



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 16, 2021 – 04:04 PM EDT

PDB ID : 7LJA
Title : Human TRAAK K⁺ channel FHEIG mutant A198E in a Tl⁺ bound conductive conformation
Authors : Rietmeijer, R.A.; Brohawn, S.G.
Deposited on : 2021-01-28
Resolution : 2.77 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 ⓘ 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	:	2.23.1
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)	:	2.23.1

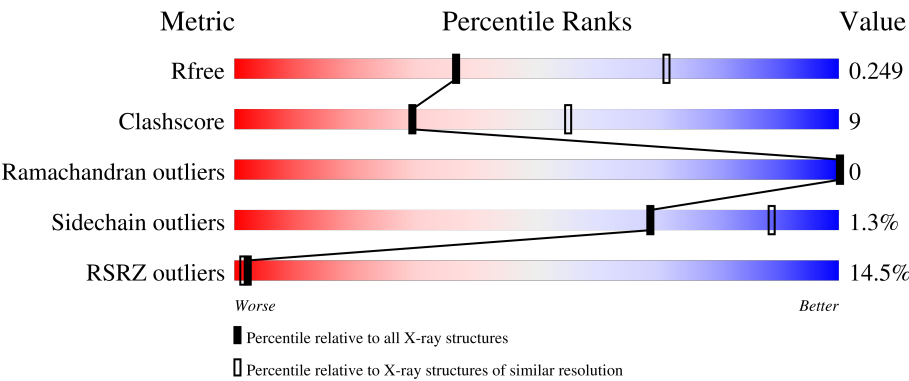
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.77 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	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

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	299	
1	B	299	
2	D	211	
2	F	211	
3	E	217	

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Mol	Chain	Length	Quality of chain
3	G	217	<div><div></div><div>7%</div><div>74%</div><div>22%</div><div>..</div></div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10651 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 Isoform 2 of Potassium channel subfamily K member 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	253	Total	C	N	O	S	0	0	0
			1967	1301	318	342	6			
1	B	255	Total	C	N	O	S	0	0	0
			1985	1310	321	348	6			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	104	GLN	ASN	engineered mutation	UNP Q9NYG8-2
A	108	GLN	ASN	engineered mutation	UNP Q9NYG8-2
A	198	GLU	ALA	engineered mutation	UNP Q9NYG8-2
A	291	SER	-	expression tag	UNP Q9NYG8-2
A	292	ASN	-	expression tag	UNP Q9NYG8-2
A	293	SER	-	expression tag	UNP Q9NYG8-2
A	294	LEU	-	expression tag	UNP Q9NYG8-2
A	295	GLU	-	expression tag	UNP Q9NYG8-2
A	296	VAL	-	expression tag	UNP Q9NYG8-2
A	297	LEU	-	expression tag	UNP Q9NYG8-2
A	298	PHE	-	expression tag	UNP Q9NYG8-2
A	299	GLN	-	expression tag	UNP Q9NYG8-2
B	104	GLN	ASN	engineered mutation	UNP Q9NYG8-2
B	108	GLN	ASN	engineered mutation	UNP Q9NYG8-2
B	198	GLU	ALA	engineered mutation	UNP Q9NYG8-2
B	291	SER	-	expression tag	UNP Q9NYG8-2
B	292	ASN	-	expression tag	UNP Q9NYG8-2
B	293	SER	-	expression tag	UNP Q9NYG8-2
B	294	LEU	-	expression tag	UNP Q9NYG8-2
B	295	GLU	-	expression tag	UNP Q9NYG8-2
B	296	VAL	-	expression tag	UNP Q9NYG8-2
B	297	LEU	-	expression tag	UNP Q9NYG8-2
B	298	PHE	-	expression tag	UNP Q9NYG8-2
B	299	GLN	-	expression tag	UNP Q9NYG8-2

- Molecule 2 is a protein called ANTI-TRAAK ANTIBODY 13E9 FAB FRAGMENT LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	211	Total	C	N	O	S	0	0	0
			1616	1003	271	333	9			
2	F	211	Total	C	N	O	S	0	0	0
			1616	1003	271	333	9			

- Molecule 3 is a protein called ANTI-TRAAK ANTIBODY 13E9 FAB FRAGMENT HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	211	Total	C	N	O	S	0	0	0
			1614	1026	261	319	8			
3	G	210	Total	C	N	O	S	0	0	0
			1605	1022	260	315	8			

- Molecule 4 is THALLIUM (I) ION (three-letter code: TL) (formula: Tl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total	Tl	0	0
			5	5		
4	B	3	Total	Tl	0	0
			3	3		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Ca	0	0
			2	2		
5	G	1	Total	Ca	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	31	Total	O	0	0
			31	31		
6	B	38	Total	O	0	0
			38	38		
6	D	35	Total	O	0	0
			35	35		

