



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:52 PM UTC

PDB ID : 9GY2 / pdb\_00009gy2  
Title : Non-Hemolytic Phospholipase C (PLC N)  
Authors : Sabharwal, N.S.; Labahn, J.L.  
Deposited on : 2024-10-01  
Resolution : 1.57 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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>.

---

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

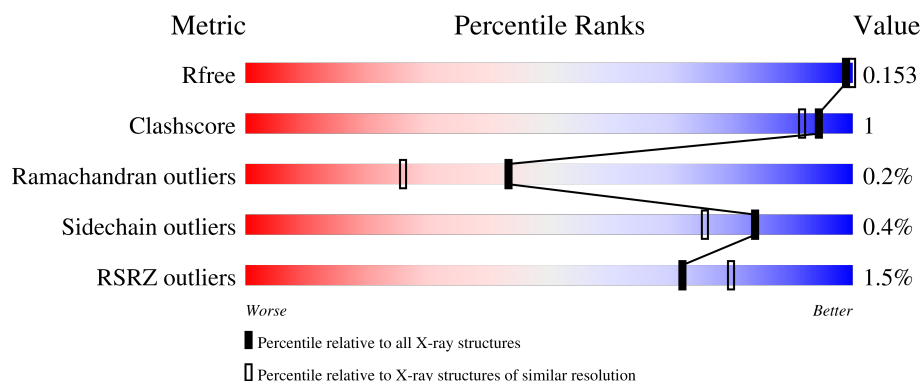
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.57 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))
$R_{free}$	180053	1094 (1.58-1.58)
Clashscore	190562	1105 (1.58-1.58)
Ramachandran outliers	187476	1082 (1.58-1.58)
Sidechain outliers	187428	1081 (1.58-1.58)
RSRZ outliers	180081	1094 (1.58-1.58)

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	706	
1	B	706	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11410 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 phospholipase C.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	643	Total	C	N	O	P	S	62	1	0
			5091	3221	913	941	1	15			
1	B	647	Total	C	N	O	P	S	81	2	0
			5137	3249	926	946	1	15			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP A0A0H2ZE19
A	-12	GLY	-	expression tag	UNP A0A0H2ZE19
A	-11	SER	-	expression tag	UNP A0A0H2ZE19
A	-10	SER	-	expression tag	UNP A0A0H2ZE19
A	-9	HIS	-	expression tag	UNP A0A0H2ZE19
A	-8	HIS	-	expression tag	UNP A0A0H2ZE19
A	-7	HIS	-	expression tag	UNP A0A0H2ZE19
A	-6	HIS	-	expression tag	UNP A0A0H2ZE19
A	-5	HIS	-	expression tag	UNP A0A0H2ZE19
A	-4	HIS	-	expression tag	UNP A0A0H2ZE19
A	-3	SER	-	expression tag	UNP A0A0H2ZE19
A	-2	GLN	-	expression tag	UNP A0A0H2ZE19
A	-1	ASP	-	expression tag	UNP A0A0H2ZE19
A	0	PRO	-	expression tag	UNP A0A0H2ZE19
A	579	ALA	ARG	conflict	UNP A0A0H2ZE19
B	-13	MET	-	initiating methionine	UNP A0A0H2ZE19
B	-12	GLY	-	expression tag	UNP A0A0H2ZE19
B	-11	SER	-	expression tag	UNP A0A0H2ZE19
B	-10	SER	-	expression tag	UNP A0A0H2ZE19
B	-9	HIS	-	expression tag	UNP A0A0H2ZE19
B	-8	HIS	-	expression tag	UNP A0A0H2ZE19
B	-7	HIS	-	expression tag	UNP A0A0H2ZE19
B	-6	HIS	-	expression tag	UNP A0A0H2ZE19
B	-5	HIS	-	expression tag	UNP A0A0H2ZE19
B	-4	HIS	-	expression tag	UNP A0A0H2ZE19

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	SER	-	expression tag	UNP A0A0H2ZE19
B	-2	GLN	-	expression tag	UNP A0A0H2ZE19
B	-1	ASP	-	expression tag	UNP A0A0H2ZE19
B	0	PRO	-	expression tag	UNP A0A0H2ZE19
B	579	ALA	ARG	conflict	UNP A0A0H2ZE19

