W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 3, 2021 – 05:04 pm GMT

PDB ID	:	7BCZ
Title	:	Structure of the 4'-phosphopantetheinyl transferase PcpS from Pseudomonas aeruginosa
Authors	:	Carivenc, C.; Mourey, L.; Pedelacq, J.D.
Deposited on	:	2020-12-21
Resolution	:	2.40 Å(reported)

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

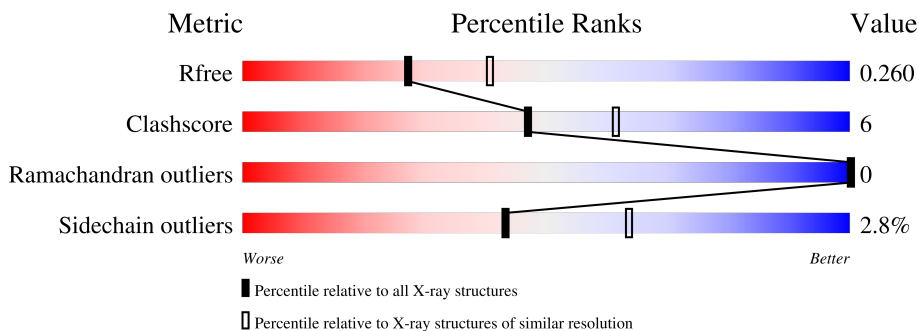|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4 (270009), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.40 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	Percentile Ranks	Value
Rfree		0.260
Clashscore		6
Ramachandran outliers		0
Sidechain outliers		2.8%

Worse   *Better*

▌ Percentile relative to all X-ray structures

◨ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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%

Mol	Chain	Length	Quality of chain
1	A	245	82% 15% ••
1	B	245	87% 9% ••
1	C	245	83% 13% • •
1	D	245	79% 19% ••

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 7843 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.
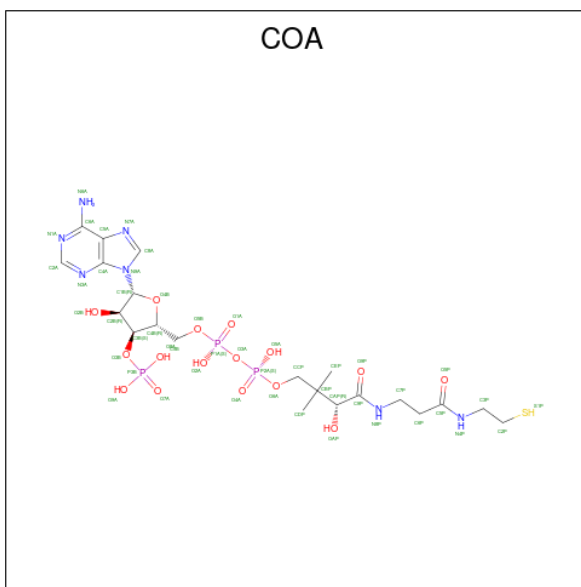
- Molecule 1 is a protein called 4'-phosphopantetheinyl transferase EntD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	242	Total	C	N	O	S	0	0	0
			1889	1204	349	332	4			
1	B	239	Total	C	N	O	S	0	0	0
			1855	1184	337	331	3			
1	C	238	Total	C	N	O	S	0	1	0
			1859	1187	344	325	3			
1	D	242	Total	C	N	O	S	0	0	0
			1885	1202	349	330	4			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP A0A6N0ZM94
A	-1	SER	-	expression tag	UNP A0A6N0ZM94
A	0	HIS	-	expression tag	UNP A0A6N0ZM94
B	-2	GLY	-	expression tag	UNP A0A6N0ZM94
B	-1	SER	-	expression tag	UNP A0A6N0ZM94
B	0	HIS	-	expression tag	UNP A0A6N0ZM94
C	-2	GLY	-	expression tag	UNP A0A6N0ZM94
C	-1	SER	-	expression tag	UNP A0A6N0ZM94
C	0	HIS	-	expression tag	UNP A0A6N0ZM94
D	-2	GLY	-	expression tag	UNP A0A6N0ZM94
D	-1	SER	-	expression tag	UNP A0A6N0ZM94
D	0	HIS	-	expression tag	UNP A0A6N0ZM94

- Molecule 2 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$) (labeled as "Ligand of Interest" by depositor).

