



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 7, 2021 – 01:04 pm GMT

PDB ID : 7A3O
Title : Crystal structure of dengue 1 virus envelope glycoprotein in complex with the scFv fragment of the broadly neutralizing human antibody EDE1 C10
Authors : Sharma, A.; Vaney, M.C.; Guardado-Calvo, P.; Duquerroy, S.; Rouvinski, A.; Rey, F.A.
Deposited on : 2020-08-18
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 following versions of software and data (see [references ⓘ](#)) 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

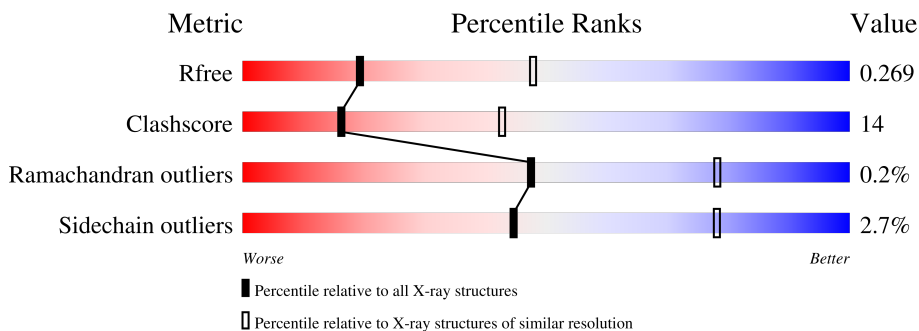
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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	A	432	58% (green), 28% (yellow), 13% (grey), 1% (red), 1% (orange)
2	H	144	67% (green), 19% (yellow), 12% (grey), 1% (red), 1% (orange)
3	L	154	51% (green), 20% (yellow), 29% (grey), 1% (red), 1% (orange)
4	B	2	100% (green)

2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 4785 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 Core protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	377	2903	1836	491	558	18	0	1	0

There are 37 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	396	ALA	-	expression tag	UNP Q9II02
A	397	ALA	-	expression tag	UNP Q9II02
A	398	ASP	-	expression tag	UNP Q9II02
A	399	ASP	-	expression tag	UNP Q9II02
A	400	ASP	-	expression tag	UNP Q9II02
A	401	ASP	-	expression tag	UNP Q9II02
A	402	LYS	-	expression tag	UNP Q9II02
A	403	ALA	-	expression tag	UNP Q9II02
A	404	GLY	-	expression tag	UNP Q9II02
A	405	TRP	-	expression tag	UNP Q9II02
A	406	SER	-	expression tag	UNP Q9II02
A	407	HIS	-	expression tag	UNP Q9II02
A	408	PRO	-	expression tag	UNP Q9II02
A	409	GLN	-	expression tag	UNP Q9II02
A	410	PHE	-	expression tag	UNP Q9II02
A	411	GLU	-	expression tag	UNP Q9II02
A	412	LYS	-	expression tag	UNP Q9II02
A	413	GLY	-	expression tag	UNP Q9II02
A	414	GLY	-	expression tag	UNP Q9II02
A	415	GLY	-	expression tag	UNP Q9II02
A	416	SER	-	expression tag	UNP Q9II02
A	417	GLY	-	expression tag	UNP Q9II02
A	418	GLY	-	expression tag	UNP Q9II02
A	419	GLY	-	expression tag	UNP Q9II02
A	420	SER	-	expression tag	UNP Q9II02
A	421	GLY	-	expression tag	UNP Q9II02
A	422	GLY	-	expression tag	UNP Q9II02

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Chain	Residue	Modelled	Actual	Comment	Reference
A	423	GLY	-	expression tag	UNP Q9II02
A	424	SER	-	expression tag	UNP Q9II02
A	425	TRP	-	expression tag	UNP Q9II02
A	426	SER	-	expression tag	UNP Q9II02
A	427	HIS	-	expression tag	UNP Q9II02
A	428	PRO	-	expression tag	UNP Q9II02
A	429	GLN	-	expression tag	UNP Q9II02
A	430	PHE	-	expression tag	UNP Q9II02
A	431	GLU	-	expression tag	UNP Q9II02
A	432	LYS	-	expression tag	UNP Q9II02

- Molecule 2 is a protein called Single chain variable fragment (scFv) from antibody EDE1 C10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	127	1021	650	169	197	5	0	0	0

- Molecule 3 is a protein called Single chain variable fragment (scFv) from antibody EDE1 C10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	110	797	494	136	164	3	0	0	0

