wwPDB X-ray Structure Validation Summary Report (i)

Jan 15, 2024 – 11:44 pm GMT

PDB ID	:	6XXG
Title	:	Structure of truncated 1-deoxy-D-xylulose 5-phosphate synthase (DXS) from Deinococcus radiodurans
Authors	:	Gierse, R.M.; Reddem, E.; Grooves, M.R.
Deposited on	:	2020-01-27
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:

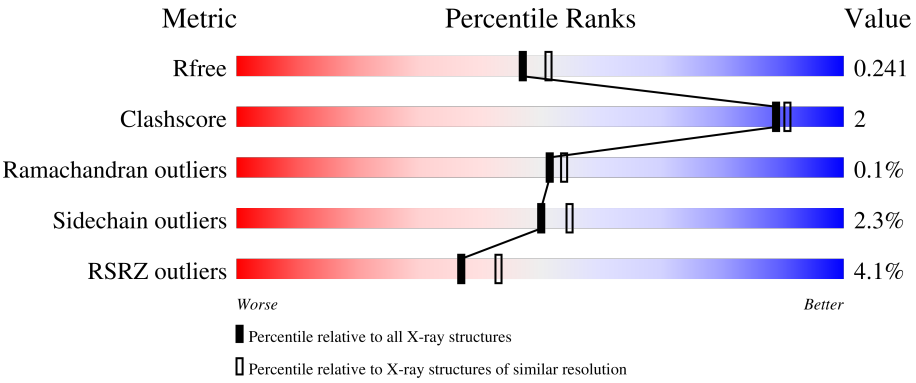
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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	AAA	594	4% 88% 6% 6%
1	BBB	594	4% 86% 9%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 17214 atoms, of which 8355 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 1-deoxy-D-xylulose-5-phosphate synthase,1-deoxy-D-xylulose-5-phosphate synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	560	Total	C	H	N	O	S	166	2	0
			8476	2676	4235	753	795	17			
1	BBB	539	Total	C	H	N	O	S	159	3	0
			8163	2567	4088	728	765	15			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-1	ALA	-	expression tag	UNP Q9RUB5
AAA	0	MET	-	expression tag	UNP Q9RUB5
AAA	1	GLY	-	expression tag	UNP Q9RUB5
AAA	200	GLY	-	linker	UNP Q9RUB5
AAA	238	GLY	-	linker	UNP Q9RUB5
AAA	239	GLY	-	linker	UNP Q9RUB5
AAA	240	GLY	-	linker	UNP Q9RUB5
AAA	241	GLY	-	linker	UNP Q9RUB5
AAA	242	GLY	-	linker	UNP Q9RUB5
AAA	243	GLY	-	linker	UNP Q9RUB5
BBB	-1	ALA	-	expression tag	UNP Q9RUB5
BBB	0	MET	-	expression tag	UNP Q9RUB5
BBB	1	GLY	-	expression tag	UNP Q9RUB5
BBB	237	GLY	-	linker	UNP Q9RUB5
BBB	238	GLY	-	linker	UNP Q9RUB5
BBB	239	GLY	-	linker	UNP Q9RUB5
BBB	240	GLY	-	linker	UNP Q9RUB5
BBB	241	GLY	-	linker	UNP Q9RUB5
BBB	242	GLY	-	linker	UNP Q9RUB5
BBB	243	GLY	-	linker	UNP Q9RUB5

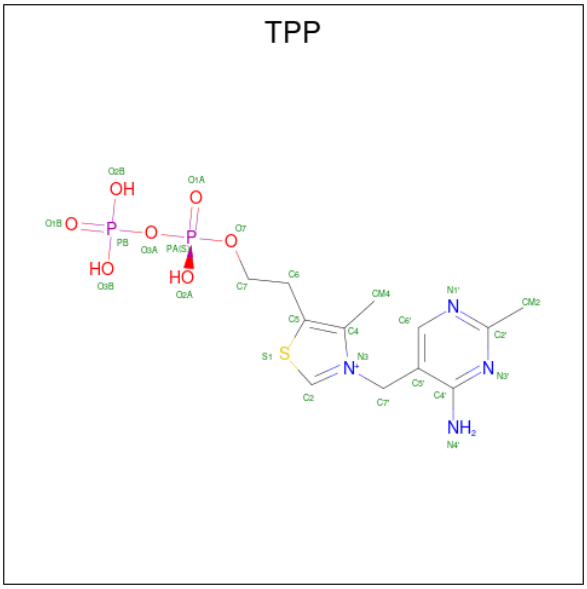
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AAA	2	Total Mg 2 2	0	0
2	BBB	3	Total Mg 3 3	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	2	Total Ca 2 2	0	0
3	BBB	4	Total Ca 4 4	0	0

- Molecule 4 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: $C_{12}H_{19}N_4O_7P_2S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	1	Total C H N O P S 42 12 16 4 7 2 1	2	0
4	BBB	1	Total C H N O P S 42 12 16 4 7 2 1	2	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	258	Total O 258 258	0	0

