



Full wwPDB X-ray Structure Validation Report ⓘ

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 : 2020-01-01
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 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 : 2.14.6
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.14.6

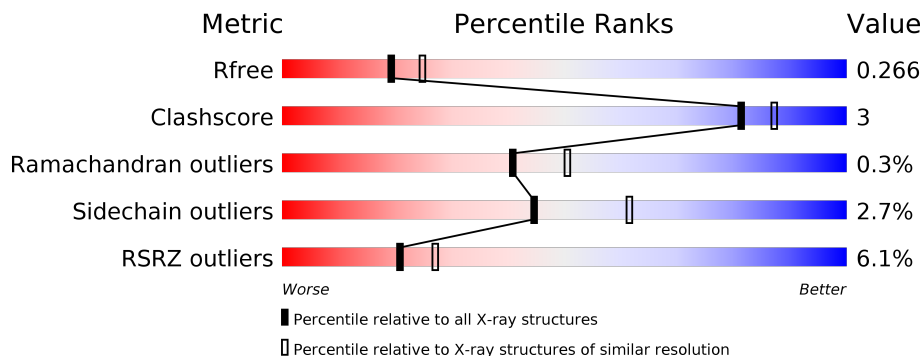
1 Overall quality at a glance

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 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 $\leq 5\%$. 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	326	
1	B	326	
1	C	326	

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.

- Molecule 1 is a protein called Annexin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	314	4987	1535	2513	446	478	15	0	0	0
1	B	314	4987	1535	2513	446	478	15	0	0	0
1	C	314	4987	1535	2513	446	478	15	0	0	0

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	178	MET	-	initiating methionine	UNP Q5XI77
A	179	LEU	-	expression tag	UNP Q5XI77
A	180	HIS	-	expression tag	UNP Q5XI77
A	181	HIS	-	expression tag	UNP Q5XI77
A	182	HIS	-	expression tag	UNP Q5XI77
A	183	HIS	-	expression tag	UNP Q5XI77
A	184	HIS	-	expression tag	UNP Q5XI77
A	185	HIS	-	expression tag	UNP Q5XI77
A	186	PRO	-	expression tag	UNP Q5XI77
A	187	MET	-	expression tag	UNP Q5XI77
A	188	GLY	-	expression tag	UNP Q5XI77
B	178	MET	-	initiating methionine	UNP Q5XI77
B	179	LEU	-	expression tag	UNP Q5XI77
B	180	HIS	-	expression tag	UNP Q5XI77
B	181	HIS	-	expression tag	UNP Q5XI77
B	182	HIS	-	expression tag	UNP Q5XI77
B	183	HIS	-	expression tag	UNP Q5XI77
B	184	HIS	-	expression tag	UNP Q5XI77
B	185	HIS	-	expression tag	UNP Q5XI77
B	186	PRO	-	expression tag	UNP Q5XI77
B	187	MET	-	expression tag	UNP Q5XI77
B	188	GLY	-	expression tag	UNP Q5XI77
C	178	MET	-	initiating methionine	UNP Q5XI77

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

- 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	B	4	Total Ca 4 4	0	0
2	A	3	Total Ca 3 3	0	0
2	C	3	Total Ca 3 3	0	0

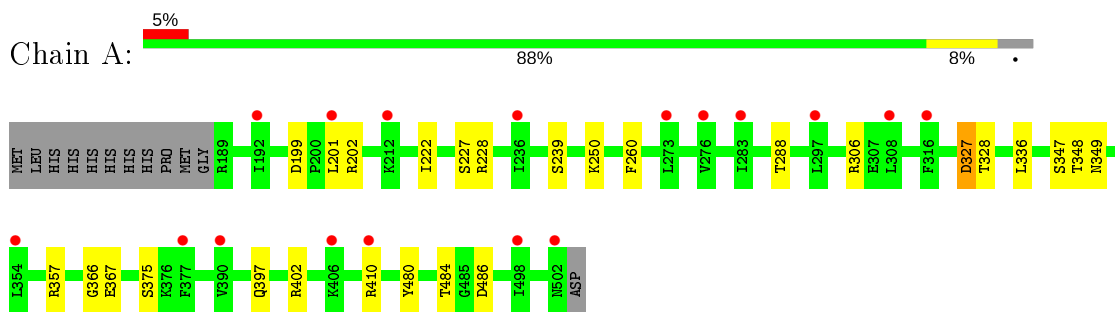
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	55	Total O 55 55	0	0
3	B	60	Total O 60 60	0	0
3	C	50	Total O 50 50	0	0

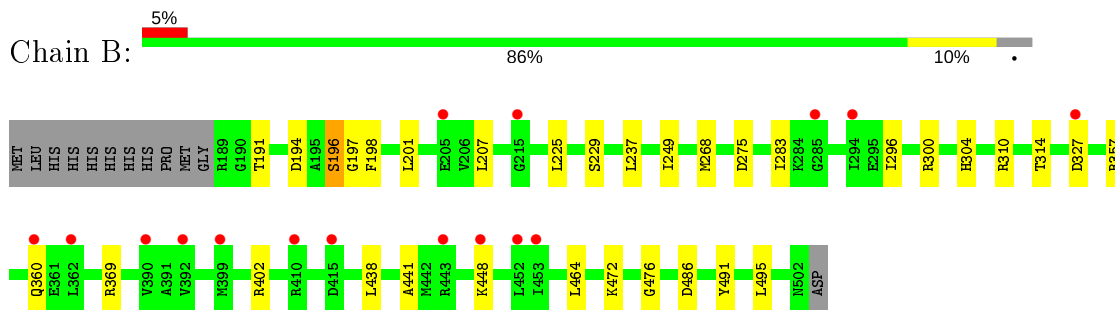
3 Residue-property plots [i](#)

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.