- Molecule 2 is CALCIUM ION (CCD ID: 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

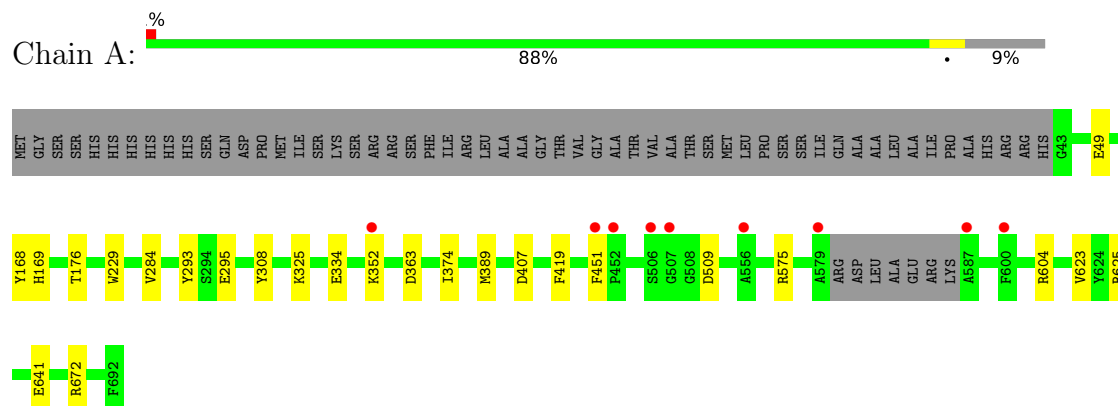
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	607	Total O 607 607	0	0
3	B	571	Total O 571 571	0	0

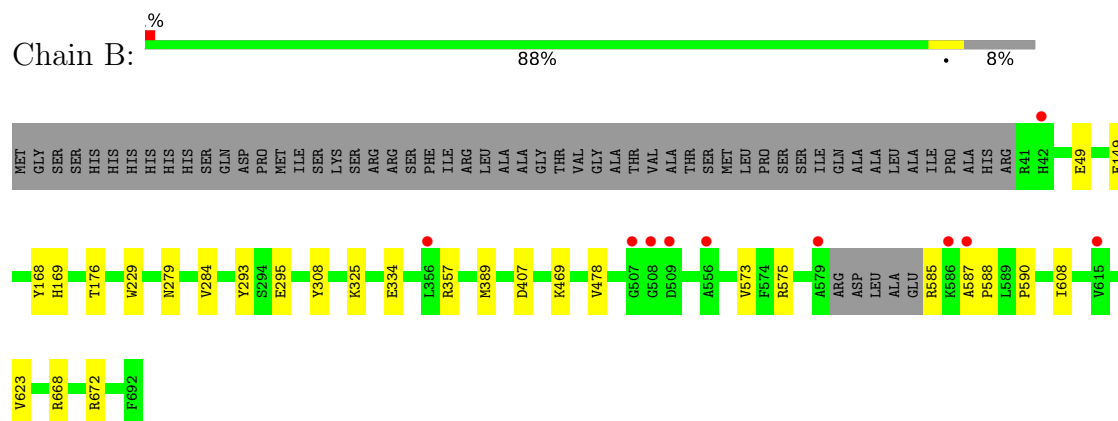
### 3 Residue-property plots

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: phospholipase C



#### • Molecule 1: phospholipase C



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.27Å 110.43Å 98.62Å 90.00° 101.03° 90.00°	Depositor
Resolution (Å)	47.96 – 1.57 47.96 – 1.57	Depositor EDS
% Data completeness (in resolution range)	95.0 (47.96-1.57) 95.0 (47.96-1.57)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.15 (at 1.57Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.152 , 0.175 0.154 , 0.153	Depositor DCC
$R_{free}$ test set	8643 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.1	Xtriage
Anisotropy	0.489	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 55.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	11410	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% 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, TPO

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	0.38	0/5235	0.58	0/7121
1	B	0.36	0/5285	0.57	0/7187
All	All	0.37	0/10520	0.58	0/14308

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	672	ARG	Sidechain
1	B	672	ARG	Sidechain

### 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	5091	0	4887	13	1
1	B	5137	0	4939	13	2
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	607	0	0	5	0
3	B	571	0	0	5	0
All	All	11410	0	9826	26	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 1.

