



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 10, 2023 – 01:46 PM EDT

PDB ID : 7L00  
Title : Streptococcus gordonii C123 Domain(s)-Structural and Functional Analysis  
Authors : Schormann, N.; Deivanayagam, C.  
Deposited on : 2020-12-11  
Resolution : 2.70 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](mailto: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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467  
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

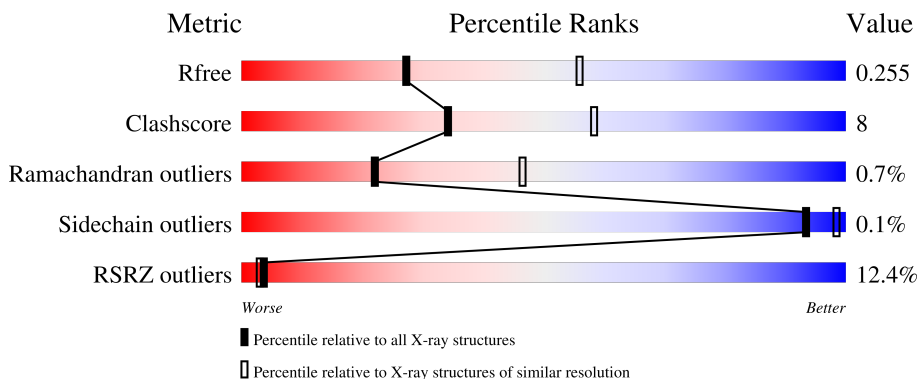
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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  $\geq 3$ , 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  $\leq 5\%$ . 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	507	
1	B	507	

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 7511 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 Agglutinin receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	479	3745	2365	608	769	3	0	0	0
1	B	476	3721	2351	602	765	3	0	0	0

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	911	MET	-	initiating methionine	UNP P16952
A	912	ALA	-	expression tag	UNP P16952
A	1407	ALA	-	expression tag	UNP P16952
A	1408	ALA	-	expression tag	UNP P16952
A	1409	ALA	-	expression tag	UNP P16952
A	1410	LEU	-	expression tag	UNP P16952
A	1411	GLU	-	expression tag	UNP P16952
A	1412	HIS	-	expression tag	UNP P16952
A	1413	HIS	-	expression tag	UNP P16952
A	1414	HIS	-	expression tag	UNP P16952
A	1415	HIS	-	expression tag	UNP P16952
A	1416	HIS	-	expression tag	UNP P16952
A	1417	HIS	-	expression tag	UNP P16952
B	911	MET	-	initiating methionine	UNP P16952
B	912	ALA	-	expression tag	UNP P16952
B	1407	ALA	-	expression tag	UNP P16952
B	1408	ALA	-	expression tag	UNP P16952
B	1409	ALA	-	expression tag	UNP P16952
B	1410	LEU	-	expression tag	UNP P16952
B	1411	GLU	-	expression tag	UNP P16952
B	1412	HIS	-	expression tag	UNP P16952
B	1413	HIS	-	expression tag	UNP P16952
B	1414	HIS	-	expression tag	UNP P16952
B	1415	HIS	-	expression tag	UNP P16952
B	1416	HIS	-	expression tag	UNP P16952

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1417	HIS	-	expression tag	UNP P16952

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Ca 2 2	0	0
2	B	2	Total Ca 2 2	0	0

