WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Oct 9, 2023 – 11:22 PM EDT

PDB ID	:	7LRY
Title	:	Structure of HIV-1 Reverse Transcriptase in complex with DNA, (-)FTC-TP, and CA(2+) ion
Authors	:	Hoang, A.; Ruiz, F.X.; Arnold, E.
Deposited on	:	2021-02-17
Resolution	:	2.45 Å(reported)

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

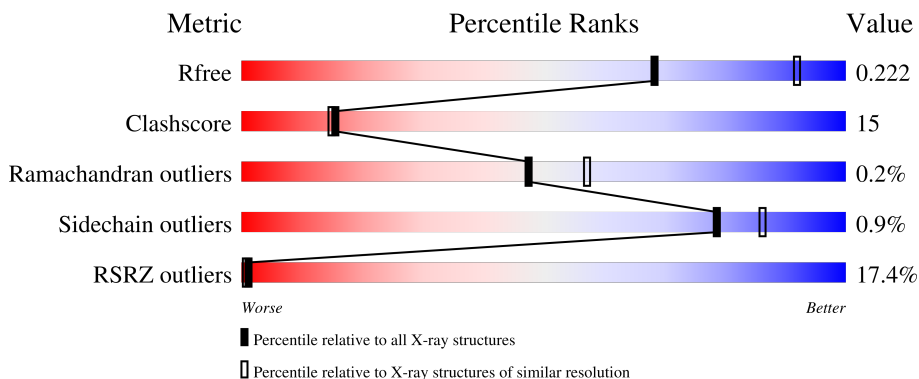|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.45 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.
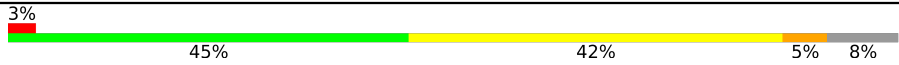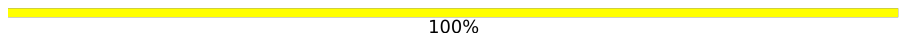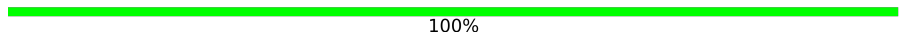
Metric	Percentile Ranks	Value
Rfree		0.222
Clashscore		15
Ramachandran outliers		0.2%
Sidechain outliers		0.9%
RSRZ outliers		17.4%

■ 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))
R_{free}	130704	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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% 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	555	13% / 68% / 31% ·
1	C	555	32% / 68% / 31% ·
2	B	429	8% / 73% / 24% ·
2	D	429	13% / 70% / 25% ·
3	E	38	53% / 37% · 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	38	3% / 45% / 42% / 5% / 8%
4	M	2	100%
4	N	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
6	GOL	A	602	-	-	-	X
7	PG4	A	603	-	-	X	-
8	NH4	A	604	-	-	-	X
8	NH4	C	602	-	-	-	X

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 17811 atoms, of which 8 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	553	Total 4510	C 2920	N 751	O 832	S 7	0	1	0
1	C	553	Total 4504	C 2916	N 750	O 831	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	415	Total 3440	C 2243	N 568	O 622	S 7	0	1	0
2	D	410	Total 3400	C 2217	N 562	O 614	S 7	0	1	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).

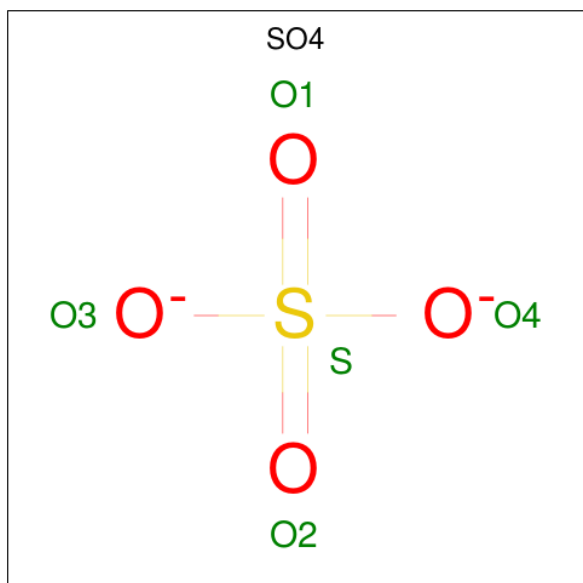| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	35	Total 721	C 340	N 130	O 216	P 35	0	0	0
3	E	35	Total 721	C 340	N 130	O 216	P 35	0	0	0

• Molecule 4 is an oligosaccharide called beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose.
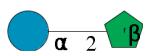
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	M	2	Total 23	C 12	O 11	0	0	0
4	N	2	Total 23	C 12	O 11	0	0	0

• Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 5	O 4	S 1	0	0
5	B	1	Total 5	O 4	S 1	0	0
5	C	1	Total 5	O 4	S 1	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
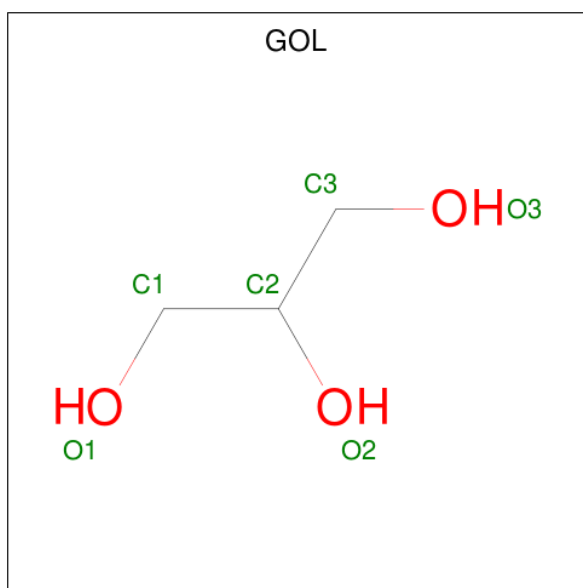
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 6	C 3	O 3	0	0
6	B	1	Total 6	C 3	O 3	0	0
6	B	1	Total 6	C 3	O 3	0	0
6	B	1	Total 6	C 3	O 3	0	0
6	B	1	Total 6	C 3	O 3	0	0
6	B	1	Total 6	C 3	O 3	0	0
6	B	1	Total 6	C 3	O 3	0	0
6	D	1	Total 6	C 3	O 3	0	0
6	D	1	Total 6	C 3	O 3	0	0
6	D	1	Total 6	C 3	O 3	0	0
6	D	1	Total 6	C 3	O 3	0	0
6	F	1	Total 6	C 3	O 3	0	0

- Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).

PG4
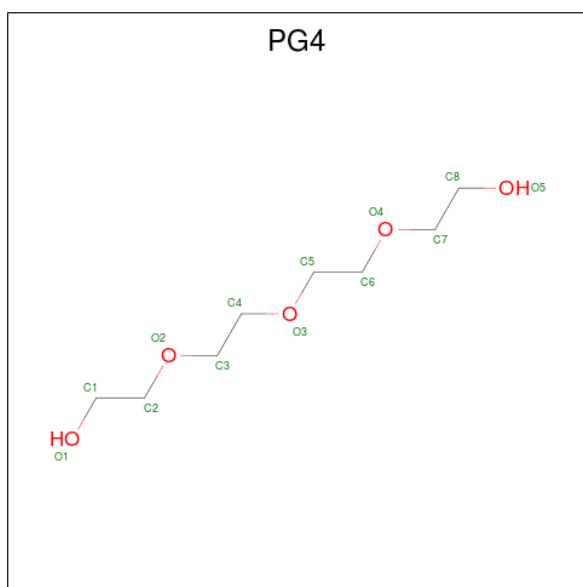
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total 13	C 8	O 5	0	0

- Molecule 8 is AMMONIUM ION (three-letter code: NH4) (formula: H_4N).