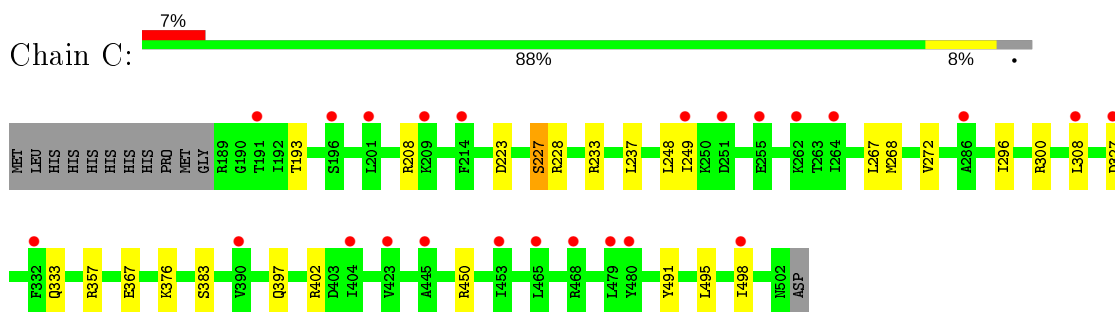
- Molecule 1: Annexin



- Molecule 1: Annexin



- Molecule 1: Annexin



4 Data and refinement statistics

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

Xtrriage'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.*

¹ Intensities estimated from amplitudes.

² 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	0.25	0/2500	0.41	0/3345
1	B	0.25	0/2500	0.42	0/3345
1	C	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

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	2474	2513	2513	11	0
1	B	2474	2513	2513	18	0
1	C	2474	2513	2513	10	0
2	A	3	0	0	0	0
2	B	4	0	0	0	0
2	C	3	0	0	0	0
3	A	55	0	0	1	0
3	B	60	0	0	2	0
3	C	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.

All (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
1:A:250:LYS:O	3:A:701:HOH:O	2.15	0.63
1:C:272:VAL:HG13	1:C:308:LEU:HD23	1.81	0.62
1:B:207:LEU:HD11	1:B:225:LEU:HD21	1.83	0.60
1:A:222:ILE:HD11	1:A:260:PHE:CE1	2.37	0.59
1:A:347:SER:OG	1:A:349:ASN:OD1	2.21	0.59
1:C:333:GLN:NE2	3:C:701:HOH:O	2.36	0.58
1:B:249:ILE:HD11	1:B:268:MET:CB	2.33	0.57
1:B:472:LYS:NZ	1:B:476:GLY:O	2.38	0.55
1:B:310:ARG:O	1:B:314:THR:HG23	2.06	0.54
1:A:367:GLU:OE2	1:A:402:ARG:NH1	2.40	0.53
1:B:237:LEU:HD11	1:B:249:ILE:HG12	1.89	0.53
1:B:275:ASP:OD2	1:B:304:HIS:NE2	2.39	0.53
1:C:228:ARG:O	1:C:233:ARG:NH1	2.43	0.51
1:A:348:THR:HG22	1:A:348:THR:O	2.10	0.51
1:A:288:THR:OG1	1:A:327:ASP:OD2	2.23	0.49
1:B:491:TYR:CZ	1:B:495:LEU:HD11	2.47	0.49
1:C:491:TYR:CZ	1:C:495:LEU:HD11	2.48	0.48
1:B:491:TYR:CE1	1:B:495:LEU:HD11	2.50	0.47
1:B:194:ASP:OD2	1:B:229:SER:OG	2.13	0.46
1:C:237:LEU:HD23	1:C:248:LEU:HB3	1.98	0.45
1:B:196:SER:O	1:B:198:PHE:N	2.50	0.45
1:C:249:ILE:HD11	1:C:268:MET:HB3	1.99	0.44
1:B:191:THR:OG1	1:B:464:LEU:HD23	2.17	0.44
1:C:296:ILE:O	1:C:300:ARG:HG2	2.18	0.43
1:A:227:SER:OG	1:A:228:ARG:NH1	2.53	0.42
1:A:328:THR:HG21	1:A:336:LEU:HD12	2.01	0.42
1:B:191:THR:HG23	1:B:464:LEU:HB3	2.01	0.42
1:C:367:GLU:OE1	1:C:402:ARG:HD2	2.20	0.42
1:A:199:ASP:OD2	1:A:202:ARG:NH1	2.53	0.42
1:A:480:TYR:O	1:A:484:THR:HG23	2.19	0.41
1:A:201:LEU:HA	1:A:239:SER:HB3	2.02	0.41
1:B:201:LEU:O	1:B:201:LEU:HD23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:296:ILE:O	1:B:300:ARG:HG2	2.21	0.41
1:B:438:LEU:O	1:B:441:ALA:HB3	2.21	0.41

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	312/326 (96%)	305 (98%)	6 (2%)	1 (0%)	41	50
1	B	312/326 (96%)	301 (96%)	9 (3%)	2 (1%)	25	31
1	C	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	B	197	GLY
1	A	366	GLY
1	B	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	A	268/279 (96%)	261 (97%)	7 (3%)	46	63
1	B	268/279 (96%)	262 (98%)	6 (2%)	52	69
1	C	268/279 (96%)	259 (97%)	9 (3%)	37	51
All	All	804/837 (96%)	782 (97%)	22 (3%)	44	61

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	306	ARG
1	A	327	ASP
1	A	357	ARG
1	A	375	SER
1	A	397	GLN
1	A	410	ARG
1	A	486	ASP
1	B	327	ASP
1	B	357	ARG
1	B	360	GLN
1	B	369	ARG
1	B	402	ARG
1	B	486	ASP
1	C	193	THR
1	C	208	ARG
1	C	227	SER
1	C	327	ASP
1	C	357	ARG
1	C	376	LYS
1	C	383	SER
1	C	397	GLN
1	C	450	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

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	314/326 (96%)	0.48	17 (5%) 25 32	33, 45, 62, 70	0
1	B	314/326 (96%)	0.56	16 (5%) 28 35	32, 48, 65, 77	0
1	C	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