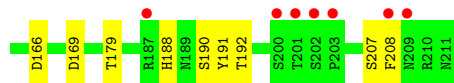
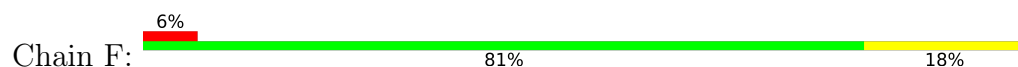
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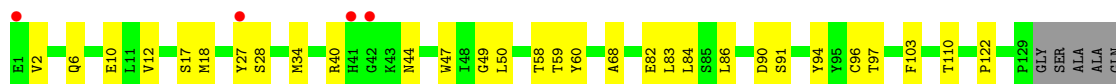
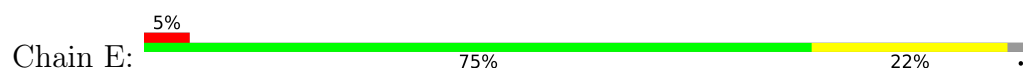
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	51	Total 51	O 51	0	0
6	F	43	Total 43	O 43	0	0
6	G	39	Total 39	O 39	0	0



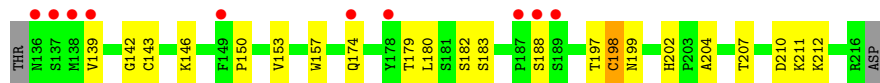
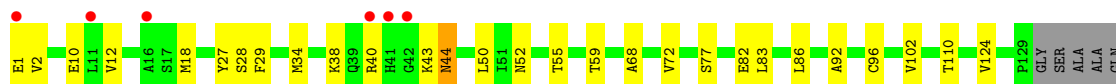
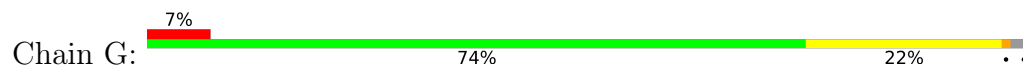
● Molecule 2: ANTI-TRAAK ANTIBODY 13E9 FAB FRAGMENT LIGHT CHAIN



● Molecule 3: ANTI-TRAAK ANTIBODY 13E9 FAB FRAGMENT HEAVY CHAIN



● Molecule 3: ANTI-TRAAK ANTIBODY 13E9 FAB FRAGMENT HEAVY CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.23Å 136.53Å 95.28Å 90.00° 94.54° 90.00°	Depositor
Resolution (Å)	47.54 – 2.77 47.49 – 2.78	Depositor EDS
% Data completeness (in resolution range)	68.6 (47.54-2.77) 68.6 (47.49-2.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.201 , 0.243 0.207 , 0.249	Depositor DCC
R_{free} test set	1755 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	67.7	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 57.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	10651	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% 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: TL, 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	0.72	0/2017	0.80	0/2750
1	B	0.74	0/2035	0.79	0/2774
2	D	0.76	0/1655	0.90	0/2247
2	F	0.81	1/1655 (0.1%)	0.92	0/2247
3	E	0.74	0/1656	0.94	0/2260
3	G	0.74	0/1647	0.92	0/2249
All	All	0.75	1/10665 (0.0%)	0.87	0/14527

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	122	GLU	CD-OE1	5.21	1.31	1.25

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	A	1967	0	1985	48	0
1	B	1985	0	2007	26	0
2	D	1616	0	1542	27	0
2	F	1616	0	1542	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	1614	0	1586	38	1
3	G	1605	0	1582	45	1
4	A	5	0	0	0	0
4	B	3	0	0	0	0
5	A	2	0	0	0	0
5	G	1	0	0	0	0
6	A	31	0	0	4	0
6	B	38	0	0	1	0
6	D	35	0	0	1	0
6	E	51	0	0	4	0
6	F	43	0	0	1	0
6	G	39	0	0	0	0
All	All	10651	0	10244	196	1

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 9.

The worst 5 of 196 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)
3:G:198:CYS:O	3:G:198:CYS:SG	2.36	0.83
2:D:99:ALA:HA	3:E:44:ASN:HB3	1.61	0.81
1:A:69:ARG:HD2	6:A:408:HOH:O	1.81	0.80
1:A:263:PHE:CZ	1:A:267:LEU:HD11	2.15	0.80
2:D:35:TYR:CD1	2:D:45:ARG:HA	2.18	0.78

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:194:GLU:OE2	3:G:10:GLU:OE1[2_556]	1.72	0.48

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	249/299 (83%)	235 (94%)	14 (6%)	0	100	100
1	B	251/299 (84%)	245 (98%)	6 (2%)	0	100	100
2	D	209/211 (99%)	202 (97%)	7 (3%)	0	100	100
2	F	209/211 (99%)	201 (96%)	8 (4%)	0	100	100
3	E	207/217 (95%)	203 (98%)	4 (2%)	0	100	100
3	G	206/217 (95%)	200 (97%)	6 (3%)	0	100	100
All	All	1331/1454 (92%)	1286 (97%)	45 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	205/243 (84%)	204 (100%)	1 (0%)	88	95
1	B	209/243 (86%)	208 (100%)	1 (0%)	88	95
2	D	184/184 (100%)	181 (98%)	3 (2%)	62	86
2	F	184/184 (100%)	181 (98%)	3 (2%)	62	86
3	E	187/190 (98%)	184 (98%)	3 (2%)	62	86
3	G	186/190 (98%)	182 (98%)	4 (2%)	52	80
All	All	1155/1234 (94%)	1140 (99%)	15 (1%)	69	89