- Molecule 4 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	B	2	24	14	1	9	0	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	L	1	Total	O	S	0	0
			5	4	1		
6	L	1	Total	O	S	0	0
			5	4	1		

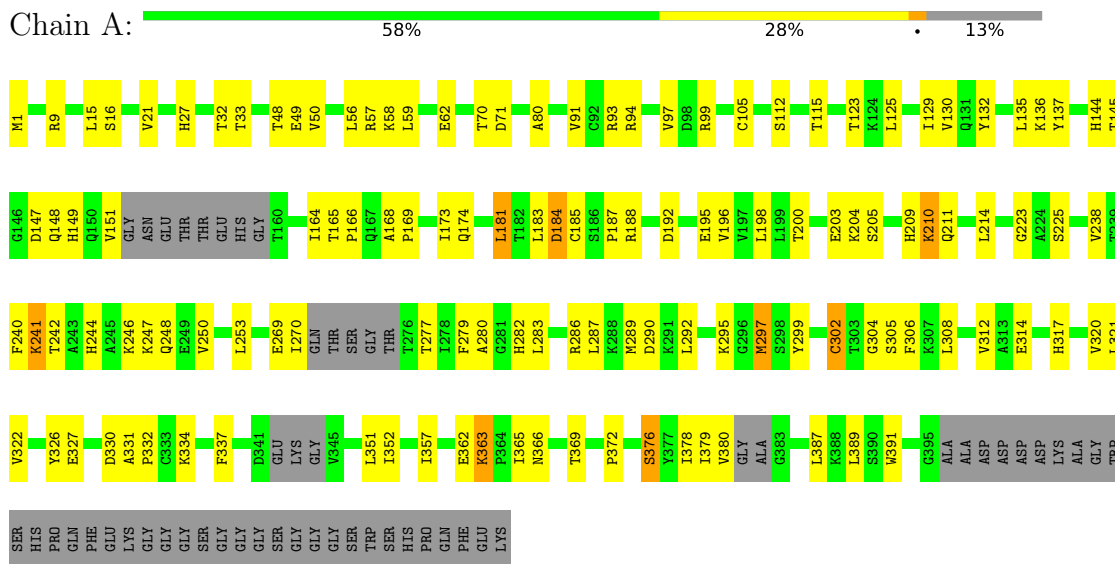
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	3	Total	O	0	0
			3	3		
7	H	1	Total	O	0	0
			1	1		

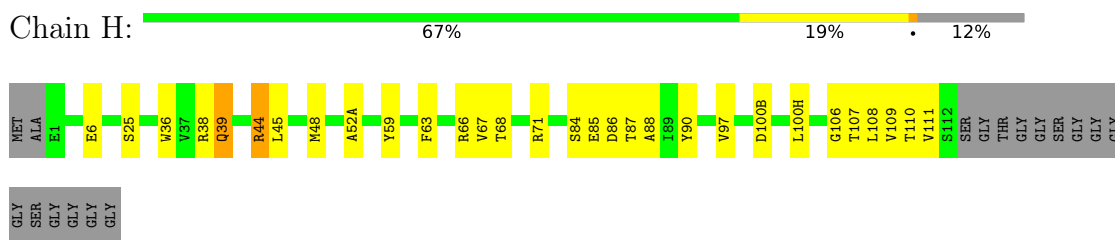
3 Residue-property plots [i](#)

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.

