



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 4, 2026 – 01:55 AM EDT

PDB ID : 9XYW / pdb_00009xyw
Title : Crystal structure of the maize chloroplastic non-photosynthetic NADP(+)-dependent malic enzyme
Authors : Klinke, S.; Schneberger, N.; Boehm, J.M.; Willms, S.; Hagelueken, G.; Geyer, M.; Maurino, V.; Alvarez, C.E.
Deposited on : 2025-08-26
Resolution : 2.55 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

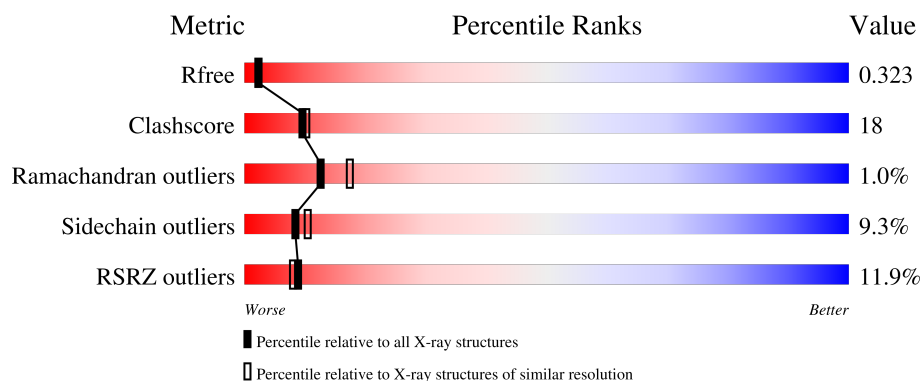
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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}	180053	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	AAA	586	
1	BBB	586	

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
3	FMT	AAA	602	-	-	X	-
3	FMT	BBB	602	-	-	X	-
4	PYR	AAA	603	-	-	X	-

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 8445 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.

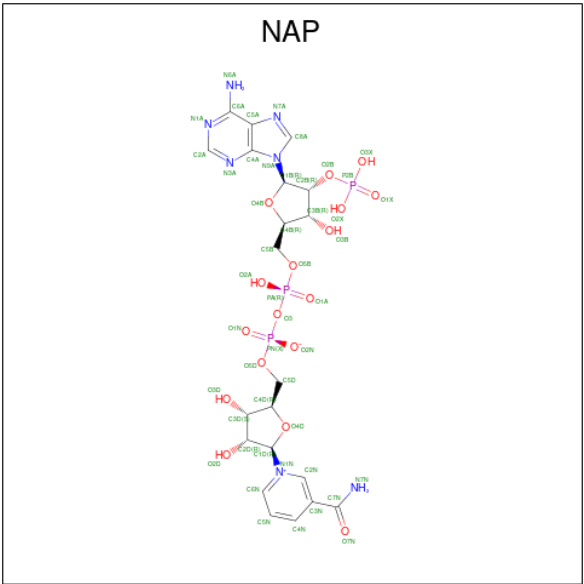
- Molecule 1 is a protein called Malic enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	553	Total	C	N	O	S	0	0	0
			4325	2771	742	795	17			
1	BBB	509	Total	C	N	O	S	0	0	0
			3991	2554	685	735	17			

There are 4 discrepancies between the modelled and reference sequences:

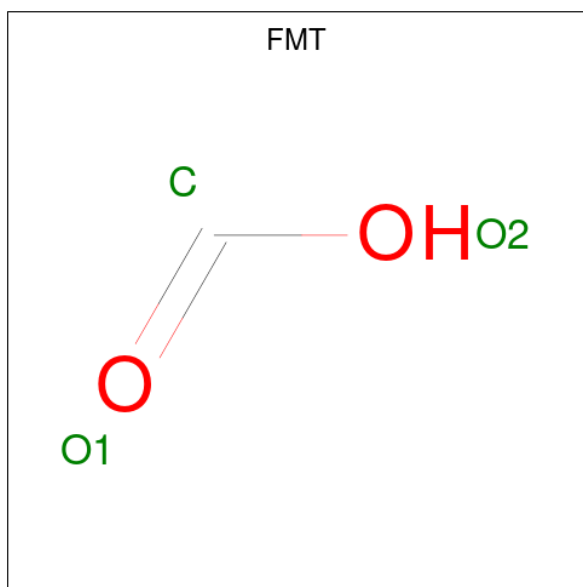
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	1	HIS	-	expression tag	UNP A0A4Y2
AAA	2	MET	-	expression tag	UNP A0A4Y2
BBB	1	HIS	-	expression tag	UNP A0A4Y2
BBB	2	MET	-	expression tag	UNP A0A4Y2

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃) (labeled as "Ligand of Interest" by depositor).



