W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Nov 24, 2021 – 01:06 pm GMT

PDB ID	:	7B0B
Title	:	Fab HbnC3t1p1_C6 bound to SARS-CoV-2 RBD
Authors	:	Borenstein-Katz, A.; Diskin, R.
Deposited on	:	2020-11-19
Resolution	:	2.98 Å(reported)

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

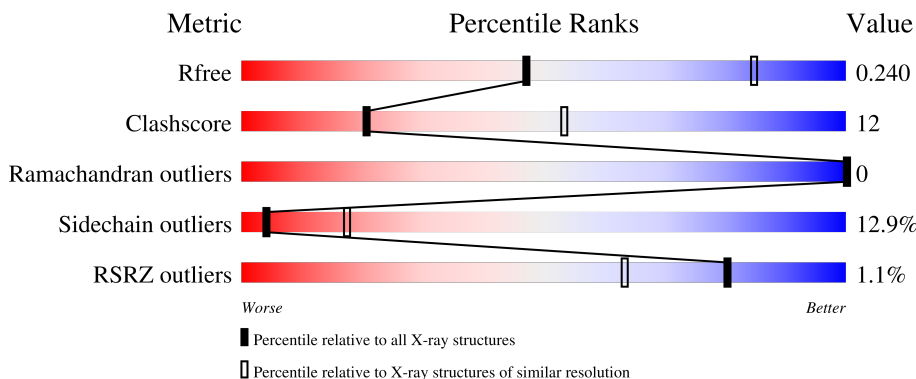|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4 (270009), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.98 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		0.240
Clashscore		12
Ramachandran outliers		0
Sidechain outliers		12.9%
RSRZ outliers		1.1%

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))
R_{free}	130704	2754 (3.00-2.96)
Clashscore	141614	3103 (3.00-2.96)
Ramachandran outliers	138981	2993 (3.00-2.96)
Sidechain outliers	138945	2996 (3.00-2.96)
RSRZ outliers	127900	2644 (3.00-2.96)

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	L	215	72% 27% •
2	H	230	60% 30% • 5%
3	F	229	3% 57% 24% • • 15%
4	A	2	100%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 4858 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 IGK@ protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	215	Total	C	N	O	S	0	0	0
			1648	1030	279	334	5			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	2	ILE	ASN	conflict	UNP Q6PIL8
L	29	VAL	LEU	conflict	UNP Q6PIL8
L	52	ALA	VAL	conflict	UNP Q6PIL8
L	79	VAL	LEU	conflict	UNP Q6PIL8
L	94	SER	THR	conflict	UNP Q6PIL8
L	?	-	ARG	deletion	UNP Q6PIL8
L	97	TRP	ILE	conflict	UNP Q6PIL8
L	104	LYS	ARG	conflict	UNP Q6PIL8
L	105	VAL	LEU	conflict	UNP Q6PIL8
L	106	GLU	ASP	conflict	UNP Q6PIL8

- Molecule 2 is a protein called Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	218	Total	C	N	O	S	0	0	0
			1639	1031	277	321	10			

- Molecule 3 is a protein called Surface glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	195	Total	C	N	O	S	0	0	0
			1543	989	257	289	8			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	542	HIS	-	expression tag	UNP A0A6M5SXU3
F	543	HIS	-	expression tag	UNP A0A6M5SXU3
F	544	HIS	-	expression tag	UNP A0A6M5SXU3
F	545	HIS	-	expression tag	UNP A0A6M5SXU3
F	546	HIS	-	expression tag	UNP A0A6M5SXU3
F	547	HIS	-	expression tag	UNP A0A6M5SXU3

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.
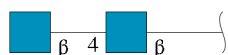
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	A	2	28	16	2	10	0	0	0

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: IGK@ protein

Chain L:

• Molecule 2: Fab heavy chain

Chain H:

• Molecule 3: Surface glycoprotein

Chain F:

• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluc opyranose

Chain A: 100%

MAG1
MAG2

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	84.41Å 109.11Å 168.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.36 – 2.98 39.36 – 2.98	Depositor EDS
% Data completeness (in resolution range)	77.2 (39.36-2.98) 77.2 (39.36-2.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.10 (at 2.95Å)	Xtriage
Refinement program	PHENIX dev_3965	Depositor
R, R_{free}	0.209 , 0.246 0.208 , 0.240	Depositor DCC
R_{free} test set	1998 reflections (7.96%)	wwPDB-VP
Wilson B-factor (Å^2)	60.7	Xtriage
Anisotropy	0.722	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	4858	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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: NAG

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	L	0.34	0/1685	0.62	0/2289
2	H	0.36	0/1677	0.59	0/2284
3	F	0.52	2/1587 (0.1%)	0.93	10/2161 (0.5%)
All	All	0.41	2/4949 (0.0%)	0.72	10/6734 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	355	ARG	CB-CG	-7.18	1.33	1.52
3	F	382	VAL	C-N	5.80	1.47	1.34

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	355	ARG	CG-CD-NE	-13.27	83.93	111.80
3	F	387	LEU	CA-CB-CG	11.64	142.06	115.30
3	F	382	VAL	C-N-CA	-7.70	102.46	121.70
3	F	355	ARG	NE-CZ-NH2	-7.42	116.59	120.30
3	F	390	LEU	CA-CB-CG	-6.62	100.08	115.30

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	L	1648	0	1595	30	0
2	H	1639	0	1606	45	1
3	F	1543	0	1459	46	1
4	A	28	0	25	2	0
All	All	4858	0	4685	117	1

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 12.