NH4

NH_4^+N
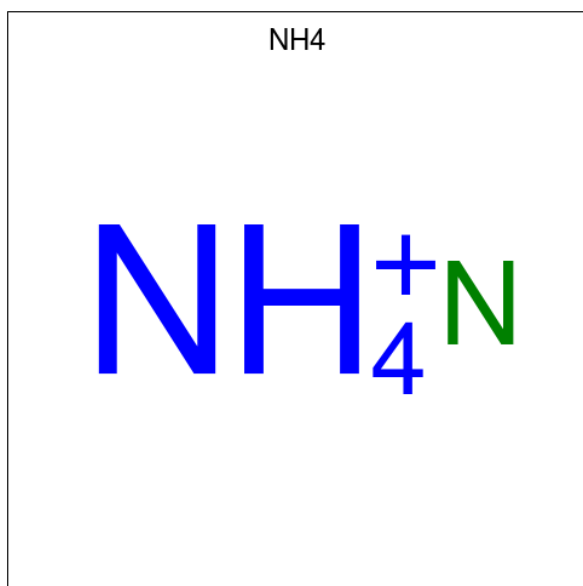
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total 5	H 4	N 1	0	0
8	C	1	Total 5	H 4	N 1	0	0

- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

W O R L D W I D E
PDB
PROTEIN DATA BANK

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

- Molecule 10 is [[(2R,5S)-5-(4-azanyl-5-fluoranyl-2-oxidanylidene-pyrimidin-1-yl)-1,3-oxathi olan-2-yl]methoxy-oxidanyl-phosphoryl] phosphono hydrogen phosphate (three-letter code: 1RY) (formula: $C_8H_{13}FN_3O_{12}P_3S$) (labeled as "Ligand of Interest" by depositor).
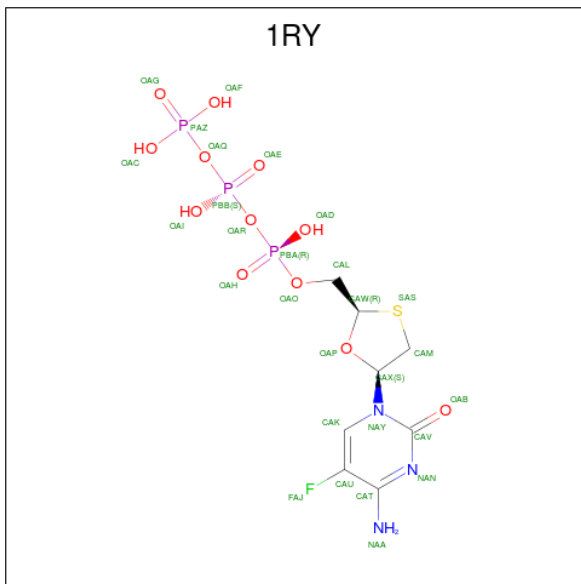
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
10	A	1	Total 28	C 8	F 1	N 3	O 12	P 3	S 1	0	0
10	C	1	Total 28	C 8	F 1	N 3	O 12	P 3	S 1	0	0