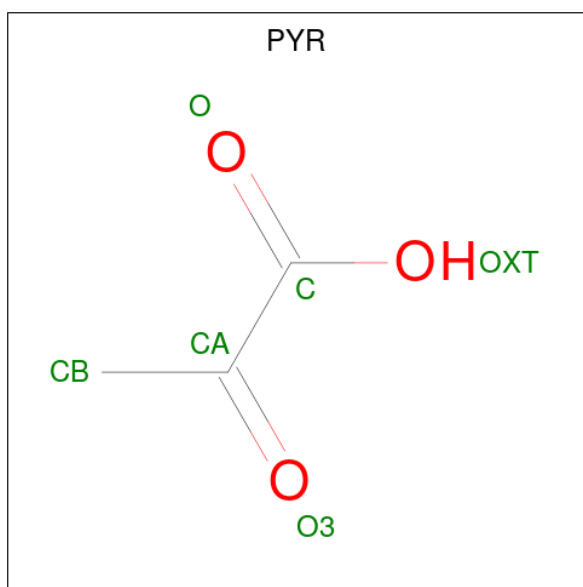
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	AAA	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	BBB	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is FORMIC ACID (CCD ID: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	AAA	1	Total	C	O	0	0
			3	1	2		
3	BBB	1	Total	C	O	0	0
			3	1	2		

- Molecule 4 is PYRUVIC ACID (CCD ID: PYR) (formula: $\text{C}_3\text{H}_4\text{O}_3$) (labeled as "Ligand of Interest" by depositor).



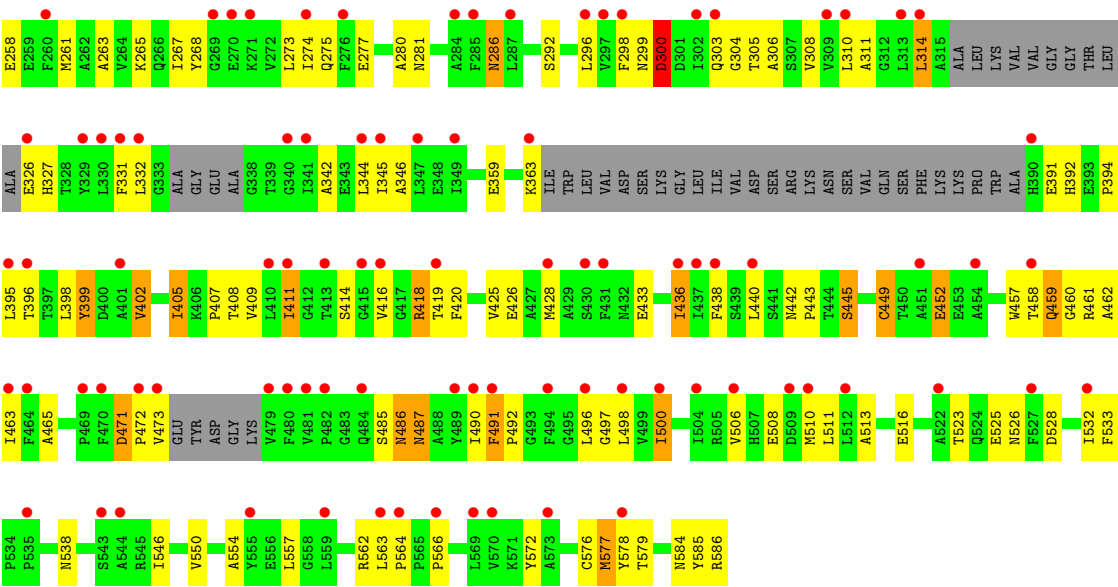
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	AAA	1	Total	C	O	0	0
			6	3	3		
4	BBB	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	1	Total	Mg	0	0
			1	1		
5	BBB	1	Total	Mg	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	AAA	11	Total	O	0	0
			11	11		
6	BBB	2	Total	O	0	0
			2	2		