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	198	CYS
3	G	143	CYS
2	F	21	MET
3	G	198	CYS
3	G	18	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
3	G	174	GLN
2	F	188	HIS
2	D	144	ASN
2	D	137	ASN
3	E	136	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 11 ligands modelled in this entry, 11 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 [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	A	253/299 (84%)	1.18	63 (24%) 0 0	46, 106, 174, 197	0
1	B	255/299 (85%)	1.96	83 (32%) 0 0	45, 107, 179, 199	0
2	D	211/211 (100%)	0.06	11 (5%) 27 22	38, 64, 104, 125	0
2	F	211/211 (100%)	0.15	12 (5%) 23 18	38, 64, 111, 127	0
3	E	211/217 (97%)	0.20	11 (5%) 27 22	34, 55, 85, 124	0
3	G	210/217 (96%)	0.24	16 (7%) 13 9	37, 60, 96, 156	0
All	All	1351/1454 (92%)	0.69	196 (14%) 2 1	34, 71, 164, 199	0

The worst 5 of 196 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	248	ALA	12.8
3	G	136	ASN	12.4
1	B	193	VAL	12.2
1	B	192	LEU	11.8
1	B	190	PRO	11.5

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

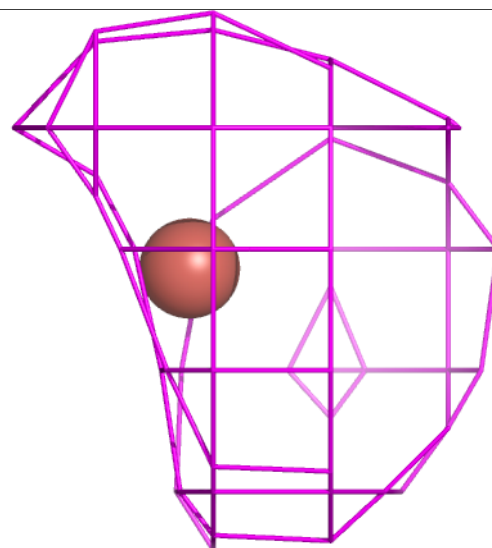
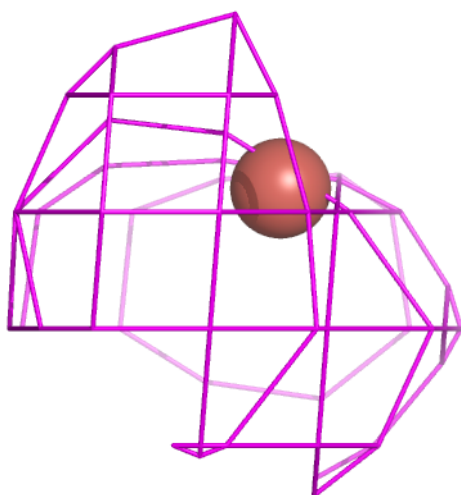
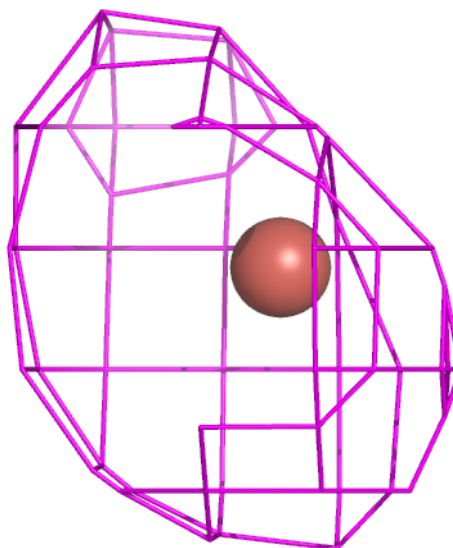
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	TL	B	303	1/1	0.53	0.16	245,245,245,245	0
4	TL	A	306	1/1	0.60	0.21	220,220,220,220	0
5	CA	A	304	1/1	0.77	0.23	102,102,102,102	0
4	TL	B	302	1/1	0.85	0.08	183,183,183,183	0
4	TL	A	307	1/1	0.86	0.21	225,225,225,225	0
5	CA	G	301	1/1	0.98	0.10	63,63,63,63	0
4	TL	A	305	1/1	0.99	0.05	88,88,88,88	0
5	CA	A	303	1/1	0.99	0.05	107,107,107,107	0
4	TL	B	301	1/1	0.99	0.05	89,89,89,89	0
4	TL	A	302	1/1	0.99	0.05	88,88,88,88	0
4	TL	A	301	1/1	1.00	0.04	85,85,85,85	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.