COA

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	C	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	D	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total	Mg	0	0
			1	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	Na	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	41	Total 41	O 41	0	0
5	B	48	Total 48	O 48	0	0
5	C	44	Total 44	O 44	0	0
5	D	28	Total 28	O 28	0	0

3 Residue-property plots ⓘ

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. 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. 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: 4'-phosphopantetheinyl transferase EntD

Chain A:

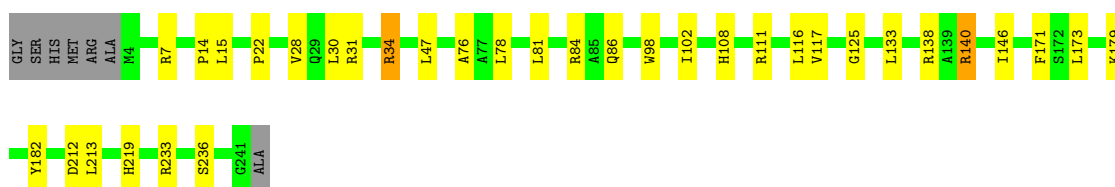• Molecule 1: 4'-phosphopantetheinyl transferase EntD

Chain B:
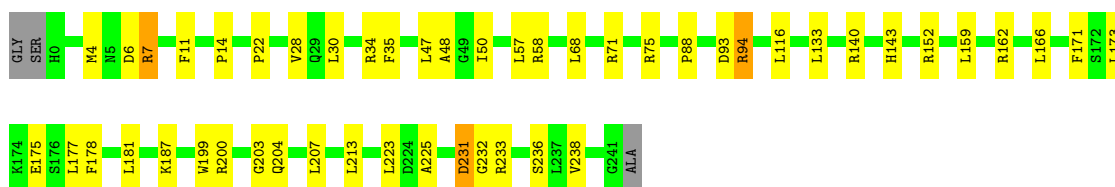
• Molecule 1: 4'-phosphopantetheinyl transferase EntD

Chain C:

• Molecule 1: 4'-phosphopantetheinyl transferase EntD

Chain D:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	44.36Å 78.87Å 81.12Å 85.62° 84.62° 73.86°	Depositor
Resolution (Å)	42.49 – 2.40 42.49 – 2.19	Depositor EDS
% Data completeness (in resolution range)	96.7 (42.49-2.40) 86.7 (42.49-2.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.29 (at 2.20Å)	Xtriage
Refinement program	PHENIX (1.17.1_3660: ???)	Depositor
R, R_{free}	0.210 , 0.262 0.211 , 0.260	Depositor DCC
R_{free} test set	2007 reflections (3.88%)	wwPDB-VP
Wilson B-factor (Å^2)	29.3	Xtriage
Anisotropy	0.611	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7843	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.15% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: MG, NA, COA

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	0.62	1/1933 (0.1%)	0.60	2/2626 (0.1%)
1	B	0.58	0/1898	0.57	0/2582
1	C	0.72	3/1902 (0.2%)	0.61	2/2585 (0.1%)
1	D	0.70	1/1929 (0.1%)	0.59	1/2621 (0.0%)
All	All	0.66	5/7662 (0.1%)	0.59	5/10414 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	213	LEU	C-O	-7.26	1.09	1.23
1	C	182	TYR	CE1-CZ	-5.65	1.31	1.38
1	D	236	SER	CB-OG	-5.56	1.35	1.42
1	C	125	GLY	C-O	-5.33	1.15	1.23
1	A	217	TRP	CE3-CZ3	-5.21	1.29	1.38

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	213	LEU	CA-CB-CG	5.82	128.68	115.30
1	C	140	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	D	47	LEU	CA-CB-CG	5.21	127.29	115.30
1	A	161	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	A	161	ARG	NE-CZ-NH1	5.10	122.85	120.30

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	1889	0	1900	29	0
1	B	1855	0	1852	15	0
1	C	1859	0	1869	18	1
1	D	1885	0	1895	41	1
2	A	48	0	32	1	0
2	B	48	0	32	1	0
2	C	48	0	32	1	0
2	D	48	0	32	1	0
3	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	41	0	0	2	0
5	B	48	0	0	1	0
5	C	44	0	0	2	0
5	D	28	0	0	1	0
All	All	7843	0	7644	95	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 6.