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	92.45Å 108.11Å 168.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.23 – 2.55 91.23 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.8 (91.23-2.55) 99.8 (91.23-2.55)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 2.55Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.243 , 0.308 0.256 , 0.323	Depositor DCC
R_{free} test set	2736 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	64.9	Xtriage
Anisotropy	0.238	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 70.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8445	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PYR, FMT, NAP, MG

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	1.14	3/4423 (0.1%)	1.55	16/5998 (0.3%)
1	BBB	1.07	0/4078	1.51	7/5525 (0.1%)
All	All	1.11	3/8501 (0.0%)	1.53	23/11523 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AAA	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	336	GLU	C-O	7.07	1.32	1.24
1	AAA	421	THR	C-O	5.27	1.29	1.23
1	AAA	340	GLY	C-O	5.20	1.30	1.23

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	509	ASP	CA-CB-CG	6.75	119.35	112.60
1	BBB	300	ASP	CA-CB-CG	6.75	119.35	112.60
1	BBB	58	LYS	CB-CA-C	6.54	121.00	109.75
1	AAA	193	ASP	CA-CB-CG	6.32	118.92	112.60
1	BBB	193	ASP	CA-CB-CG	5.99	118.59	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AAA	380	SER	Peptide

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	4325	0	4349	132	0
1	BBB	3991	0	3992	172	0
2	AAA	48	0	25	7	0
2	BBB	48	0	25	3	0
3	AAA	3	0	1	3	0
3	BBB	3	0	1	2	0
4	AAA	6	0	0	5	0
4	BBB	6	0	0	1	0
5	AAA	1	0	0	0	0
5	BBB	1	0	0	0	0
6	AAA	11	0	0	0	0
6	BBB	2	0	0	1	0
All	All	8445	0	8393	300	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 18.

The worst 5 of 300 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:BBB:459:GLN:HA	1:BBB:459:GLN:HE21	1.33	0.92
1:BBB:471:ASP:HB2	1:BBB:472:PRO:HD2	1.48	0.92
1:BBB:277:GLU:OE2	6:BBB:701:HOH:O	1.88	0.91
1:AAA:55:HIS:NE2	3:AAA:602:FMT:O2	2.04	0.90
1:BBB:186:GLU:HG2	1:BBB:280:ALA:HB2	1.54	0.90

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	551/586 (94%)	487 (88%)	58 (10%)	6 (1%)	11	15
1	BBB	499/586 (85%)	437 (88%)	57 (11%)	5 (1%)	12	17
All	All	1050/1172 (90%)	924 (88%)	115 (11%)	11 (1%)	12	17

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	376	SER
1	AAA	445	SER
1	BBB	314	LEU
1	BBB	445	SER
1	AAA	188	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	460/482 (95%)	426 (93%)	34 (7%)	13	17
1	BBB	425/482 (88%)	377 (89%)	48 (11%)	5	6
All	All	885/964 (92%)	803 (91%)	82 (9%)	8	10

5 of 82 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BBB	314	LEU

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Mol	Chain	Res	Type
1	BBB	471	ASP
1	BBB	399	TYR
1	BBB	436	ILE
1	BBB	506	VAL

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	FMT	AAA	602	-	2,2,2	0.54	0	1,1,1	0.03	0
2	NAP	BBB	601	-	50,52,52	1.27	6 (12%)	71,80,80	1.98	19 (26%)
3	FMT	BBB	602	-	2,2,2	0.41	0	1,1,1	0.04	0
2	NAP	AAA	601	-	50,52,52	1.48	8 (16%)	71,80,80	2.86	33 (46%)
4	PYR	BBB	603	5	5,5,5	3.33	2 (40%)	3,6,6	1.07	0
4	PYR	AAA	603	5	5,5,5	3.71	2 (40%)	3,6,6	1.65	1 (33%)

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
2	NAP	AAA	601	-	-	5/35/67/67	0/5/5/5
2	NAP	BBB	601	-	-	16/35/67/67	0/5/5/5
4	PYR	BBB	603	5	-	0/4/4/4	-
4	PYR	AAA	603	5	-	0/4/4/4	-

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	AAA	603	PYR	CA-C	-7.84	1.28	1.54
4	BBB	603	PYR	CA-C	-6.94	1.31	1.54
2	BBB	601	NAP	C5A-C4A	4.97	1.48	1.39
2	AAA	601	NAP	PA-O3	4.93	1.64	1.59
2	AAA	601	NAP	O4D-C1D	3.78	1.45	1.40

