wwPDB X-ray Structure Validation Summary Report (i)

Jan 24, 2023 – 03:21 pm GMT

PDB ID	:	8A7X
Title	:	NaK C-DI F92A mutant soaked in Cs+
Authors	:	Minniberger, S.; Plested, A.J.R.
Deposited on	:	2022-06-21
Resolution	:	2.10 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

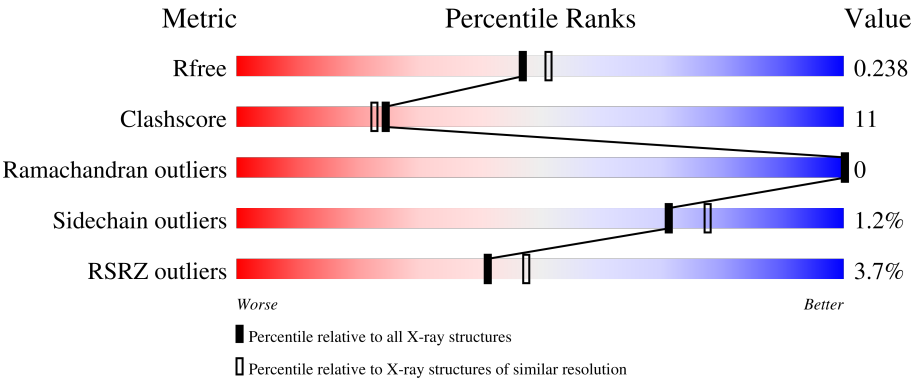
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.3
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 <=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	96	4% 76% 20% .
1	B	96	3% 84% 14% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CS	B	203	-	-	-	X
3	MPD	B	212	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3415 atoms, of which 1780 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 Potassium channel protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	92	Total	C	H	N	O	S	0	0	0
			1459	478	748	105	127	1			
1	B	95	Total	C	H	N	O	S	0	1	0
			1522	496	780	113	132	1			

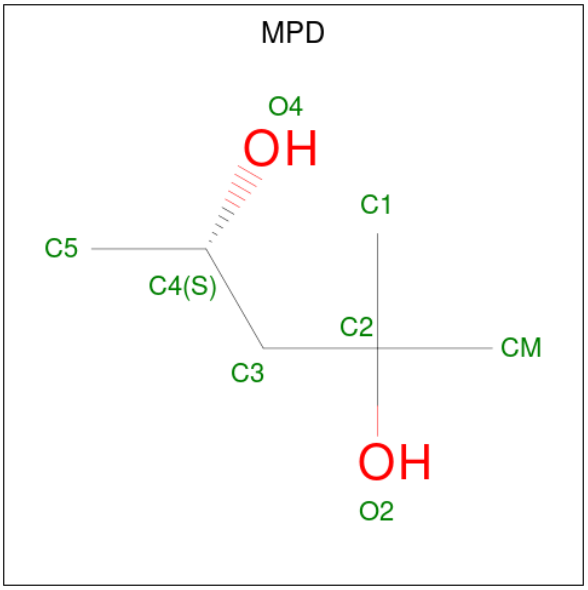
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	MET	-	initiating methionine	UNP Q81HW2
A	66	CYS	ASP	engineered mutation	UNP Q81HW2
A	?	-	GLY	deletion	UNP Q81HW2
A	67	ASP	ASN	engineered mutation	UNP Q81HW2
A	68	ILE	PHE	engineered mutation	UNP Q81HW2
A	91	ALA	PHE	engineered mutation	UNP Q81HW2
A	110	LEU	-	expression tag	UNP Q81HW2
A	111	VAL	-	expression tag	UNP Q81HW2
A	112	PRO	-	expression tag	UNP Q81HW2
A	113	ARG	-	expression tag	UNP Q81HW2
B	18	MET	-	initiating methionine	UNP Q81HW2
B	66	CYS	ASP	engineered mutation	UNP Q81HW2
B	?	-	GLY	deletion	UNP Q81HW2
B	67	ASP	ASN	engineered mutation	UNP Q81HW2
B	68	ILE	PHE	engineered mutation	UNP Q81HW2
B	91	ALA	PHE	engineered mutation	UNP Q81HW2
B	110	LEU	-	expression tag	UNP Q81HW2
B	111	VAL	-	expression tag	UNP Q81HW2
B	112	PRO	-	expression tag	UNP Q81HW2
B	113	ARG	-	expression tag	UNP Q81HW2

- Molecule 2 is CESIUM ION (three-letter code: CS) (formula: Cs) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cs 2 2	0	1
2	B	3	Total Cs 3 3	0	0

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C H O 22 6 14 2	0	0
3	A	1	Total C H O 22 6 14 2	0	0
3	A	1	Total C H O 22 6 14 2	0	0
3	A	1	Total C H O 22 6 14 2	0	0
3	A	1	Total C H O 22 6 14 2	0	0
3	A	1	Total C H O 22 6 14 2	0	0
3	A	1	Total C H O 22 6 14 2	0	0
3	B	1	Total C H O 22 6 14 2	0	0
3	B	1	Total C H O 22 6 14 2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
3	B	1	22	6	14	2	0	0
3	B	1	22	6	14	2	0	0
3	B	1	22	6	14	2	0	0
3	B	1	22	6	14	2	0	0
3	B	1	22	6	14	2	0	0
3	B	1	22	6	14	2	0	0
3	B	1	22	6	14	2	0	0
3	B	1	22	6	14	2	0	0
3	B	1	22	6	14	2	0	0

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	K		
4	A	4	4	4	0	0
4	B	1	1	1	0	0

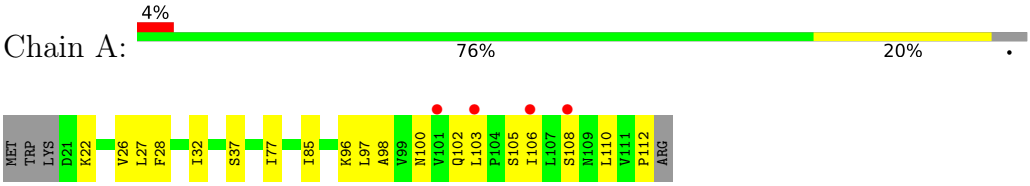
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	15	15	15	0	0
5	B	13	13	13	0	0