The worst 5 of 95 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:D:4:MET:HA	1:D:7:ARG:HH22	1.31	0.94
1:D:7:ARG:NE	1:D:7:ARG:HA	1.95	0.82
1:D:7:ARG:HA	1:D:7:ARG:HE	1.45	0.81
1:C:34:ARG:NH2	1:D:34:ARG:HD3	1.99	0.78
1:A:210:LEU:O	1:A:219:HIS:ND1	2.20	0.74

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:C:138:ARG:NH1	1:D:6:ASP:OD1[1_455]	2.16	0.04

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	240/245 (98%)	231 (96%)	9 (4%)	0	100	100
1	B	237/245 (97%)	230 (97%)	7 (3%)	0	100	100
1	C	237/245 (97%)	232 (98%)	5 (2%)	0	100	100
1	D	240/245 (98%)	226 (94%)	14 (6%)	0	100	100
All	All	954/980 (97%)	919 (96%)	35 (4%)	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	187/189 (99%)	180 (96%)	7 (4%)	34	53
1	B	183/189 (97%)	178 (97%)	5 (3%)	44	65
1	C	183/189 (97%)	179 (98%)	4 (2%)	52	71
1	D	186/189 (98%)	181 (97%)	5 (3%)	44	65
All	All	739/756 (98%)	718 (97%)	21 (3%)	43	63

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	108	HIS
1	D	57	LEU
1	D	231	ASP

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Mol	Chain	Res	Type
1	D	94	ARG
1	D	7	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	29	GLN
1	B	219	HIS