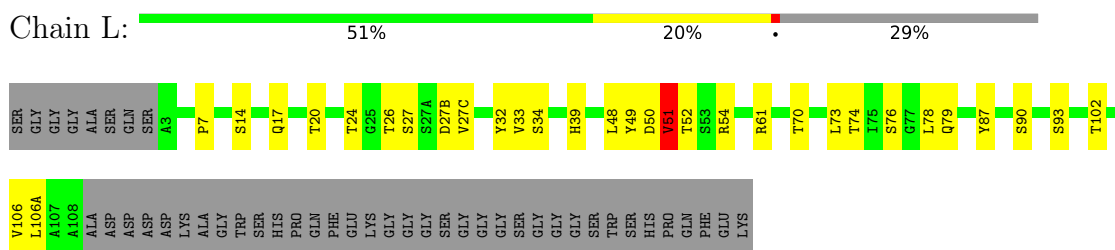
- Molecule 1: Core protein



- Molecule 2: Single chain variable fragment (scFv) from antibody EDE1 C10



- Molecule 3: Single chain variable fragment (scFv) from antibody EDE1 C10



- Molecule 4: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:  100%

3463
FUC2

4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	135.56Å 135.56Å 160.27Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.76 – 2.80 19.76 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.3 (19.76-2.80) 99.3 (19.76-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 2.79Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.218 , 0.268 0.218 , 0.269	Depositor DCC
R_{free} test set	1097 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	90.8	Xtriage
Anisotropy	0.209	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4785	wwPDB-VP
Average B, all atoms (Å ²)	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.27% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SO4, FUC, 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	A	0.33	0/2953	0.60	2/4005 (0.0%)
2	H	0.32	0/1050	0.53	0/1427
3	L	0.35	0/815	0.55	0/1107
All	All	0.33	0/4818	0.58	2/6539 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	181	LEU	CA-CB-CG	5.29	127.47	115.30
1	A	247	LYS	CD-CE-NZ	-5.23	99.67	111.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2903	0	2903	95	2
2	H	1021	0	960	20	0
3	L	797	0	760	25	1
4	B	24	0	22	0	0
5	A	6	0	8	0	0
6	A	20	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	L	10	0	0	0	0
7	A	3	0	0	0	0
7	H	1	0	0	0	0
All	All	4785	0	4653	136	2

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 14.

The worst 5 of 136 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:L:33:VAL:HG22	3:L:51:VAL:HG12	1.49	0.94
2:H:6:GLU:HG3	2:H:107:THR:HG23	1.56	0.85
1:A:241:LYS:HE3	1:A:242:THR:H	1.47	0.78
1:A:362:GLU:OE2	3:L:54:ARG:NH2	2.17	0.77
3:L:34:SER:HB3	3:L:49:TYR:HA	1.67	0.77

All (2) 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)
1:A:184:ASP:OD1	1:A:286:ARG:NH1[11_654]	2.09	0.11
1:A:71:ASP:OD1	3:L:93:SER:OG[10_554]	2.14	0.06

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	368/432 (85%)	350 (95%)	18 (5%)	0	100 100
2	H	125/144 (87%)	120 (96%)	5 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	L	108/154 (70%)	102 (94%)	5 (5%)	1 (1%)	17	46
All	All	601/730 (82%)	572 (95%)	28 (5%)	1 (0%)	47	78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	51	VAL

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	A	324/364 (89%)	315 (97%)	9 (3%)	43	77
2	H	107/112 (96%)	104 (97%)	3 (3%)	43	77
3	L	88/116 (76%)	86 (98%)	2 (2%)	50	82
All	All	519/592 (88%)	505 (97%)	14 (3%)	44	78

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	363	LYS
1	A	376	SER
3	L	51	VAL
2	H	44	ARG
3	L	39	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](#)

2 monosaccharides are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

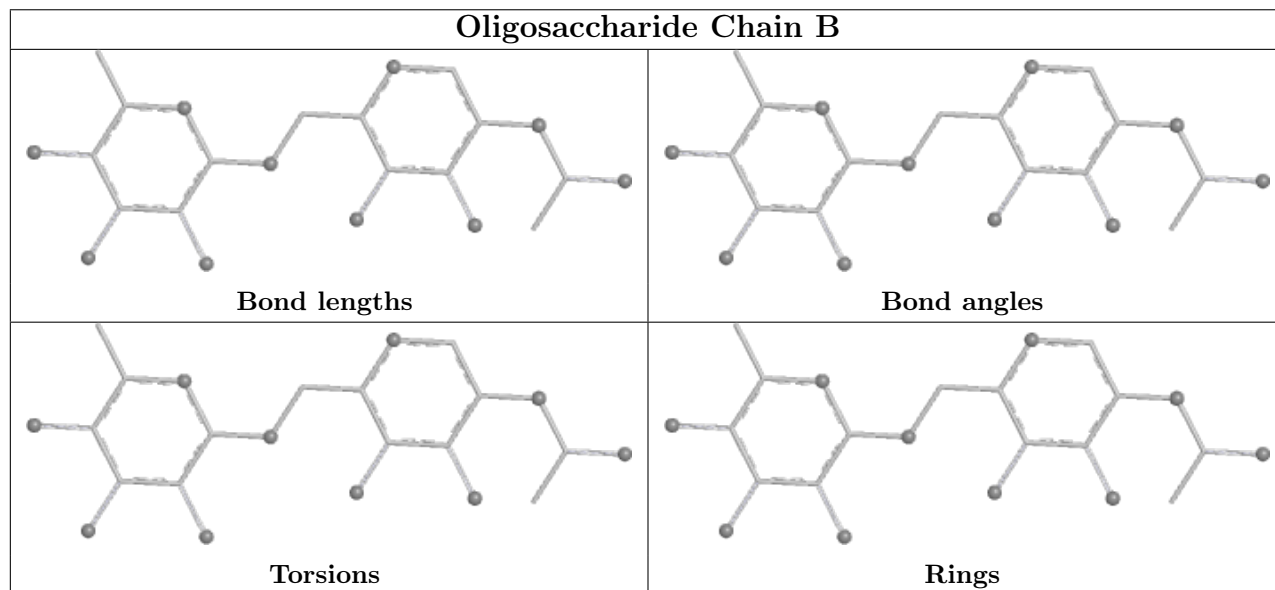
There are no chirality outliers.