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	214	PHE	6.8
1	A	201	LEU	4.9
1	C	327	ASP	4.9
1	C	251	ASP	4.6
1	C	480	TYR	4.4
1	A	498	ILE	3.9
1	C	445	ALA	3.8
1	A	410	ARG	3.6
1	C	196	SER	3.4
1	A	308	LEU	3.3
1	C	191	THR	3.2
1	B	327	ASP	3.2
1	C	264	ILE	3.2
1	C	209	LYS	3.1
1	C	390	VAL	3.0
1	B	399	MET	3.0
1	C	308	LEU	2.9
1	A	502	ASN	2.8
1	A	354	LEU	2.8
1	C	262	LYS	2.7
1	C	201	LEU	2.7
1	C	332	PHE	2.7
1	A	297	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	410	ARG	2.6
1	B	294	ILE	2.6
1	A	406	LYS	2.5
1	C	468	ARG	2.5
1	B	452	LEU	2.5
1	A	192	ILE	2.5
1	A	316	PHE	2.5
1	C	498	ILE	2.4
1	B	215	GLY	2.4
1	B	360	GLN	2.4
1	B	443	ARG	2.4
1	C	255	GLU	2.4
1	B	448	LYS	2.3
1	A	377	PHE	2.3
1	B	390	VAL	2.3
1	B	415	ASP	2.3
1	C	465	LEU	2.3
1	B	362	LEU	2.2
1	B	205	GLU	2.2
1	A	273	LEU	2.2
1	C	479	LEU	2.2
1	B	453	ILE	2.2
1	A	390	VAL	2.2
1	A	212	LYS	2.2
1	B	285	GLY	2.1
1	A	236	ILE	2.1
1	A	283	ILE	2.1
1	C	286	ALA	2.1
1	C	453	ILE	2.1
1	A	276	VAL	2.1
1	B	392	VAL	2.1
1	C	404	ILE	2.0
1	C	423	VAL	2.0
1	C	249	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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](#)

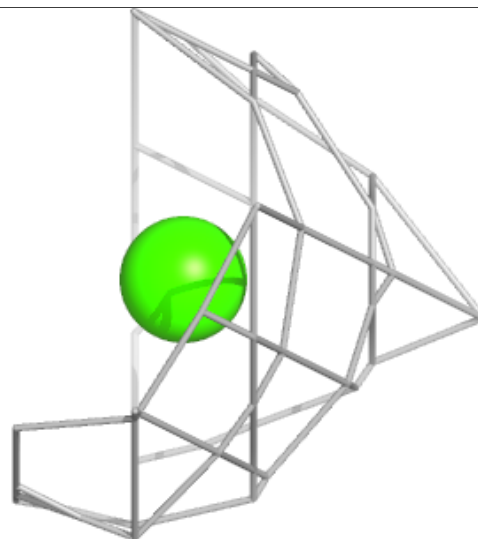
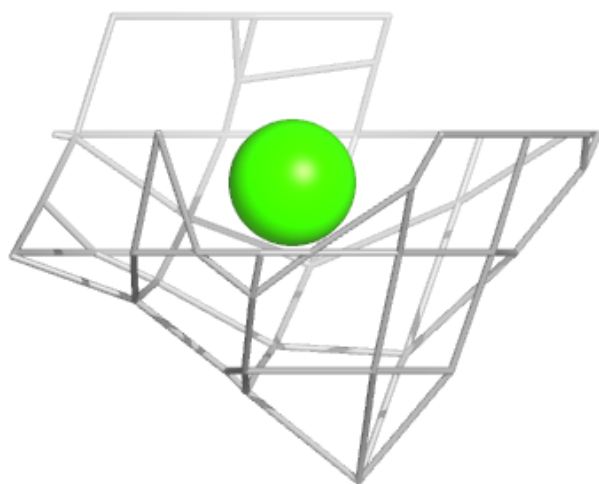
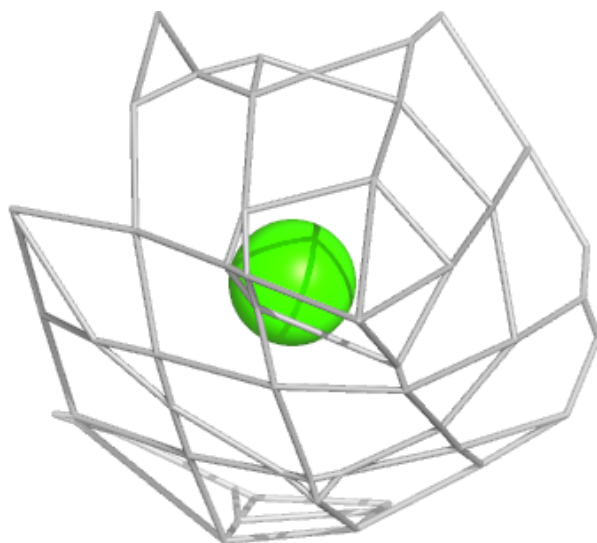
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	A	601	1/1	0.47	0.10	69,69,69,69	0
2	CA	B	601	1/1	0.57	0.09	72,72,72,72	0
2	CA	C	601	1/1	0.73	0.14	82,82,82,82	0
2	CA	B	602	1/1	0.75	0.13	75,75,75,75	0
2	CA	A	602	1/1	0.81	0.09	66,66,66,66	0
2	CA	C	602	1/1	0.85	0.06	51,51,51,51	0
2	CA	C	603	1/1	0.90	0.09	85,85,85,85	0
2	CA	B	604	1/1	0.91	0.09	82,82,82,82	0
2	CA	B	603	1/1	0.93	0.09	70,70,70,70	0
2	CA	A	603	1/1	0.93	0.11	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.

