

wwPDB X-ray Structure Validation Summary Report (i)

Nov 9, 2020 – 12:07 PM GMT

PDB ID	:	6TU2
Title	:	Crystal structure of rat annexin A11
Authors	:	Raasakka, A.; Lillebostad, P.; Vedeler, A.; Kursula, P.
Deposited on		
Resolution	:	2.30 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

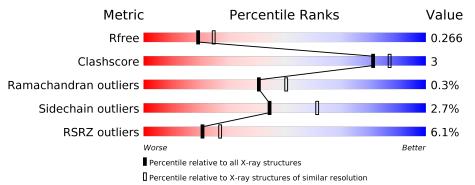
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
$\operatorname{CCP4}$:	$7.0.044 (\mathrm{Gargrove})$
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

1 Overall quality at a glance (i)

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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries},{ m resolution\ range}({ m \AA}))$
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 on 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	А	326	5% 88%	8%	·
1	В	326	5%	10%	•
1	С	326	88%	8%	·



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 15136 atoms, of which 7539 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.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace		
1	А	314	Total	С	Н	Ν	Ο	\mathbf{S}	0	Ο	Ο
	11	011	4987	1535	2513	446	478	15	0	0	0
1	В	314	Total	\mathbf{C}	Η	Ν	Ο	\mathbf{S}	0	0	0
	D	014	4987	1535	2513	446	478	15	0	0	0
1	C	314	Total	С	Η	Ν	0	S	0	0	0
L	U	014	4987	1535	2513	446	478	15	0	0	0

• Molecule 1 is a protein called Annexin.

There are 33 discrepancies between the modelled and reference sequences:

Residue	Modelled	Actual	Comment	Reference
178	MET	-	initiating methionine	UNP Q5XI77
179	LEU	-	expression tag	UNP Q5XI77
180	HIS	-	expression tag	UNP Q5XI77
181	HIS	-	expression tag	UNP Q5XI77
182	HIS	-	expression tag	UNP Q5XI77
183	HIS	-	expression tag	UNP Q5XI77
184	HIS	-	expression tag	UNP Q5XI77
185	HIS	-	expression tag	UNP Q5XI77
186	PRO	-	expression tag	UNP Q5XI77
187	MET	-	expression tag	UNP Q5XI77
188	GLY	-	expression tag	UNP Q5XI77
178	MET	-	initiating methionine	UNP Q5XI77
179	LEU	-	expression tag	UNP Q5XI77
180	HIS	-	expression tag	UNP Q5XI77
181	HIS	-	expression tag	UNP Q5XI77
182	HIS	-	expression tag	UNP Q5XI77
183	HIS	-	expression tag	UNP Q5XI77
184	HIS	-	expression tag	UNP Q5XI77
185	HIS	-	expression tag	UNP Q5XI77
186	PRO	-	expression tag	UNP Q5XI77
187	MET	-	expression tag	UNP Q5XI77
188	GLY	-	expression tag	UNP Q5XI77
178	MET	-	initiating methionine	UNP Q5XI77
	$\begin{array}{c} 178 \\ 179 \\ 180 \\ 181 \\ 182 \\ 183 \\ 184 \\ 185 \\ 186 \\ 187 \\ 188 \\ 178 \\ 179 \\ 180 \\ 181 \\ 182 \\ 183 \\ 181 \\ 182 \\ 183 \\ 184 \\ 185 \\ 186 \\ 187 \\ 188 \\ \end{array}$	178 MET 179 LEU 180 HIS 181 HIS 182 HIS 183 HIS 184 HIS 185 HIS 186 PRO 187 MET 188 GLY 179 LEU 180 HIS 181 HIS 182 HIS 183 GLY 178 MET 184 HIS 185 HIS 181 HIS 182 HIS 183 HIS 184 HIS 185 HIS 184 HIS 185 HIS 186 PRO 187 MET 188 GLY	178 MET - 179 LEU - 180 HIS - 181 HIS - 181 HIS - 182 HIS - 183 HIS - 184 HIS - 185 HIS - 186 PRO - 187 MET - 188 GLY - 178 MET - 188 GLY - 189 HIS - 180 HIS - 181 HIS - 182 HIS - 183 HIS - 184 HIS - 183 HIS - 184 HIS - 185 HIS - 186 PRO - 187 MET - 188 GLY -	178MET-initiating methionine179LEU-expression tag180HIS-expression tag181HIS-expression tag182HIS-expression tag183HIS-expression tag184HIS-expression tag185HIS-expression tag186PRO-expression tag187MET-expression tag188GLY-expression tag179LEU-expression tag181HIS-expression tag182HIS-expression tag184HIS-expression tag185HIS-expression tag181HIS-expression tag182HIS-expression tag183HIS-expression tag184HIS-expression tag185HIS-expression tag186PRO-expression tag187MET-expression tag188GLY-expression tag188GLY-expression tag