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AAA	601	NAP	C4D-O4D-C1D	-10.14	100.64	109.92
2	AAA	601	NAP	N3A-C4A-N9A	5.85	137.12	127.17
2	AAA	601	NAP	C4A-N9A-C8A	5.83	111.86	105.74
2	AAA	601	NAP	O2A-PA-O1A	5.67	138.81	112.44
2	BBB	601	NAP	N3A-C2A-N1A	-5.49	120.28	128.58

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

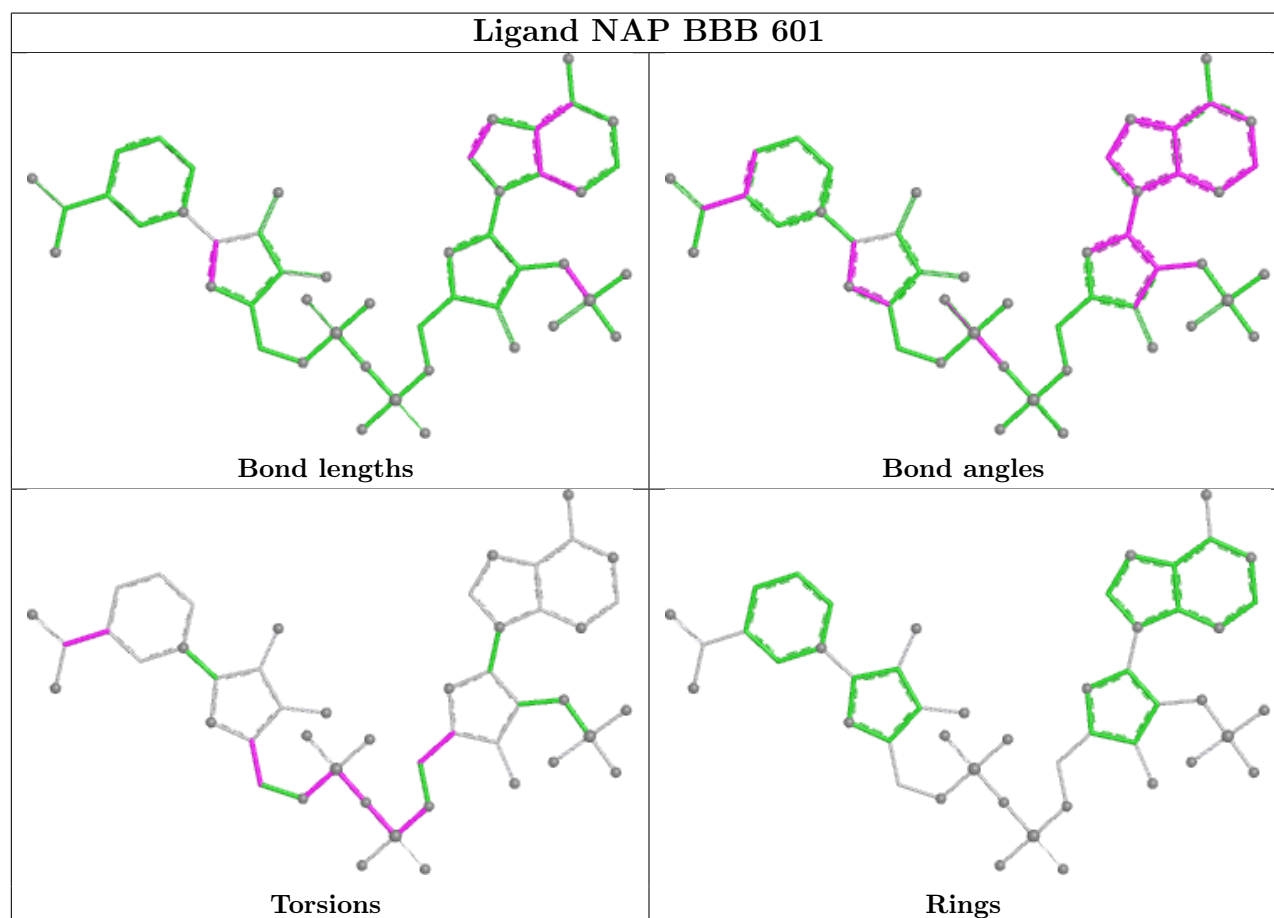
Mol	Chain	Res	Type	Atoms
2	AAA	601	NAP	C5B-O5B-PA-O2A
2	AAA	601	NAP	O4D-C1D-N1N-C6N
2	BBB	601	NAP	C5B-O5B-PA-O1A
2	BBB	601	NAP	C5B-O5B-PA-O2A
2	BBB	601	NAP	C5B-O5B-PA-O3