The worst 5 of 117 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:F:493:GLN:HE21	3:F:494:SER:H	1.11	0.95
1:L:80:GLU:HG3	1:L:81:PRO:HD2	1.53	0.89
3:F:503:VAL:HA	3:F:506:GLN:HE21	1.46	0.79
2:H:2:MET:HB2	2:H:26:GLY:HA3	1.63	0.77
1:L:84:PHE:CD1	1:L:107:ILE:HG22	2.22	0.75

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:220:ARG:NH1	3:F:369:TYR:O[2_454]	2.19	0.01

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	L	213/215 (99%)	201 (94%)	12 (6%)	0	100	100
2	H	214/230 (93%)	208 (97%)	6 (3%)	0	100	100
3	F	193/229 (84%)	181 (94%)	12 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	620/674 (92%)	590 (95%)	30 (5%)	0	100 100

There are no Ramachandran outliers to report.

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	L	186/186 (100%)	161 (87%)	25 (13%)	4	16
2	H	187/198 (94%)	154 (82%)	33 (18%)	2	9
3	F	168/202 (83%)	156 (93%)	12 (7%)	14	44
All	All	541/586 (92%)	471 (87%)	70 (13%)	4	17

5 of 70 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	219	LYS
3	F	369	TYR
3	F	443	SER
1	L	207	THR
1	L	203	SER

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

Mol	Chain	Res	Type
2	H	174	HIS
3	F	409	GLN
3	F	493	GLN
3	F	501	ASN

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.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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.

Oligosaccharide Chain A — Bond lengths, Bond angles, Torsions, Rings
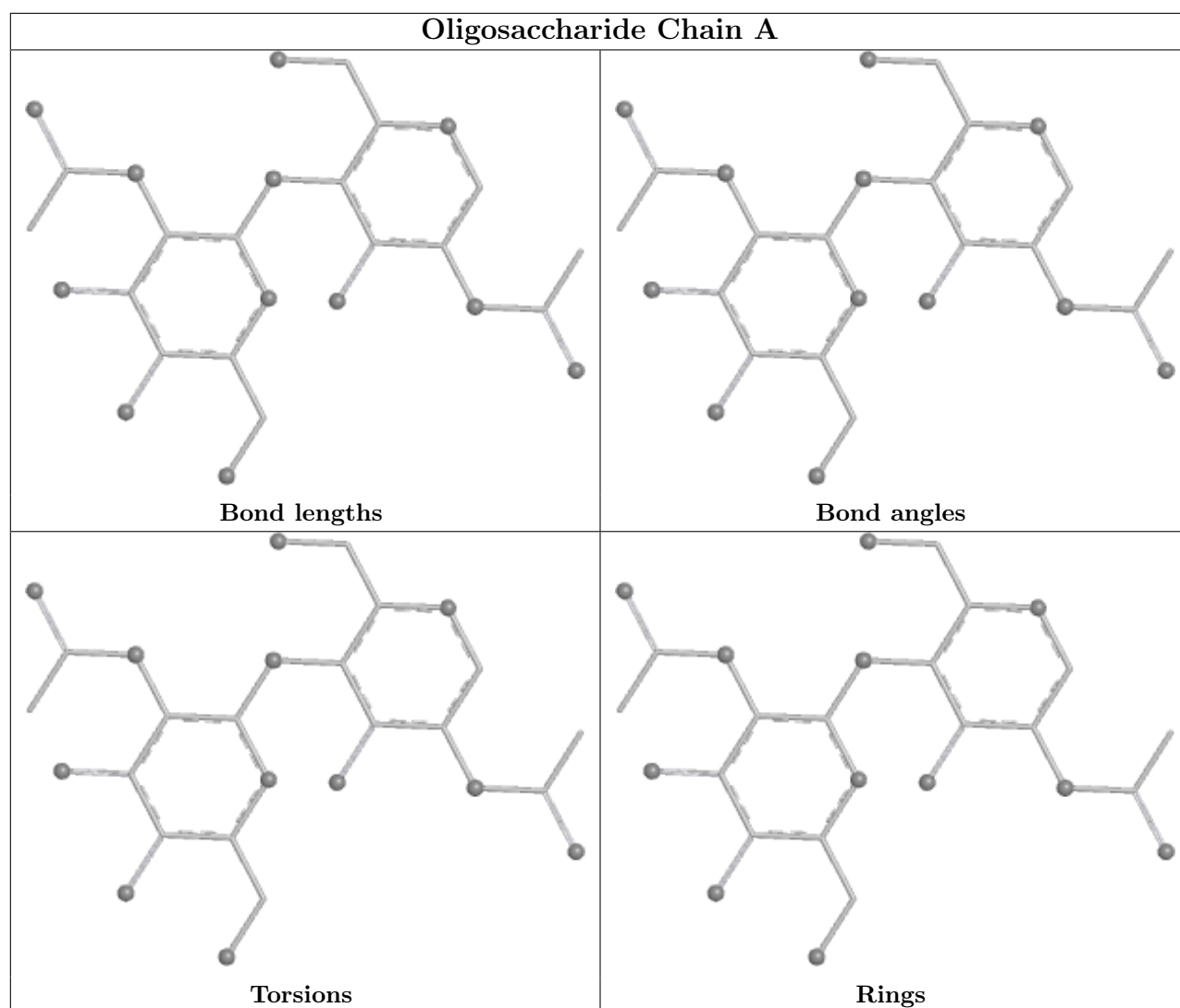
5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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	L	215/215 (100%)	-0.26	0	100	100	30, 52, 75, 105	0
2	H	218/230 (94%)	-0.31	0	100	100	33, 51, 82, 103	0
3	F	195/229 (85%)	-0.03	7 (3%)	42	26	40, 71, 116, 149	0
All	All	628/674 (93%)	-0.21	7 (1%)	80	63	30, 56, 98, 149	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	519	HIS	3.3
3	F	334	ASN	2.6
3	F	520	ALA	2.4
3	F	333	THR	2.3
3	F	335	LEU	2.2