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Chain	Residue	Modelled	Actual	Comment	Reference
С	179	LEU	-	expression tag	UNP Q5XI77
С	180	HIS	-	expression tag	UNP Q5XI77
С	181	HIS	-	expression tag	UNP Q5XI77
С	182	HIS	-	expression tag	UNP Q5XI77
С	183	HIS	-	expression tag	UNP Q5XI77
С	184	HIS	-	expression tag	UNP Q5XI77
С	185	HIS	-	expression tag	UNP Q5XI77
С	186	PRO	-	expression tag	UNP Q5XI77
С	187	MET	-	expression tag	UNP Q5XI77
С	188	GLY	-	expression tag	UNP Q5XI77

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	В	4	Total Ca 4 4	0	0
2	А	3	Total Ca 3 3	0	0
2	С	3	Total Ca 3 3	0	0

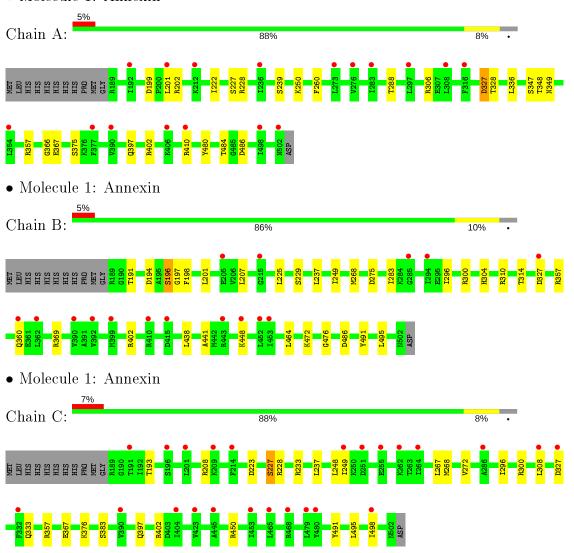
• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	55	$\begin{array}{cc} {\rm Total} & {\rm O} \\ 55 & 55 \end{array}$	0	0
3	В	60	Total O 60 60	0	0
3	С	50	$\begin{array}{cc} {\rm Total} & {\rm O} \\ 50 & 50 \end{array}$	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: Annexin



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	39.07Å 86.69 Å 87.30 Å	Depositor
a, b, c, α , β , γ	114.00° 101.98° 97.21°	Depositor
Resolution (Å)	50.00 - 2.30	Depositor
Resolution (A)	45.11 - 2.30	EDS
% Data completeness	95.4(50.00-2.30)	Depositor
(in resolution range)	$95.6\ (45.11 - 2.30)$	EDS
R _{merge}	(Not available)	Depositor
R _{sym}	0.17	Depositor
$< I/\sigma(I) > 1$	$1.38 (at 2.29 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.16-3549	Depositor
R, R_{free}	0.228 , 0.266	Depositor
n, n_{free}	0.228 , 0.266	DCC
R_{free} test set	2023 reflections $(4.79%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	40.0	Xtriage
Anisotropy	0.706	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.40 , 35.0	EDS
L-test for twinning ²	$< L >=0.51, < L^2>=0.34$	Xtriage
Estimated twinning fraction	0.011 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	15136	wwPDB-VP
Average B, all atoms $(Å^2)$	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 9.24% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: 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		
	Cham	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.25	0/2500	0.41	0/3345	
1	В	0.25	0/2500	0.42	0/3345	
1	С	0.25	0/2500	0.41	0/3345	
All	All	0.25	0/7500	0.41	0/10035	

