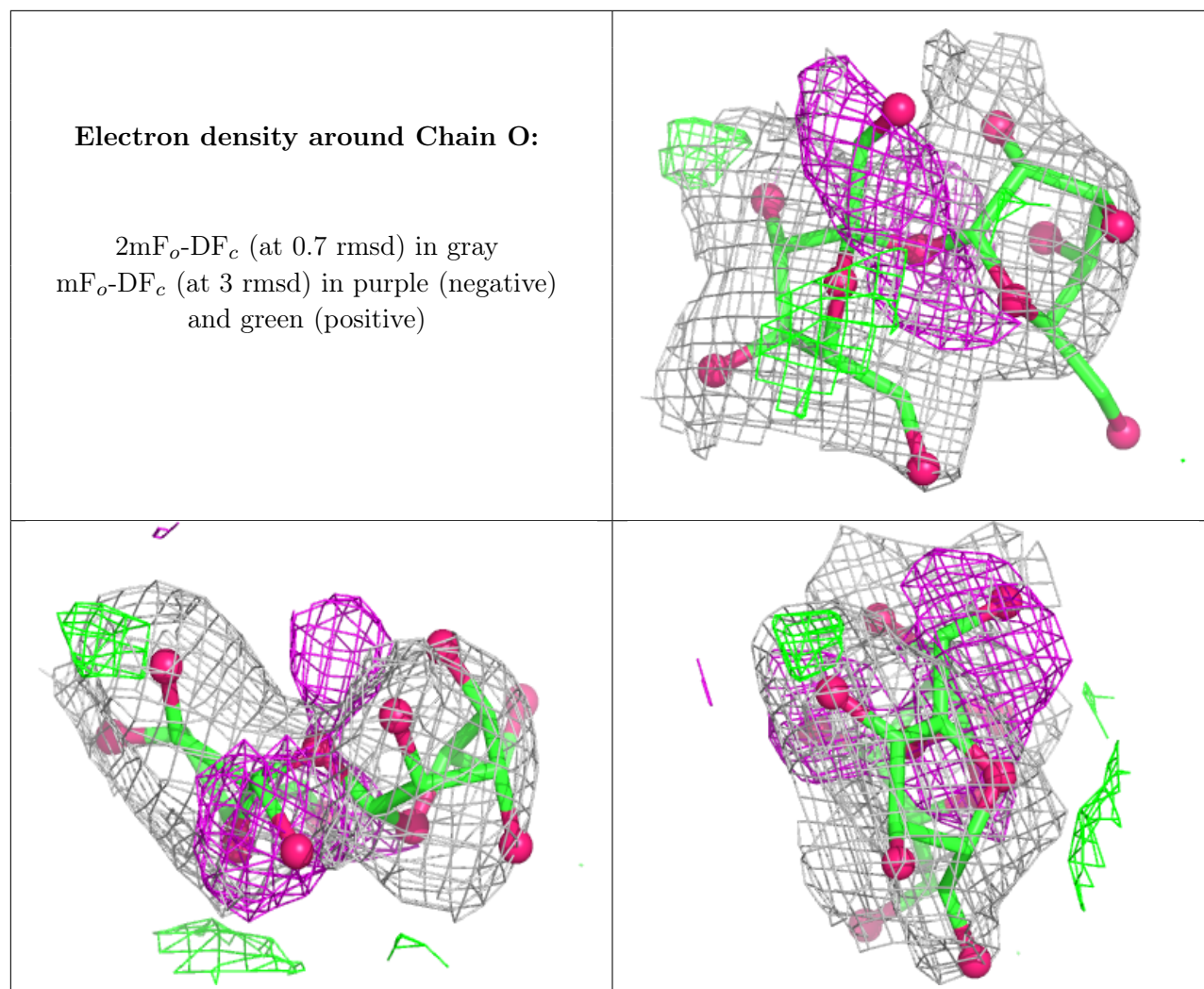
6.2   Non-standard residues in protein, DNA, RNA chains ⓘ

EDS failed to run properly - this section is therefore empty.

6.3   Carbohydrates ⓘ

EDS failed to run properly - this section is therefore empty.

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.
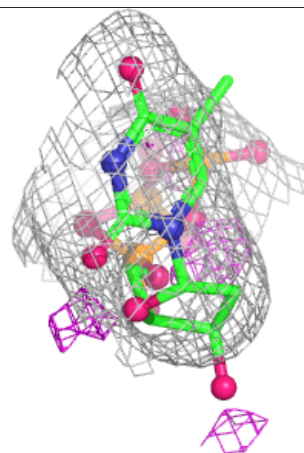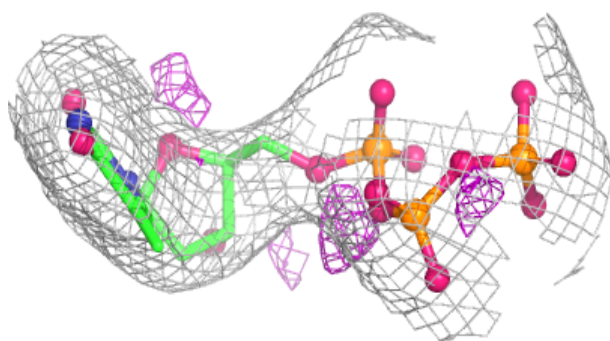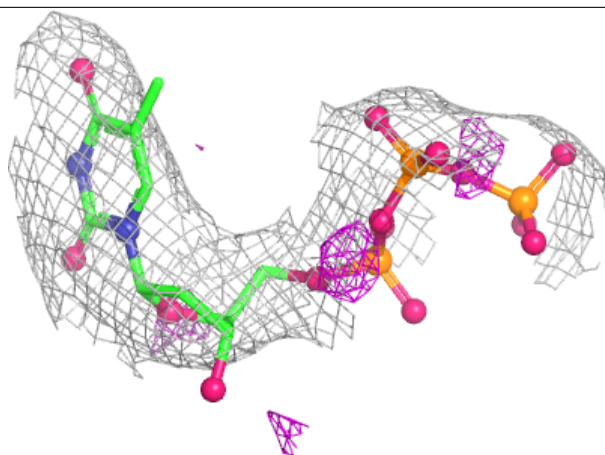