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 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand COA A 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand COA B 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand COA C 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand COA D 301	
 Bond lengths	 Bond angles
 Torsions	 Rings
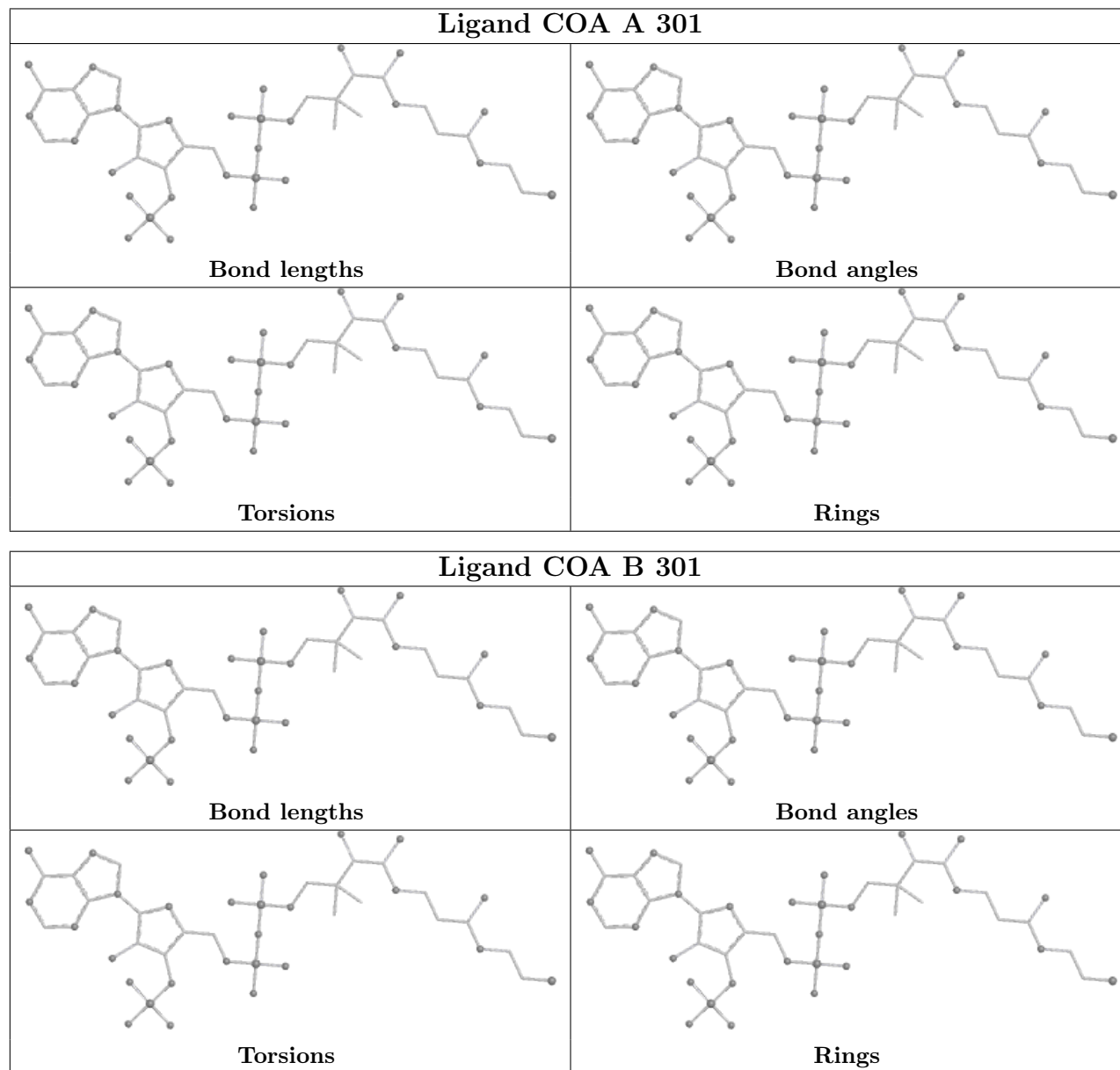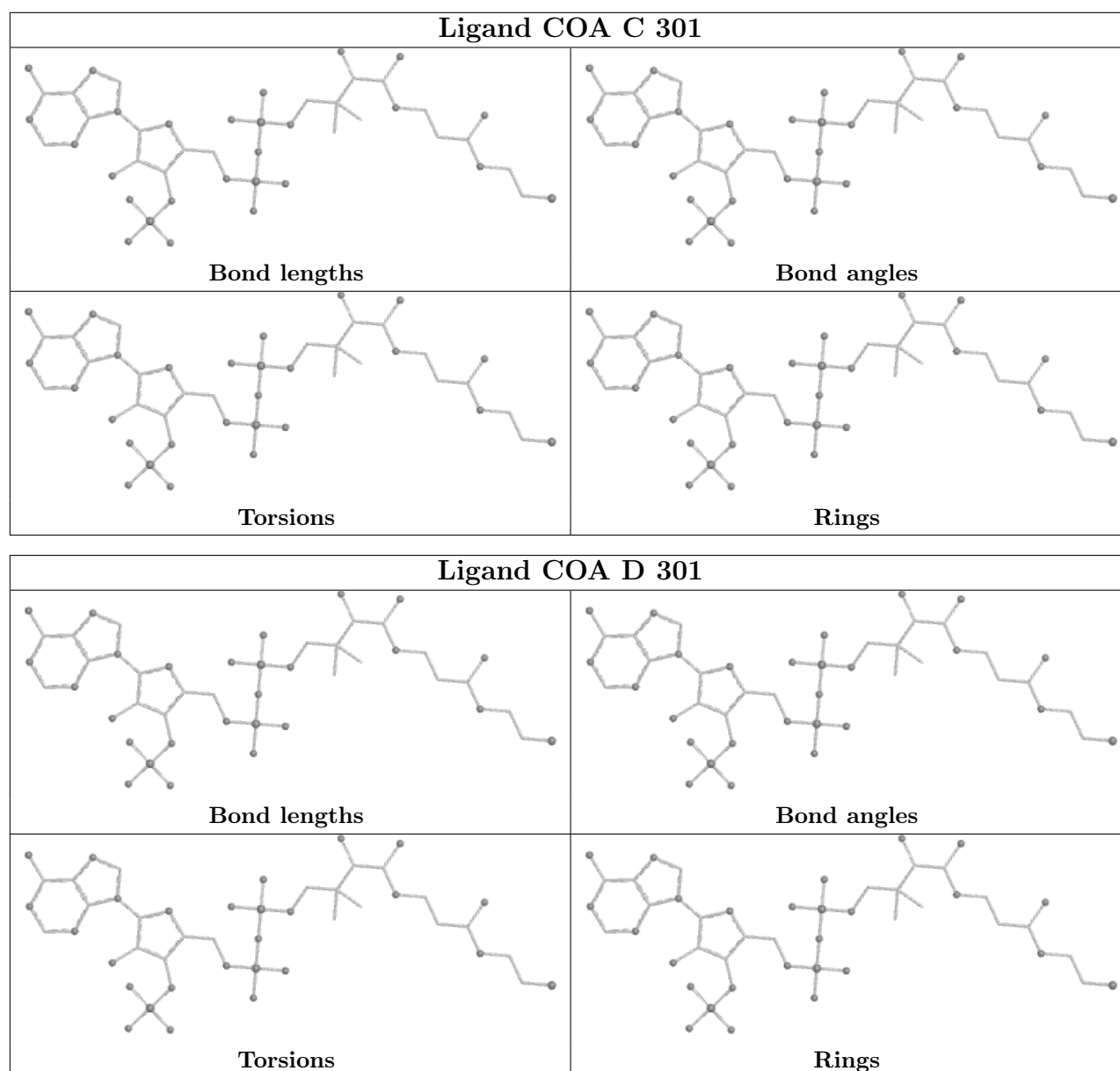
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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.