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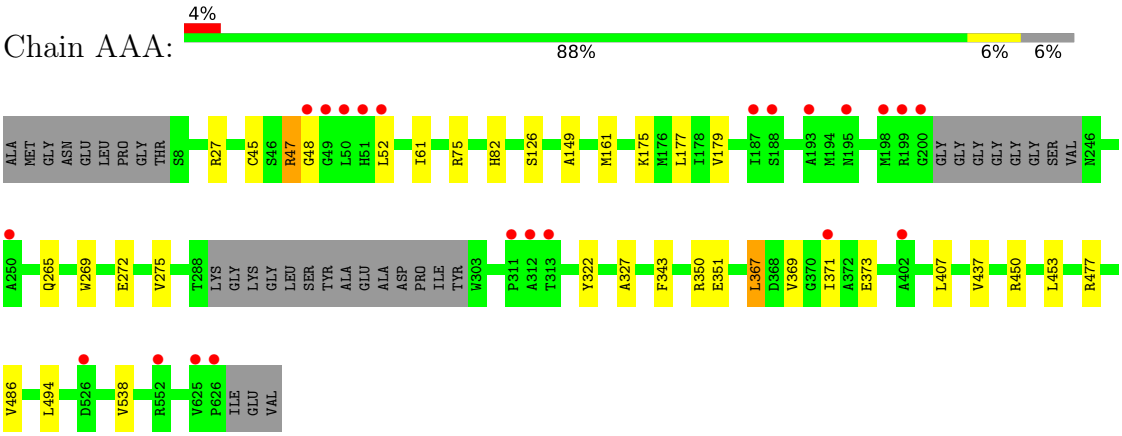
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	BBB	222	Total O 222 222	0	0

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.

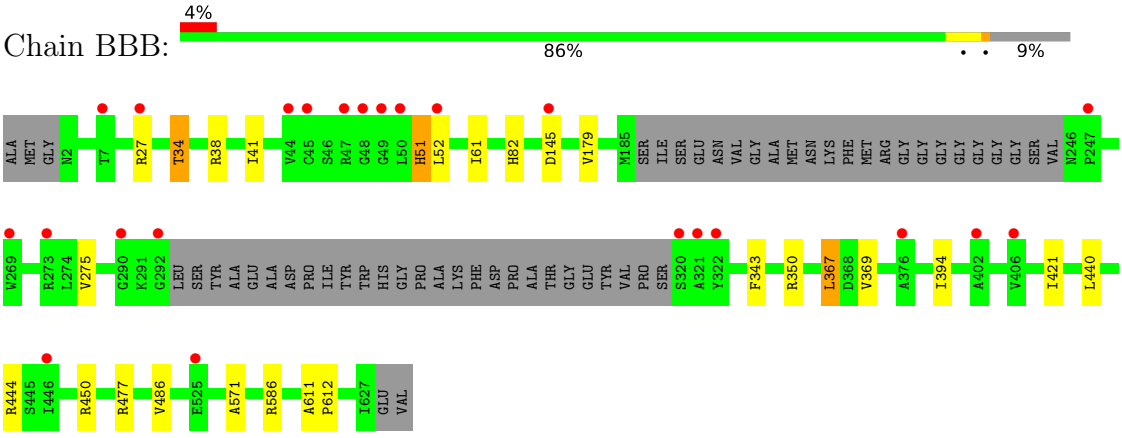
• Molecule 1: 1-deoxy-D-xylulose-5-phosphate synthase,1-deoxy-D-xylulose-5-phosphate synthase

Chain AAA:



• Molecule 1: 1-deoxy-D-xylulose-5-phosphate synthase,1-deoxy-D-xylulose-5-phosphate synthase

Chain BBB:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	72.32Å 87.37Å 181.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.55 – 2.10 47.50 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.0 (47.55-2.10) 99.0 (47.50-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.95 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.191 , 0.236 0.198 , 0.241	Depositor DCC
R_{free} test set	3427 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	25.5	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 41.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	17214	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% 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: CA, MG, TPP

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	AAA	0.66	0/4327	0.78	0/5877
1	BBB	0.66	0/4153	0.78	0/5640
All	All	0.66	0/8480	0.78	0/11517

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	AAA	4241	4235	4206	18	0
1	BBB	4075	4088	4056	11	0
2	AAA	2	0	0	0	0
2	BBB	3	0	0	0	0
3	AAA	2	0	0	0	0
3	BBB	4	0	0	0	0
4	AAA	26	16	16	2	0
4	BBB	26	16	16	1	0
5	AAA	258	0	0	0	0
5	BBB	222	0	0	2	0
All	All	8859	8355	8294	31	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 2.

The worst 5 of 31 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:AAA:350:ARG:NH1	1:AAA:351:GLU:OE2	2.19	0.75
1:BBB:41:ILE:HG22	1:BBB:52:LEU:CD1	2.34	0.57
1:BBB:51:HIS:CG	1:BBB:82:HIS:HB2	2.40	0.57
1:AAA:367:LEU:HD13	1:AAA:369:VAL:HG13	1.87	0.56
1:BBB:61:ILE:HG12	1:BBB:179:VAL:HG11	1.86	0.56

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	AAA	556/594 (94%)	546 (98%)	9 (2%)	1 (0%)	47 49
1	BBB	536/594 (90%)	524 (98%)	12 (2%)	0	100 100
All	All	1092/1188 (92%)	1070 (98%)	21 (2%)	1 (0%)	51 54

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	371	ILE

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	AAA	437/458 (95%)	428 (98%)	9 (2%)	53 59
1	BBB	420/458 (92%)	409 (97%)	11 (3%)	46 50
All	All	857/916 (94%)	837 (98%)	20 (2%)	50 55

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BBB	343	PHE
1	BBB	450	ARG
1	BBB	486	VAL
1	BBB	477	ARG
1	AAA	477	ARG

Sometimes 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 13 ligands modelled in this entry, 11 are monoatomic - leaving 2 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	$\#\|Z\|>2$
4	TPP	AAA	703	2	22,27,27	0.63	0	29,40,40	0.77	1 (3%)
4	TPP	BBB	705	2	22,27,27	0.72	0	29,40,40	0.98	2 (6%)