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 (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	А	2474	2513	2513	11	0
1	В	2474	2513	2513	18	0
1	С	2474	2513	2513	10	0
2	А	3	0	0	0	0
2	В	4	0	0	0	0
2	С	3	0	0	0	0
3	А	55	0	0	1	0
3	В	60	0	0	2	0
3	С	50	0	0	1	0
All	All	7597	7539	7539	39	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 3.

The worst 5 of 39 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:C:223:ASP:O	1:C:227:SER:OG	2.12	0.68
1:B:448:LYS:NZ	3:B:702:HOH:O	2.26	0.68
1:B:283:ILE:O	3:B:701:HOH:O	2.11	0.68
1:C:267:LEU:HD11	1:C:498:ILE:HD11	1.75	0.65
1:B:249:ILE:HD11	1:B:268:MET:HB3	1.79	0.65

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	А	312/326~(96%)	305~(98%)	6(2%)	1 (0%)	41 50
1	В	312/326~(96%)	301~(96%)	9(3%)	2(1%)	25 31
1	С	312/326~(96%)	304 (97%)	8 (3%)	0	100 100
All	All	936/978~(96%)	910~(97%)	23 (2%)	3 (0%)	41 50

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	197	GLY
1	А	366	GLY
1	В	196	SER



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	А	268/279~(96%)	261~(97%)	7(3%)	46 63
1	В	268/279~(96%)	262~(98%)	6 (2%)	52 69
1	С	268/279~(96%)	259~(97%)	9(3%)	37 51
All	All	804/837~(96%)	782~(97%)	22 (3%)	44 61

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	360	GLN
1	В	486	ASP
1	С	397	GLN
1	В	369	ARG
1	В	402	ARG

Some 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 10 ligands modelled in this entry, 10 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, 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	А	314/326~(96%)	0.48	17 (5%) 25 32	33, 45, 62, 70	0
1	В	314/326~(96%)	0.56	16 (5%) 28 35	32, 48, 65, 77	0
1	С	314/326~(96%)	0.61	24 (7%) 13 18	31, 48, 71, 87	0
All	All	942/978~(96%)	0.55	57 (6%) 21 27	31, 47, 65, 87	0

The worst 5 of 57 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	С	214	PHE	6.8
1	А	201	LEU	4.9
1	С	327	ASP	4.9
1	С	251	ASP	4.6
1	С	480	TYR	4.4

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)

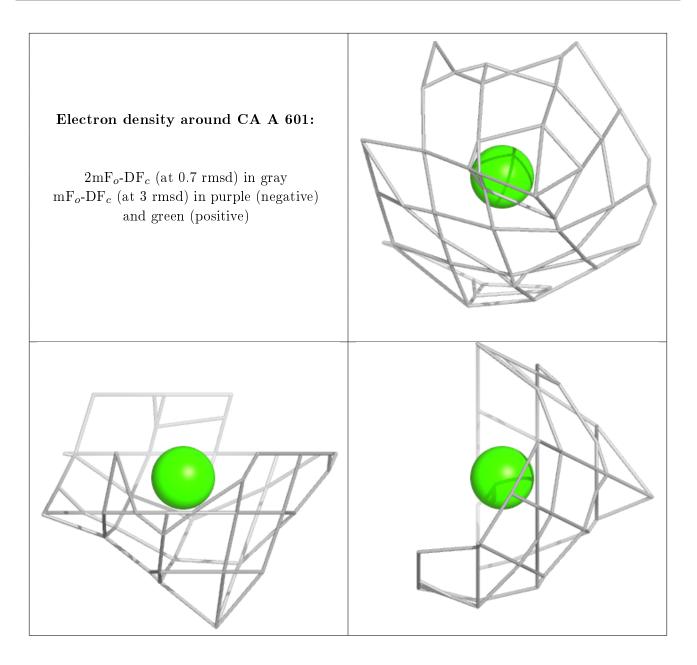
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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



