



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2023 – 02:00 AM EDT

PDB ID : 8DEO
Title : Structure of AAP A domain and B-repeats (residues 351-813) from *Staphylococcus epidermidis*
Authors : Harris, G.; Whelan, F.; Clark, L.; Turkenburg, J.P.; Potts, J.R.
Deposited on : 2022-06-21
Resolution : 2.30 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

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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

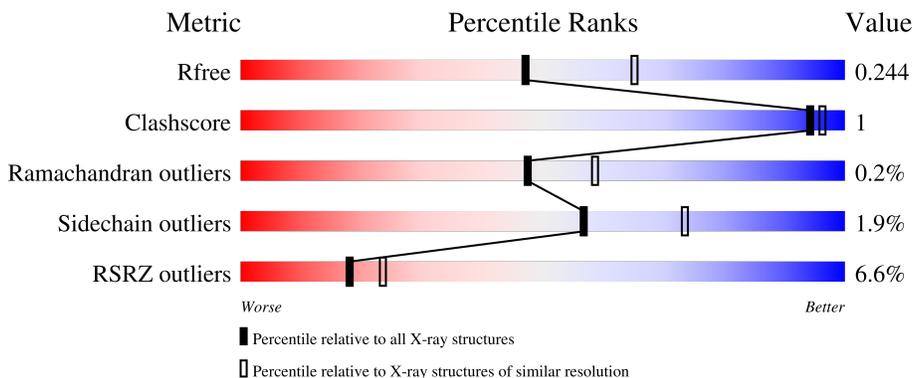
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 $\leq 5\%$. 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	467	
1	B	467	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6876 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 Accumulation associated protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	454	3309	2050	567	690	2	0	1	0
1	B	454	3395	2109	579	705	2	0	1	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	347	GLY	-	expression tag	UNP Q5HKE8
A	348	PRO	-	expression tag	UNP Q5HKE8
A	349	ALA	-	expression tag	UNP Q5HKE8
A	350	MET	-	expression tag	UNP Q5HKE8
B	347	GLY	-	expression tag	UNP Q5HKE8
B	348	PRO	-	expression tag	UNP Q5HKE8
B	349	ALA	-	expression tag	UNP Q5HKE8
B	350	MET	-	expression tag	UNP Q5HKE8

- 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	1	Total	Ca	0	0
			1	1		
2	B	1	Total	Ca	0	0
			1	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Cl 1 1	0	0

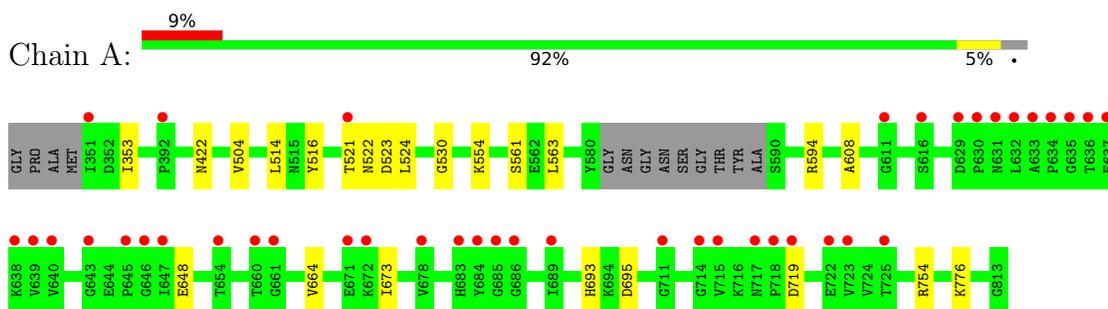
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	87	Total O 87 87	0	0
4	B	81	Total O 81 81	0	0

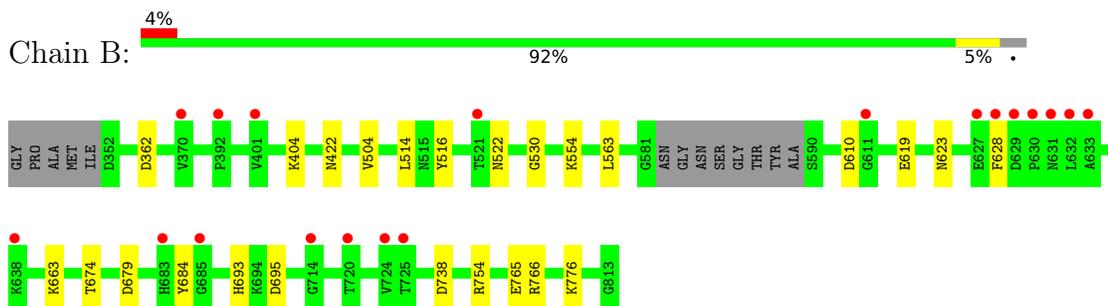
3 Residue-property plots [i](#)