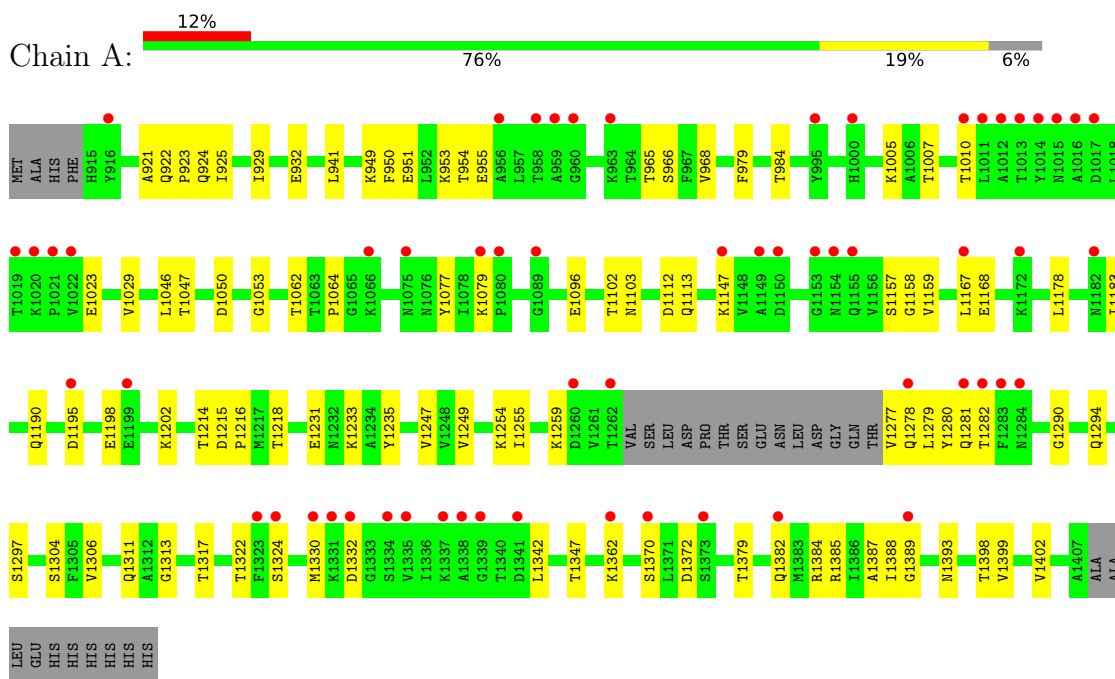
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	21	Total O 21 21	0	0
3	B	20	Total O 20 20	0	0

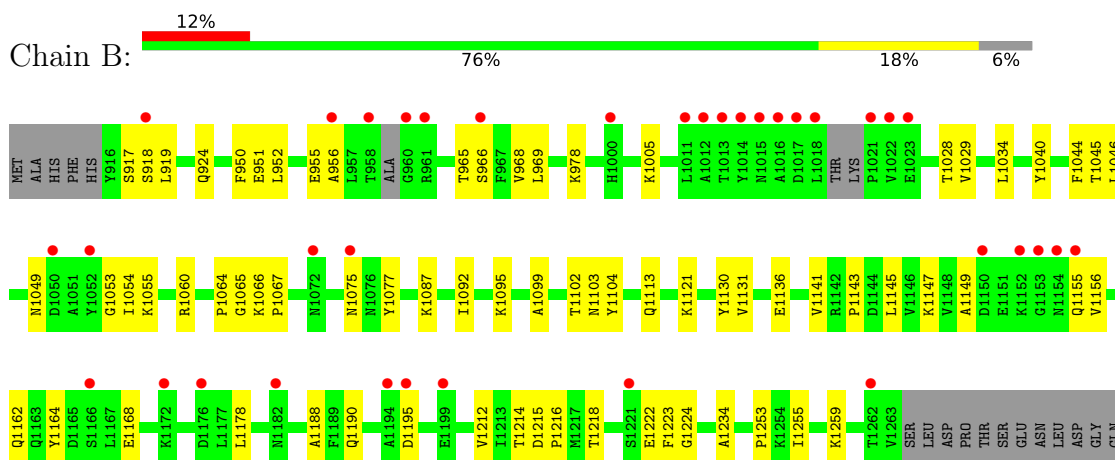
### 3 Residue-property plots [i](#)

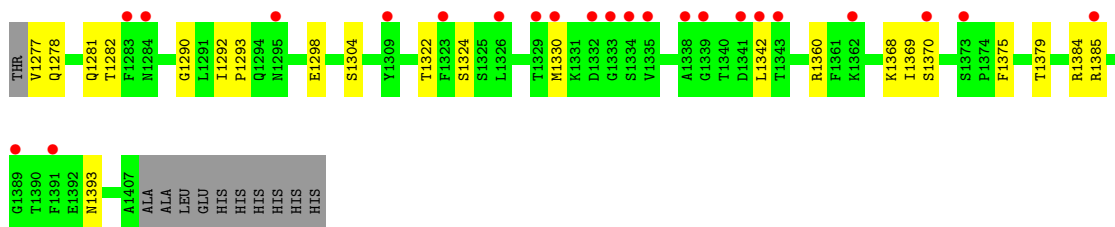
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Agglutinin receptor



- Molecule 1: Agglutinin receptor





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	100.05Å 109.14Å 204.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.59 – 2.70 48.59 – 2.70	Depositor EDS
% Data completeness (in resolution range)	96.4 (48.59-2.70) 96.7 (48.59-2.70)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.69 (at 2.69Å)	Xtrriage
Refinement program	PHENIX 1.14_3228	Depositor
R, $R_{free}$	0.218 , 0.255 0.221 , 0.255	Depositor DCC
$R_{free}$ test set	2854 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	58.1	Xtrriage
Anisotropy	0.923	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 52.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7511	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	89.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	0/3816	0.54	0/5187
1	B	0.31	0/3789	0.53	0/5147
All	All	0.32	0/7605	0.54	0/10334

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	3745	0	3646	66	0
1	B	3721	0	3621	59	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	21	0	0	2	0
3	B	20	0	0	0	0
All	All	7511	0	7267	124	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 8.