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	82	Total O 82 82		0	0
11	B	71	Total O 71 71		0	0
11	C	76	Total O 76 76		0	0
11	D	54	Total O 54 54		0	0
11	F	8	Total O 8 8		0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	E	10	Total 10	O 10	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: Reverse transcriptase p66
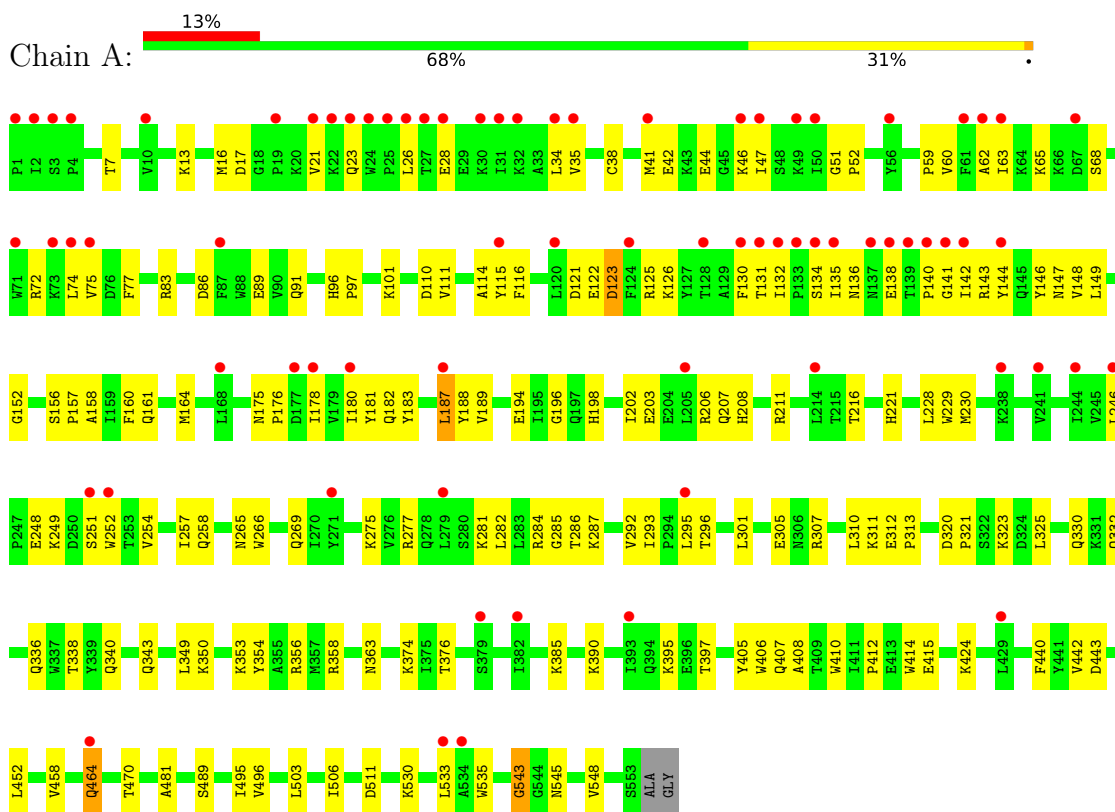
• Molecule 1: Reverse transcriptase p66
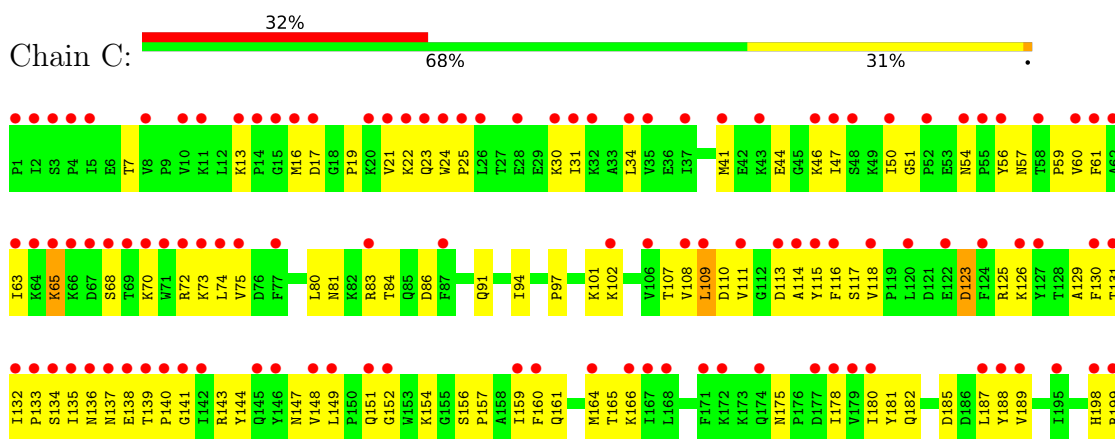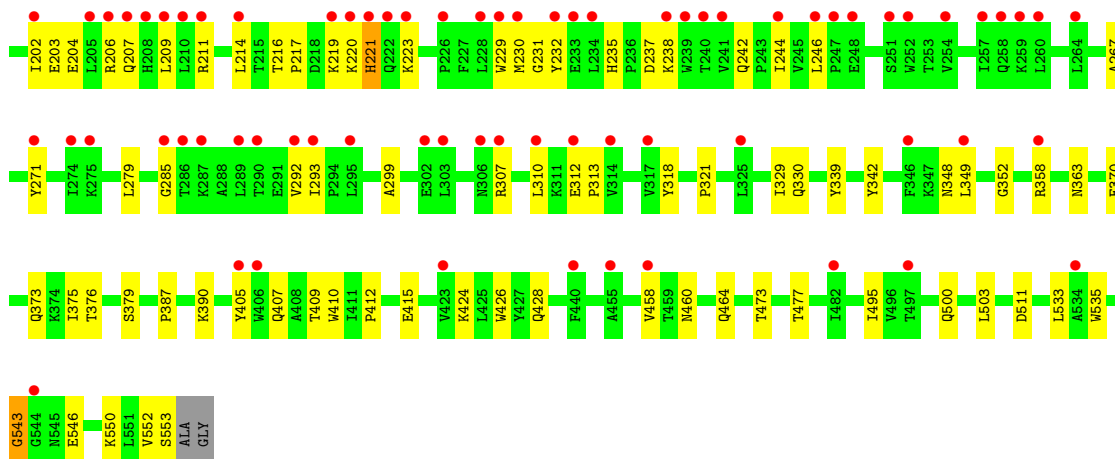
- Molecule 2: Reverse transcriptase p51
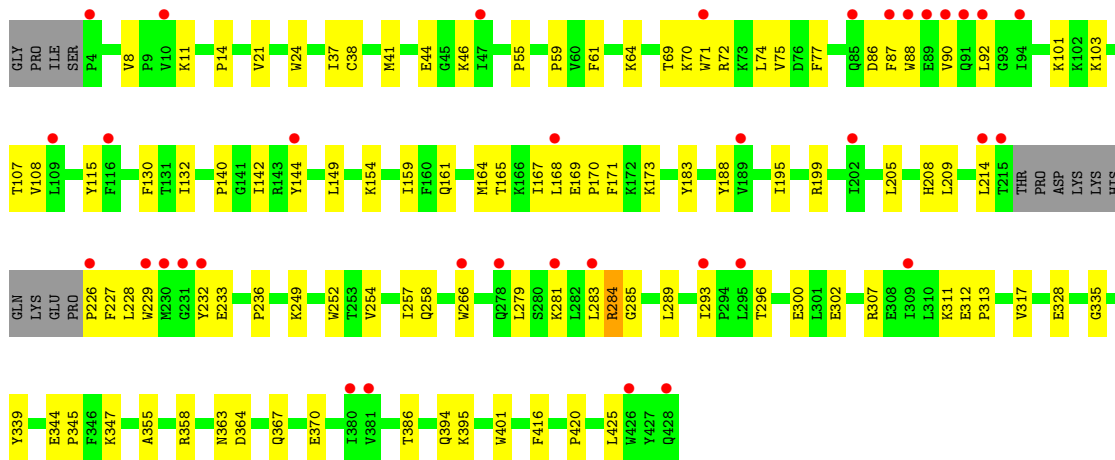
- Molecule 2: Reverse transcriptase p51
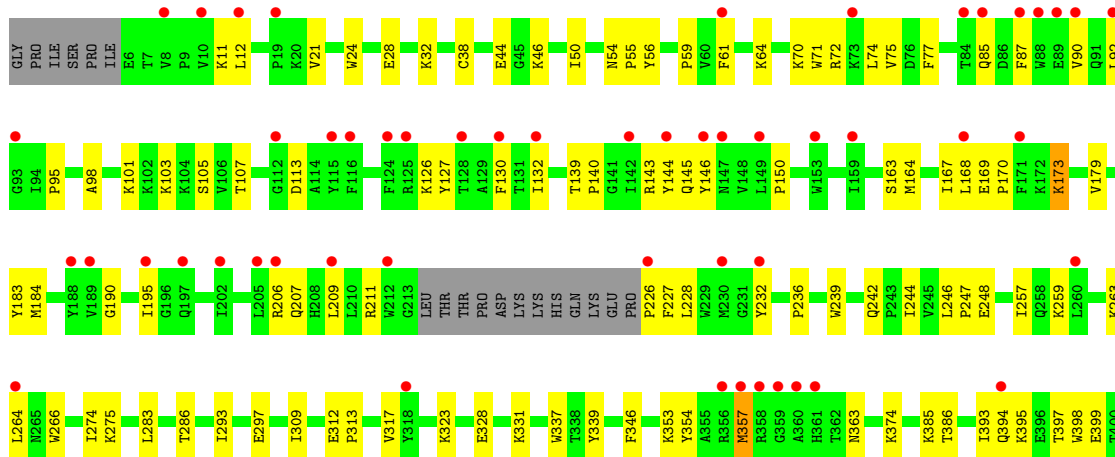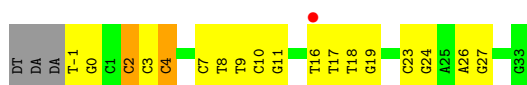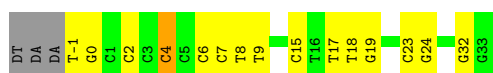
W401 F416 L422 V423 K424 L425 W426 Y427 GLN

• Molecule 3: DNA/RNA (38-MER)

Chain F:

3%

45% 42% 5% 8%

DT DA DA T-1 G0 C1 C2 C3 C4 C7 T8 T9 C10 G11 T16 T17 T18 G19 C23 G24 A25 A26 G27 G33

• Molecule 3: DNA/RNA (38-MER)

Chain E:

53% 37% • 8%

DT DA DA T-1 G0 C1 C2 C3 C4 C5 C6 C7 T8 T9 C15 T16 T17 T18 G19 C23 G24 G32 G33

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

Chain M:

100%

GLC1 FRU2

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

Chain N:

100%

GLC1 FRU2

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	90.26Å 129.19Å 131.32Å 90.00° 100.86° 90.00°	Depositor
Resolution (Å)	91.27 – 2.45 91.27 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.6 (91.27-2.45) 99.6 (91.27-2.45)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.25 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.190 , 0.222 0.190 , 0.222	Depositor DCC
R_{free} test set	1993 reflections (1.84%)	wwPDB-VP
Wilson B-factor (Å^2)	71.0	Xtriage
Anisotropy	0.349	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 81.1	EDS
L-test for twinning[2]	$< |L| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	17811	wwPDB-VP
Average B, all atoms (Å^2)	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[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: GOL, SO4, PG4, OMC, FRU, GLC, CA, NH4, 1RY