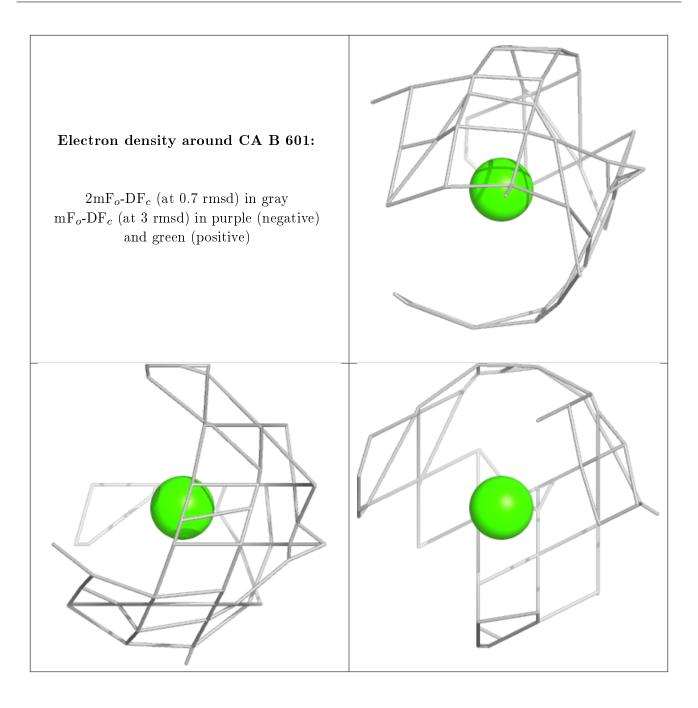
Mol	Type	Chain	Res	Atoms	RSCC	\mathbf{RSR}	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
2	CA	А	601	1/1	0.47	0.10	$69,\!69,\!69,\!69$	0
2	CA	В	601	1/1	0.57	0.09	72,72,72,72	0
2	CA	С	601	1/1	0.73	0.14	82,82,82,82	0
2	CA	В	602	1/1	0.75	0.13	75,75,75,75	0
2	CA	А	602	1/1	0.81	0.09	$66,\!66,\!66,\!66$	0
2	CA	С	602	1/1	0.85	0.06	$51,\!51,\!51,\!51$	0
2	CA	С	603	1/1	0.90	0.09	85,85,85,85	0
2	CA	В	604	1/1	0.91	0.09	82,82,82,82	0
2	CA	В	603	1/1	0.93	0.09	70,70,70,70	0
2	CA	А	603	1/1	0.93	0.11	59, 59, 59, 59, 59	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.