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: Accumulation associated protein



- Molecule 1: Accumulation associated protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	58.48Å 66.56Å 66.87Å 84.69° 80.49° 89.66°	Depositor
Resolution (Å)	39.71 – 2.30 39.68 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.5 (39.71-2.30) 87.0 (39.68-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 2.29Å)	Xtrriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.198 , 0.243 0.203 , 0.244	Depositor DCC
R_{free} test set	1895 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	37.7	Xtrriage
Anisotropy	0.780	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 41.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6876	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.11% 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: CL, 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	0.41	0/3388	0.75	1/4625 (0.0%)
1	B	0.42	0/3472	0.76	0/4728
All	All	0.42	0/6860	0.76	1/9353 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	594	ARG	NE-CZ-NH2	-7.06	116.77	120.30

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	3309	0	2985	8	0
1	B	3395	0	3141	9	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	87	0	0	0	0
4	B	81	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6876	0	6126	17	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 1.

All (17) 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:522:ASN:O	1:A:524:LEU:N	2.28	0.65
1:B:623:ASN:HB2	1:B:679:ASP:OD1	2.04	0.57
1:B:362:ASP:O	1:B:404:LYS:HE3	2.08	0.53
1:A:504:VAL:HG21	1:A:563:LEU:HD23	1.91	0.52
1:B:504:VAL:HG21	1:B:563:LEU:HD23	1.92	0.52
1:A:693:HIS:HE1	1:A:695:ASP:OD1	1.94	0.51
1:B:754:ARG:HH11	1:B:754:ARG:HG2	1.76	0.50
1:B:628:PHE:HB2	1:B:684:TYR:CE1	2.50	0.46
1:B:765:GLU:O	1:B:766:ARG:HD3	2.16	0.46
1:B:514:LEU:HD21	1:B:554:LYS:HD3	1.98	0.45
1:A:353:ILE:HD11	1:A:608:ALA:HB2	2.00	0.43
1:A:514:LEU:HD21	1:A:554:LYS:HD3	2.00	0.43
1:A:648:GLU:HG3	1:A:673:ILE:HG13	1.99	0.43
1:A:754:ARG:HH11	1:A:754:ARG:HG2	1.83	0.42
1:A:516:TYR:O	1:A:530:GLY:HA3	2.19	0.42
1:B:693:HIS:HE1	1:B:695:ASP:OD1	2.02	0.42
1:B:516:TYR:O	1:B:530:GLY:HA3	2.20	0.41

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	451/467 (97%)	434 (96%)	16 (4%)	1 (0%)	47	58
1	B	451/467 (97%)	432 (96%)	18 (4%)	1 (0%)	47	58
All	All	902/934 (97%)	866 (96%)	34 (4%)	2 (0%)	47	58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	523	ASP
1	B	522	ASN

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	335/393 (85%)	329 (98%)	6 (2%)	59	75
1	B	355/393 (90%)	348 (98%)	7 (2%)	55	72
All	All	690/786 (88%)	677 (98%)	13 (2%)	57	73

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	422	ASN
1	A	521	THR
1	A	561	SER
1	A	664	VAL
1	A	719	ASP
1	A	776	LYS
1	B	422	ASN
1	B	610	ASP
1	B	619	GLU
1	B	663	LYS
1	B	674	THR
1	B	738	ASP
1	B	776	LYS

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	405	ASN
1	A	406	GLN
1	A	631	ASN
1	A	659	ASN
1	B	406	GLN
1	B	448	ASN