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	0.26	0/4631	0.44	0/6291
1	C	0.25	0/4622	0.44	0/6279
2	B	0.26	0/3543	0.45	0/4812
2	D	0.25	0/3502	0.44	0/4757
3	E	0.53	0/760	0.87	0/1172
3	F	0.53	0/760	0.88	0/1172
All	All	0.29	0/17818	0.50	0/24483

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	4510	0	4575	150	0
1	C	4504	0	4567	163	0
2	B	3440	0	3474	91	0
2	D	3400	0	3429	105	0
3	E	721	0	397	15	0
3	F	721	0	397	19	0
4	M	23	0	21	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	N	23	0	21	0	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
5	C	5	0	0	0	0
6	A	6	0	8	1	0
6	B	36	0	48	5	0
6	D	24	0	32	6	0
6	F	6	0	8	0	0
7	A	13	0	18	7	0
8	A	1	4	0	0	0
8	C	1	4	0	0	0
9	A	1	0	0	0	0
9	C	1	0	0	0	0
10	A	28	0	12	2	0
10	C	28	0	11	2	0
11	A	82	0	0	11	0
11	B	71	0	0	5	0
11	C	76	0	0	11	0
11	D	54	0	0	6	0
11	E	10	0	0	2	0
11	F	8	0	0	2	0
All	All	17803	8	17018	510	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 15.

The worst 5 of 510 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)
2:B:281:LYS:HE3	2:B:284:ARG:NH2	1.43	1.34
2:D:257:ILE:HD12	2:D:293:ILE:HD11	1.35	1.08
1:A:208:HIS:HA	1:A:211:ARG:HE	1.14	1.06
1:C:246:LEU:HD11	1:C:310:LEU:HD12	1.38	1.03
1:A:458:VAL:HG23	1:A:464[B]:GLN:HG2	1.41	0.99

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	532 (96%)	18 (3%)	2 (0%)	34	41
1	C	551/555 (99%)	534 (97%)	16 (3%)	1 (0%)	47	57
2	B	412/429 (96%)	398 (97%)	14 (3%)	0	100	100
2	D	407/429 (95%)	393 (97%)	14 (3%)	0	100	100
All	All	1922/1968 (98%)	1857 (97%)	62 (3%)	3 (0%)	47	57

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	543	GLY
1	C	543	GLY
1	A	140	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	496/495 (100%)	489 (99%)	7 (1%)	67	77
1	C	495/495 (100%)	489 (99%)	6 (1%)	71	81
2	B	378/390 (97%)	377 (100%)	1 (0%)	92	95
2	D	373/390 (96%)	371 (100%)	2 (0%)	88	93
All	All	1742/1770 (98%)	1726 (99%)	16 (1%)	78	86

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

Mol	Chain	Res	Type
2	D	173	LYS
1	C	428	GLN
1	C	65	LYS
1	C	330	GLN
2	B	284	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	161	GLN
1	C	182	GLN
2	D	242	GLN
1	A	221	HIS
1	A	91	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	2	3	19,22,23	3.06	7 (36%)	26,31,34	0.75	0
3	OMC	F	4	3	19,22,23	3.05	7 (36%)	26,31,34	0.73	0
3	OMC	E	4	3	19,22,23	3.04	7 (36%)	26,31,34	0.70	0
3	OMC	E	2	3	19,22,23	3.05	7 (36%)	26,31,34	0.77	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	2	3	-	1/9/27/28	0/2/2/2
3	OMC	F	4	3	-	0/9/27/28	0/2/2/2
3	OMC	E	4	3	-	1/9/27/28	0/2/2/2
3	OMC	E	2	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	E	2	OMC	C6-C5	6.53	1.50	1.35
3	E	4	OMC	C6-C5	6.51	1.50	1.35
3	F	2	OMC	C6-C5	6.47	1.50	1.35
3	F	2	OMC	C2-N3	6.45	1.49	1.36
3	F	4	OMC	C6-C5	6.43	1.50	1.35

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	4	OMC	C1'-C2'-O2'-CM2
3	F	2	OMC	C1'-C2'-O2'-CM2

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	2	OMC	1	0
3	F	4	OMC	3	0
3	E	4	OMC	1	0

5.5 Carbohydrates (i)

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	M	1	4	11,11,12	0.60	0	15,15,17	0.71	0
4	FRU	M	2	4	11,12,12	0.51	0	10,18,18	0.58	0
4	GLC	N	1	4	11,11,12	0.66	0	15,15,17	0.73	0
4	FRU	N	2	4	11,12,12	0.52	0	10,18,18	0.84	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
4	GLC	M	1	4	-	1/2/19/22	0/1/1/1
4	FRU	M	2	4	-	5/5/24/24	0/1/1/1
4	GLC	N	1	4	-	0/2/19/22	0/1/1/1
4	FRU	N	2	4	-	5/5/24/24	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	M	2	FRU	O1-C1-C2-O2
4	N	2	FRU	O1-C1-C2-O2
4	M	2	FRU	O5-C5-C6-O6
4	N	2	FRU	O5-C5-C6-O6
4	M	2	FRU	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	M	1	GLC	1	0
4	M	2	FRU	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 oligosaccharide.