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
4	TPP	AAA	703	2	-	2/16/17/17	0/2/2/2
4	TPP	BBB	705	2	-	7/16/17/17	0/2/2/2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	BBB	705	TPP	C6-C5-C4	3.19	129.99	127.43
4	AAA	703	TPP	C7'-N3-C2	-2.28	121.23	125.35
4	BBB	705	TPP	C7'-N3-C2	-2.15	121.47	125.35

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	AAA	703	TPP	C4'-C5'-C7'-N3
4	BBB	705	TPP	C4'-C5'-C7'-N3
4	BBB	705	TPP	C5-C6-C7-O7
4	BBB	705	TPP	C7-O7-PA-O3A
4	BBB	705	TPP	PA-O3A-PB-O3B

There are no ring outliers.

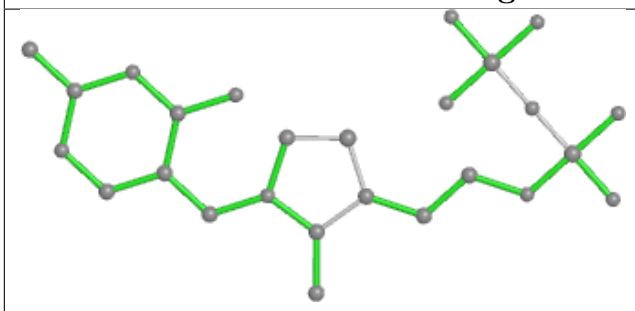
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	AAA	703	TPP	2	0
4	BBB	705	TPP	1	0

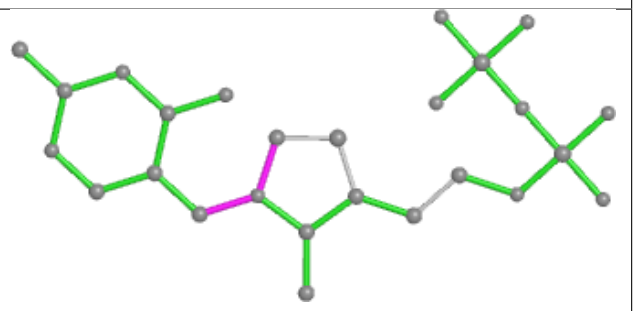
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