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

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	454/467 (97%)	0.41	41 (9%) 9 12	30, 52, 112, 139	0
1	B	454/467 (97%)	0.24	19 (4%) 36 43	29, 52, 94, 115	0
All	All	908/934 (97%)	0.33	60 (6%) 18 23	29, 52, 106, 139	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	632	LEU	6.2
1	A	634	PRO	5.6
1	A	686	GLY	5.6
1	A	637	GLU	4.6
1	A	685	GLY	4.5
1	A	630	PRO	4.3
1	A	684	TYR	4.1
1	B	631	ASN	3.8
1	A	521	THR	3.7
1	A	645	PRO	3.7
1	A	714	GLY	3.7
1	A	633	ALA	3.5
1	B	392	PRO	3.5
1	A	640	VAL	3.5
1	A	683	HIS	3.5
1	B	638	LYS	3.5
1	A	629	ASP	3.5
1	B	683	HIS	3.4
1	A	632	LEU	3.4
1	A	631	ASN	3.3
1	A	723	VAL	3.3
1	A	636	THR	3.3
1	A	616	SER	3.3
1	A	638	LYS	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	715	VAL	3.1
1	A	660	THR	3.1
1	A	717	ASN	3.0
1	B	521	THR	2.9
1	A	719	ASP	2.9
1	A	725	THR	2.9
1	A	711	GLY	2.9
1	A	689	ILE	2.8
1	B	628	PHE	2.8
1	B	633	ALA	2.8
1	A	639	VAL	2.7
1	A	646	GLY	2.7
1	B	724	VAL	2.7
1	B	685	GLY	2.7
1	A	718	PRO	2.6
1	B	611	GLY	2.6
1	A	643	GLY	2.6
1	A	647	ILE	2.5
1	B	725	THR	2.5
1	A	671	GLU	2.4
1	B	401	VAL	2.4
1	A	635	GLY	2.4
1	B	714	GLY	2.3
1	B	630	PRO	2.3
1	A	611	GLY	2.3
1	A	351	ILE	2.3
1	A	661	GLY	2.2
1	A	654	THR	2.2
1	A	392	PRO	2.2
1	B	627	GLU	2.2
1	B	370	VAL	2.2
1	A	722	GLU	2.1
1	B	629	ASP	2.1
1	B	720	THR	2.1
1	A	672	LYS	2.1
1	A	678	VAL	2.1

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](#)

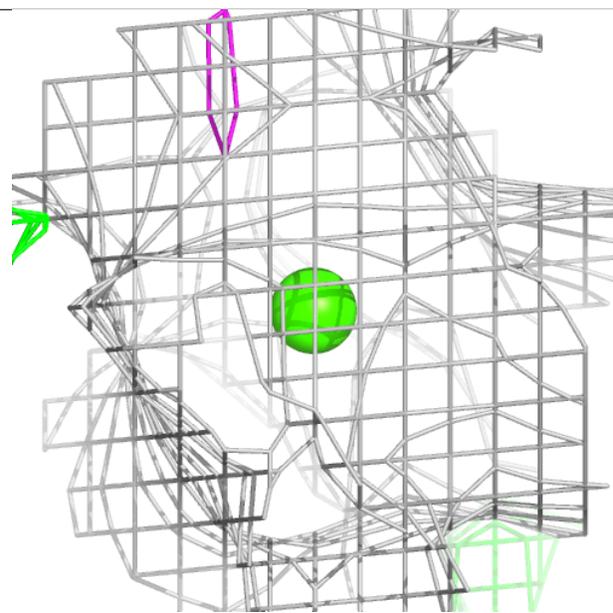
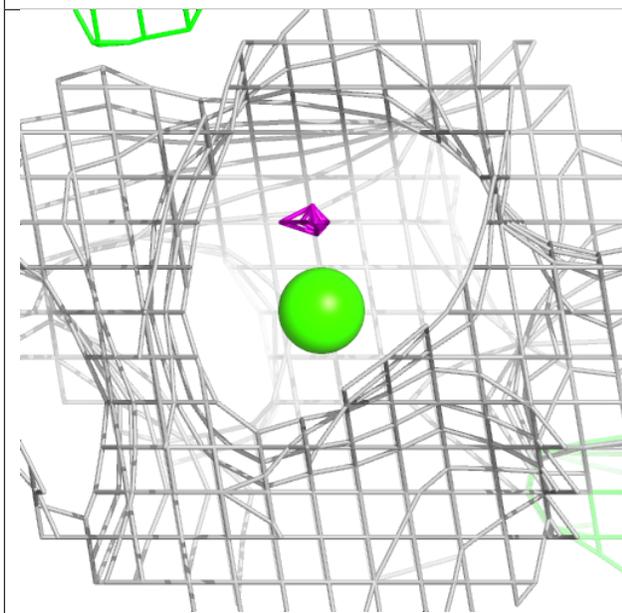
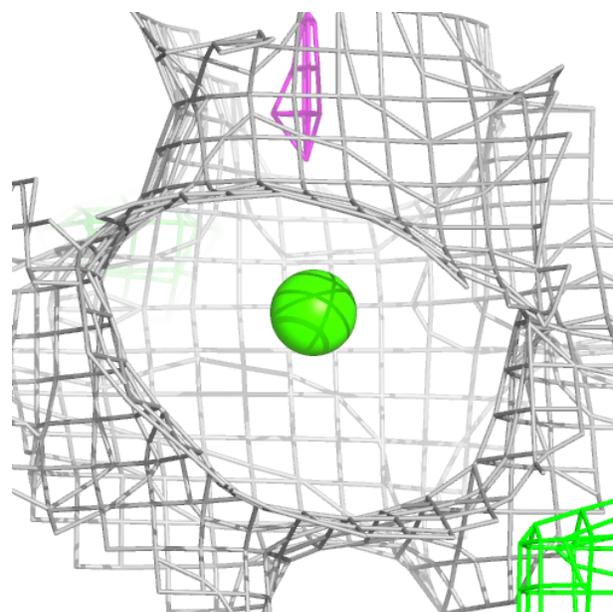
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