Oligosaccharide Chain M

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain N

Bond lengths

Bond angles

Torsions

Rings
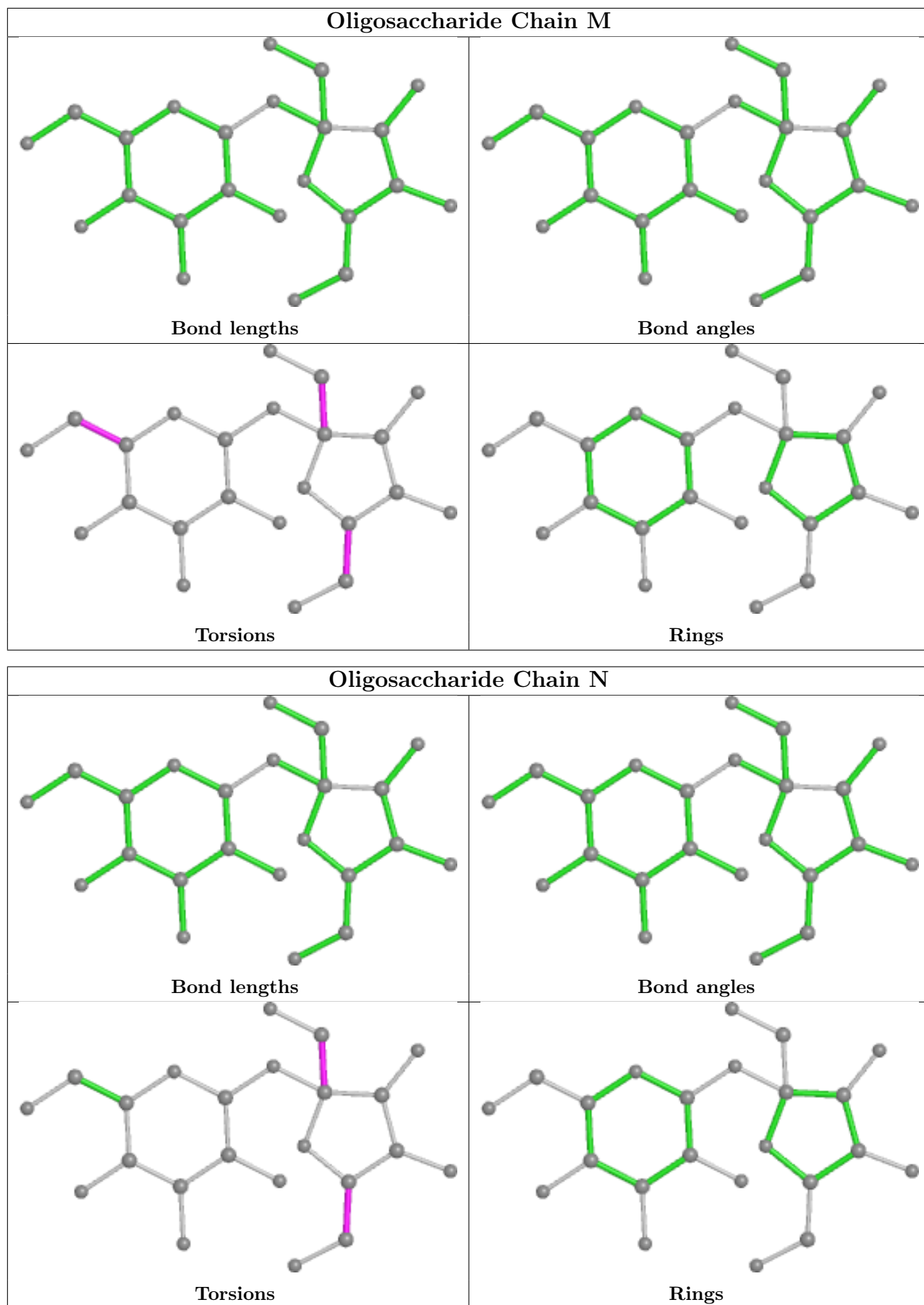
5.6 Ligand geometry ⓘ

Of 22 ligands modelled in this entry, 2 are modelled with single atom and 2 are monoatomic - leaving 18 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	$\#|Z| > 2$
5	SO4	B	506	-	4,4,4	0.13	0	6,6,6	0.05	0
6	GOL	A	602	-	5,5,5	0.96	0	5,5,5	0.97	0
5	SO4	A	601	-	4,4,4	0.13	0	6,6,6	0.06	0
6	GOL	B	504	-	5,5,5	1.03	0	5,5,5	0.97	0
6	GOL	B	507	-	5,5,5	0.96	0	5,5,5	0.92	0
6	GOL	F	101	-	5,5,5	0.89	0	5,5,5	0.99	0
6	GOL	D	504	-	5,5,5	0.91	0	5,5,5	0.98	0
5	SO4	C	601	-	4,4,4	0.15	0	6,6,6	0.05	0
10	1RY	C	604	9	25,29,29	0.41	0	35,45,45	0.94	1 (2%)
6	GOL	B	503	-	5,5,5	0.94	0	5,5,5	0.94	0
6	GOL	B	501	-	5,5,5	0.91	0	5,5,5	1.03	0
6	GOL	B	505	-	5,5,5	0.99	0	5,5,5	0.92	0
6	GOL	D	501	-	5,5,5	1.08	0	5,5,5	0.87	0
6	GOL	D	502	-	5,5,5	0.96	0	5,5,5	0.97	0
7	PG4	A	603	-	12,12,12	0.53	0	11,11,11	0.25	0
10	1RY	A	606	9	25,29,29	0.54	0	35,45,45	0.92	1 (2%)
6	GOL	D	503	-	5,5,5	0.90	0	5,5,5	1.00	0
6	GOL	B	502	-	5,5,5	0.95	0	5,5,5	0.93	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	GOL	A	602	-	-	3/4/4/4	-
6	GOL	B	507	-	-	3/4/4/4	-
6	GOL	B	504	-	-	2/4/4/4	-
6	GOL	F	101	-	-	2/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	D	504	-	-	0/4/4/4	-
10	1RY	C	604	9	-	8/22/31/31	0/2/2/2
6	GOL	B	503	-	-	2/4/4/4	-
6	GOL	B	501	-	-	2/4/4/4	-
6	GOL	B	505	-	-	1/4/4/4	-
6	GOL	D	501	-	-	2/4/4/4	-
6	GOL	D	502	-	-	0/4/4/4	-
7	PG4	A	603	-	-	7/10/10/10	-
10	1RY	A	606	9	-	5/22/31/31	0/2/2/2
6	GOL	D	503	-	-	4/4/4/4	-
6	GOL	B	502	-	-	4/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	C	604	1RY	OAO-PBA-OAH	4.08	125.01	109.07
10	A	606	1RY	OAO-PBA-OAH	3.63	123.27	109.07

There are no chirality outliers.

5 of 45 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	602	GOL	O1-C1-C2-C3
6	B	502	GOL	O1-C1-C2-C3
6	B	502	GOL	C1-C2-C3-O3
6	D	501	GOL	O1-C1-C2-O2
6	D	501	GOL	O1-C1-C2-C3

There are no ring outliers.

11 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	602	GOL	1	0
6	B	507	GOL	1	0
6	D	504	GOL	2	0
10	C	604	1RY	2	0
6	B	501	GOL	1	0
6	B	505	GOL	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	501	GOL	2	0
6	D	502	GOL	2	0
7	A	603	PG4	7	0
10	A	606	1RY	2	0
6	B	502	GOL	2	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 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 1RY C 604