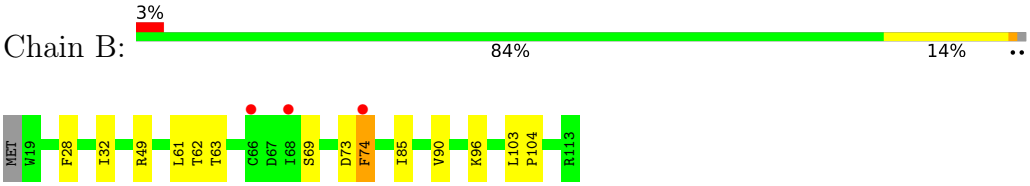
3 Residue-property plots (i)

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: Potassium channel protein



• Molecule 1: Potassium channel protein



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α, β, γ	68.16Å 68.16Å 90.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.12 – 2.10 45.12 – 2.10	Depositor EDS
% Data completeness (in resolution range)	96.1 (45.12-2.10) 98.7 (45.12-2.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.41 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.197 , 0.240 0.201 , 0.238	Depositor DCC
R_{free} test set	598 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	50.3	Xtriage
Anisotropy	0.217	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 76.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.063 for -h,k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	3415	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.11% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MPD, CS, K

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	0.63	0/726	0.80	1/992 (0.1%)
1	B	0.53	0/757	0.67	0/1032
All	All	0.58	0/1483	0.74	1/2024 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	27	LEU	CB-CG-CD2	5.96	121.13	111.00

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	711	748	747	14	0
1	B	742	780	779	9	1
2	A	2	0	0	0	0
2	B	3	0	0	0	0
3	A	56	98	98	8	0
3	B	88	154	154	15	0
4	A	4	0	0	0	0
4	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	15	0	0	1	0
5	B	13	0	0	1	0
All	All	1635	1780	1778	37	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 11.

The worst 5 of 37 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:96:LYS:NZ	5:B:301:HOH:O	2.24	0.71
1:A:22:LYS:O	1:A:26:VAL:HG23	1.90	0.70
3:B:214:MPD:H52	3:B:214:MPD:HM2	1.74	0.70
1:B:85:ILE:HD13	3:B:214:MPD:H13	1.75	0.67
3:A:207:MPD:H12	3:A:207:MPD:H52	1.79	0.65

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)
1:B:49:ARG:HH12	1:B:73:ASP:OD1[4_555]	1.58	0.02

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	90/96 (94%)	89 (99%)	1 (1%)	0	100	100
1	B	94/96 (98%)	93 (99%)	1 (1%)	0	100	100
All	All	184/192 (96%)	182 (99%)	2 (1%)	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	82/86 (95%)	81 (99%)	1 (1%)	71 77
1	B	85/86 (99%)	84 (99%)	1 (1%)	71 77
All	All	167/172 (97%)	165 (99%)	2 (1%)	71 77

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	PRO
1	B	74	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 28 ligands modelled in this entry, 10 are monoatomic - leaving 18 for Mogul analysis.

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	$\#\|Z\| > 2$
3	MPD	A	203	-	7,7,7	1.34	0	9,10,10	0.59	0
3	MPD	B	211	-	7,7,7	0.97	0	9,10,10	0.64	0
3	MPD	A	207	-	7,7,7	0.90	0	9,10,10	0.56	0
3	MPD	A	202	4	7,7,7	0.92	0	9,10,10	0.85	0
3	MPD	B	214	-	7,7,7	1.04	0	9,10,10	0.51	0
3	MPD	B	206	-	7,7,7	1.21	1 (14%)	9,10,10	0.59	0
3	MPD	B	204	-	7,7,7	1.24	0	9,10,10	0.55	0
3	MPD	B	213	-	7,7,7	1.08	0	9,10,10	0.52	0
3	MPD	A	206	-	7,7,7	1.38	1 (14%)	9,10,10	0.68	0
3	MPD	A	204	-	7,7,7	1.01	0	9,10,10	0.39	0
3	MPD	B	207	-	7,7,7	1.20	0	9,10,10	0.71	0
3	MPD	B	209	-	7,7,7	1.04	0	9,10,10	0.81	0
3	MPD	B	205	-	7,7,7	1.14	0	9,10,10	0.79	0
3	MPD	B	212	-	7,7,7	1.10	0	9,10,10	0.42	0
3	MPD	B	208	-	7,7,7	1.07	0	9,10,10	0.51	0
3	MPD	A	205	-	7,7,7	0.97	0	9,10,10	0.61	0
3	MPD	B	210	-	7,7,7	0.98	0	9,10,10	0.46	0
3	MPD	A	208	-	7,7,7	1.02	0	9,10,10	0.65	0

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
3	MPD	A	203	-	-	1/5/5/5	-
3	MPD	B	211	-	-	3/5/5/5	-
3	MPD	A	207	-	-	2/5/5/5	-
3	MPD	A	202	4	-	1/5/5/5	-
3	MPD	B	214	-	-	2/5/5/5	-
3	MPD	B	206	-	-	0/5/5/5	-
3	MPD	B	204	-	-	2/5/5/5	-
3	MPD	B	213	-	-	2/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MPD	A	206	-	-	4/5/5/5	-
3	MPD	A	204	-	-	1/5/5/5	-
3	MPD	B	207	-	-	3/5/5/5	-
3	MPD	B	209	-	-	2/5/5/5	-
3	MPD	B	205	-	-	0/5/5/5	-
3	MPD	B	212	-	-	2/5/5/5	-
3	MPD	B	208	-	-	1/5/5/5	-
3	MPD	A	205	-	-	1/5/5/5	-
3	MPD	B	210	-	-	5/5/5/5	-
3	MPD	A	208	-	-	4/5/5/5	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	206	MPD	O2-C2	-2.04	1.39	1.44
3	B	206	MPD	C1-C2	2.01	1.58	1.52

There are no bond angle outliers.

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	206	MPD	O2-C2-C3-C4
3	A	206	MPD	CM-C2-C3-C4
3	A	206	MPD	C2-C3-C4-O4
3	B	207	MPD	C2-C3-C4-O4
3	B	209	MPD	C2-C3-C4-O4

There are no ring outliers.