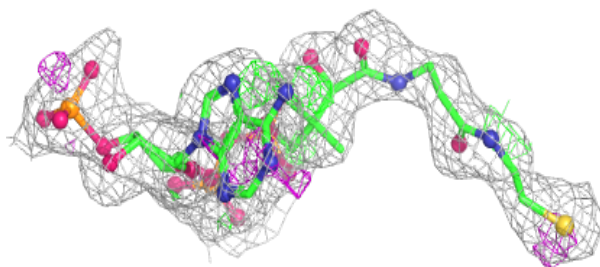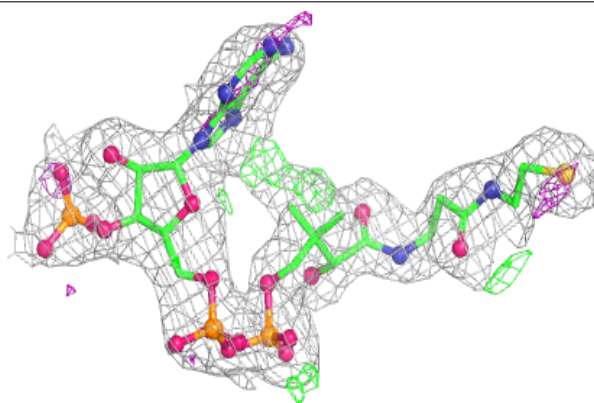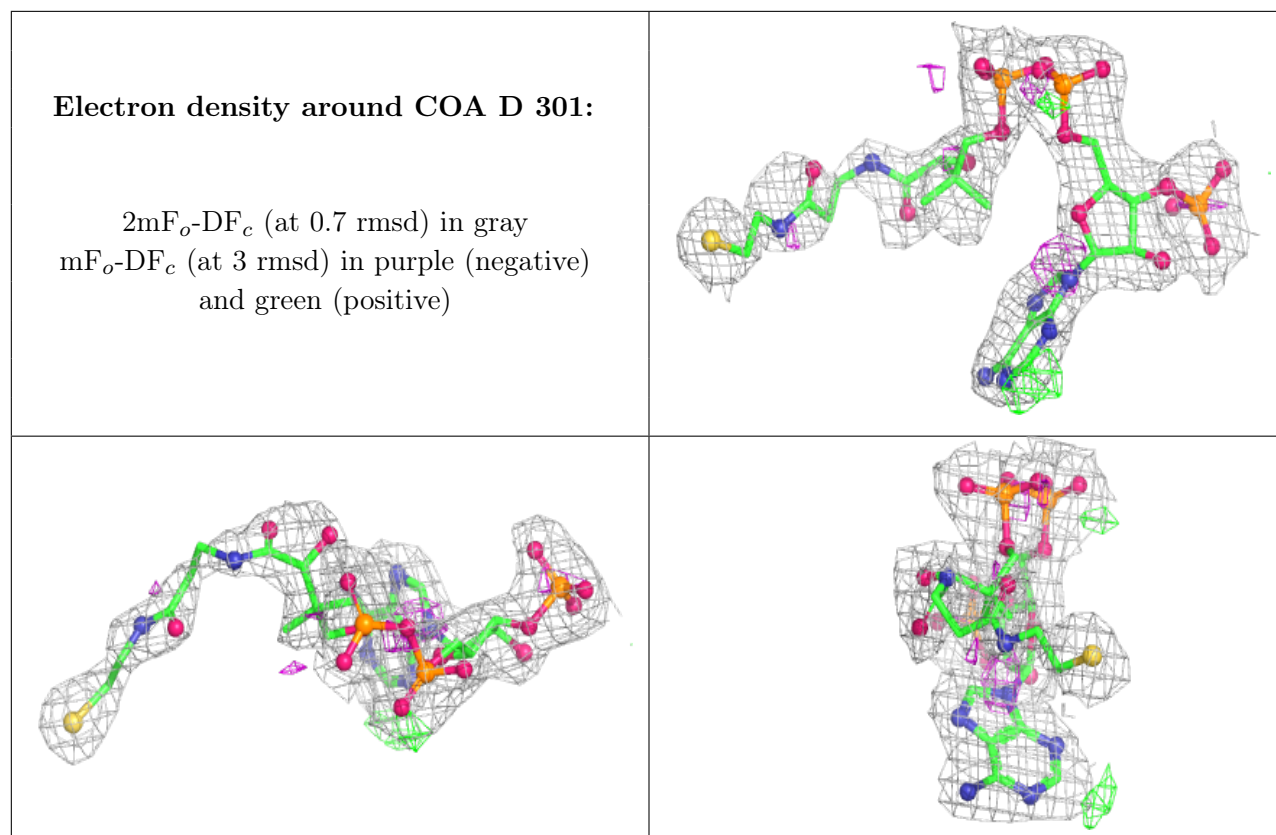
Electron density around COA A 301:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
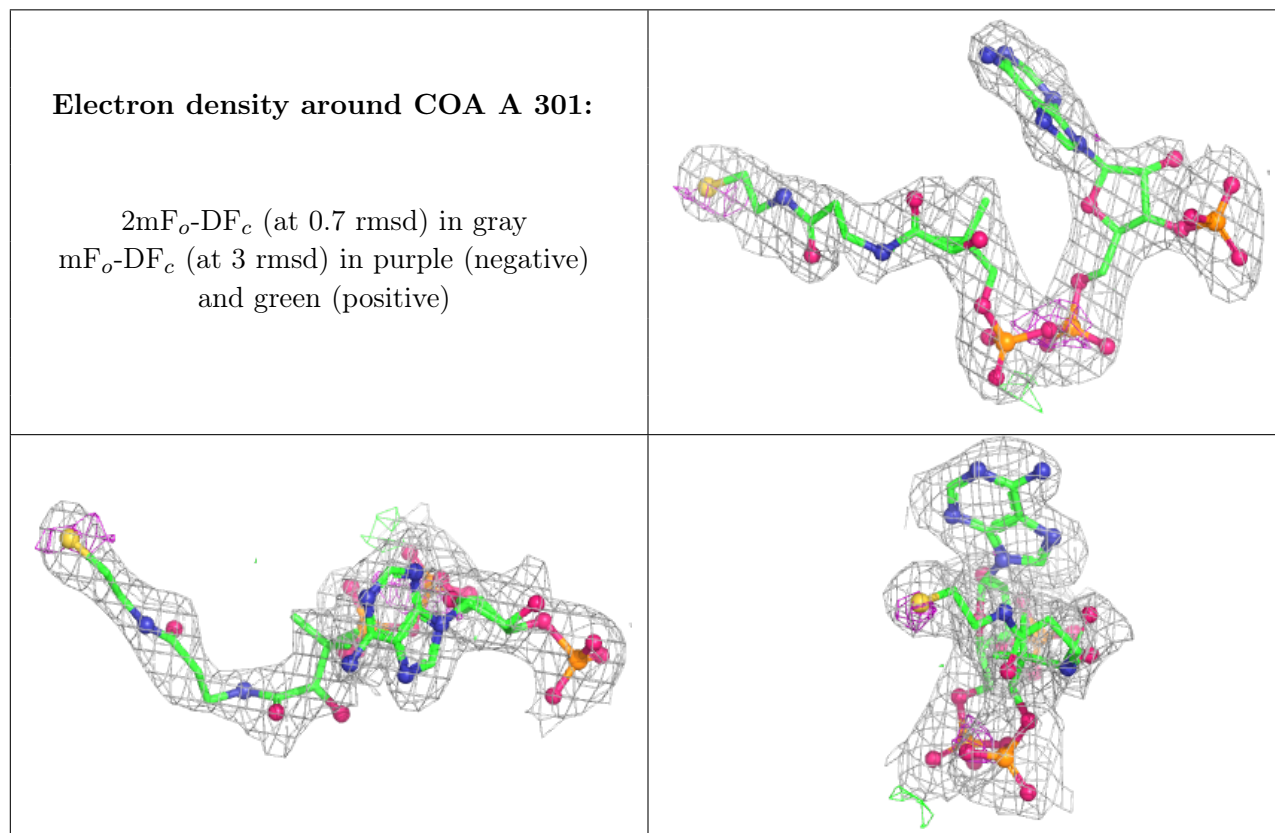
Electron density around COA B 301:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