Bond lengths

Bond angles

Torsions

Rings

Ligand 1RY A 606

Bond lengths

Bond angles

Torsions

Rings
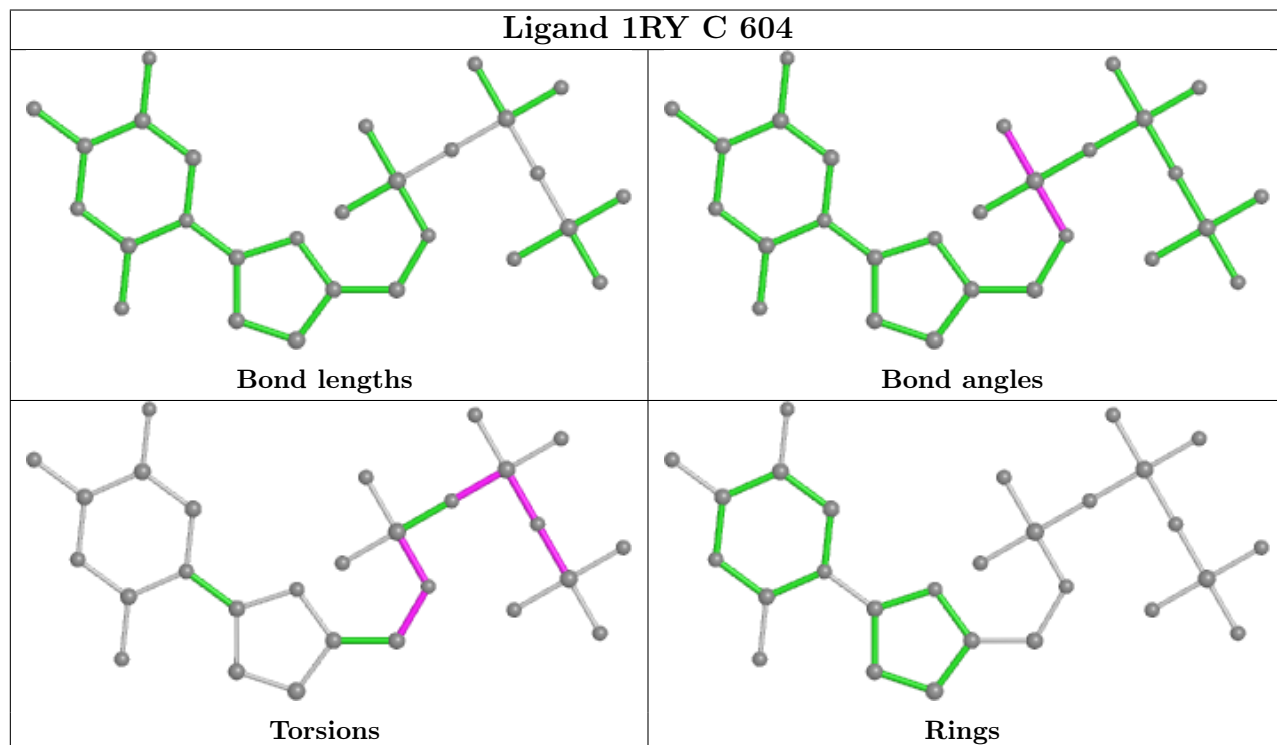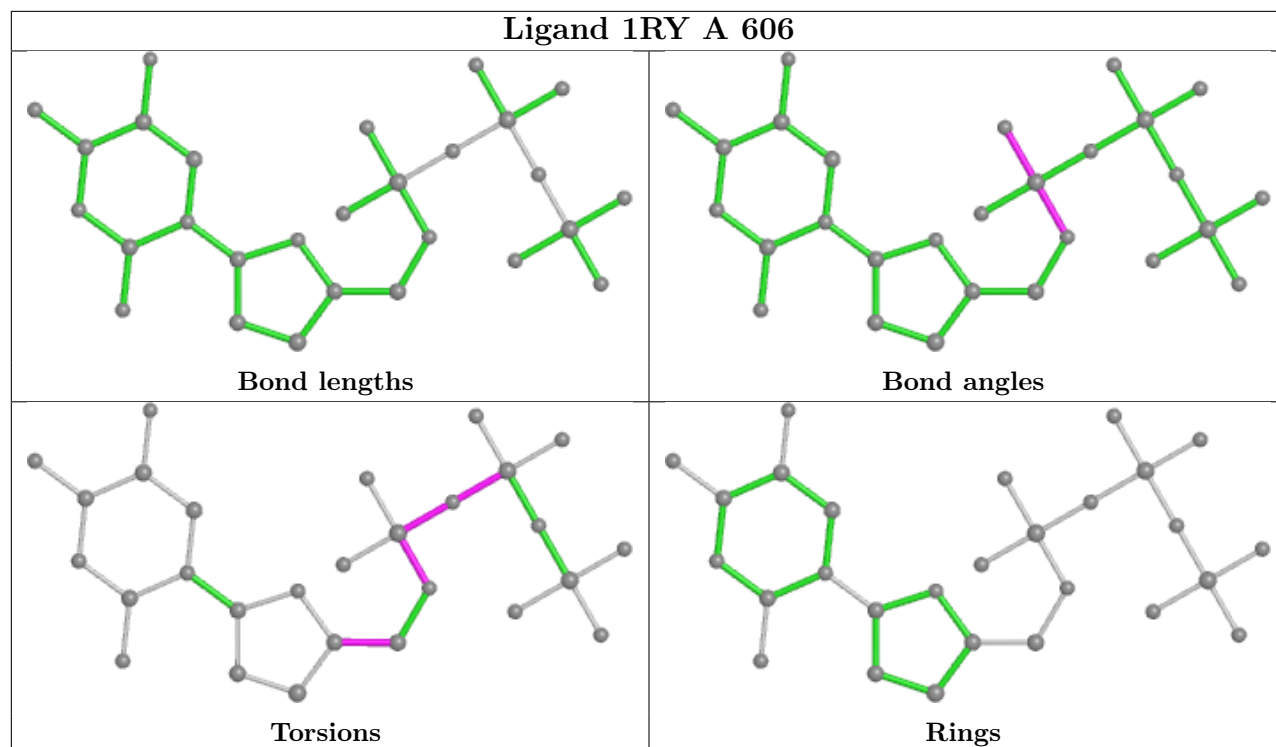
5.7 Other polymers ⓘ

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 ⓘ

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	553/555 (99%)	1.12	74 (13%)	3	2	53, 117, 193, 276	0
1	C	553/555 (99%)	1.82	180 (32%)	0	0	56, 138, 236, 297	0
2	B	415/429 (96%)	0.85	36 (8%)	10	7	55, 98, 159, 212	0
2	D	410/429 (95%)	1.10	56 (13%)	3	2	59, 118, 185, 267	0
3	E	33/38 (86%)	0.02	0	100	100	90, 121, 151, 180	0
3	F	33/38 (86%)	0.02	1 (3%)	50	46	90, 135, 172, 197	0
All	All	1997/2044 (97%)	1.22	347 (17%)	1	1	53, 115, 210, 297	0

The worst 5 of 347 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	133	PRO	16.4
1	C	133	PRO	16.4
1	C	137	ASN	14.4
1	C	26	LEU	13.9
1	A	2	ILE	13.8

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

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
3	OMC	F	2	21/22	0.90	0.16	128,137,147,150	0
3	OMC	E	2	21/22	0.91	0.19	102,122,132,136	0
3	OMC	F	4	21/22	0.93	0.15	104,115,129,141	0
3	OMC	E	4	21/22	0.97	0.18	81,91,103,105	0