12 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	207	MPD	2	0
3	B	214	MPD	5	0
3	B	204	MPD	1	0
3	A	206	MPD	1	0
3	A	204	MPD	1	0
3	B	207	MPD	2	0
3	B	209	MPD	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	205	MPD	2	0
3	B	208	MPD	3	0
3	A	205	MPD	1	0
3	B	210	MPD	1	0
3	A	208	MPD	3	0

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, 95^{th} 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	92/96 (95%)	0.31	4 (4%)	35	41	33, 49, 104, 122	0
1	B	95/96 (98%)	0.17	3 (3%)	47	54	35, 54, 98, 122	0
All	All	187/192 (97%)	0.24	7 (3%)	41	48	33, 52, 102, 122	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	108	SER	6.7
1	B	74	PHE	4.2
1	B	66	CYS	4.2
1	A	106	ILE	3.6
1	B	68	ILE	3.2

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

There are no monosaccharides in this entry.

6.4 Ligands

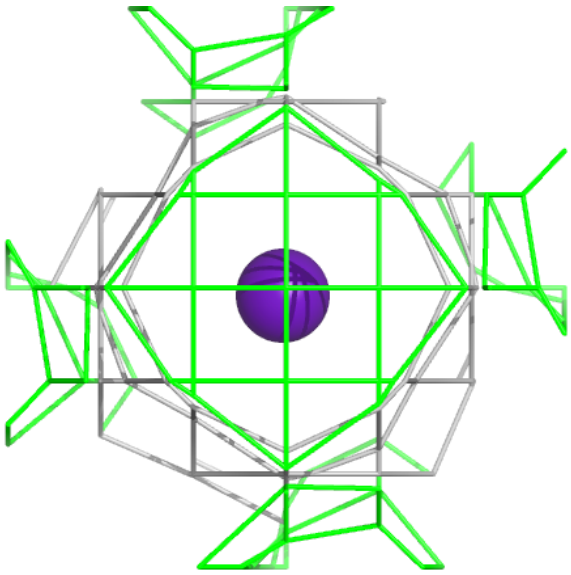
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

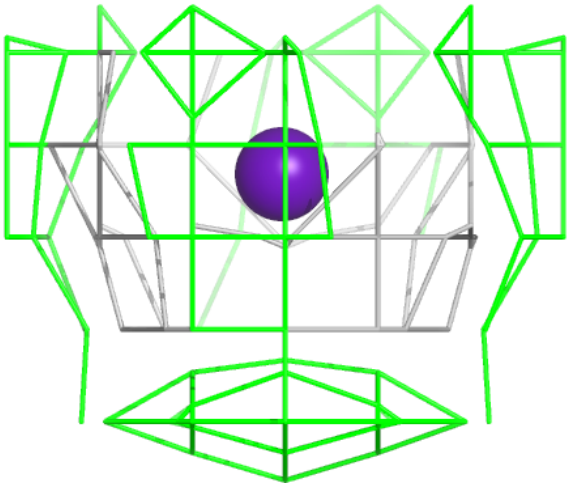
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CS	B	203	1/1	-0.31	0.73	112,112,112,112	1
3	MPD	A	206	8/8	0.44	0.39	94,121,141,142	0
3	MPD	B	209	8/8	0.70	0.37	84,109,120,131	0
4	K	A	209	1/1	0.71	0.35	75,75,75,75	1
3	MPD	B	211	8/8	0.72	0.39	76,100,130,130	0
3	MPD	B	207	8/8	0.74	0.24	87,116,126,128	0
3	MPD	B	212	8/8	0.77	0.52	87,113,136,136	0
3	MPD	A	203	8/8	0.77	0.26	66,94,113,113	0
3	MPD	B	214	8/8	0.81	0.40	81,97,116,116	0
3	MPD	B	206	8/8	0.82	0.35	76,92,106,110	0
3	MPD	B	213	8/8	0.83	0.45	65,93,108,108	0
3	MPD	A	208	8/8	0.84	0.51	77,106,126,130	0
3	MPD	B	208	8/8	0.85	0.53	92,122,139,139	0
3	MPD	A	205	8/8	0.90	0.35	61,86,103,106	0
3	MPD	A	207	8/8	0.90	0.52	68,98,105,129	0
3	MPD	B	205	8/8	0.91	0.23	42,61,85,90	0
3	MPD	B	210	8/8	0.93	0.28	69,93,108,131	0
3	MPD	A	204	8/8	0.93	0.24	75,92,115,115	0
3	MPD	B	204	8/8	0.94	0.14	65,81,98,99	0
3	MPD	A	202	8/8	0.94	0.11	64,90,118,118	0
4	K	B	215	1/1	0.96	0.24	64,64,64,64	1
2	CS	B	202	1/1	0.97	0.24	48,48,48,48	1
4	K	A	210	1/1	0.98	0.28	38,38,38,38	1
4	K	A	212	1/1	0.99	0.24	62,62,62,62	0
4	K	A	211	1/1	0.99	0.15	65,65,65,65	1
2	CS	A	201[B]	1/1	1.00	0.26	30,30,30,30	1
2	CS	B	201	1/1	1.00	0.30	53,53,53,53	1
2	CS	A	201[A]	1/1	1.00	0.26	31,31,31,31	1

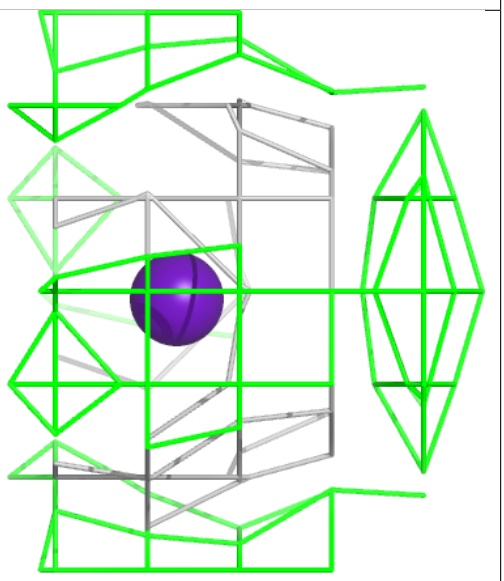
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around CS B 203:

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

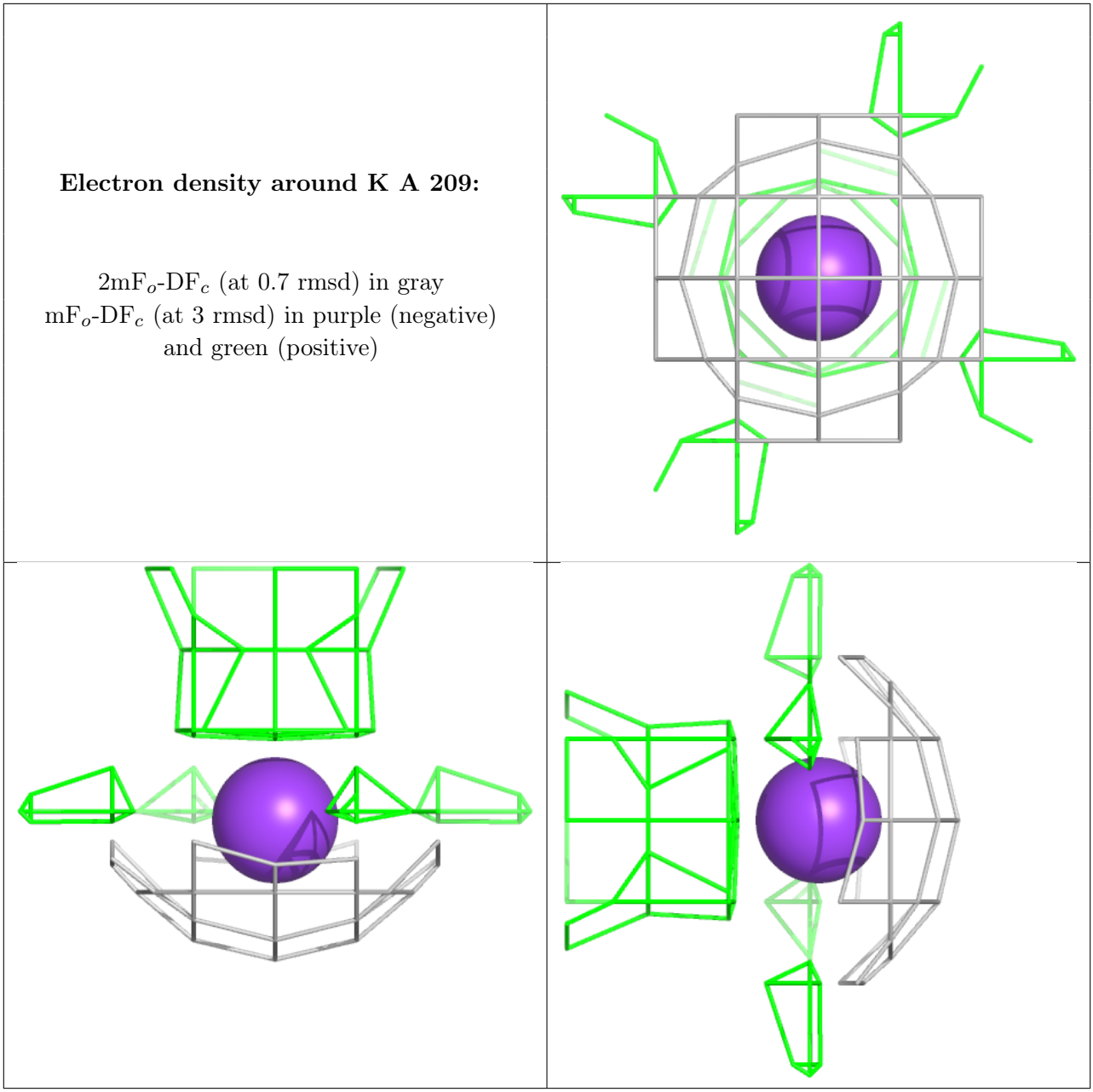






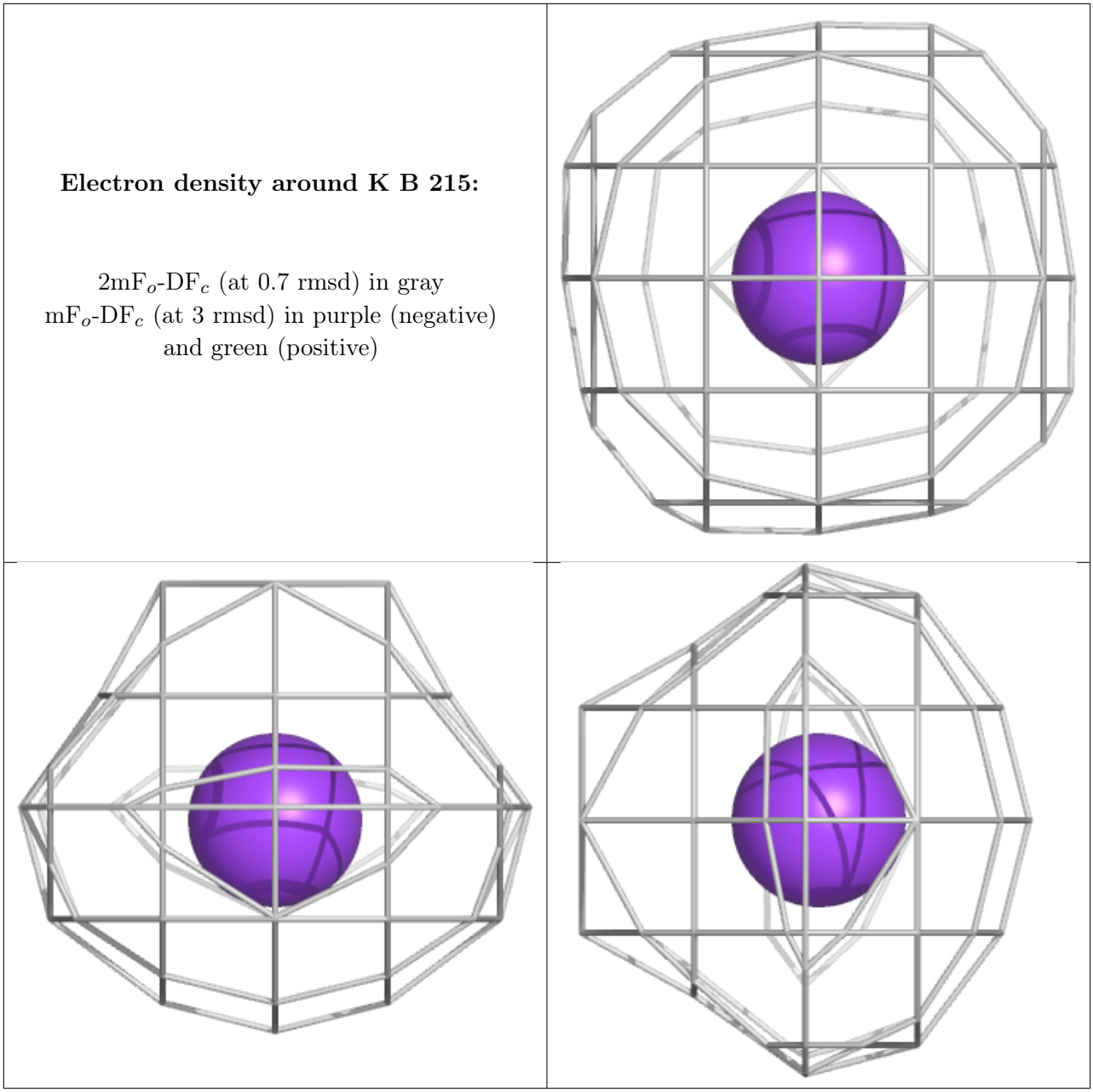
Electron density around K A 209:

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



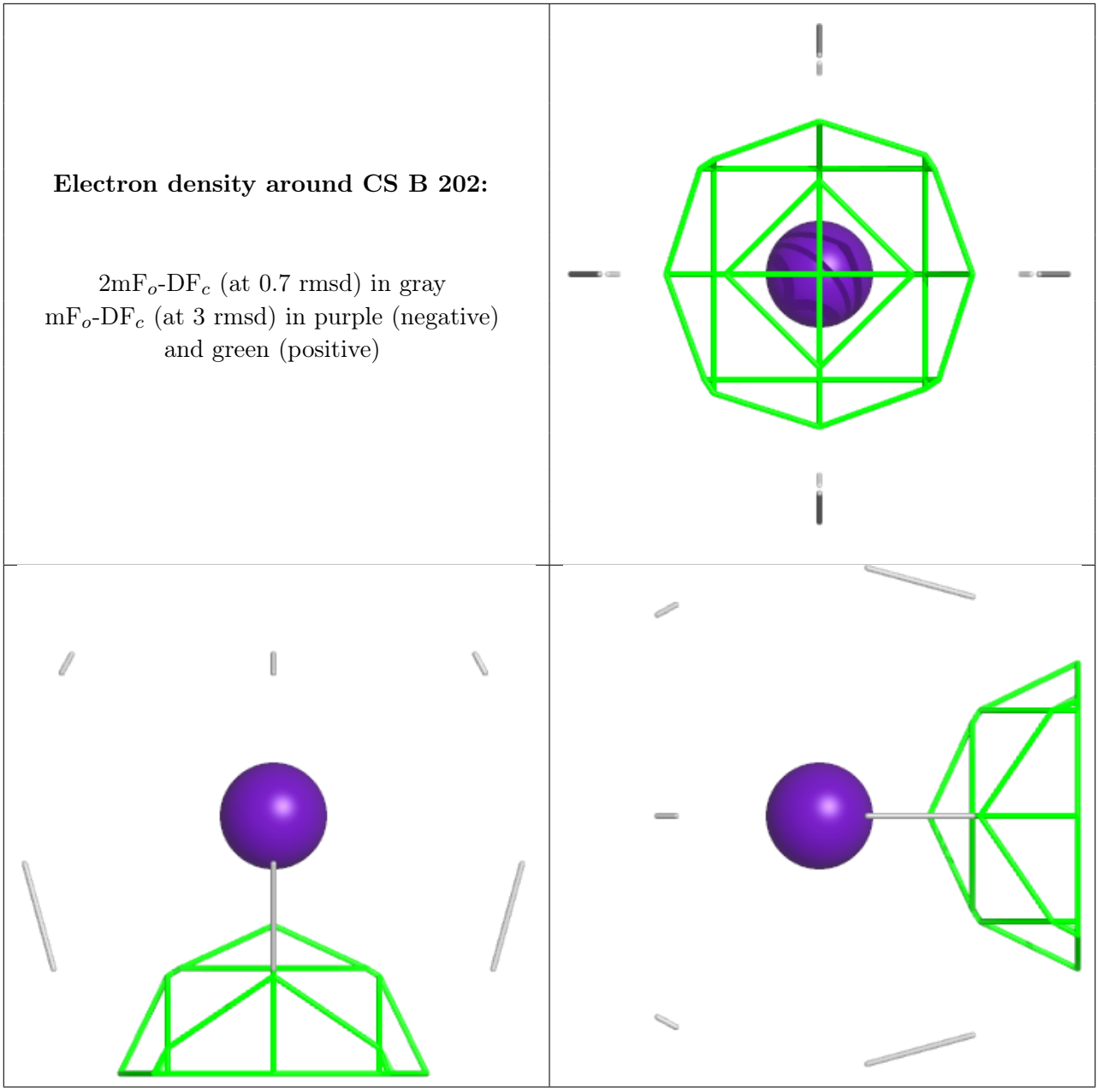
Electron density around K B 215:

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



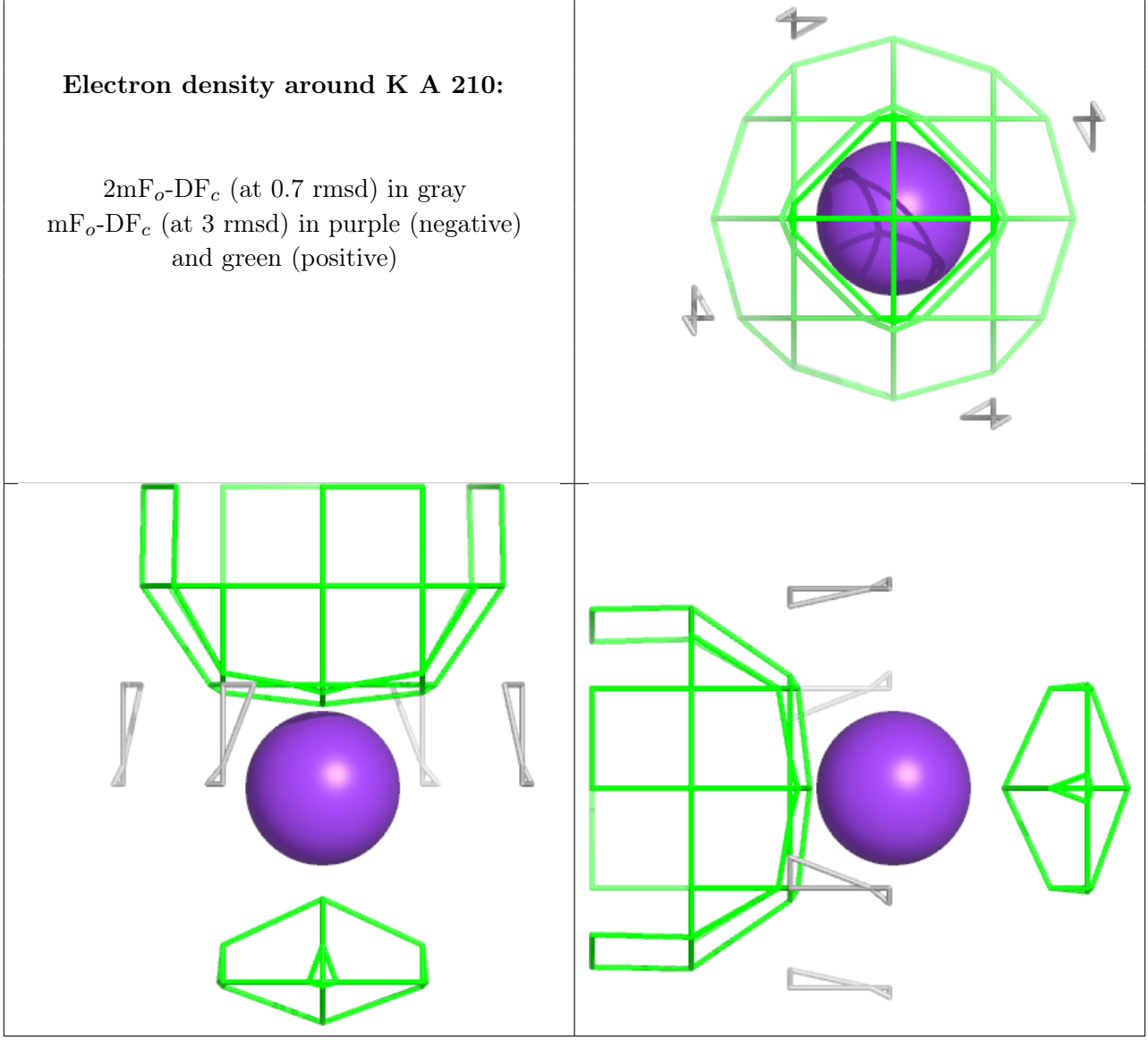
Electron density around CS B 202:

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



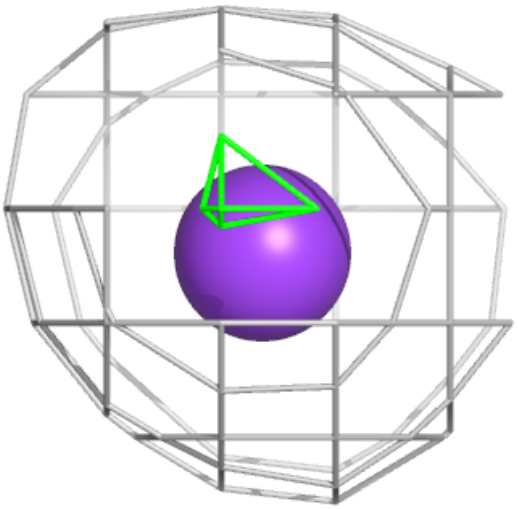
Electron density around K A 210:

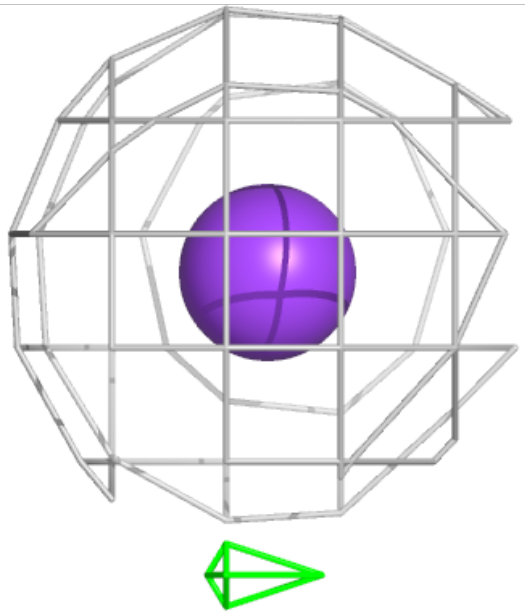
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

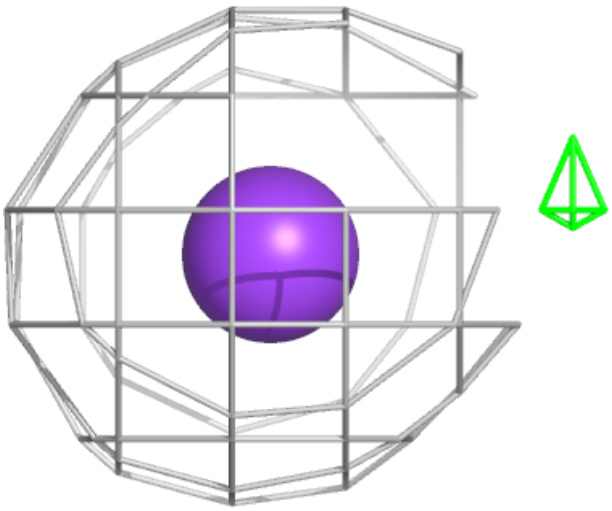


Electron density around K A 212:

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

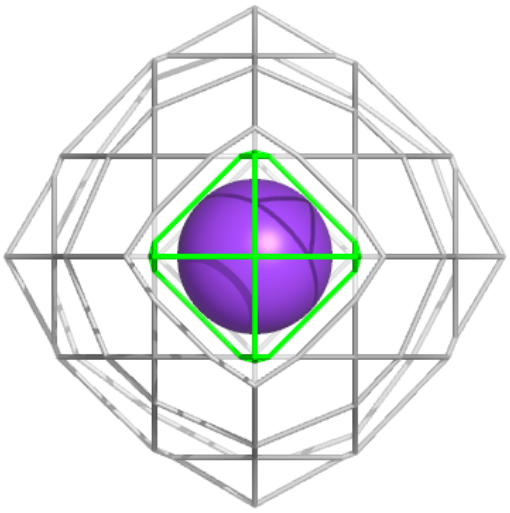


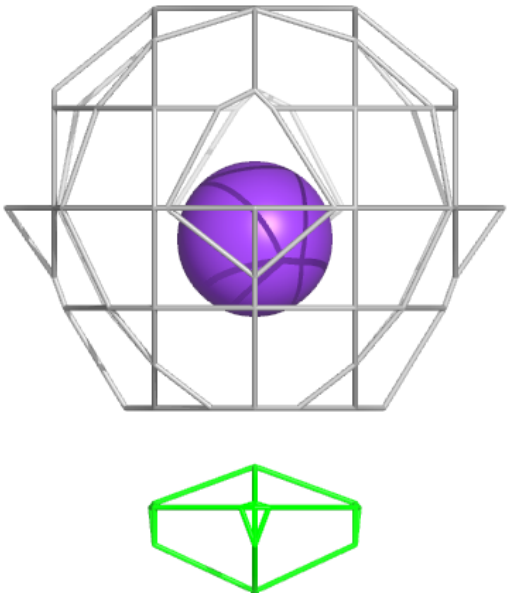


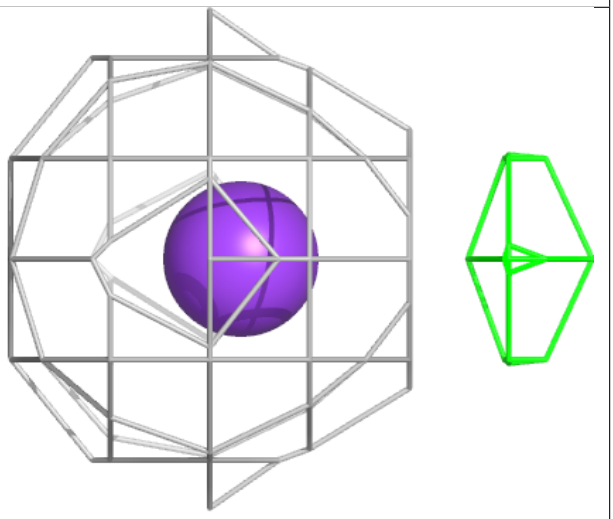


Electron density around K A 211:

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

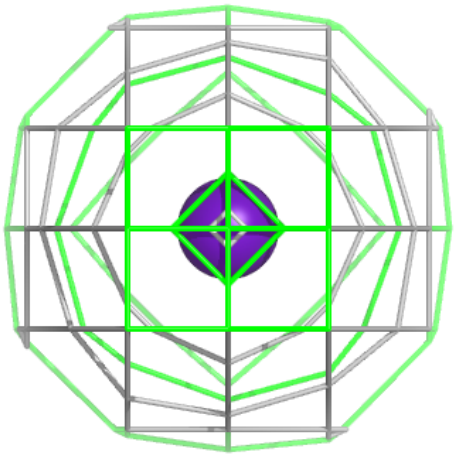


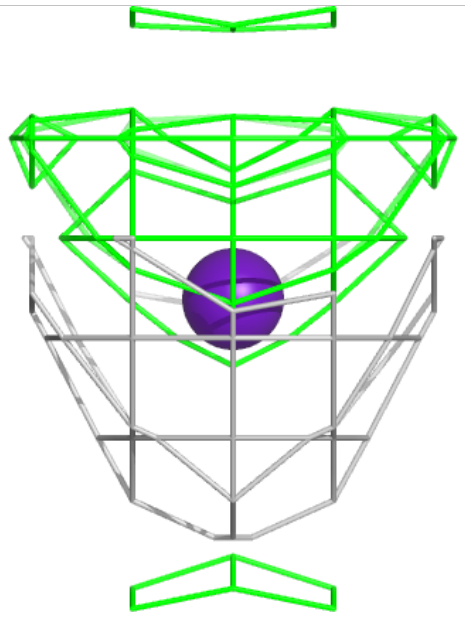


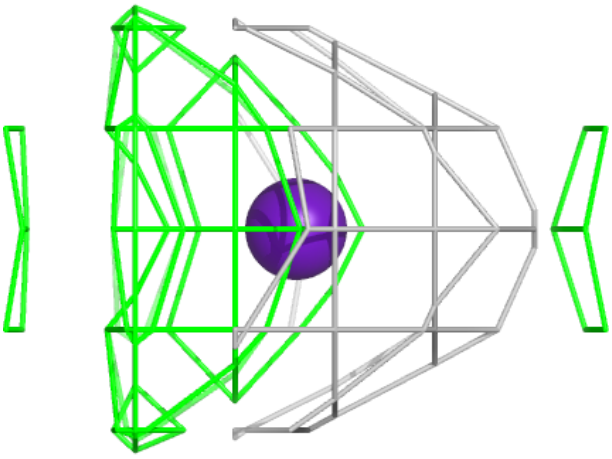


Electron density around CS A 201 (B):