The worst 5 of 124 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:922:GLN:CG	1:A:923:PRO:HD3	1.63	1.28
1:A:922:GLN:HG2	1:A:923:PRO:CD	1.63	1.25
1:A:1306:VAL:HG21	1:B:1222:GLU:OE1	1.76	0.86
1:A:923:PRO:HD2	1:A:955:GLU:HG3	1.58	0.83
1:A:1112:ASP:OD1	1:A:1113:GLN:N	2.14	0.80

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	475/507 (94%)	446 (94%)	24 (5%)	5 (1%)	14	34
1	B	468/507 (92%)	438 (94%)	28 (6%)	2 (0%)	34	60
All	All	943/1014 (93%)	884 (94%)	52 (6%)	7 (1%)	22	46

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	921	ALA
1	A	1158	GLY
1	B	956	ALA
1	B	1195	ASP
1	A	924	GLN

#### 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	415/439 (94%)	415 (100%)	0	100	100
1	B	413/439 (94%)	412 (100%)	1 (0%)	93	98
All	All	828/878 (94%)	827 (100%)	1 (0%)	93	98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1223	PHE

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](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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 [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	479/507 (94%)	0.87	59 (12%) 4 3	54, 86, 128, 157	0
1	B	476/507 (93%)	0.87	59 (12%) 4 3	54, 86, 130, 154	0
All	All	955/1014 (94%)	0.87	118 (12%) 4 3	54, 86, 128, 157	0

The worst 5 of 118 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1323	PHE	4.9
1	A	956	ALA	4.8
1	B	1339	GLY	4.7
1	B	1338	ALA	4.6
1	B	1021	PRO	4.3

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

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

### 6.3 Carbohydrates [i](#)

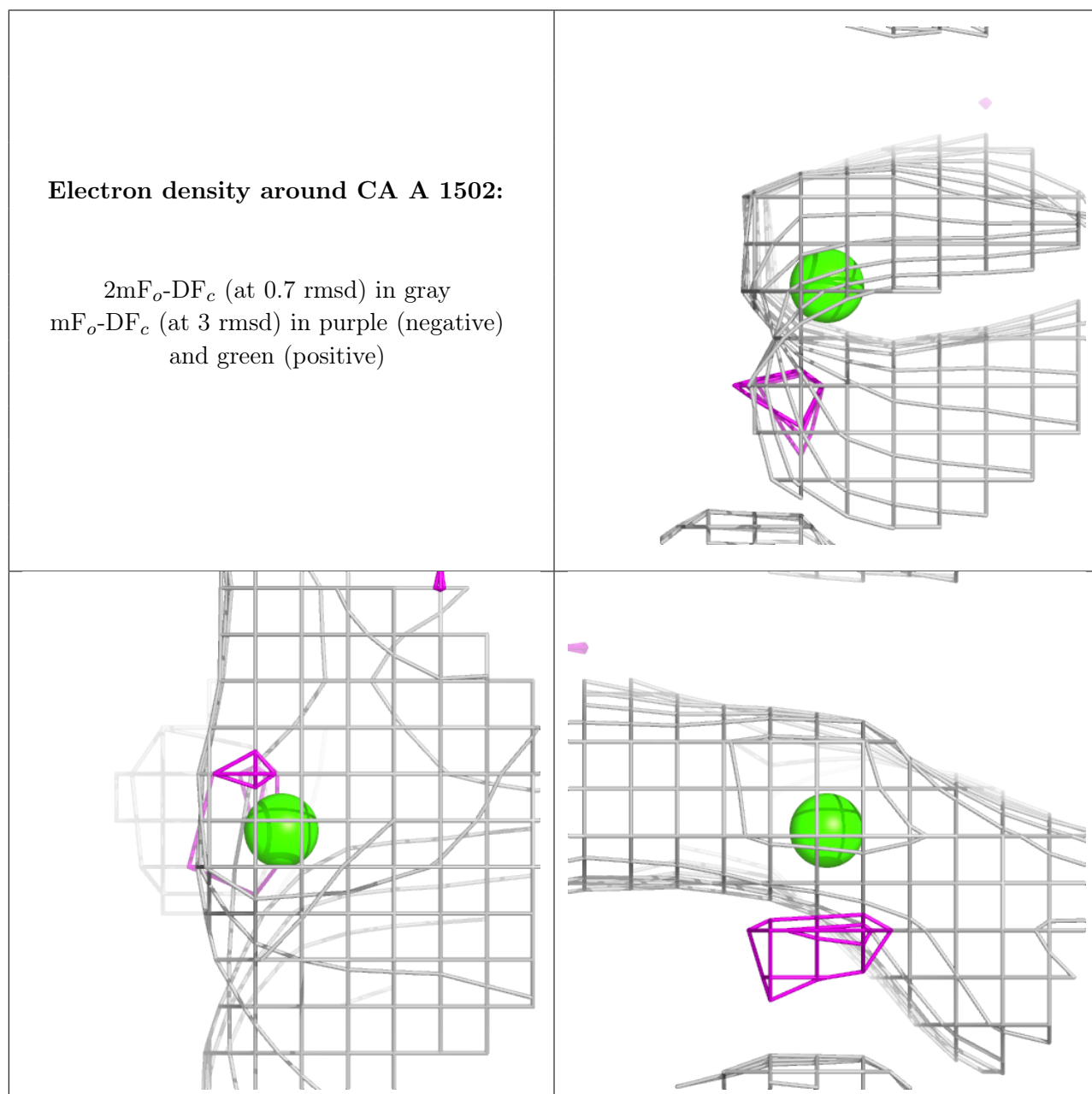
There are no monosaccharides in this entry.