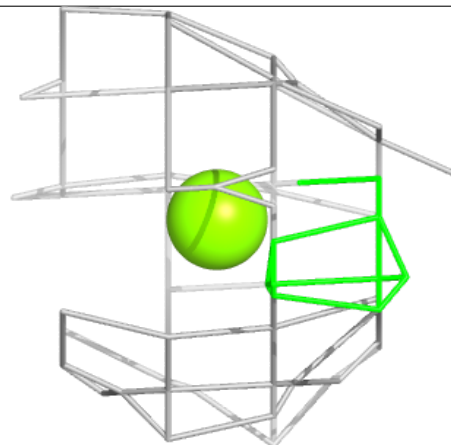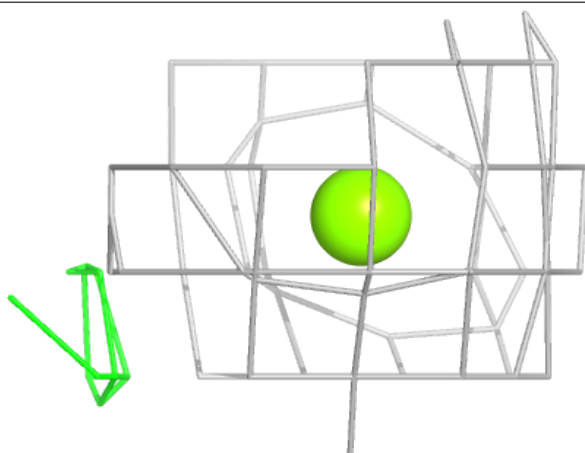and green (positive)
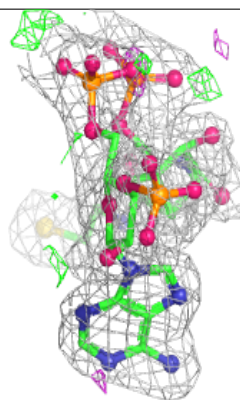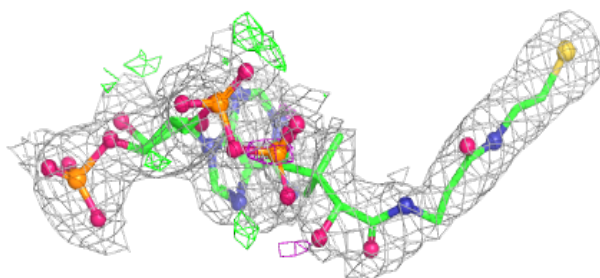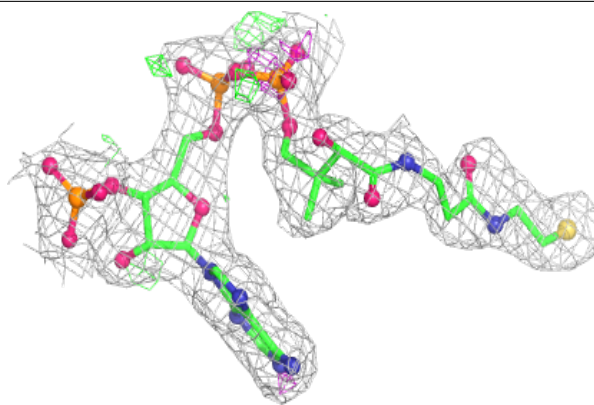
Electron density around COA C 301:

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

Electron density around COA D 301:

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

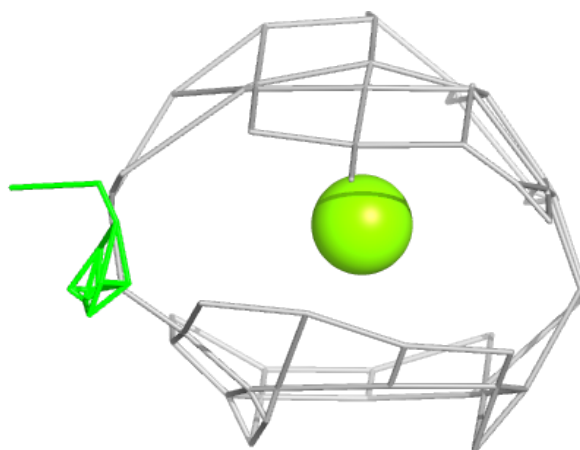**Electron density around MG C 302:**

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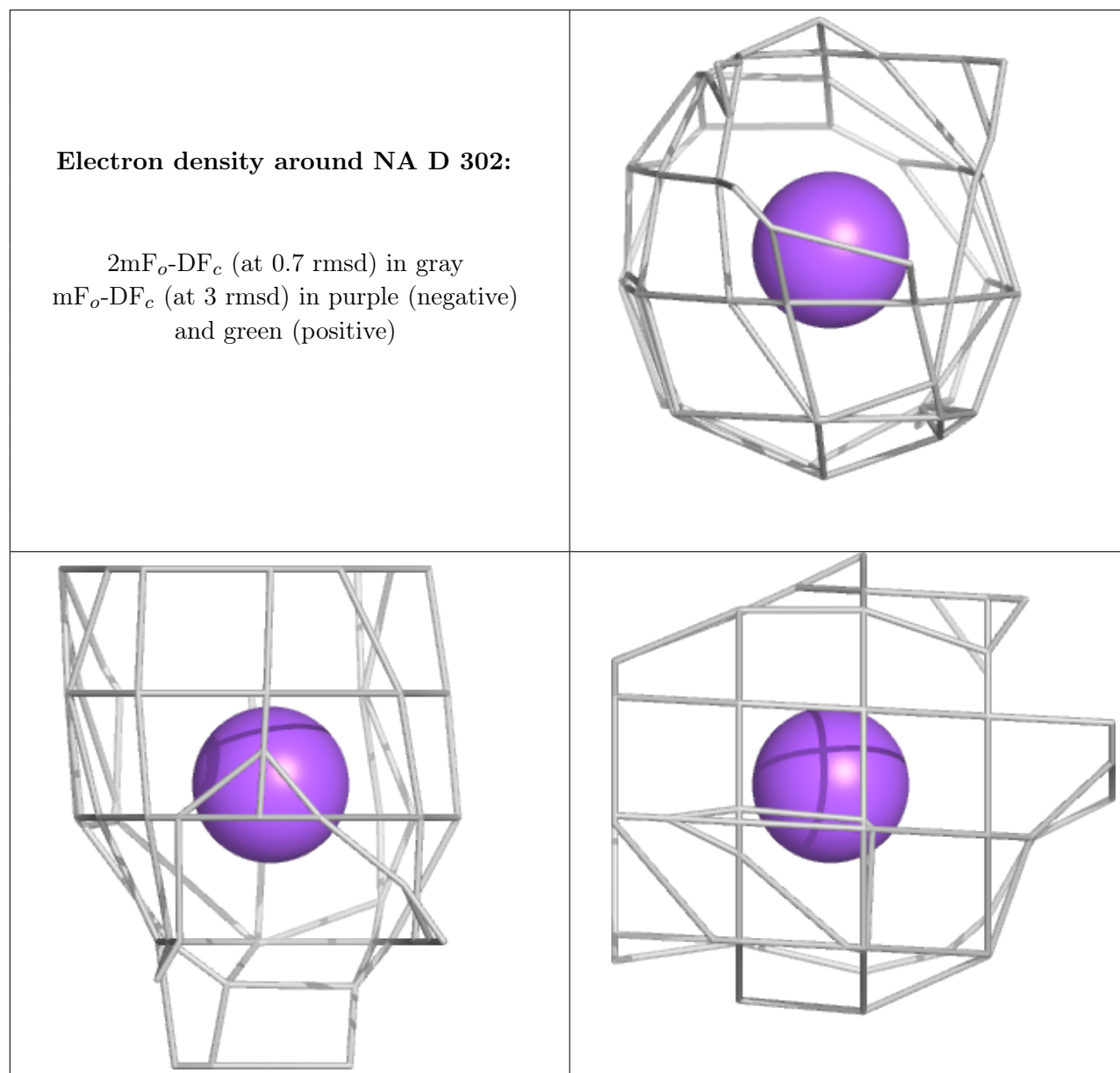mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around NA D 302:

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

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.