All (26) 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:B:357:ARG:O	3:B:801:HOH:O	2.03	0.75
1:B:279:ASN:OD1	3:B:802:HOH:O	2.06	0.72
1:B:478:VAL:O	3:B:803:HOH:O	2.15	0.63
1:A:352:LYS:HD2	1:A:352:LYS:H	1.65	0.61
1:B:575:ARG:NH2	3:B:808:HOH:O	2.36	0.54
1:A:363:ASP:OD2	3:A:801:HOH:O	2.18	0.51
1:A:229:TRP:HA	1:A:284:VAL:O	2.13	0.49
1:B:168:TYR:CE2	1:B:389:MET:HE2	2.48	0.49
1:B:229:TRP:HA	1:B:284:VAL:O	2.13	0.48
1:A:604:ARG:NE	1:A:641:GLU:OE2	2.46	0.48
1:A:293:TYR:HB3	1:A:308:TYR:HB2	1.96	0.47
1:B:587:ALA:HB1	1:B:588:PRO:CD	2.46	0.46
1:B:293:TYR:HB3	1:B:308:TYR:HB2	1.99	0.45
1:B:149:GLU:OE2	3:B:804:HOH:O	2.21	0.45
1:A:168:TYR:CE2	1:A:389:MET:HE2	2.52	0.43
1:A:374:ILE:C	1:A:374:ILE:HD12	2.44	0.43
1:A:49:GLU:HG3	1:A:325:LYS:HD3	2.00	0.42
1:A:169:HIS:O	1:A:407:ASP:HA	2.20	0.42
1:A:419:PHE:HB2	3:A:879:HOH:O	2.20	0.42
1:B:49:GLU:HG3	1:B:325:LYS:HD3	2.01	0.42
1:B:169:HIS:O	1:B:407:ASP:HA	2.19	0.42
1:A:625:ARG:HD2	3:A:1289:HOH:O	2.19	0.42
1:A:575:ARG:NH2	3:A:814:HOH:O	2.50	0.41
1:B:573:VAL:HB	1:B:668:ARG:HB3	2.02	0.41
1:A:451:PHE:N	3:A:802:HOH:O	2.25	0.40
1:B:590:PRO:HA	1:B:608:ILE:O	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-



metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:478:VAL:CG2	1:B:585:ARG:NH2[2_454]	1.98	0.22
1:A:509:ASP:OD2	1:B:469:LYS:NZ[2_445]	2.08	0.12

## 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	639/706 (90%)	622 (97%)	16 (2%)	1 (0%)	43 26
1	B	644/706 (91%)	625 (97%)	18 (3%)	1 (0%)	43 26
All	All	1283/1412 (91%)	1247 (97%)	34 (3%)	2 (0%)	43 26

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	623	VAL
1	B	623	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	535/585 (92%)	533 (100%)	2 (0%)	84 75
1	B	540/585 (92%)	538 (100%)	2 (0%)	84 75
All	All	1075/1170 (92%)	1071 (100%)	4 (0%)	84 75

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	295	GLU
1	A	334	GLU
1	B	295	GLU
1	B	334	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	GLN
1	A	379	GLN
1	A	448	ASN
1	B	91	GLN
1	B	111	GLN
1	B	448	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	$\# Z  > 2$
1	TPO	A	176	1,2	8,10,11	1.11	1 (12%)	10,14,16	1.26	1 (10%)
1	TPO	B	176	1,2	8,10,11	1.32	1 (12%)	10,14,16	1.50	2 (20%)

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
1	TPO	A	176	1,2	-	1/9/11/13	-
1	TPO	B	176	1,2	-	1/9/11/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	176	TPO	P-OG1	2.62	1.64	1.59
1	A	176	TPO	P-OG1	2.06	1.63	1.59

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	176	TPO	P-OG1-CB	-2.78	115.78	123.33
1	B	176	TPO	P-OG1-CB	-2.71	115.97	123.33
1	B	176	TPO	CG2-CB-CA	-2.24	108.89	113.26