### 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, 95<sup>th</sup> 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.

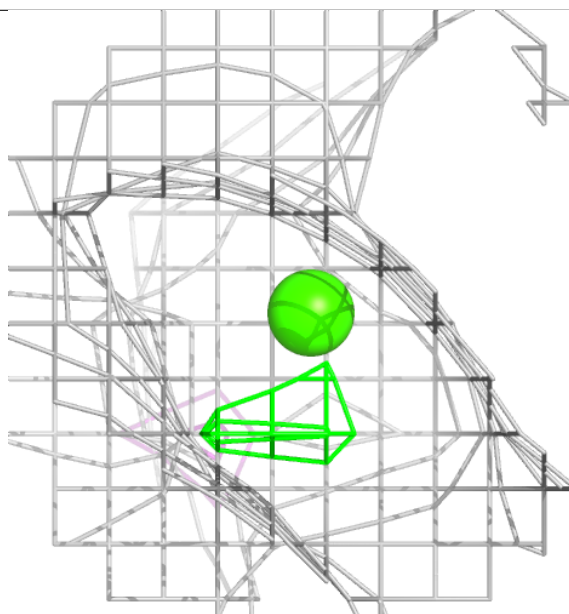
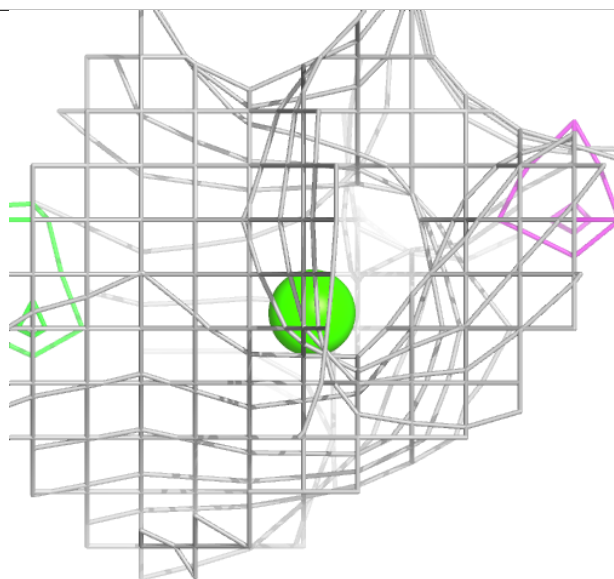
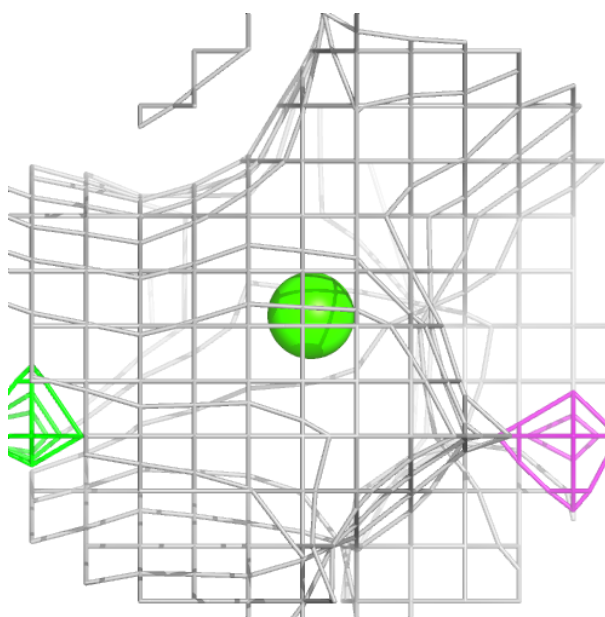
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CA	A	1502	1/1	0.75	0.30	122,122,122,122	0
2	CA	B	1501	1/1	0.78	0.33	135,135,135,135	0
2	CA	B	1502	1/1	0.78	0.15	133,133,133,133	0
2	CA	A	1501	1/1	0.82	0.31	111,111,111,111	0