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.



5.6 Ligand geometry [i](#)

7 ligands 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.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

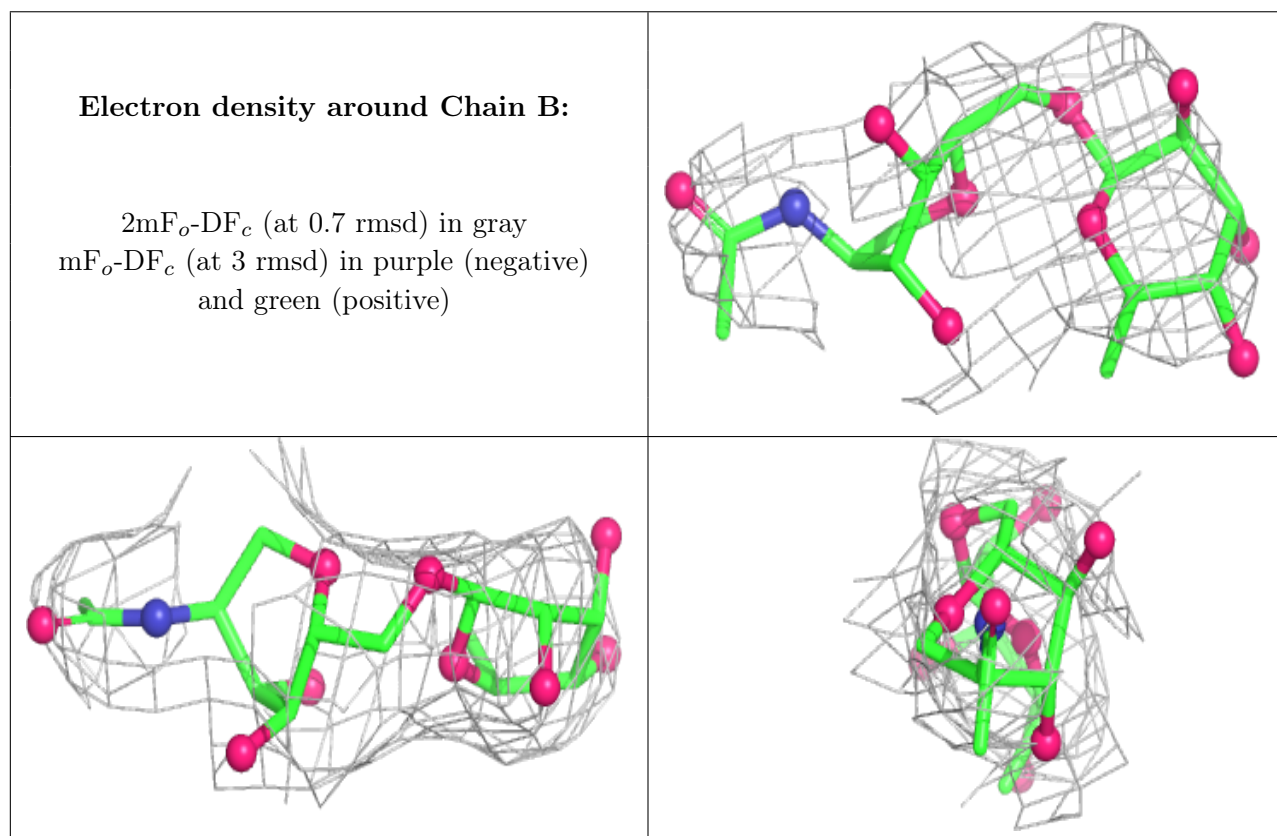
6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

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 for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



6.4 Ligands [i](#)

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

6.5 Other polymers

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