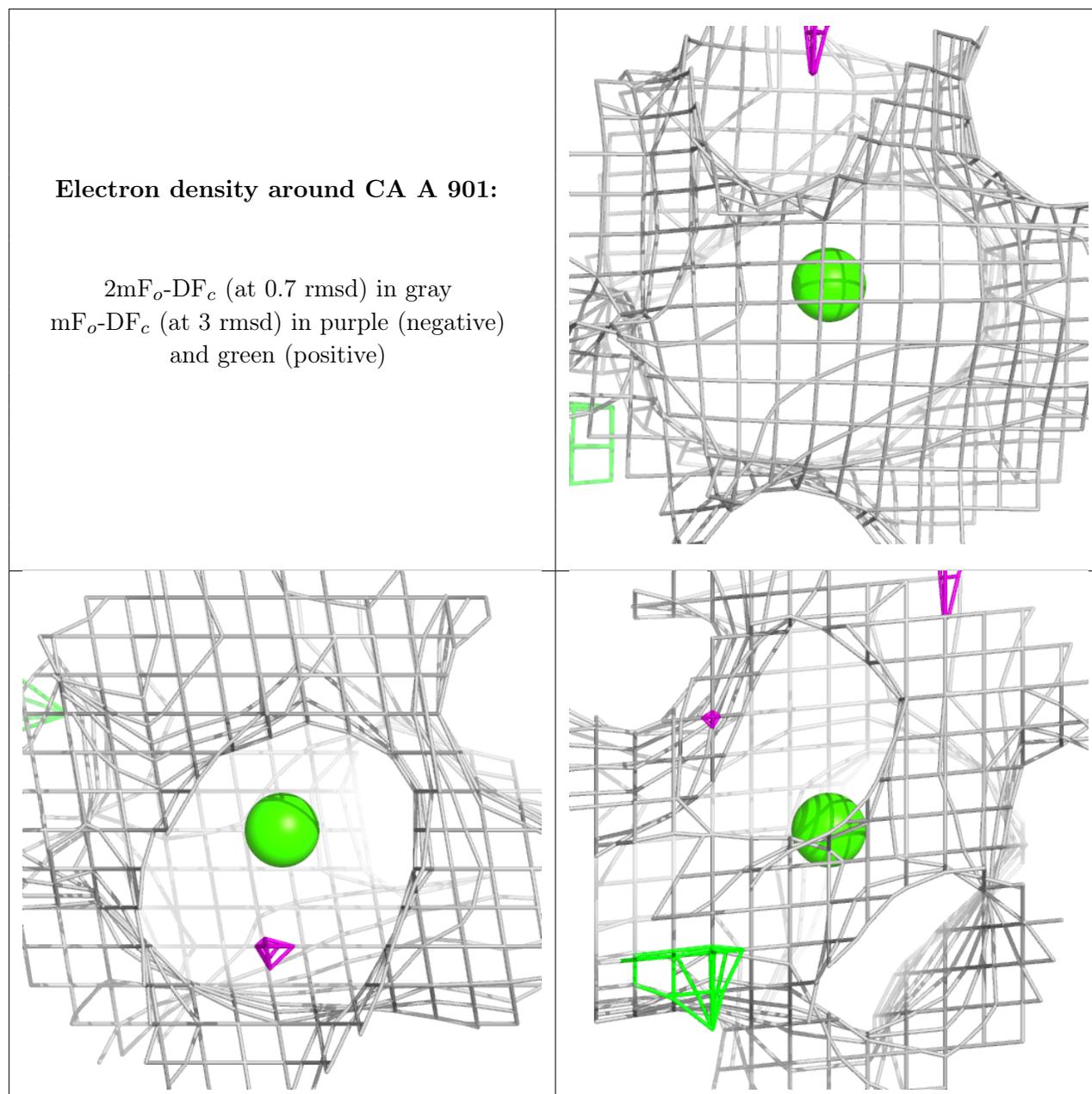
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CA	B	901	1/1	0.97	0.12	31,31,31,31	0
3	CL	A	902	1/1	0.98	0.08	45,45,45,45	0
3	CL	B	902	1/1	0.98	0.08	44,44,44,44	0
2	CA	A	901	1/1	0.99	0.15	30,30,30,30	0

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 901:

$2mF_o-DF_c$ (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.