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.



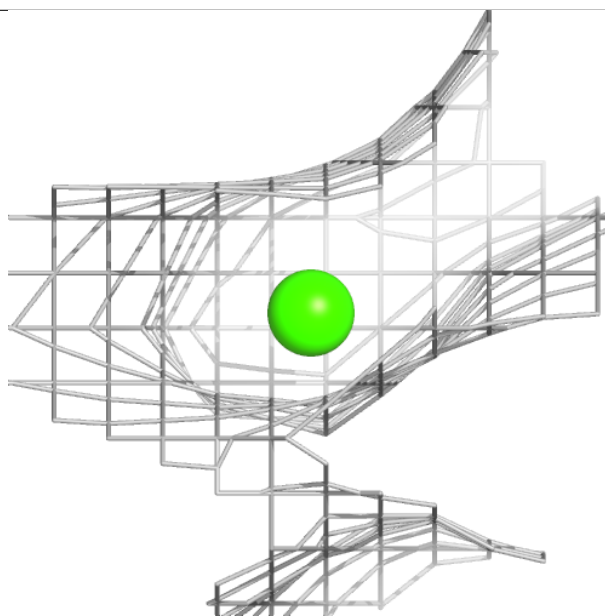
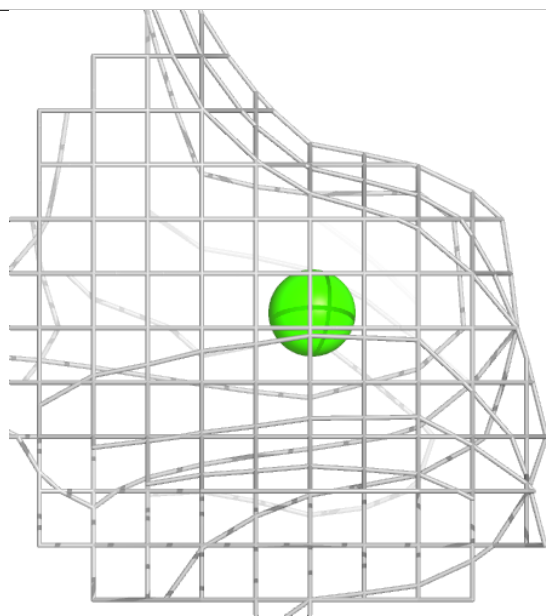
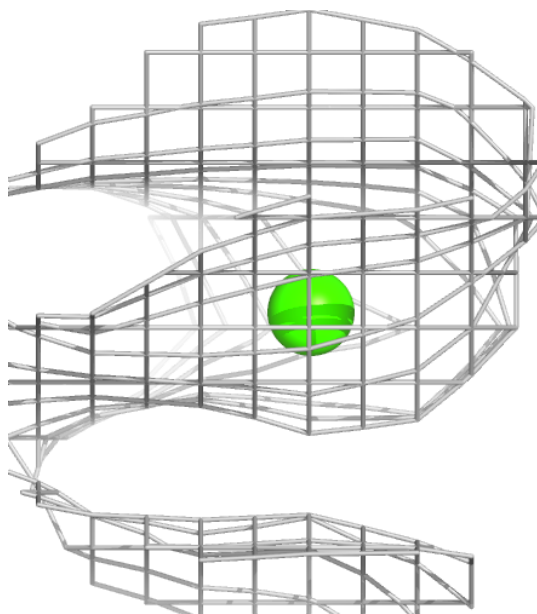
**Electron density around CA B 1501:**