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, 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.
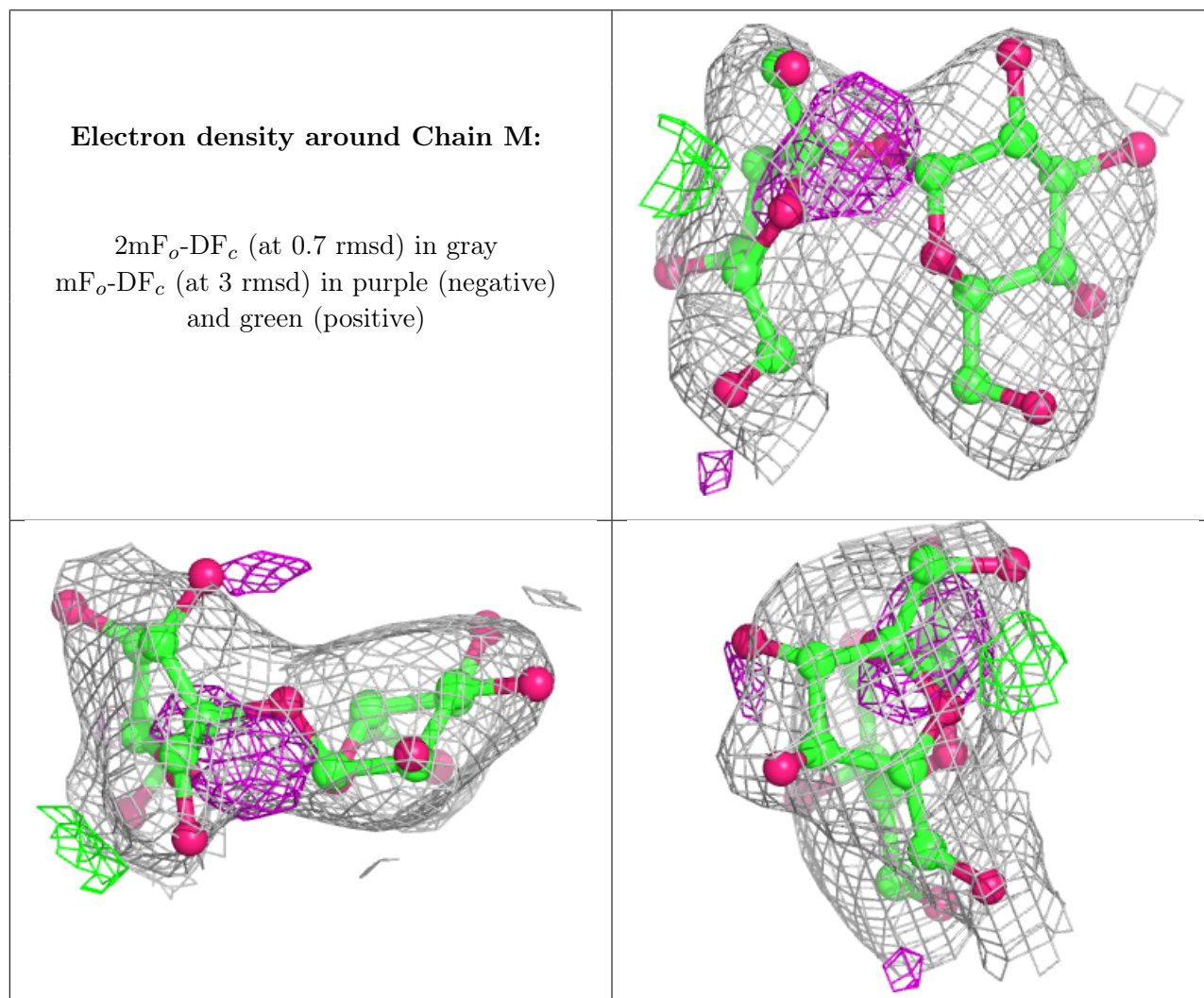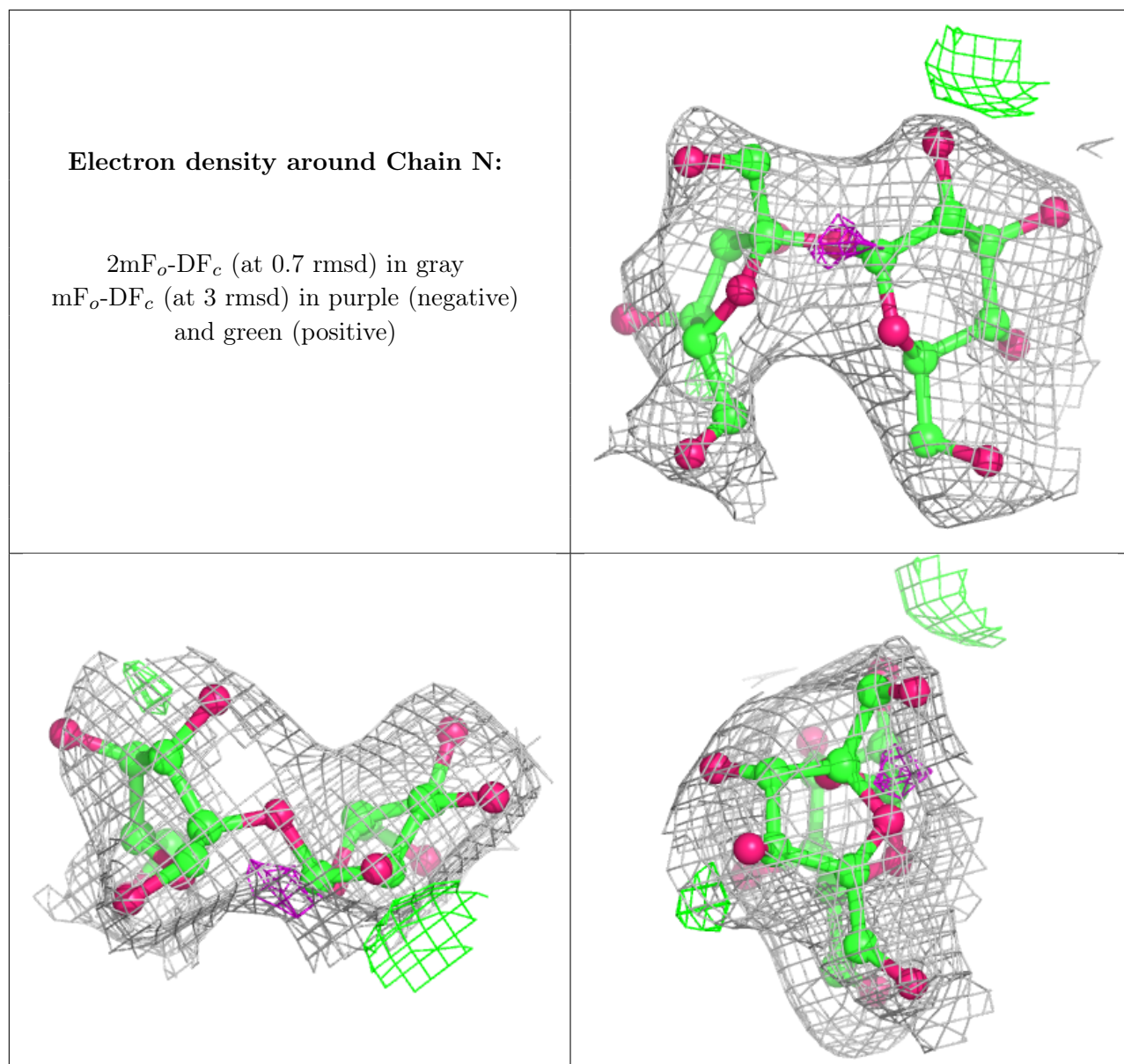
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	FRU	N	2	12/12	0.84	0.18	92,126,129,130	0
4	GLC	N	1	11/12	0.89	0.19	91,111,125,129	0
4	GLC	M	1	11/12	0.90	0.25	78,104,114,114	0
4	FRU	M	2	12/12	0.90	0.23	79,116,126,127	0

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.

Electron density around Chain M:

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

Electron density around 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)