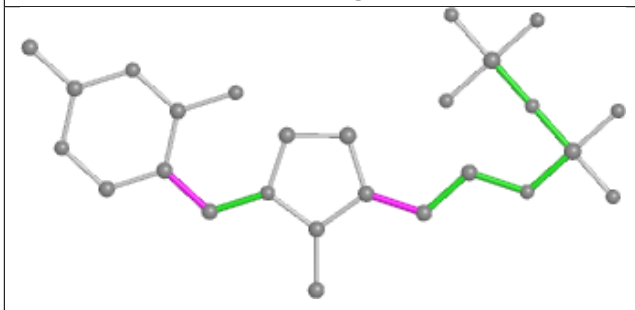
Ligand TPP AAA 703



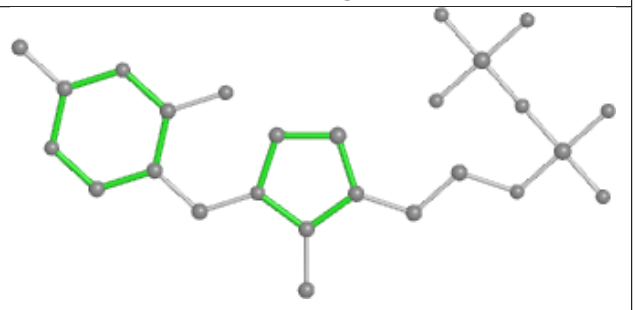
Bond lengths



Bond angles

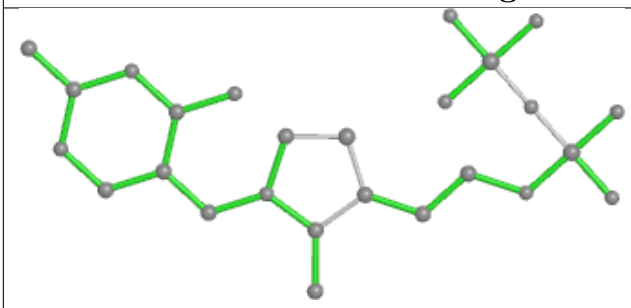


Torsions

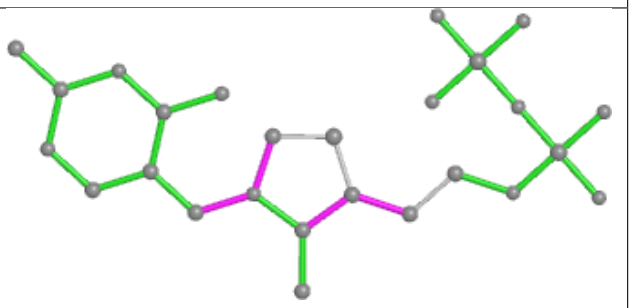


Rings

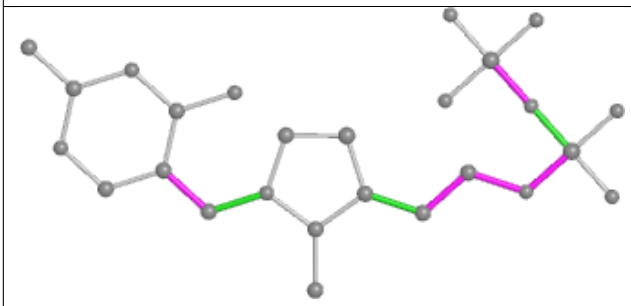
Ligand TPP BBB 705



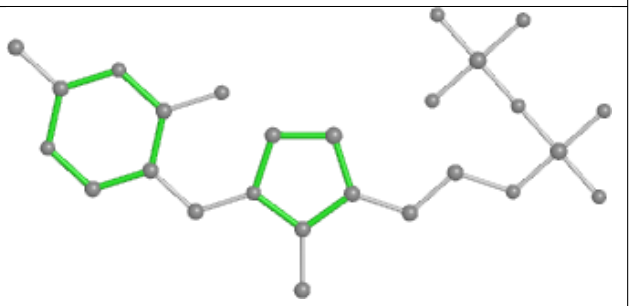
Bond lengths



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

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	AAA	560/594 (94%)	0.36	22 (3%)	39	45	17, 27, 52, 69	0
1	BBB	539/594 (90%)	0.43	23 (4%)	35	41	16, 28, 55, 97	0
All	All	1099/1188 (92%)	0.39	45 (4%)	37	43	16, 27, 54, 97	0

The worst 5 of 45 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	312	ALA	6.3
1	BBB	320	SER	5.5
1	BBB	49	GLY	5.4
1	BBB	321	ALA	5.3
1	BBB	269	TRP	5.0

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

There are no monosaccharides in this entry.

6.4 Ligands

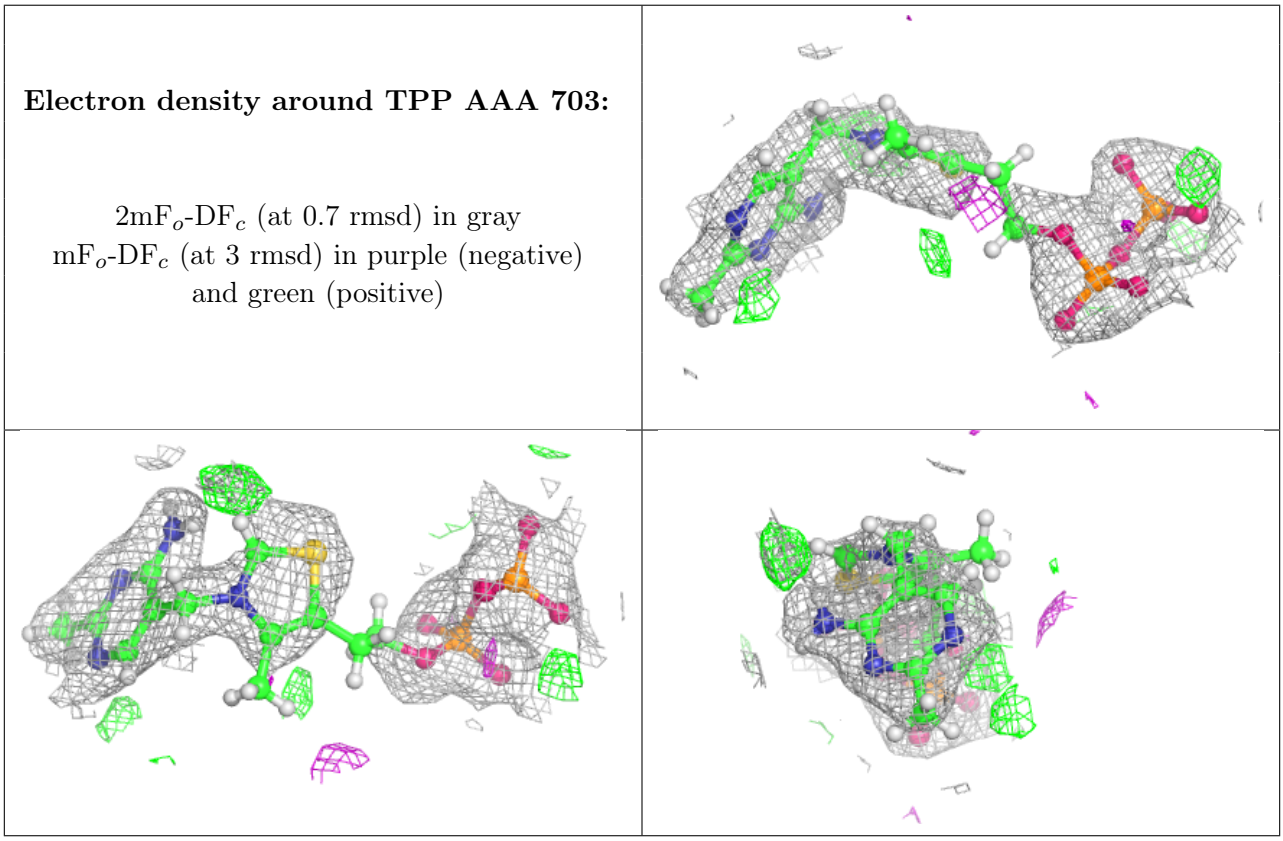
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
3	CA	BBB	708	1/1	0.89	0.14	64,64,64,64	0
4	TPP	AAA	703	26/26	0.91	0.16	31,53,67,72	2
4	TPP	BBB	705	26/26	0.91	0.15	28,46,58,61	2
3	CA	AAA	702	1/1	0.94	0.07	53,53,53,53	0
2	MG	BBB	704	1/1	0.94	0.10	34,34,34,34	0
3	CA	BBB	702	1/1	0.96	0.30	69,69,69,69	0
3	CA	AAA	704	1/1	0.98	0.08	44,44,44,44	0
3	CA	BBB	706	1/1	0.98	0.06	50,50,50,50	0
3	CA	BBB	707	1/1	0.98	0.15	59,59,59,59	0
2	MG	AAA	705	1/1	0.99	0.10	18,18,18,18	0
2	MG	BBB	701	1/1	0.99	0.12	27,27,27,27	0
2	MG	BBB	703	1/1	0.99	0.08	13,13,13,13	0
2	MG	AAA	701	1/1	0.99	0.13	24,24,24,24	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.