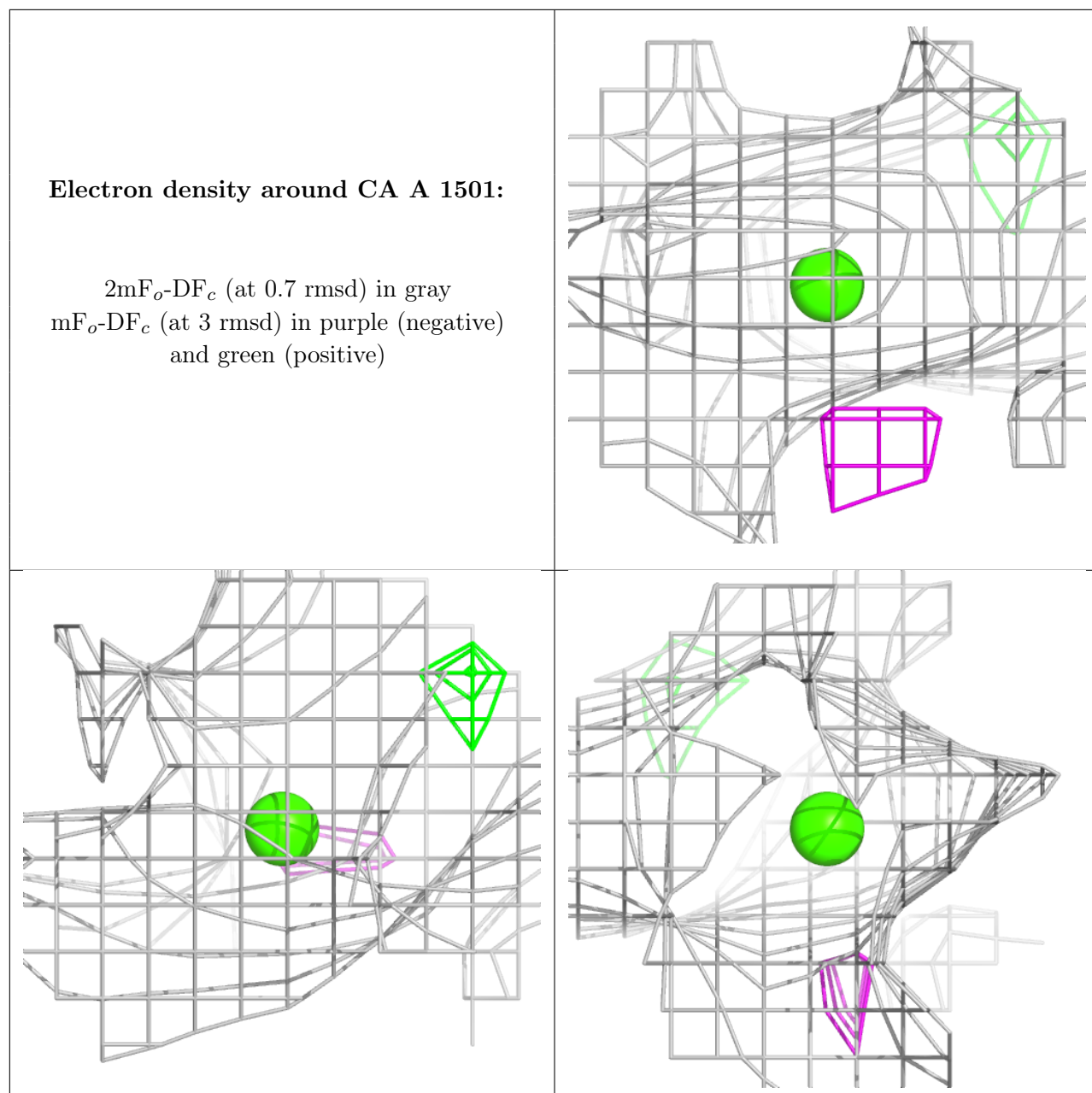
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CA B 1502:**

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





## 6.5 Other polymers ⓘ

There are no such residues in this entry.