Electron density around Chain N:

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

Electron density around Chain O:

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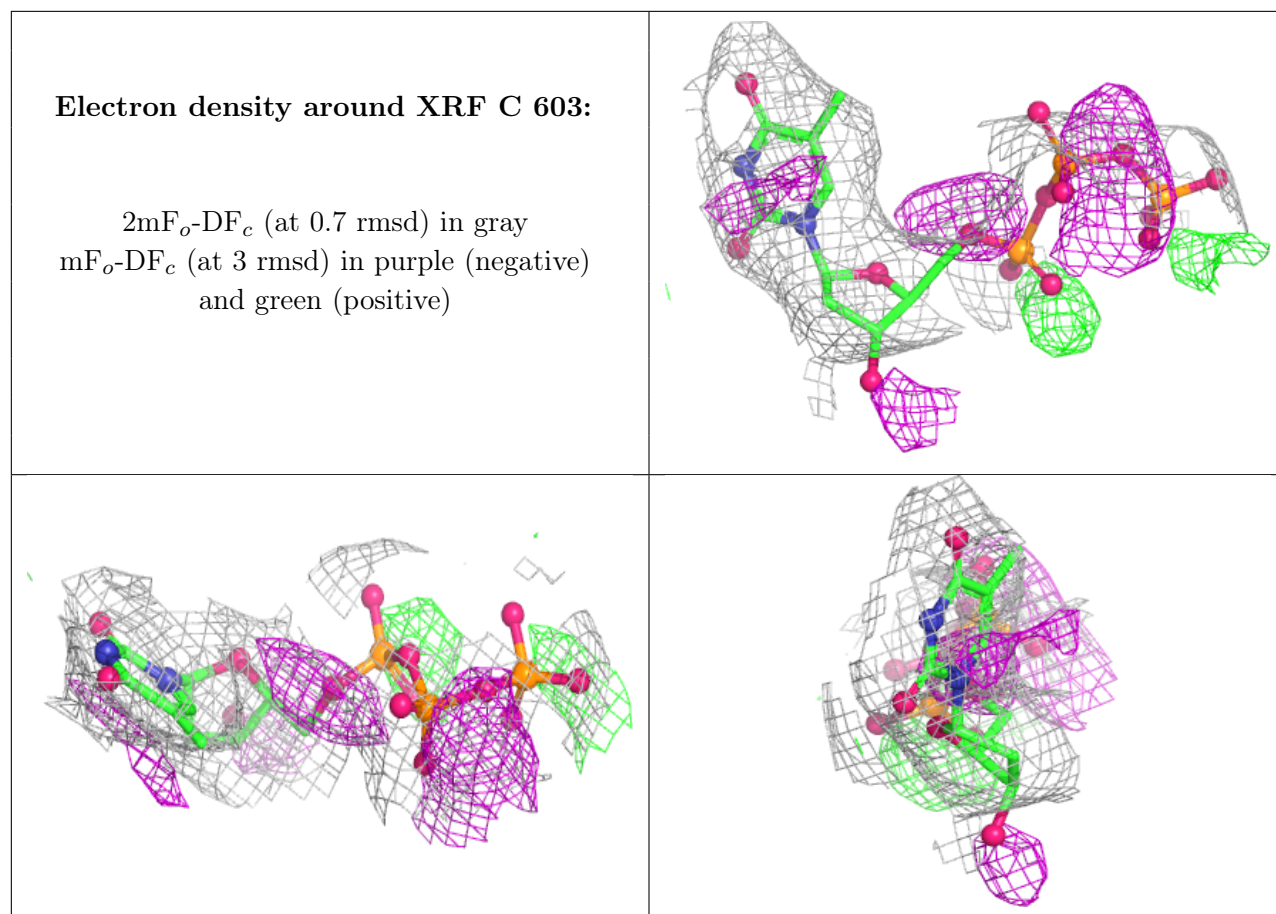and green (positive)

6.4 Ligands ⓘ

EDS failed to run properly - 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.

Electron density around XRF A 605:

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

Electron density around XRF C 603:

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

6.5   Other polymers ⓘ

EDS failed to run properly - this section is therefore empty.