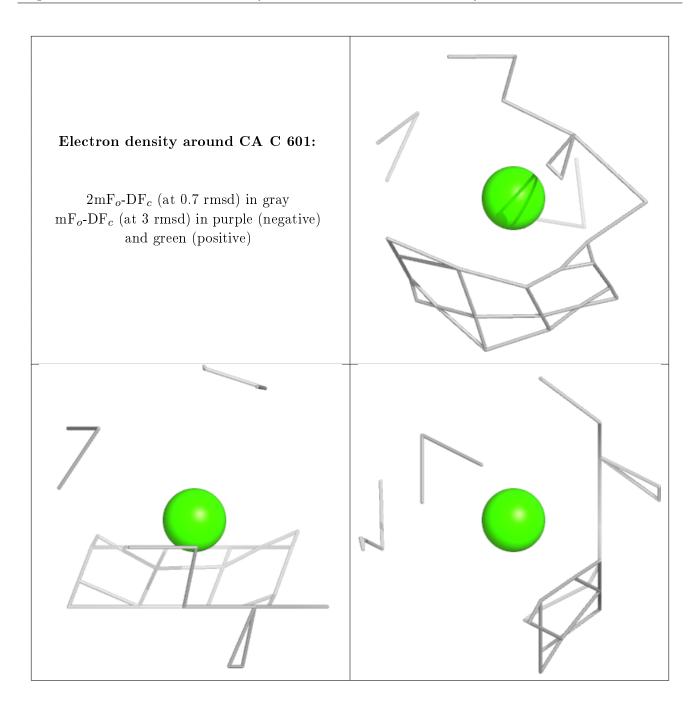




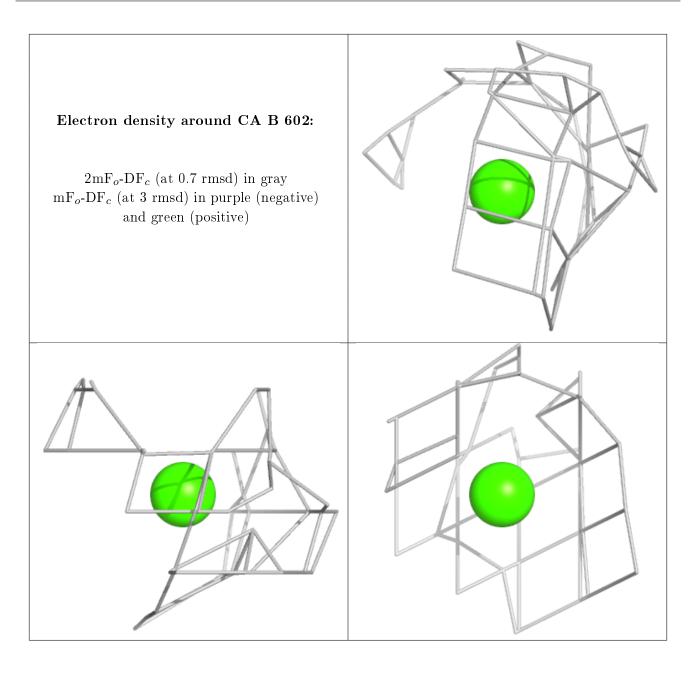




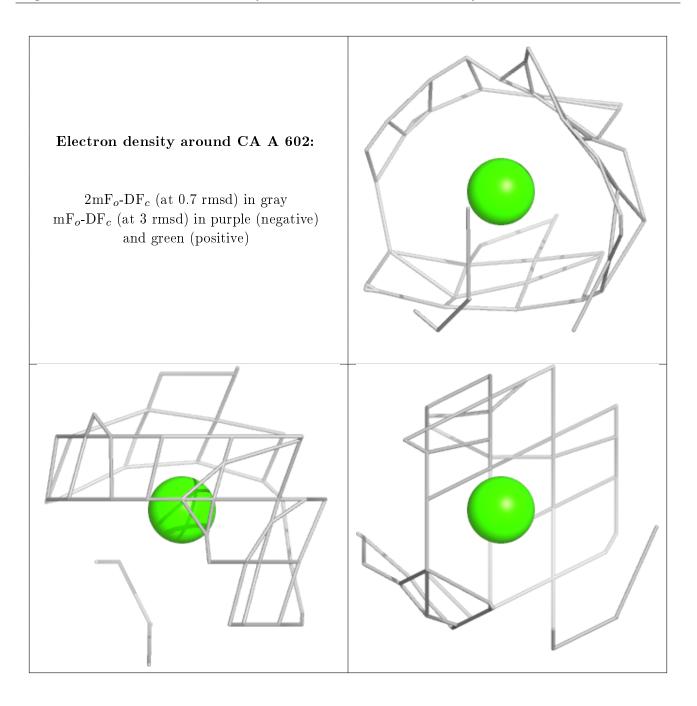