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	176	TPO	O-C-CA-CB
1	B	176	TPO	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	642/706 (90%)	-0.06	9 (1%) 73 81	13, 21, 36, 62	32 (4%)
1	B	646/706 (91%)	-0.02	10 (1%) 72 80	14, 22, 39, 77	43 (6%)
All	All	1288/1412 (91%)	-0.04	19 (1%) 72 80	13, 22, 37, 77	75 (5%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	451	PHE	4.0
1	A	579	ALA	3.5
1	A	507	GLY	3.2
1	A	506	SER	3.2
1	B	579	ALA	3.2
1	A	600	PHE	3.2
1	B	587	ALA	3.1
1	B	556	ALA	3.0
1	B	507	GLY	2.9
1	B	42	HIS	2.7
1	A	587	ALA	2.6
1	A	452	PRO	2.5
1	B	508	GLY	2.4
1	A	352	LYS	2.3
1	B	615	VAL	2.2
1	B	586	LYS	2.2
1	B	356	LEU	2.1
1	B	509	ASP	2.1
1	A	556	ALA	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains [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(Å <sup>2</sup> )	Q<0.9
1	TPO	B	176	11/12	0.97	0.06	15,17,21,22	0
1	TPO	A	176	11/12	0.98	0.05	14,16,19,20	0

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

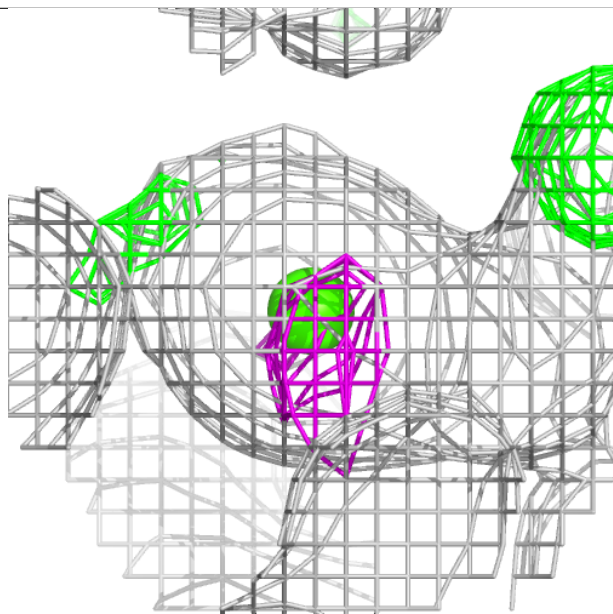
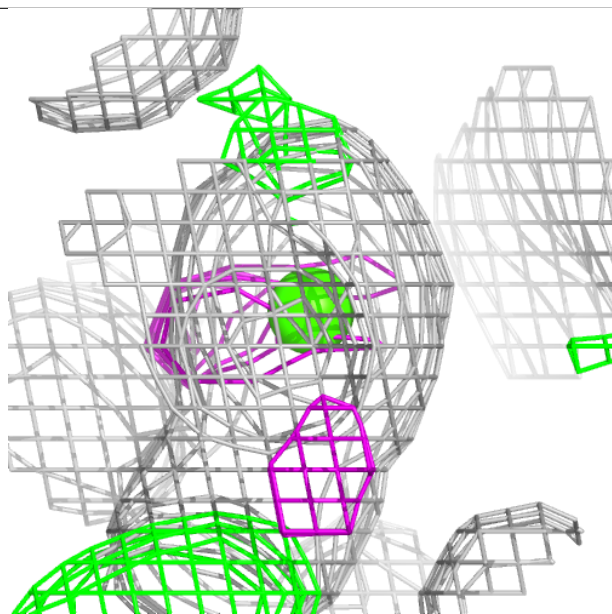
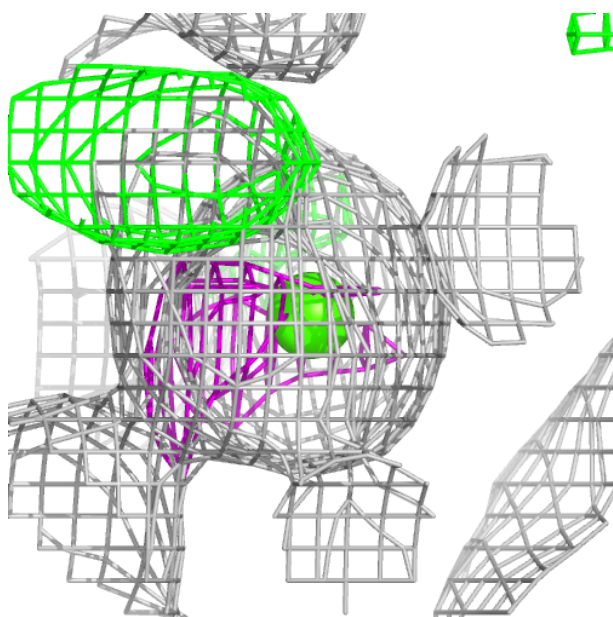
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	CA	A	702	1/1	0.98	0.07	27,27,27,27	0
2	CA	B	701	1/1	0.99	0.04	19,19,19,19	0
2	CA	B	702	1/1	0.99	0.05	23,23,23,23	0
2	CA	A	701	1/1	1.00	0.04	18,18,18,18	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 A 702:**