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

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

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	NAG	A	2	14/15	0.72	0.36	88,124,142,142	0
4	NAG	A	1	14/15	0.84	0.19	67,102,119,126	0

The following is a graphical depiction of the model fit to experimental electron density for oligosac-

charide. Each fit is shown from different orientation to approximate a three-dimensional view.
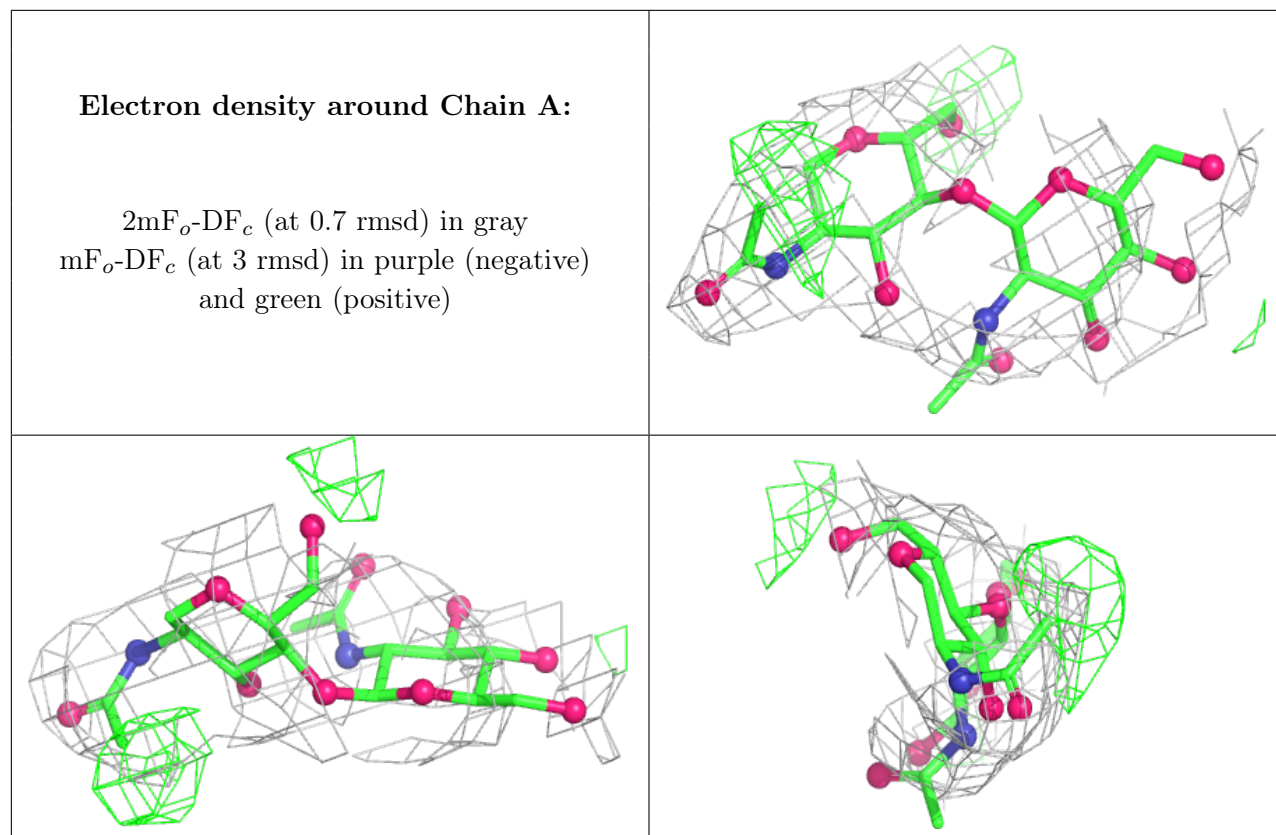
6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.