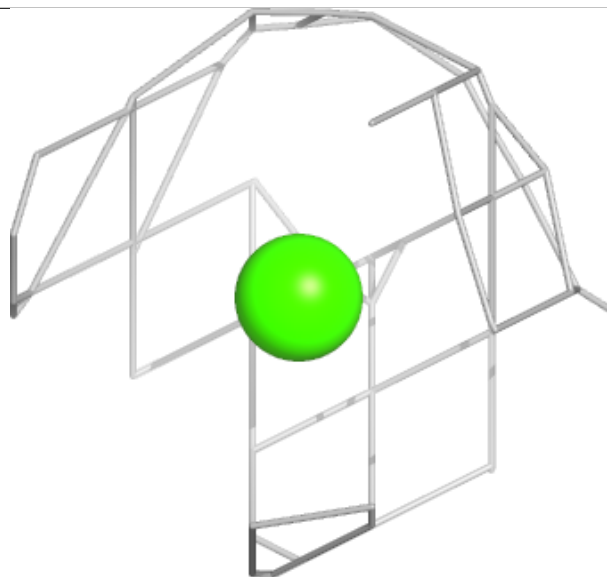
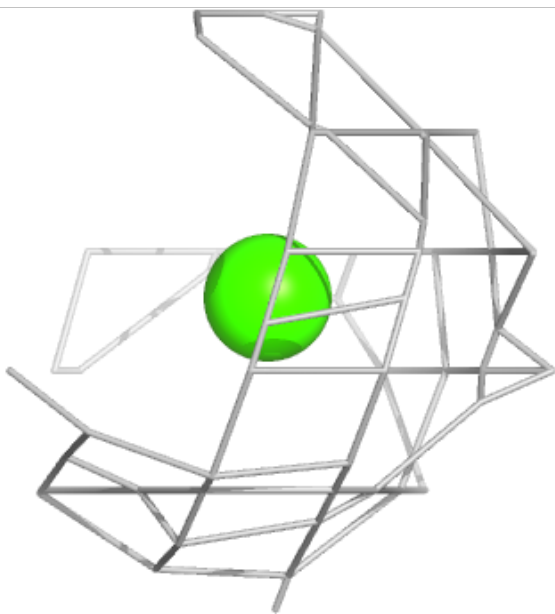
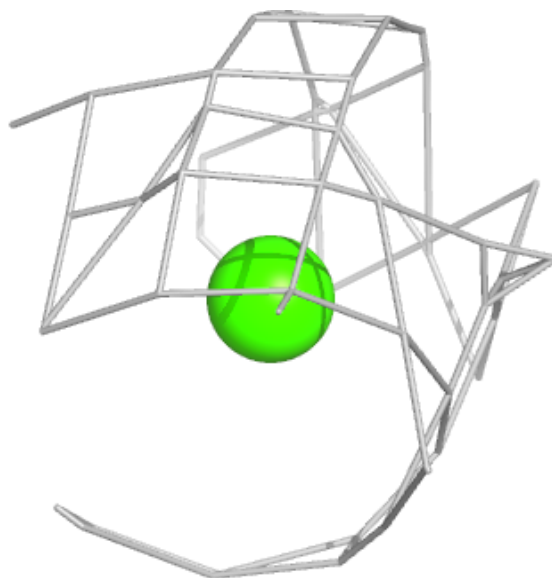
Electron density around CA A 601:

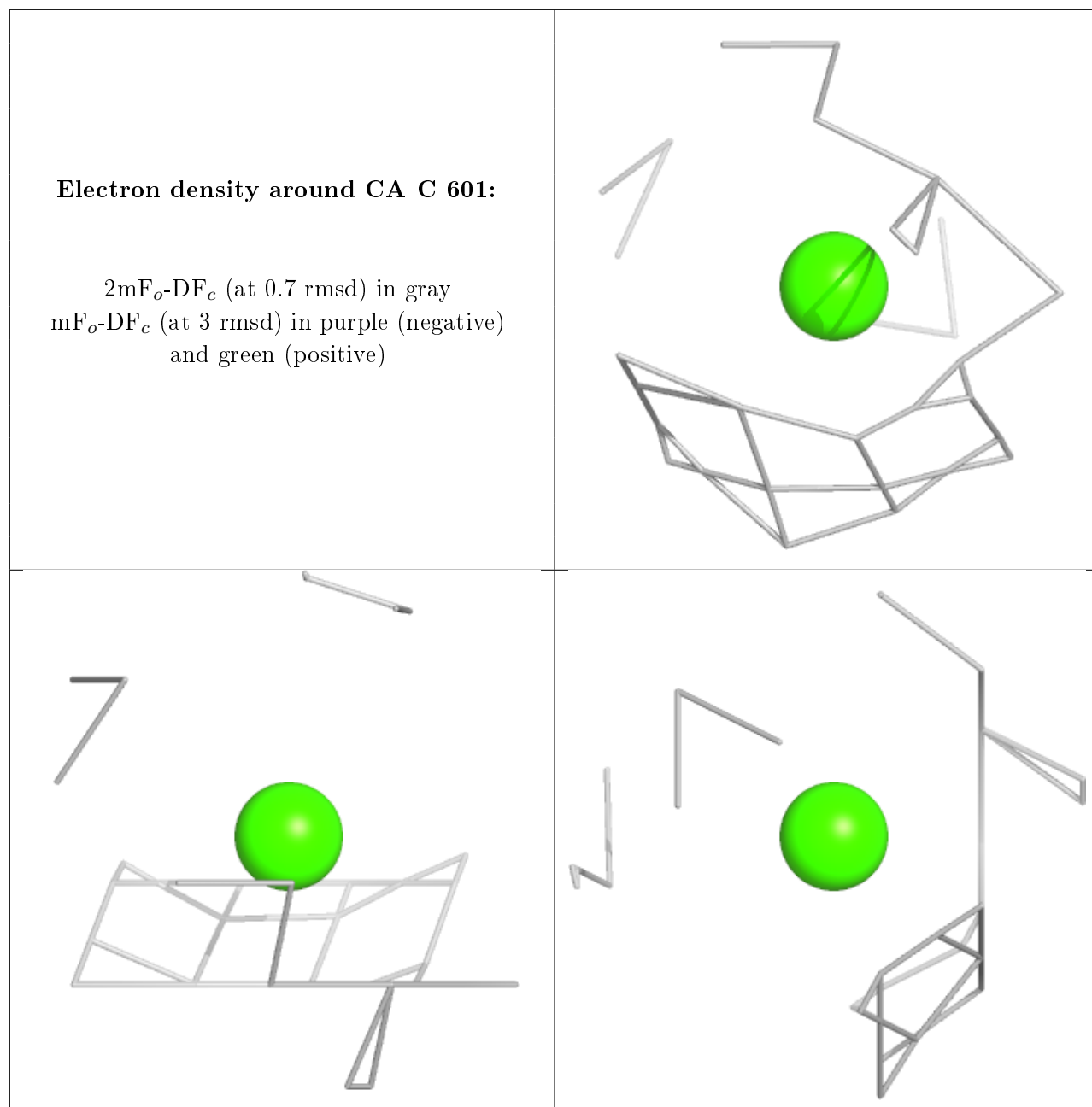
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CA B 601:

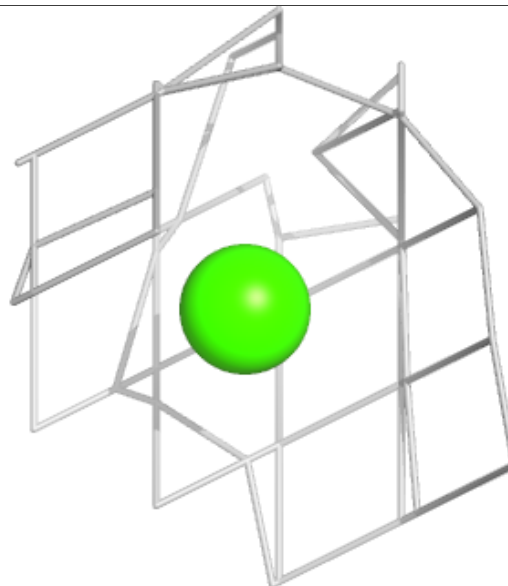
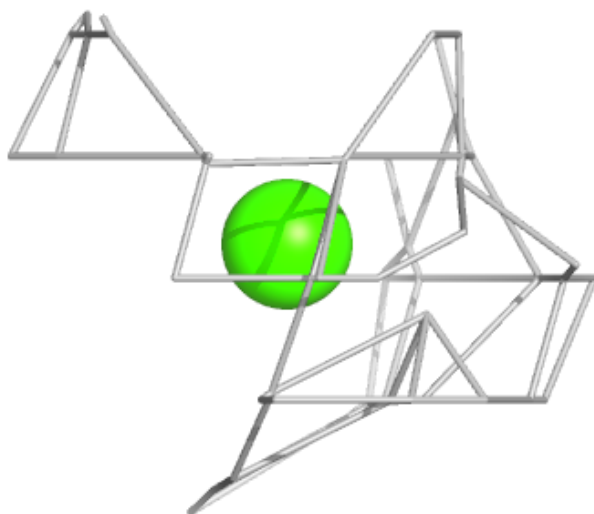
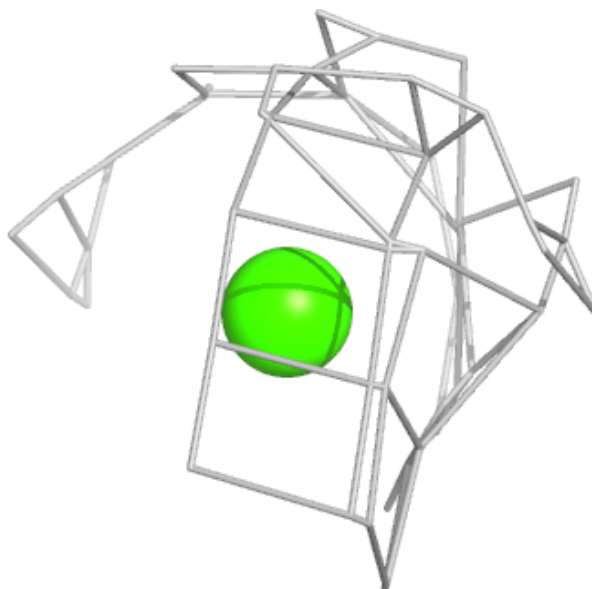
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





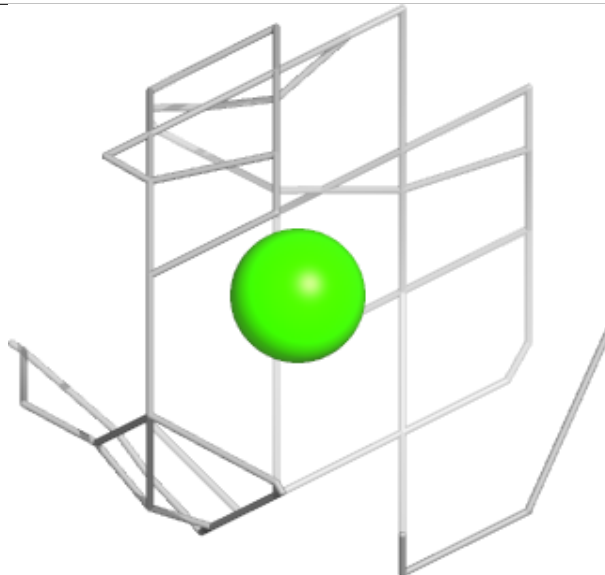
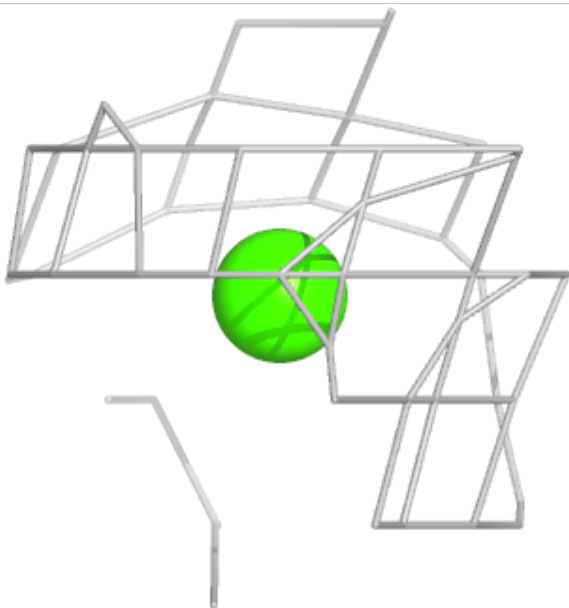
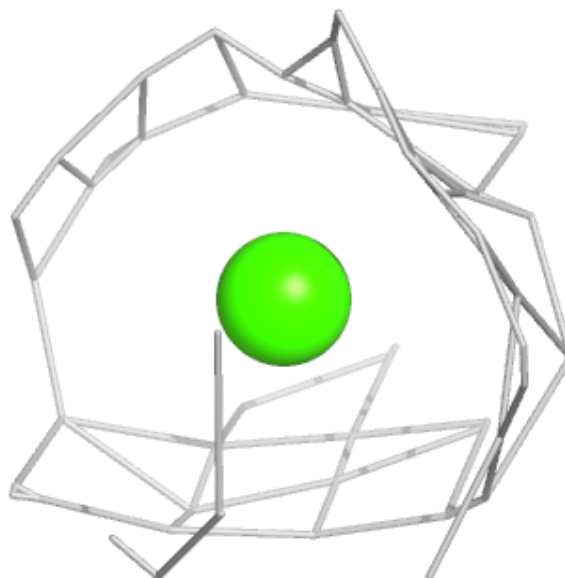
Electron density around CA B 602:

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



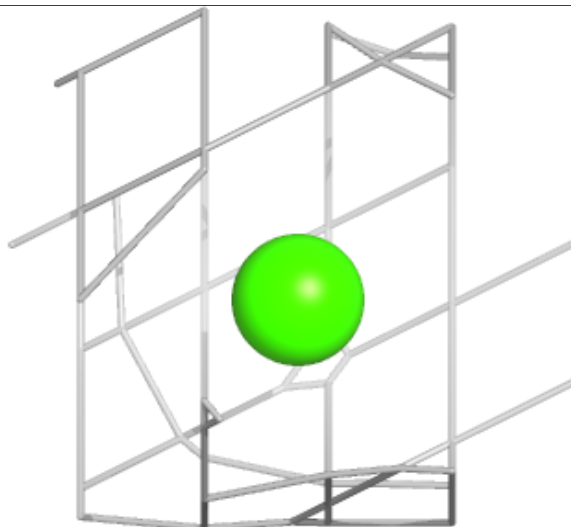
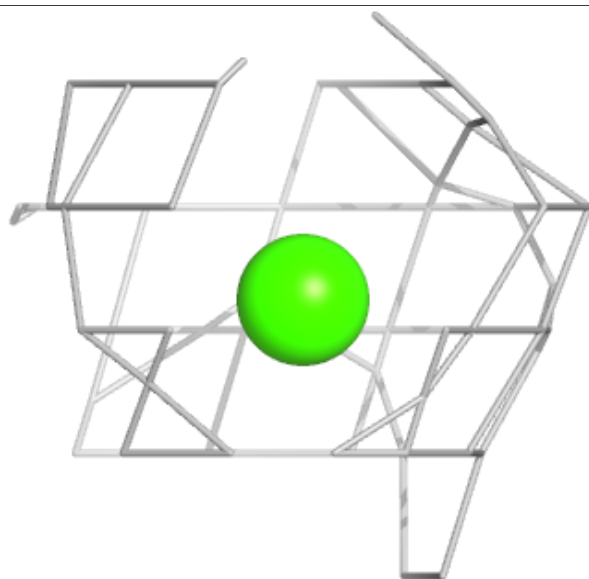
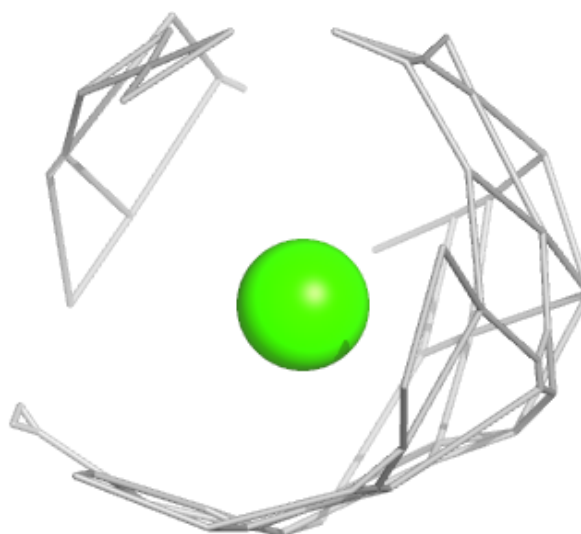
Electron density around CA A 602:

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



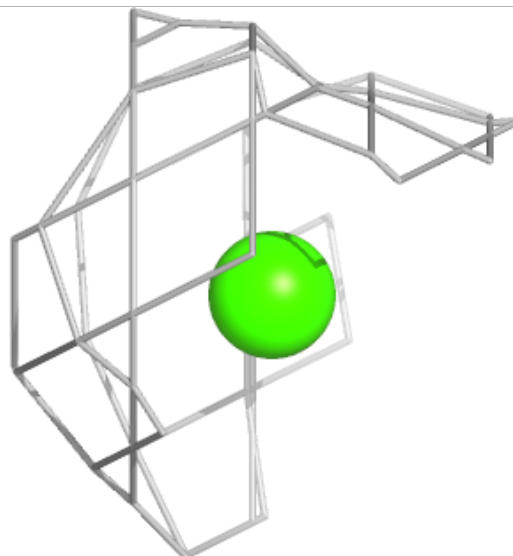
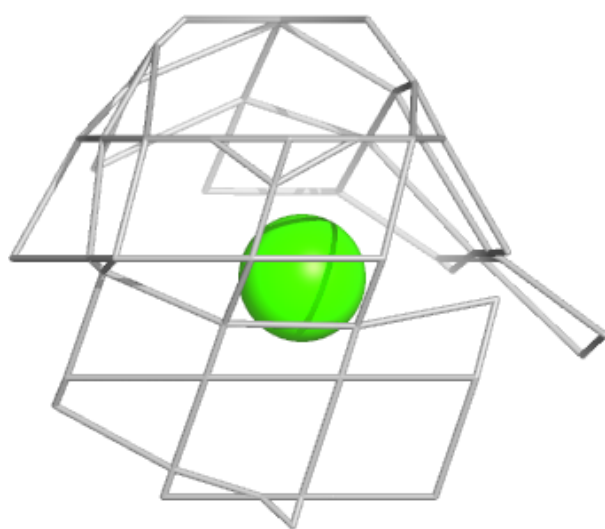
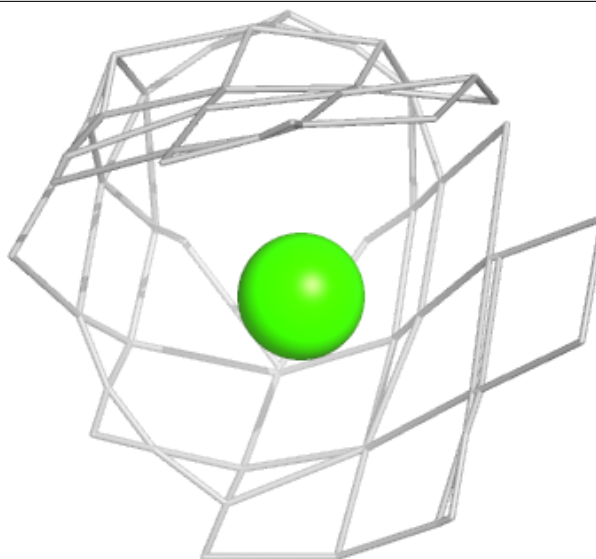
Electron density around CA C 602:

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



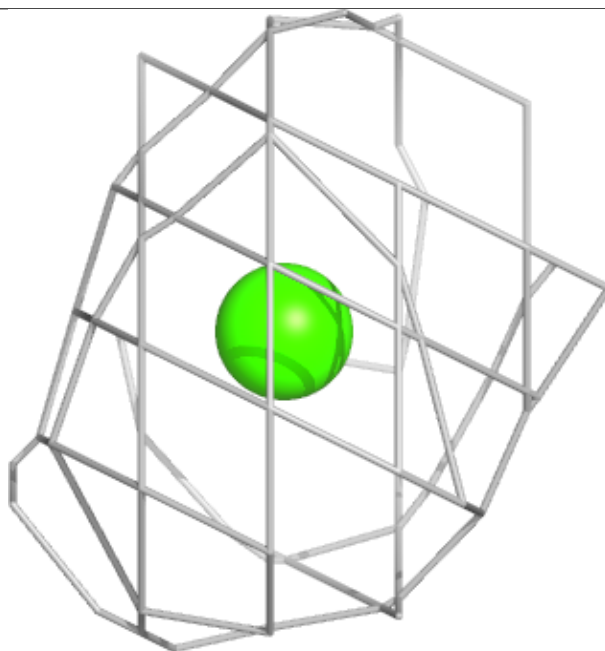
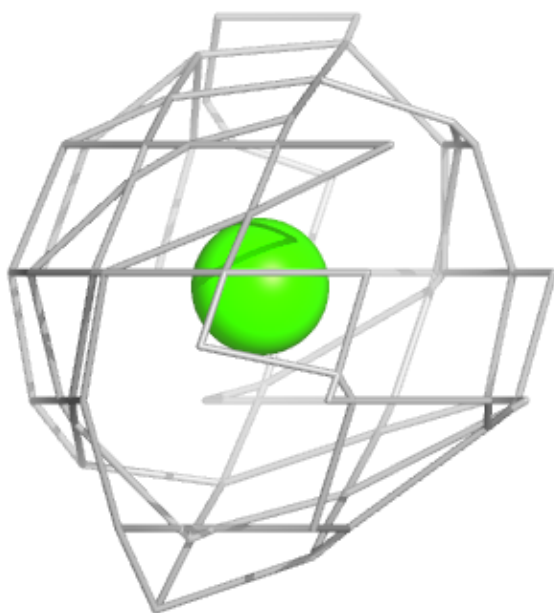
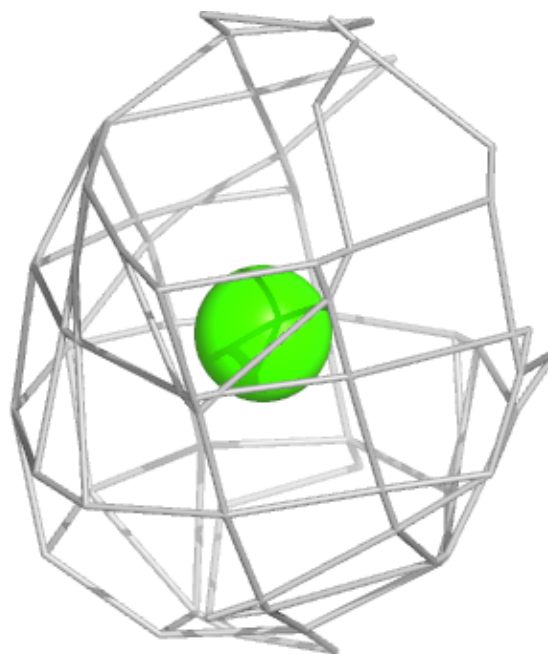
Electron density around CA C 603:

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



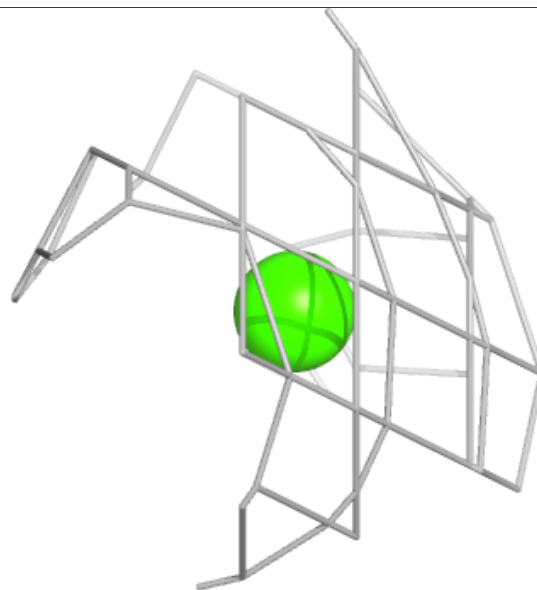
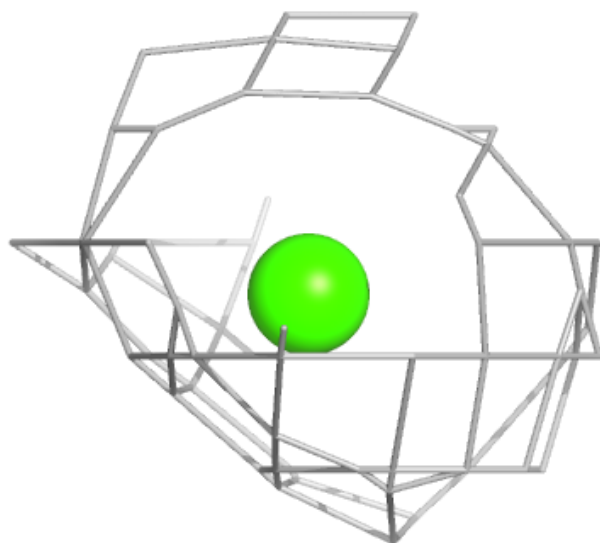
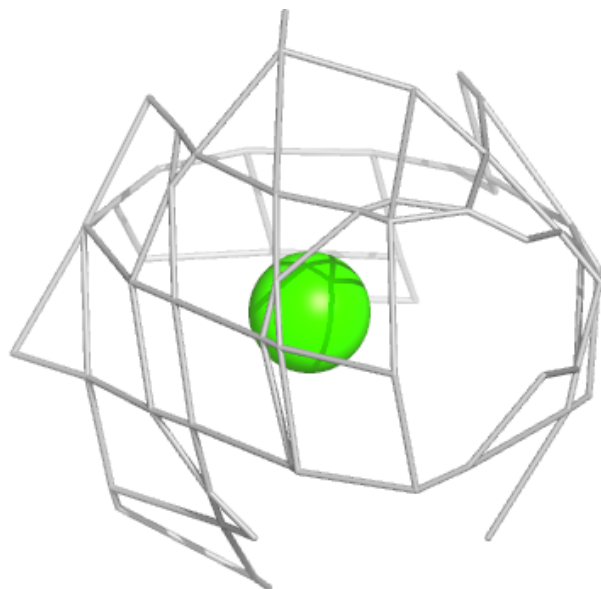
Electron density around CA B 604:

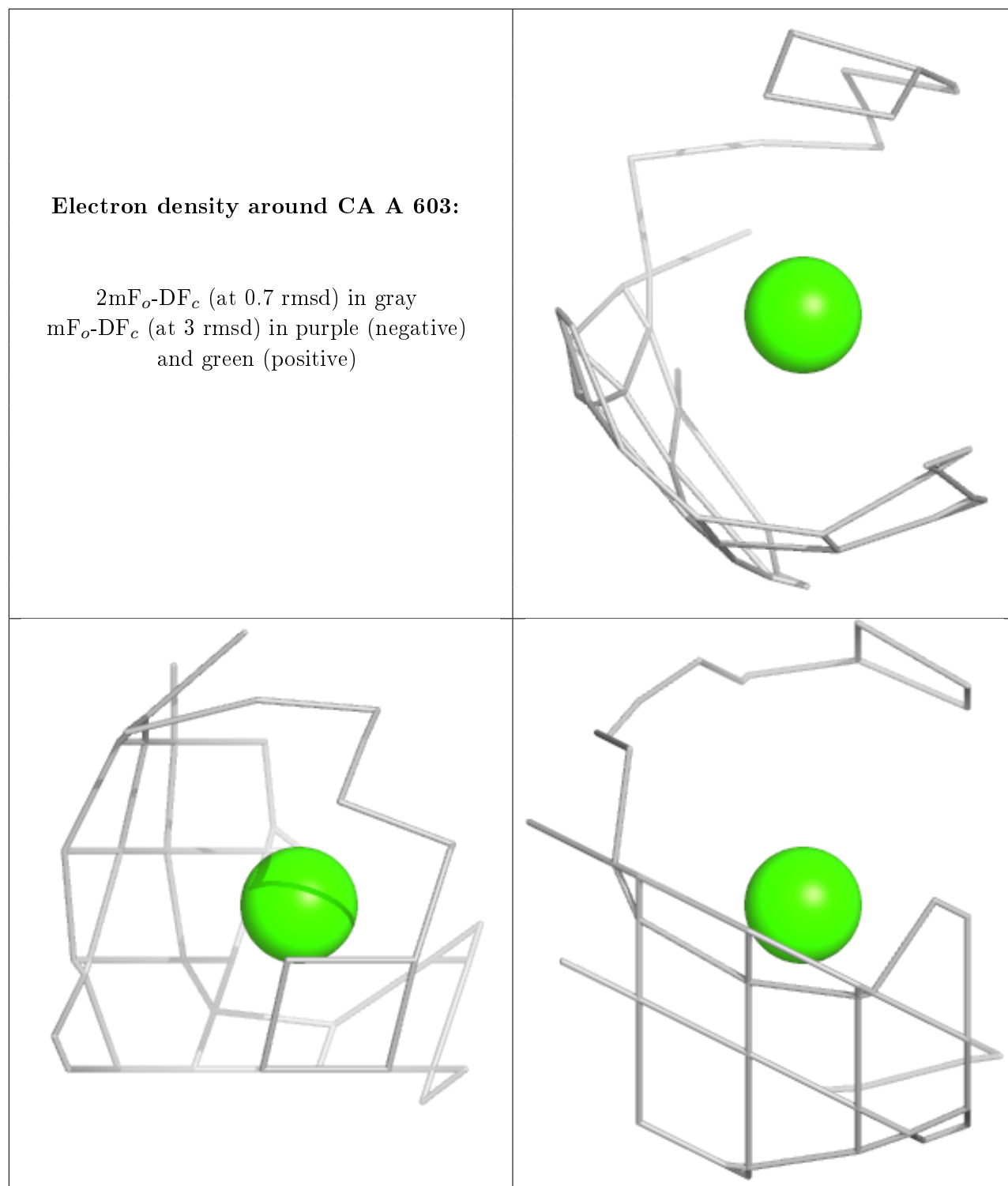
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CA B 603:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.