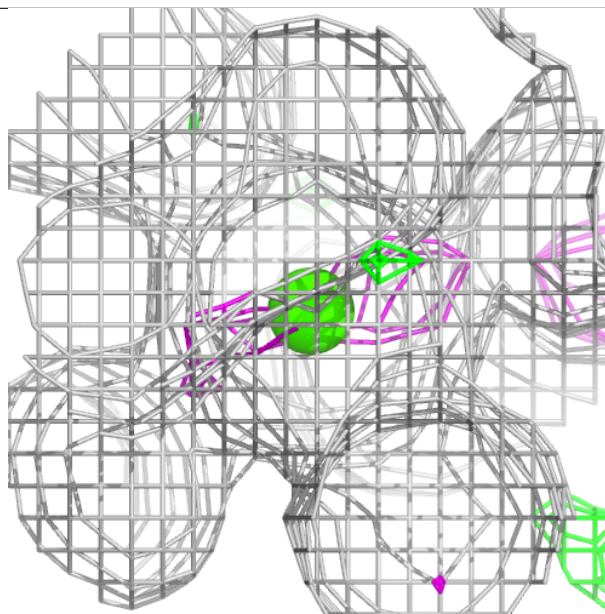
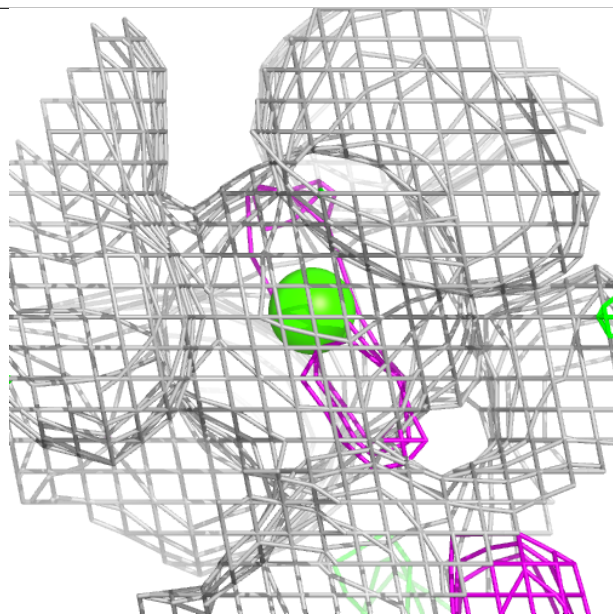
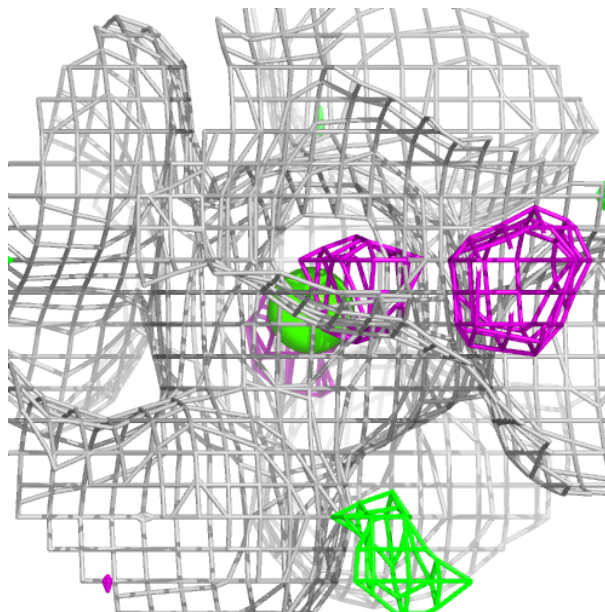
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CA B 701:**