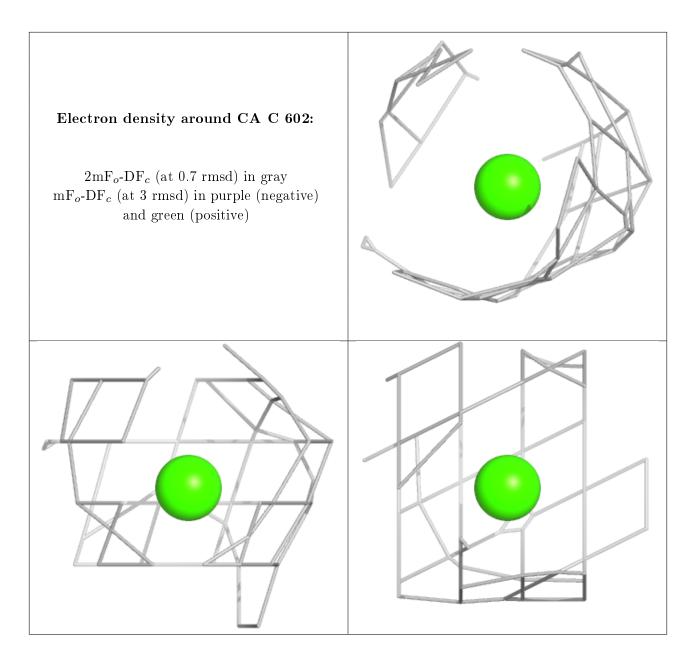




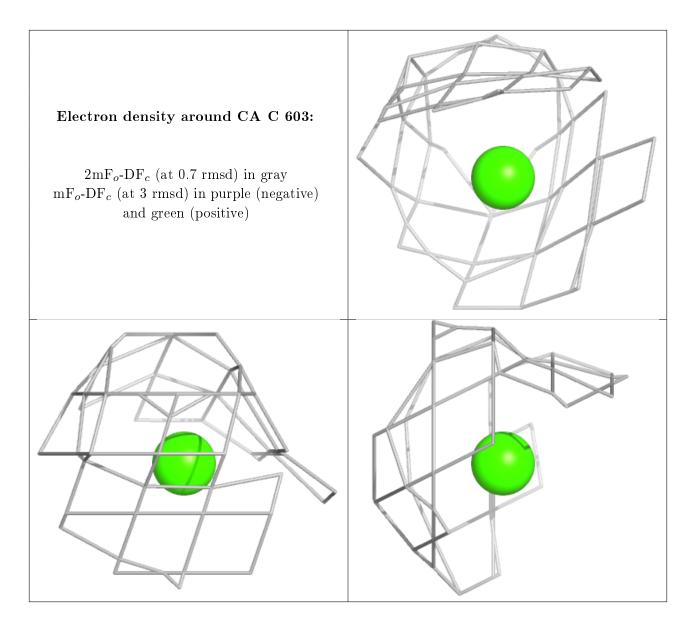




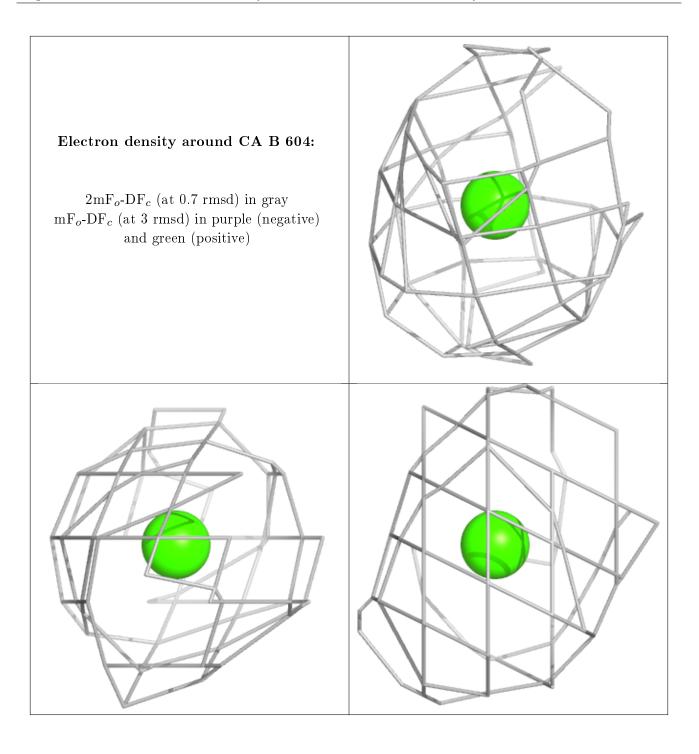