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.
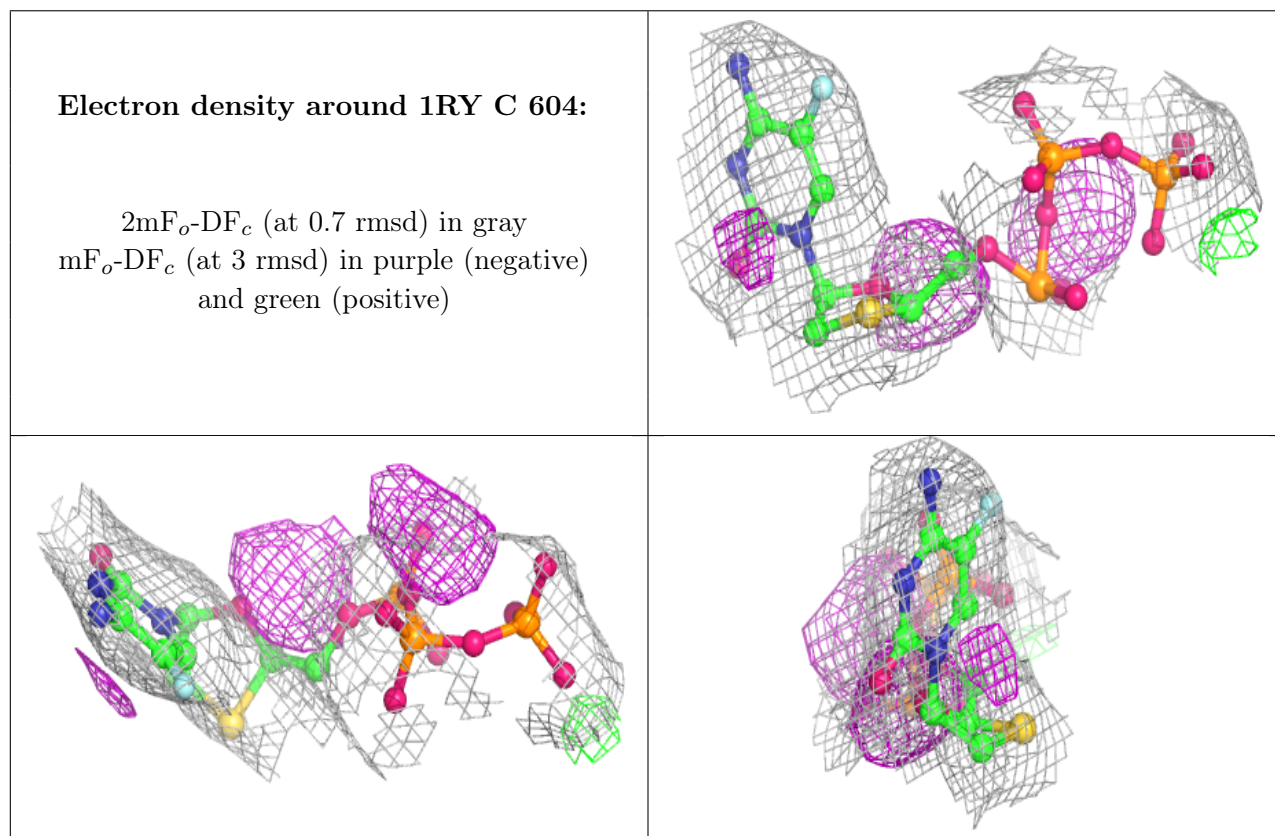
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	NH4	A	604	1/1	0.63	0.46	108,130,130,130	0
8	NH4	C	602	1/1	0.66	0.50	70,84,84,84	0
7	PG4	A	603	13/13	0.75	0.32	101,109,117,122	0
6	GOL	A	602	6/6	0.76	0.68	64,104,117,126	0
6	GOL	D	504	6/6	0.77	0.38	100,104,111,115	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	GOL	D	501	6/6	0.80	0.53	76,82,93,97	0
6	GOL	B	505	6/6	0.80	0.30	69,90,94,107	0
6	GOL	F	101	6/6	0.80	0.38	116,121,125,128	0
10	1RY	C	604	28/28	0.81	0.17	142,181,211,216	0
6	GOL	B	503	6/6	0.84	0.24	80,91,94,103	0
6	GOL	B	507	6/6	0.86	0.23	90,97,101,102	0
10	1RY	A	606	28/28	0.87	0.14	127,143,171,175	0
5	SO4	A	601	5/5	0.88	0.18	93,115,128,139	0
9	CA	A	605	1/1	0.88	0.10	146,146,146,146	0
6	GOL	B	501	6/6	0.89	0.19	74,83,100,107	0
6	GOL	D	502	6/6	0.89	0.27	87,96,105,105	0
6	GOL	B	502	6/6	0.91	0.19	77,89,93,94	0
6	GOL	D	503	6/6	0.91	0.23	95,104,111,113	0
9	CA	C	603	1/1	0.92	0.08	186,186,186,186	0
5	SO4	B	506	5/5	0.93	0.25	136,146,161,164	0
6	GOL	B	504	6/6	0.97	0.22	63,71,80,84	0
5	SO4	C	601	5/5	0.98	0.15	98,101,111,123	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 1RY C 604:

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

Electron density around 1RY A 606:

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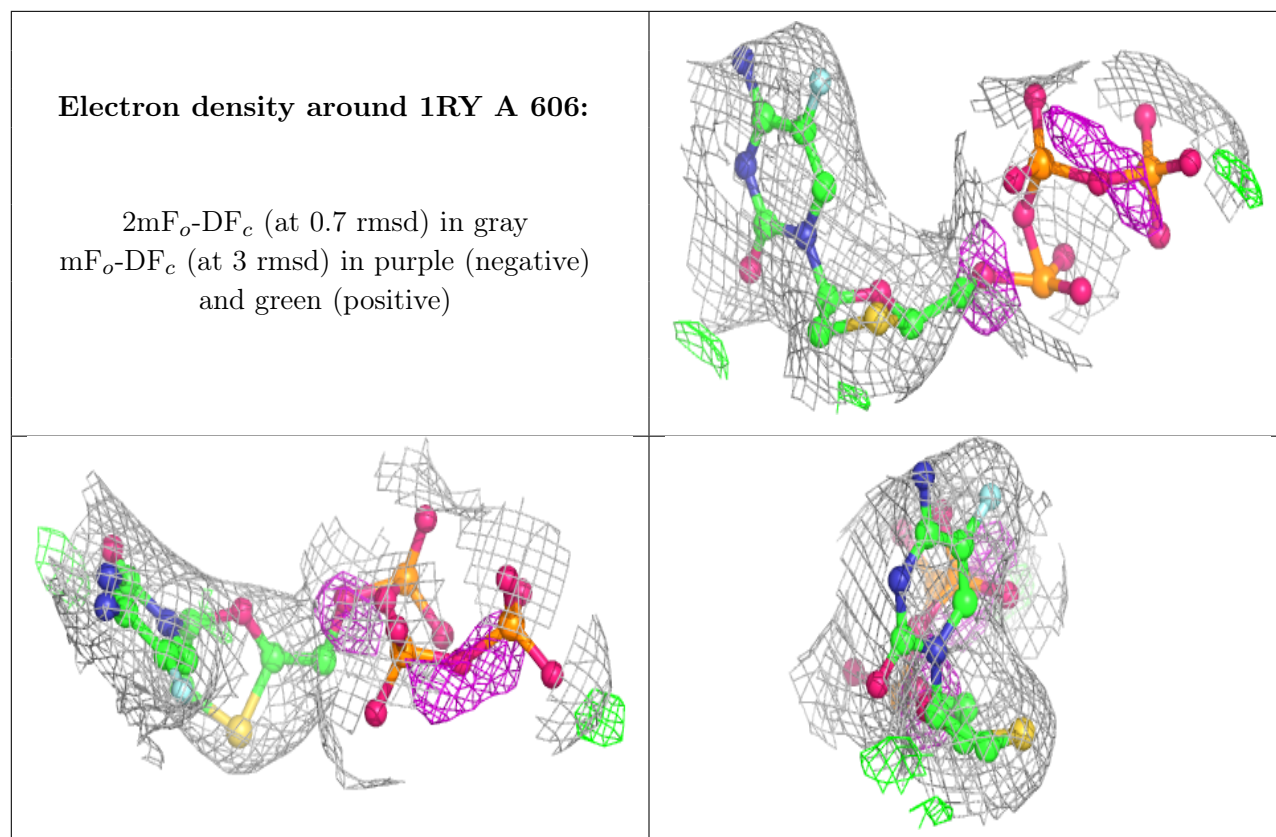
6.5 Other polymers (i)

There are no such residues in this entry.