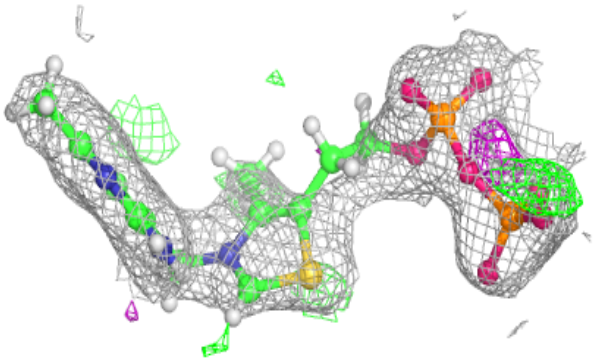
Electron density around TPP AAA 703:

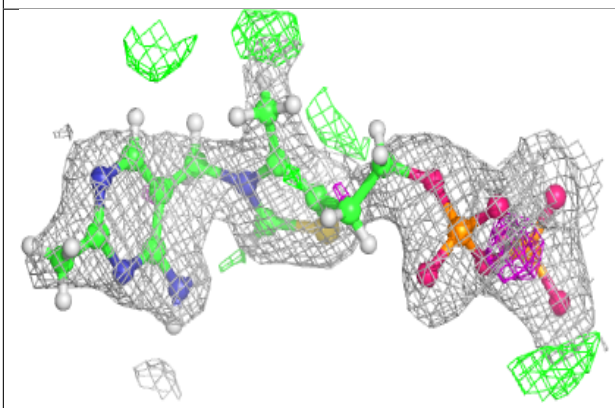
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

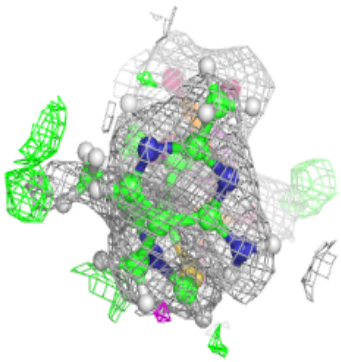


Electron density around TPP BBB 705:

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

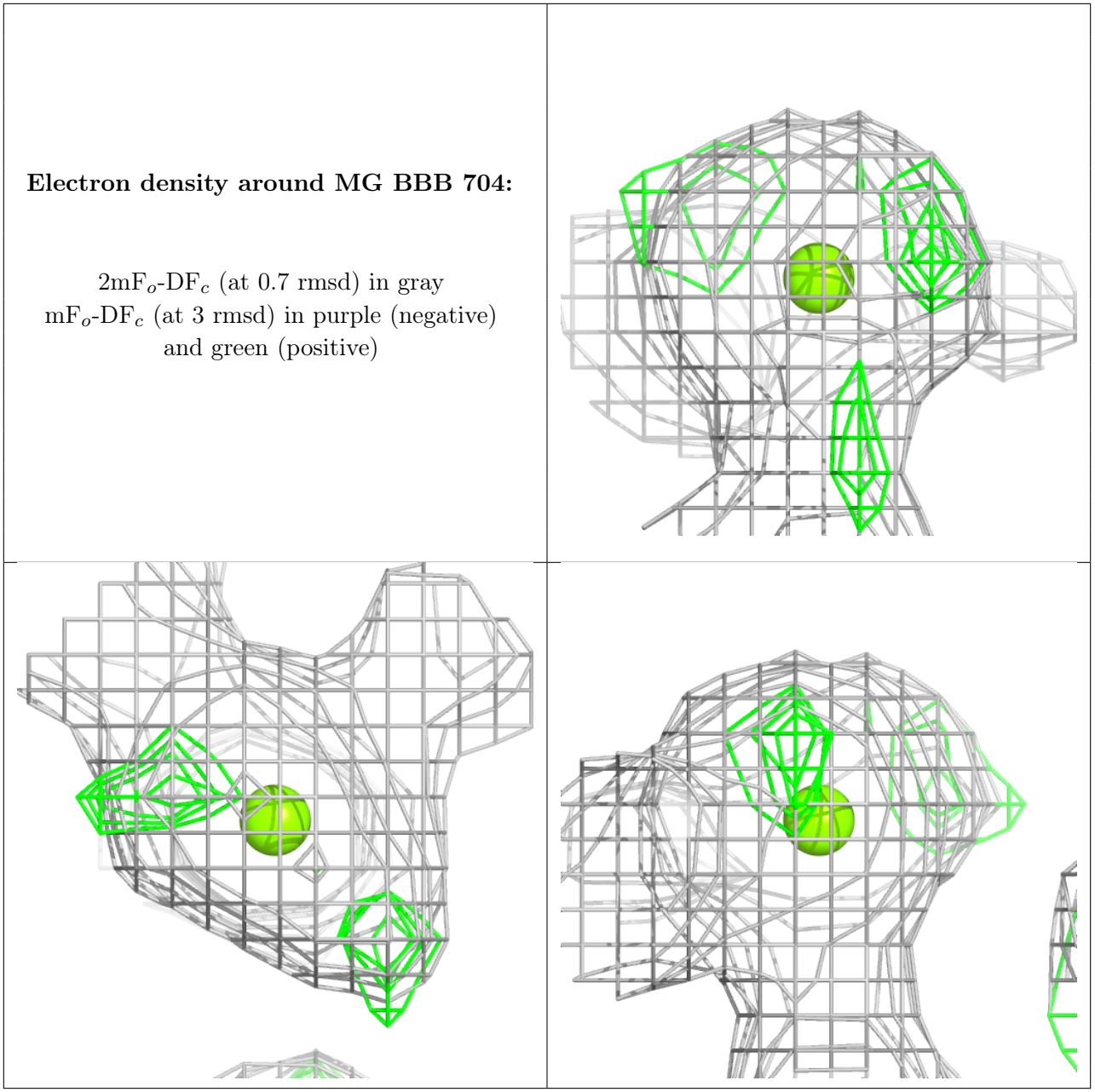






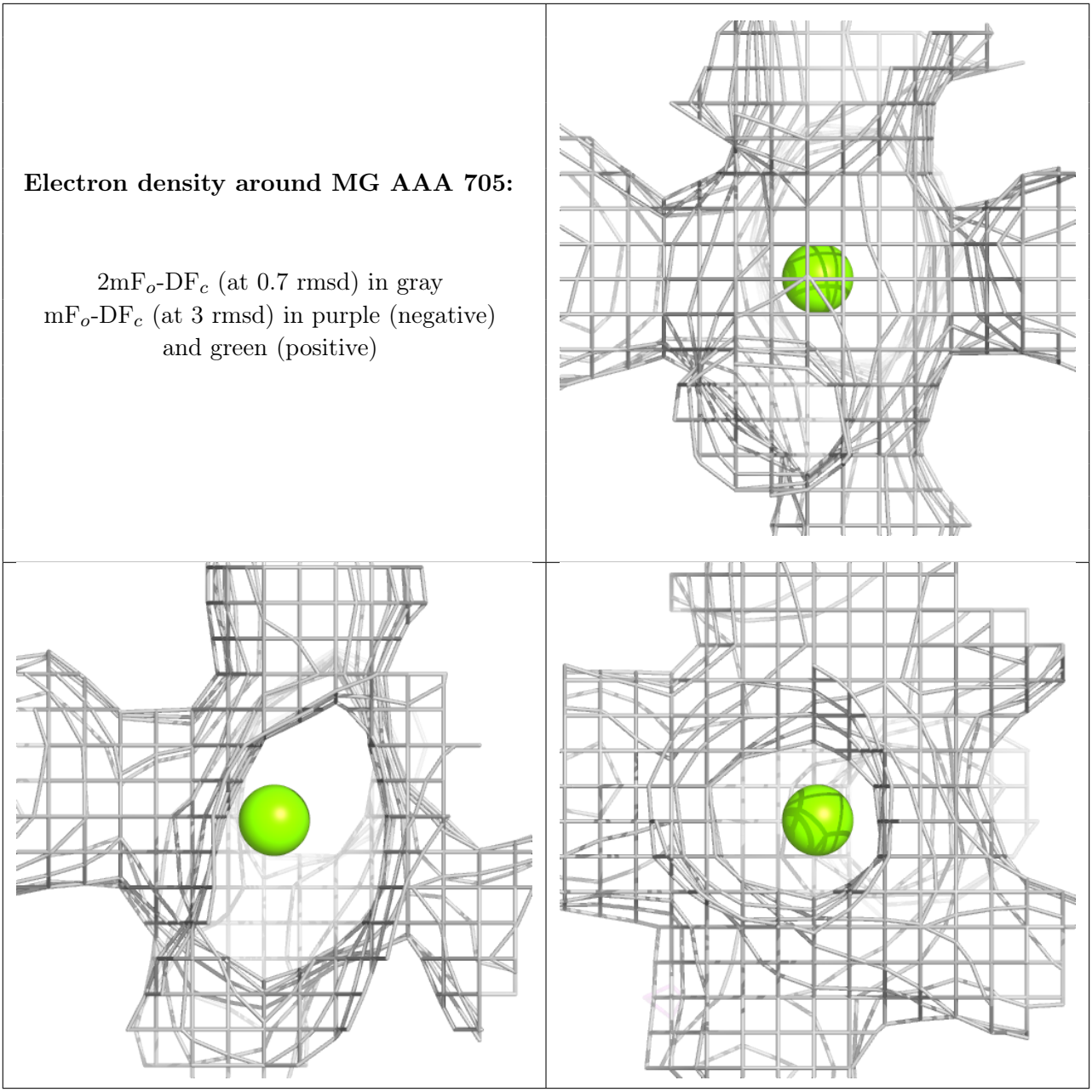
Electron density around MG BBB 704:

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



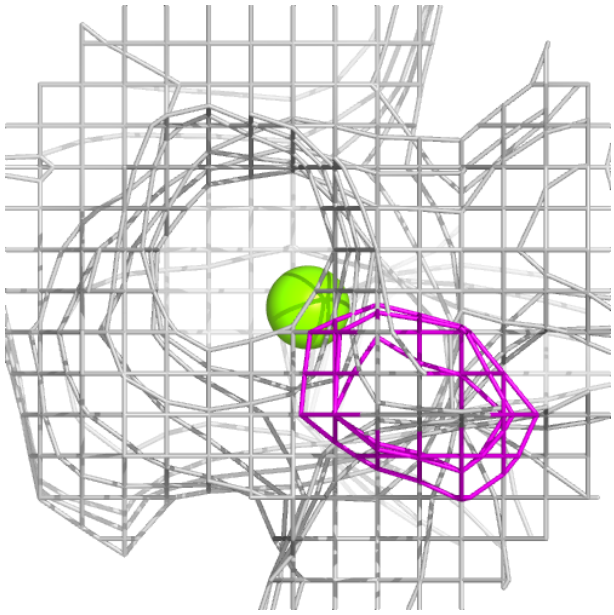
Electron density around MG AAA 705:

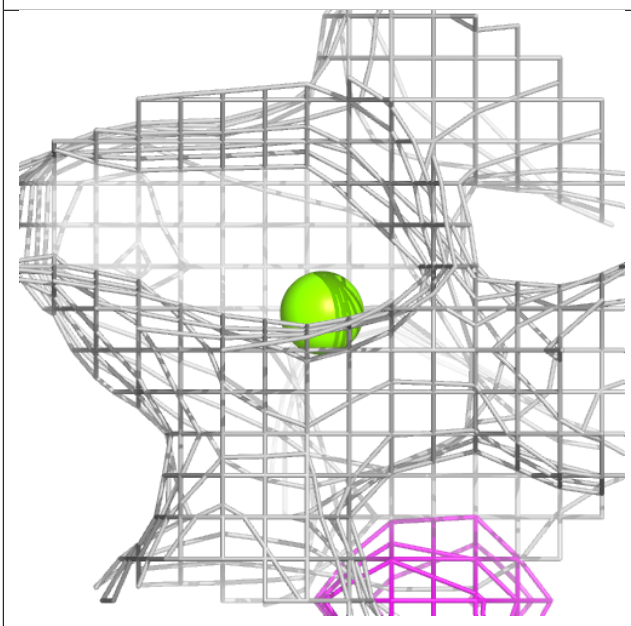
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

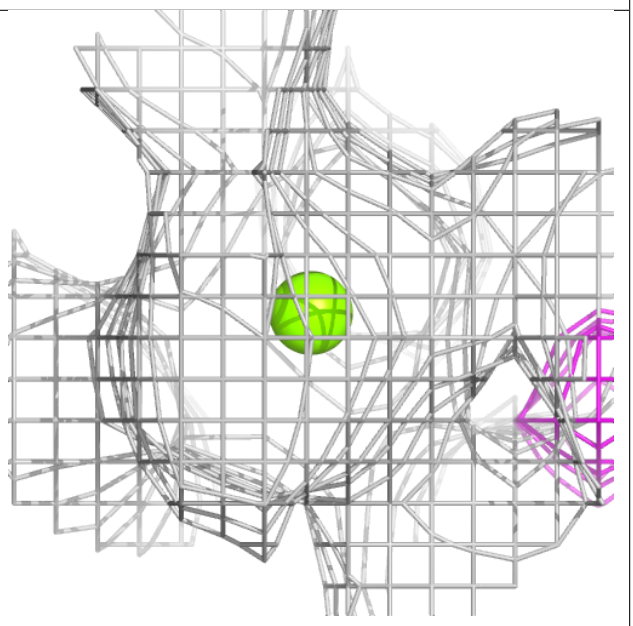


Electron density around MG BBB 701:

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

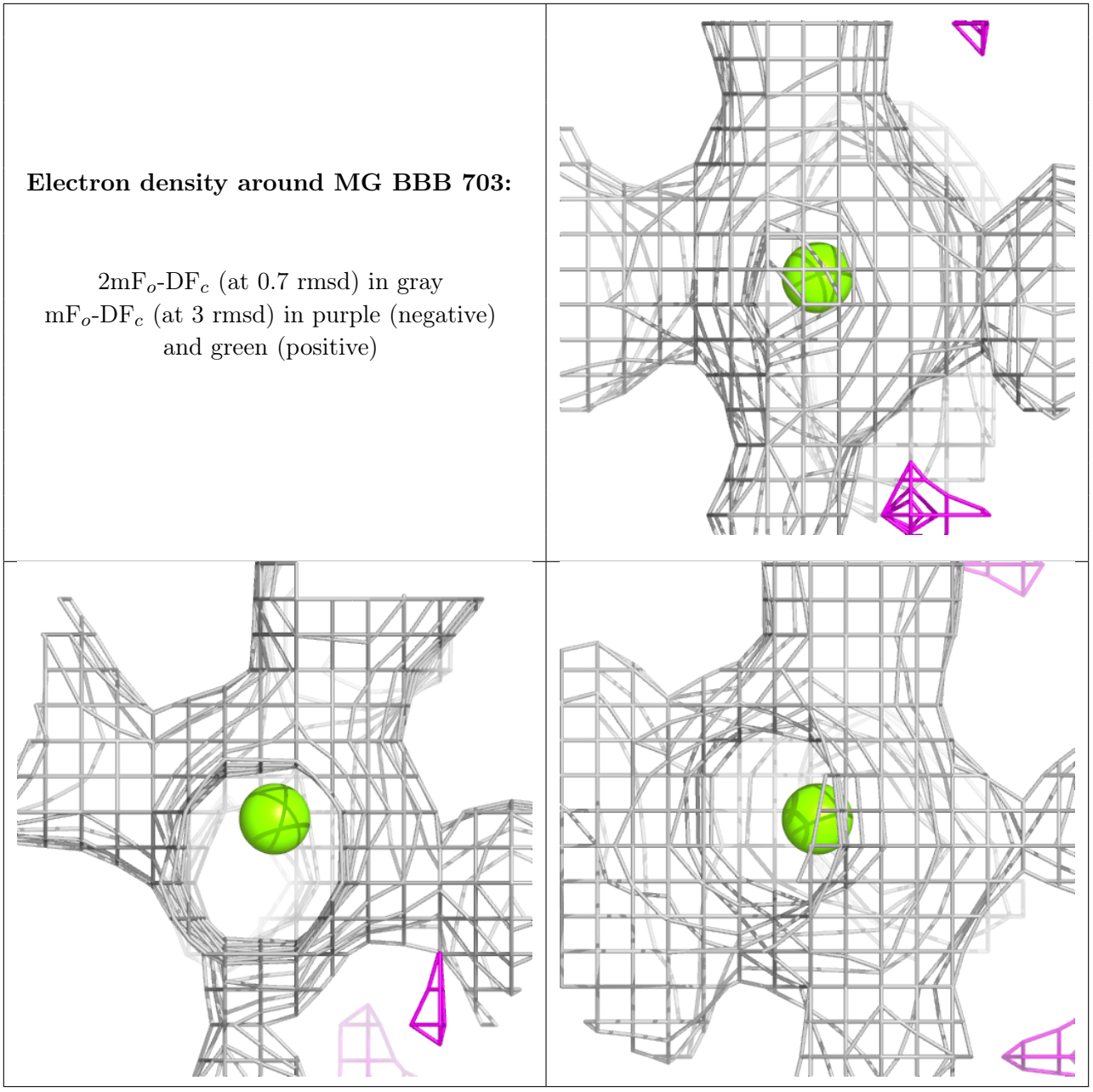






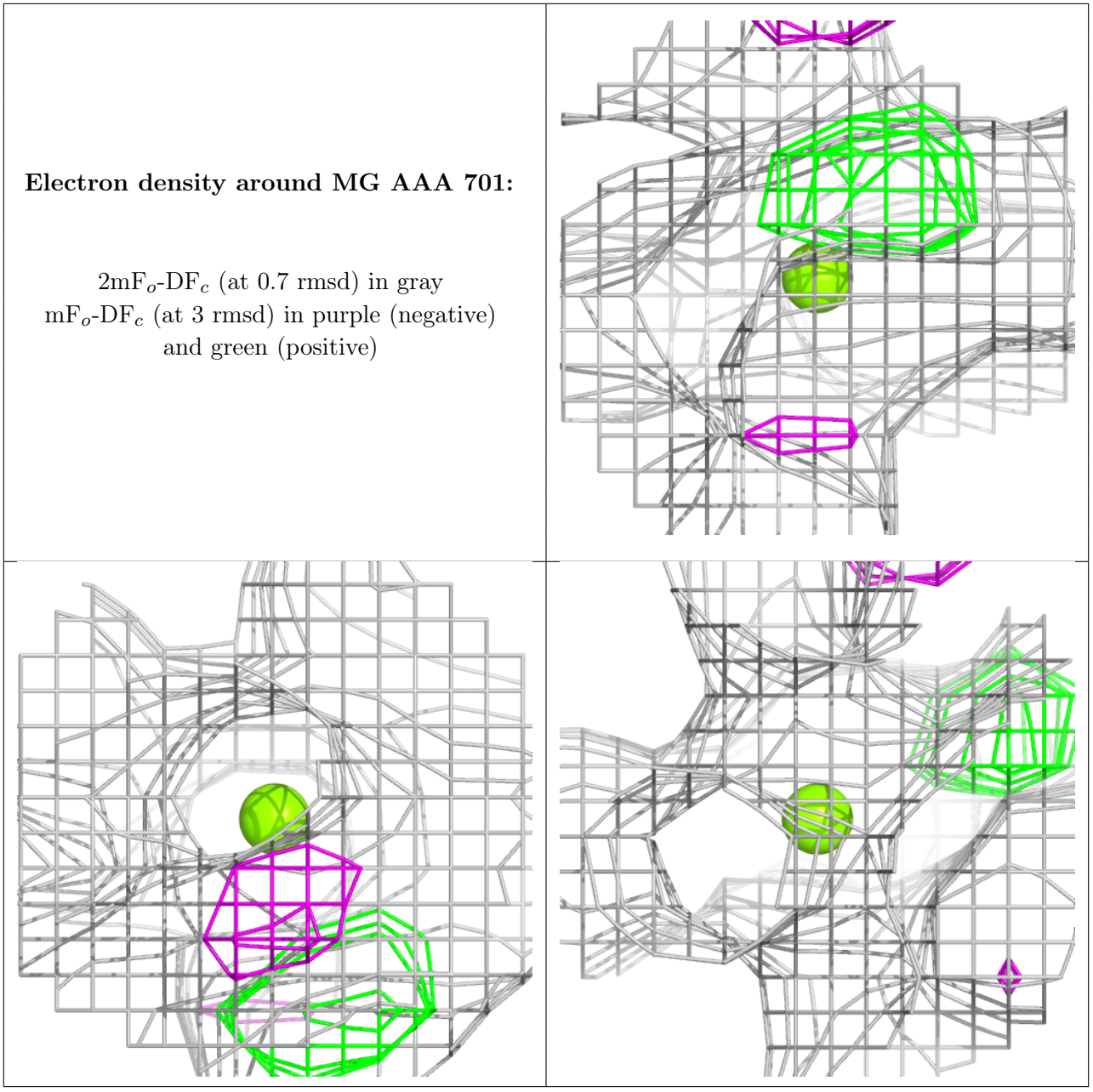
Electron density around MG BBB 703:

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



Electron density around MG AAA 701:

$2mF_o$-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.