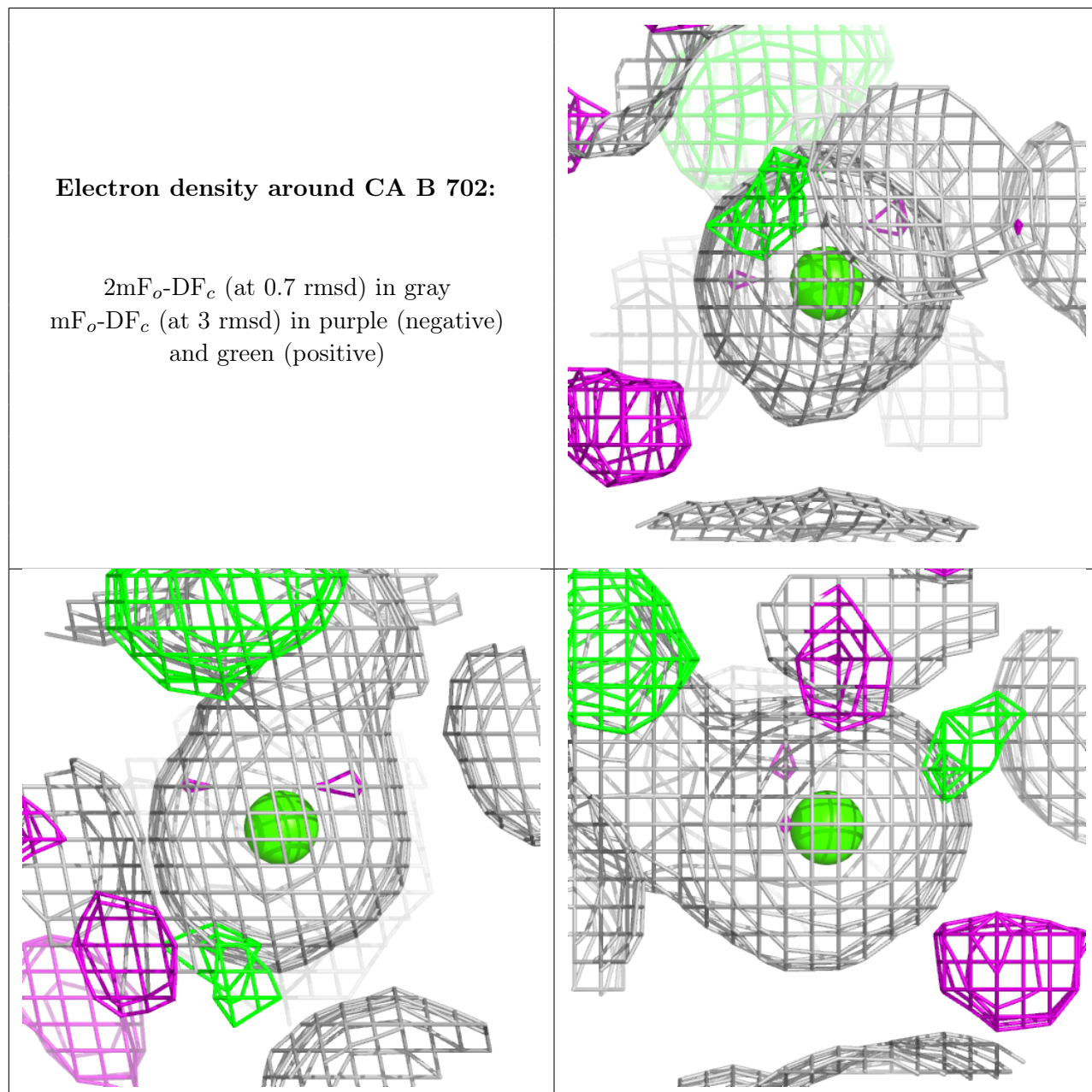
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