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

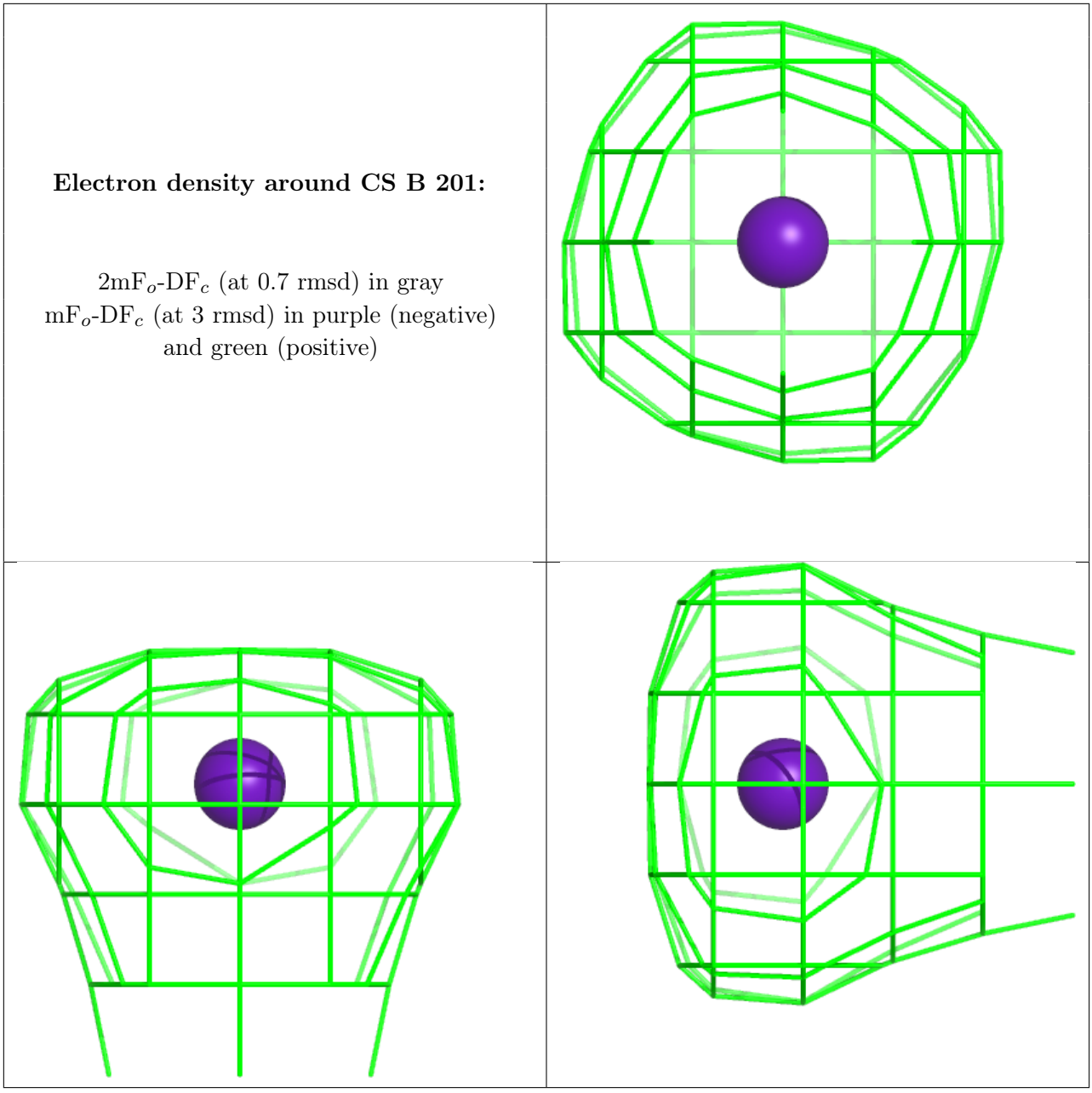






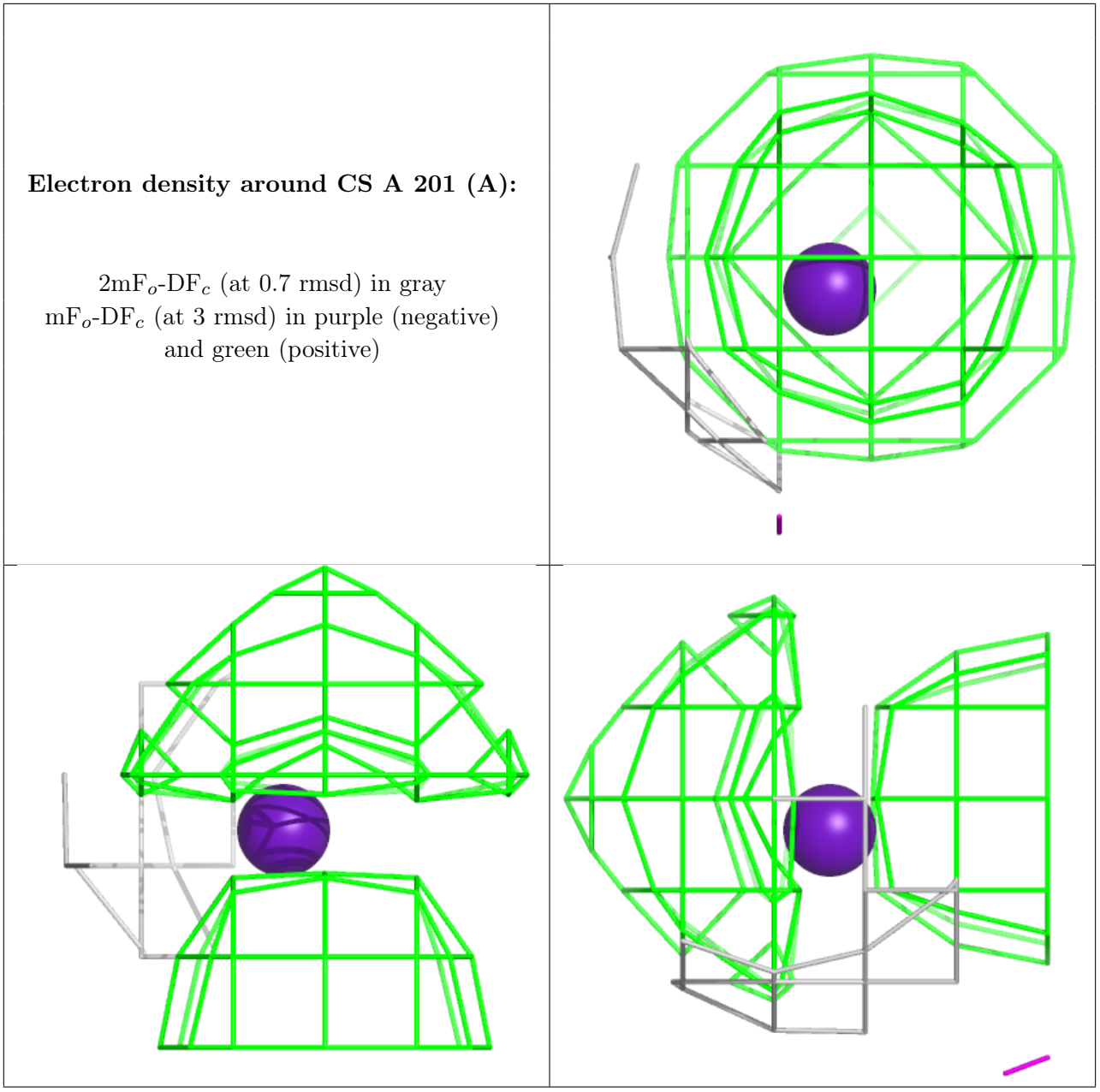
Electron density around CS B 201:

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



Electron density around CS A 201 (A):

$2mF_o$-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.