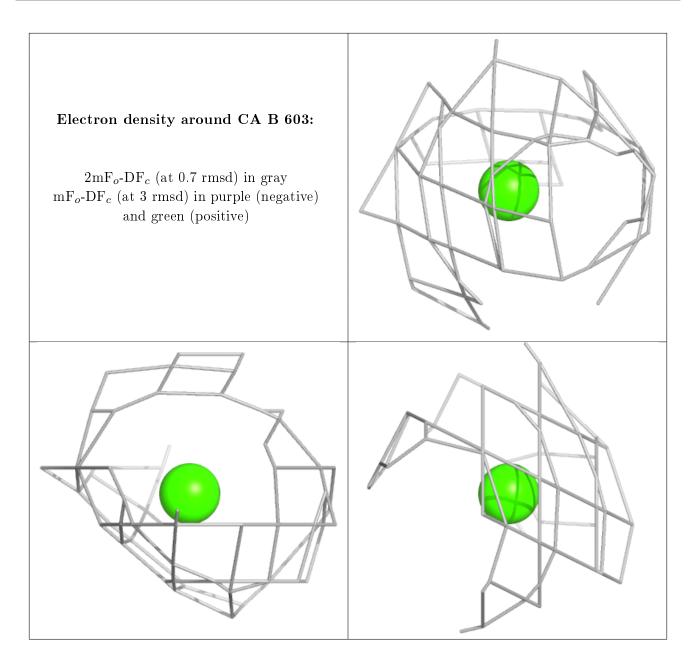




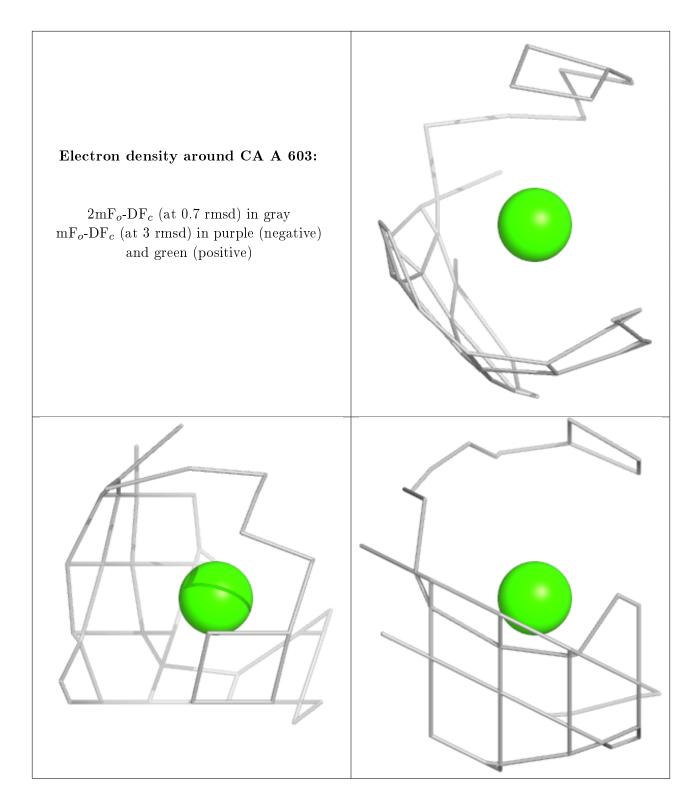












6.5 Other polymers (i)

There are no such residues in this entry.