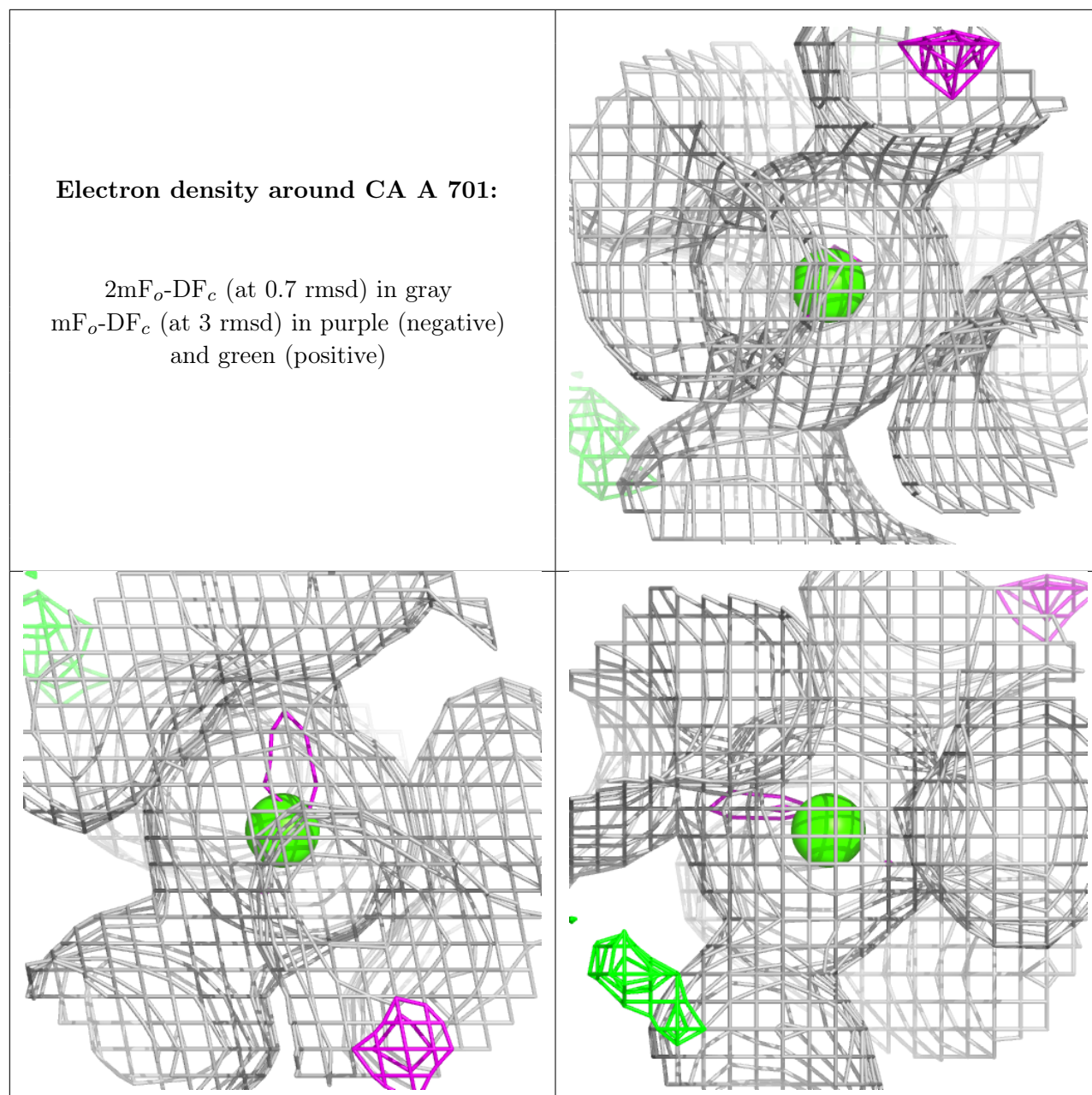




**Electron density around CA B 702:**

$2mF_o-DF_c$  (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.