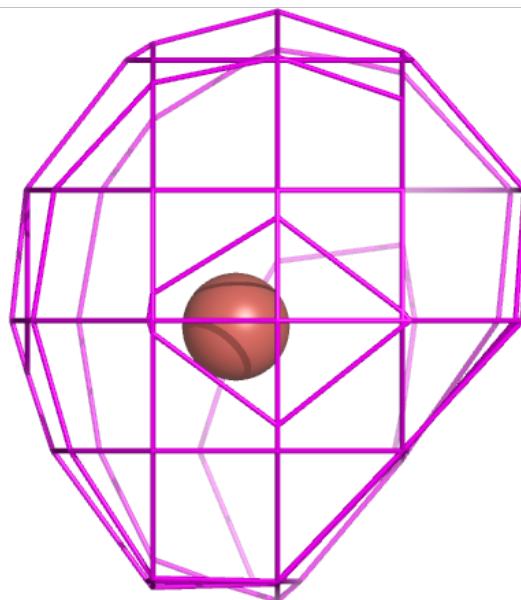
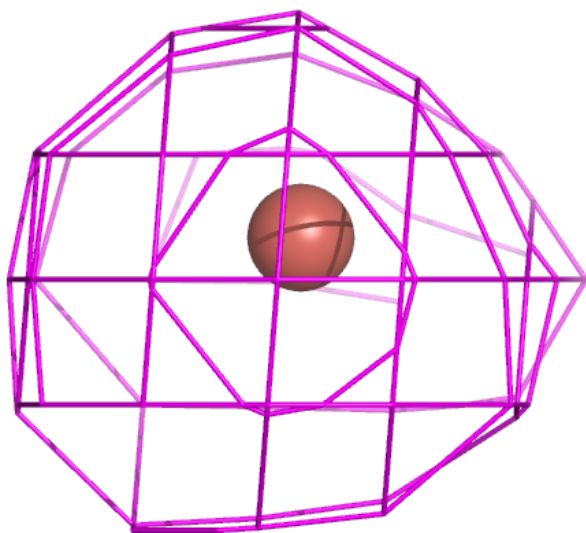
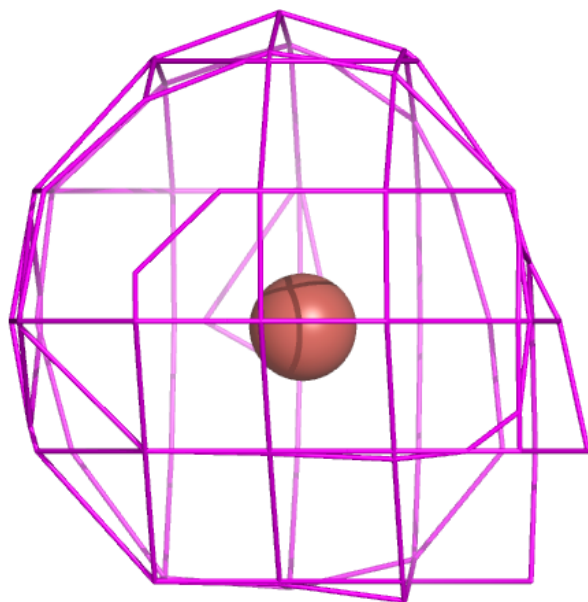
Electron density around TL B 303:

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



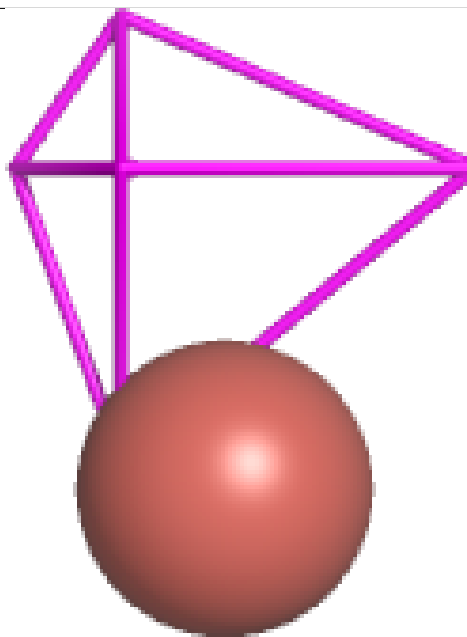
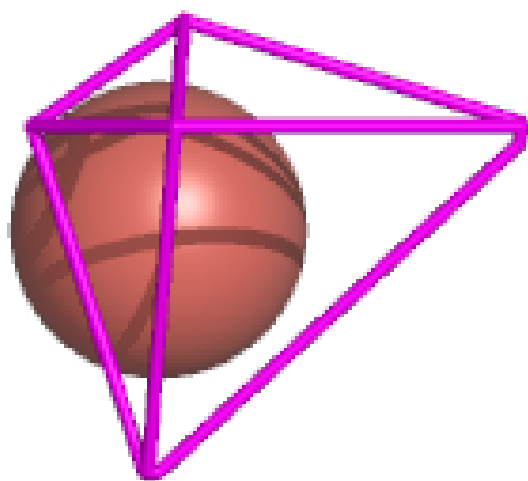
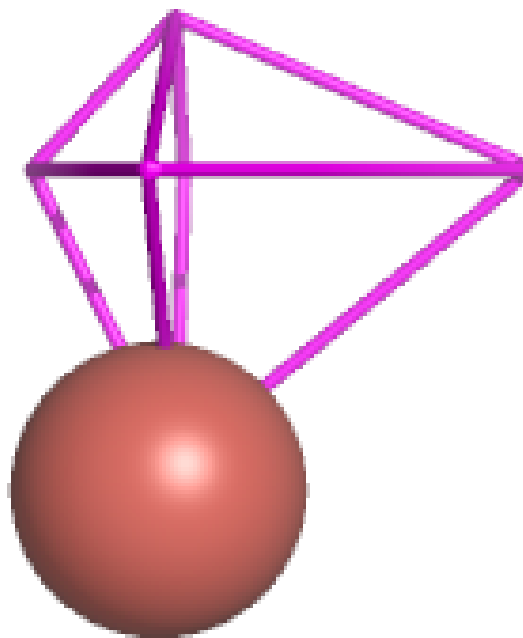
Electron density around TL A 306:

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



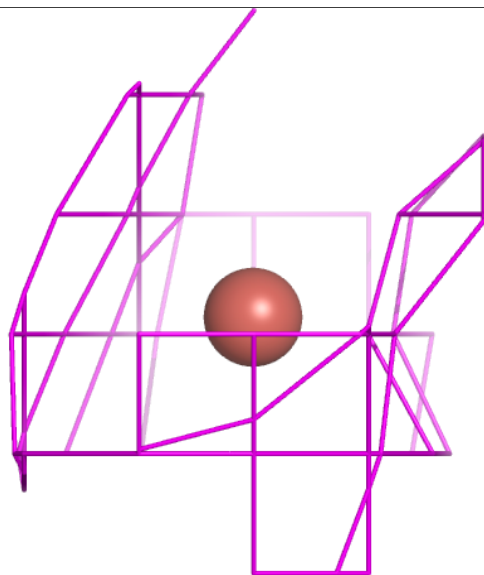
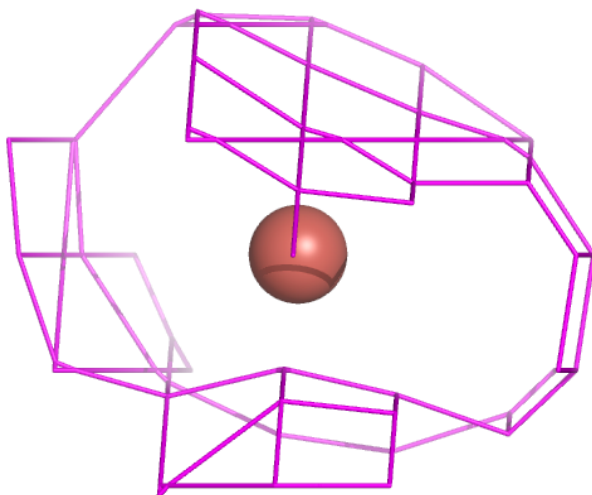
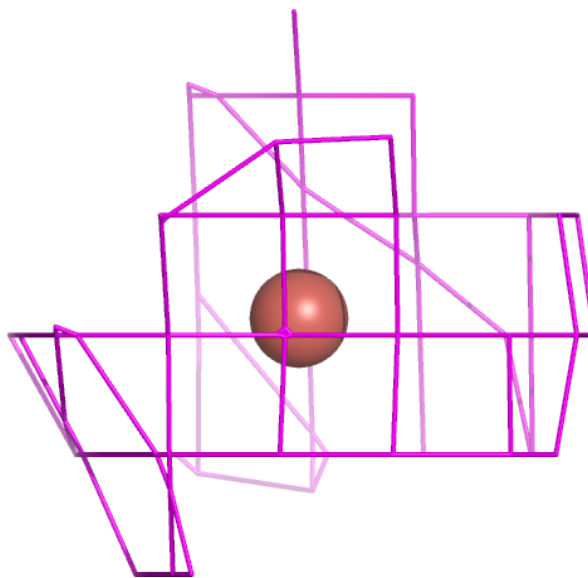
Electron density around TL B 302:

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



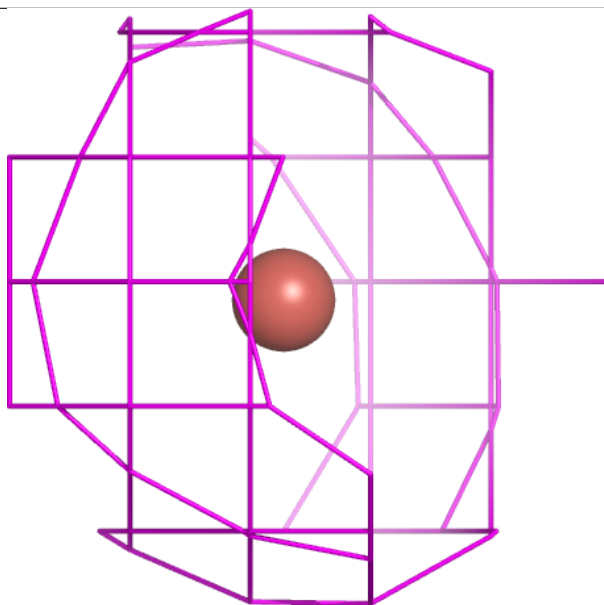
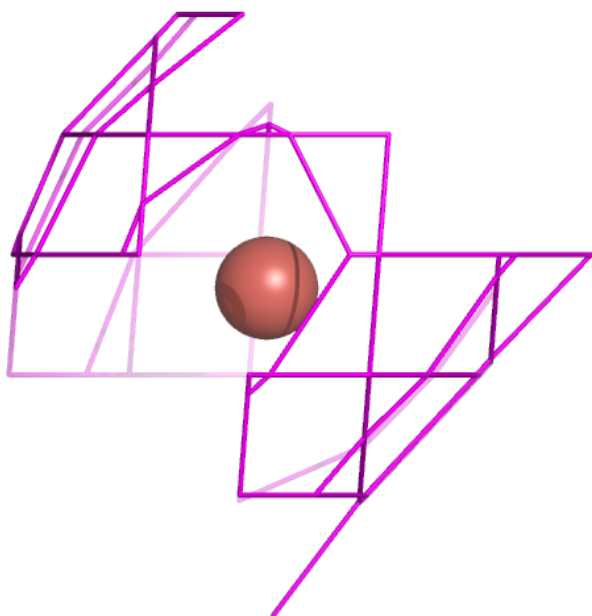
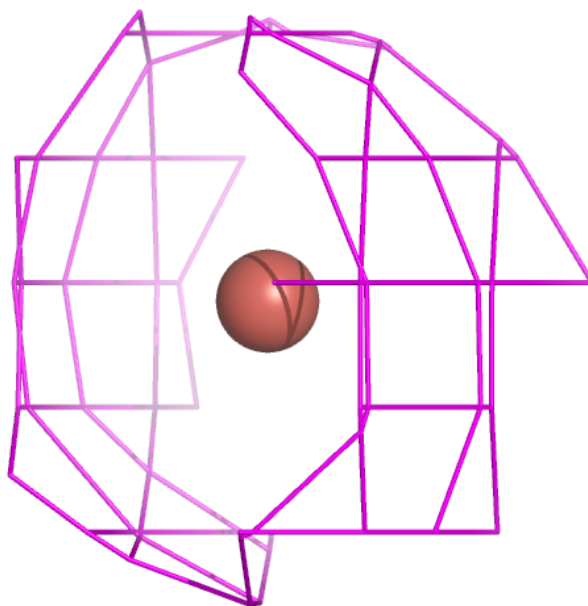
Electron density around TL A 307:

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



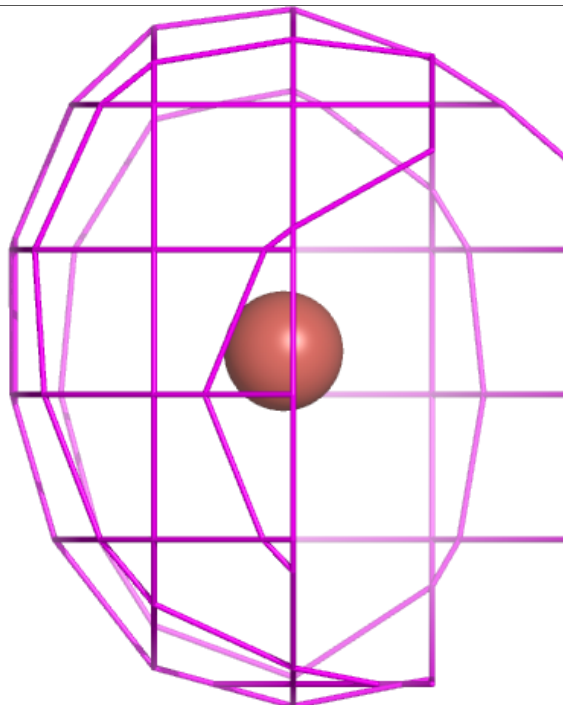
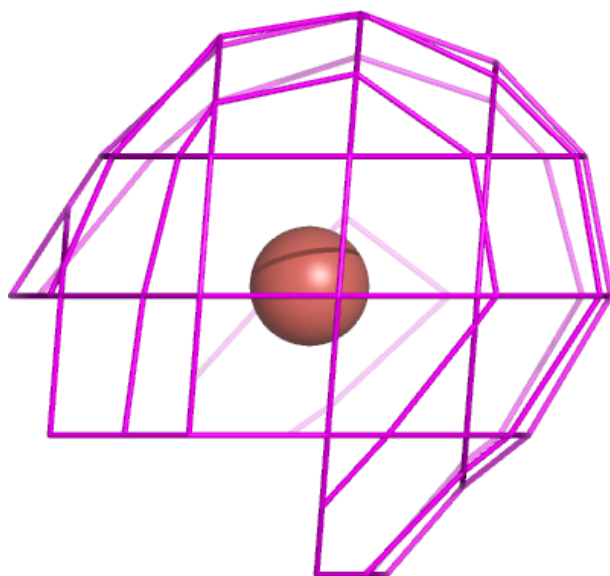
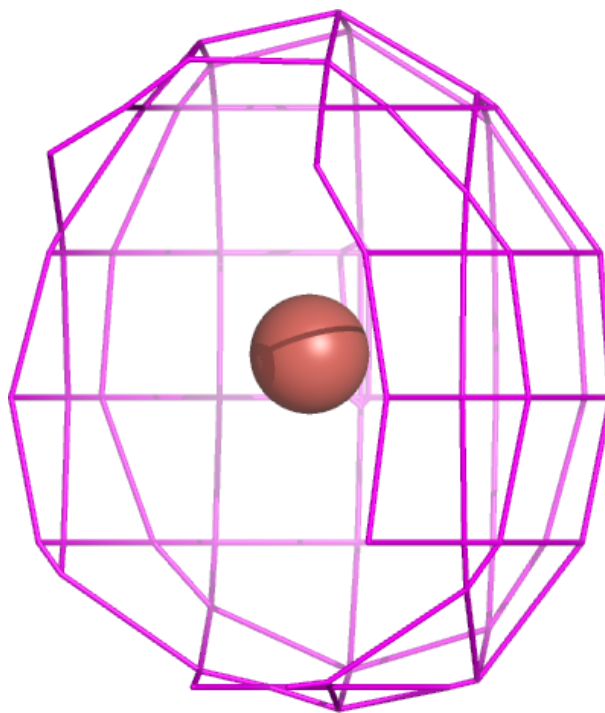
Electron density around TL A 305:

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



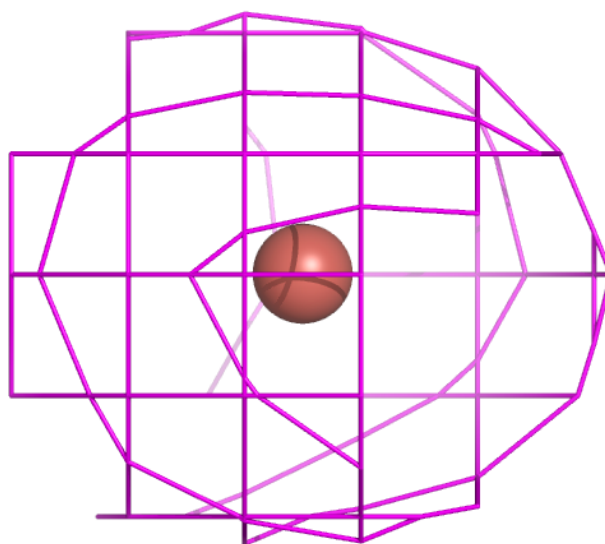
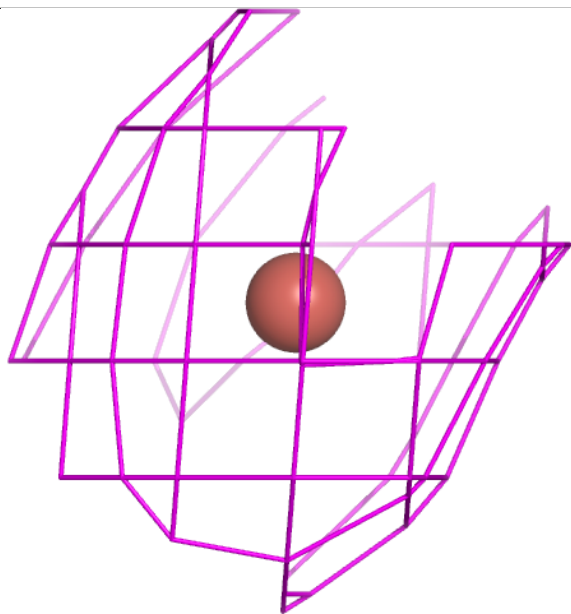
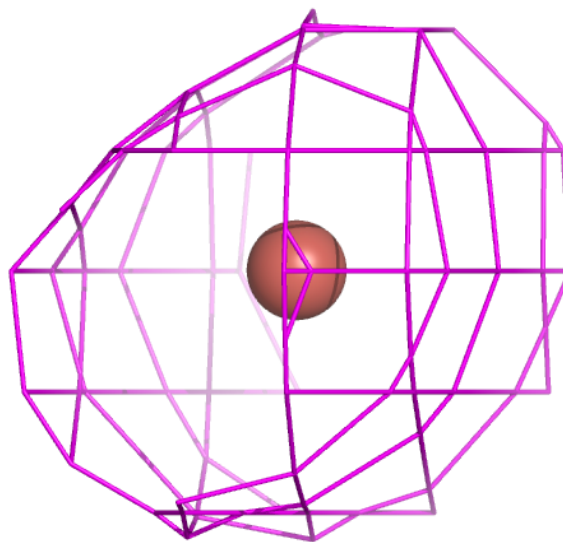
Electron density around TL B 301:

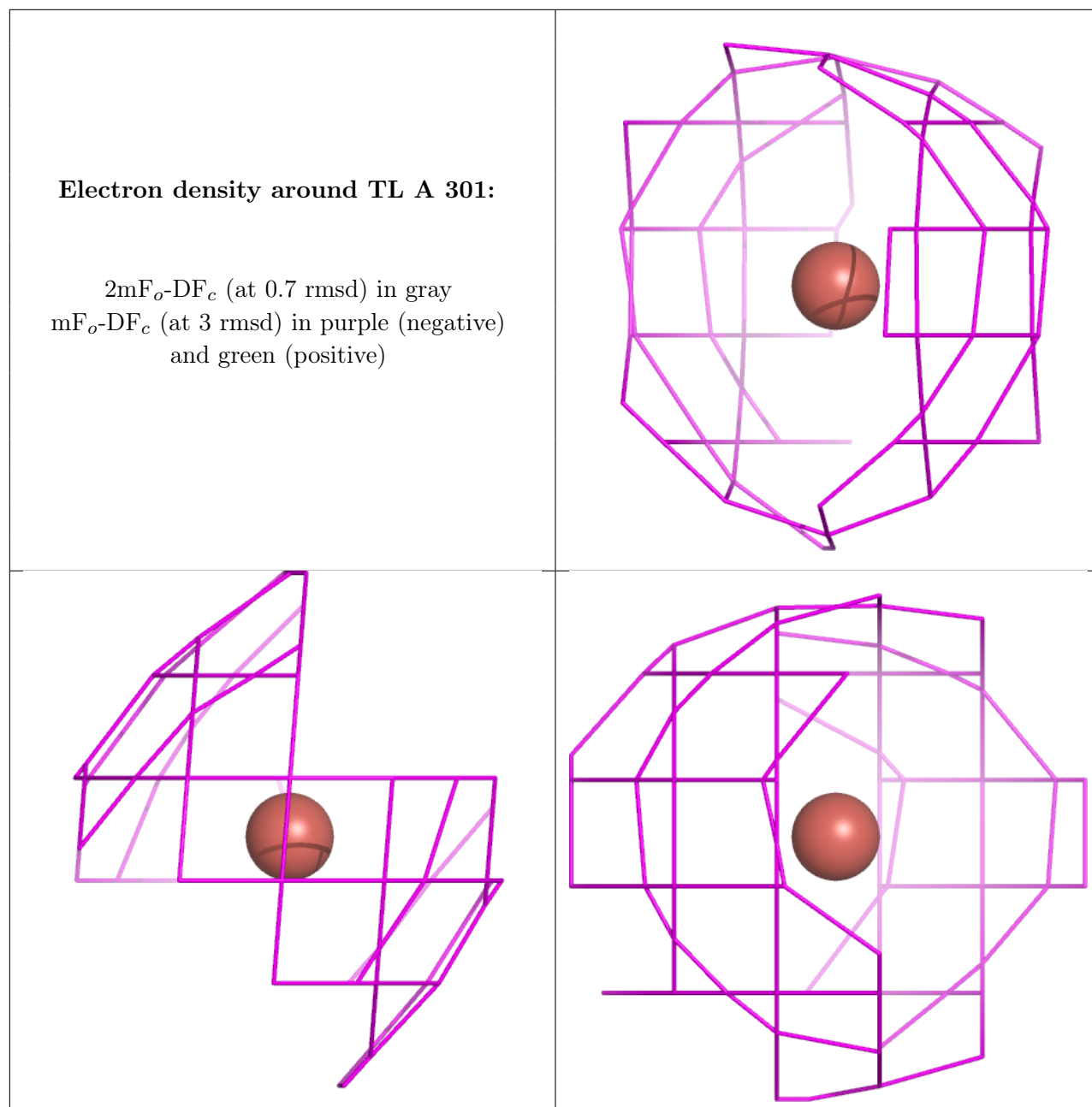
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around TL A 302:

$2mF_o-DF_c$ (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.