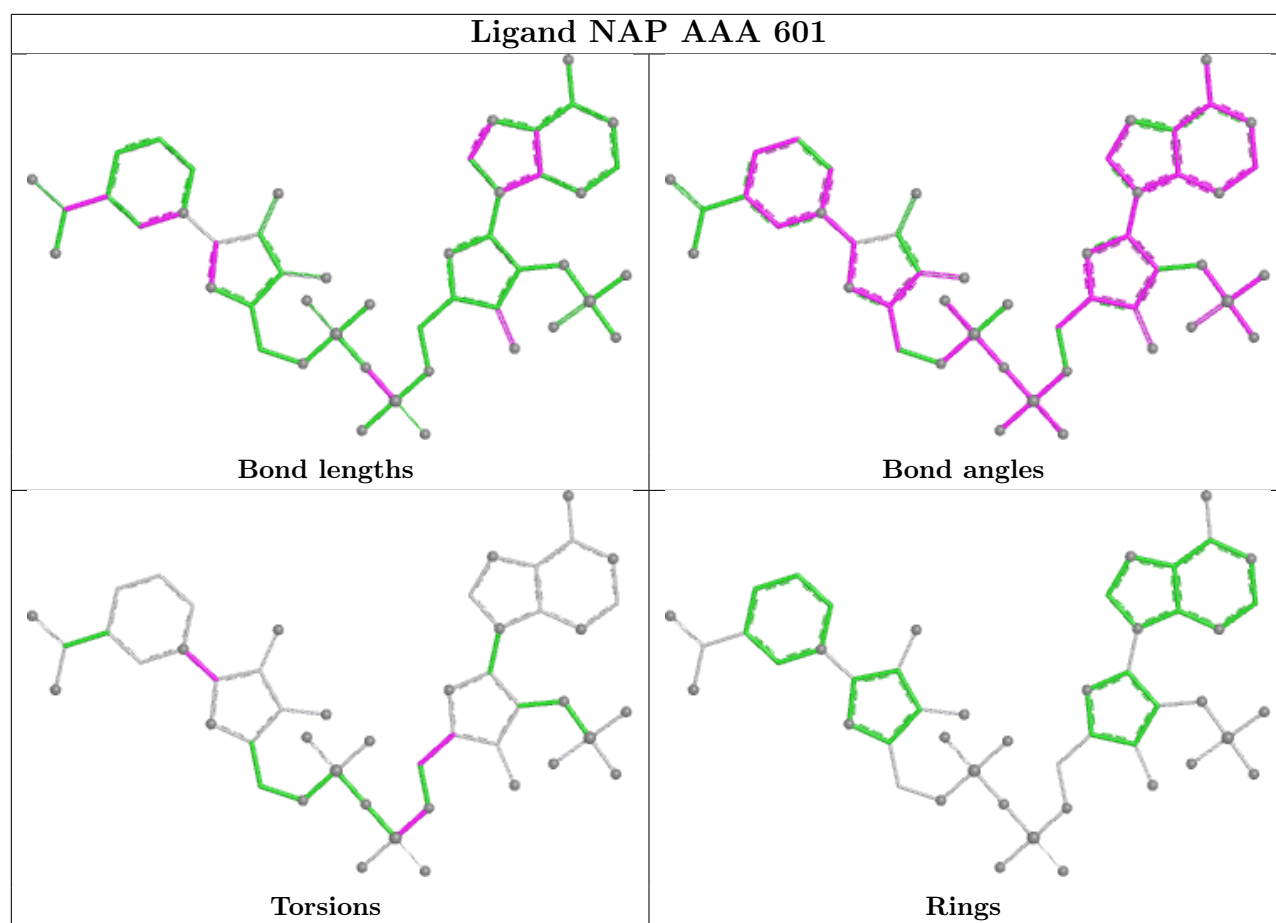
There are no ring outliers.

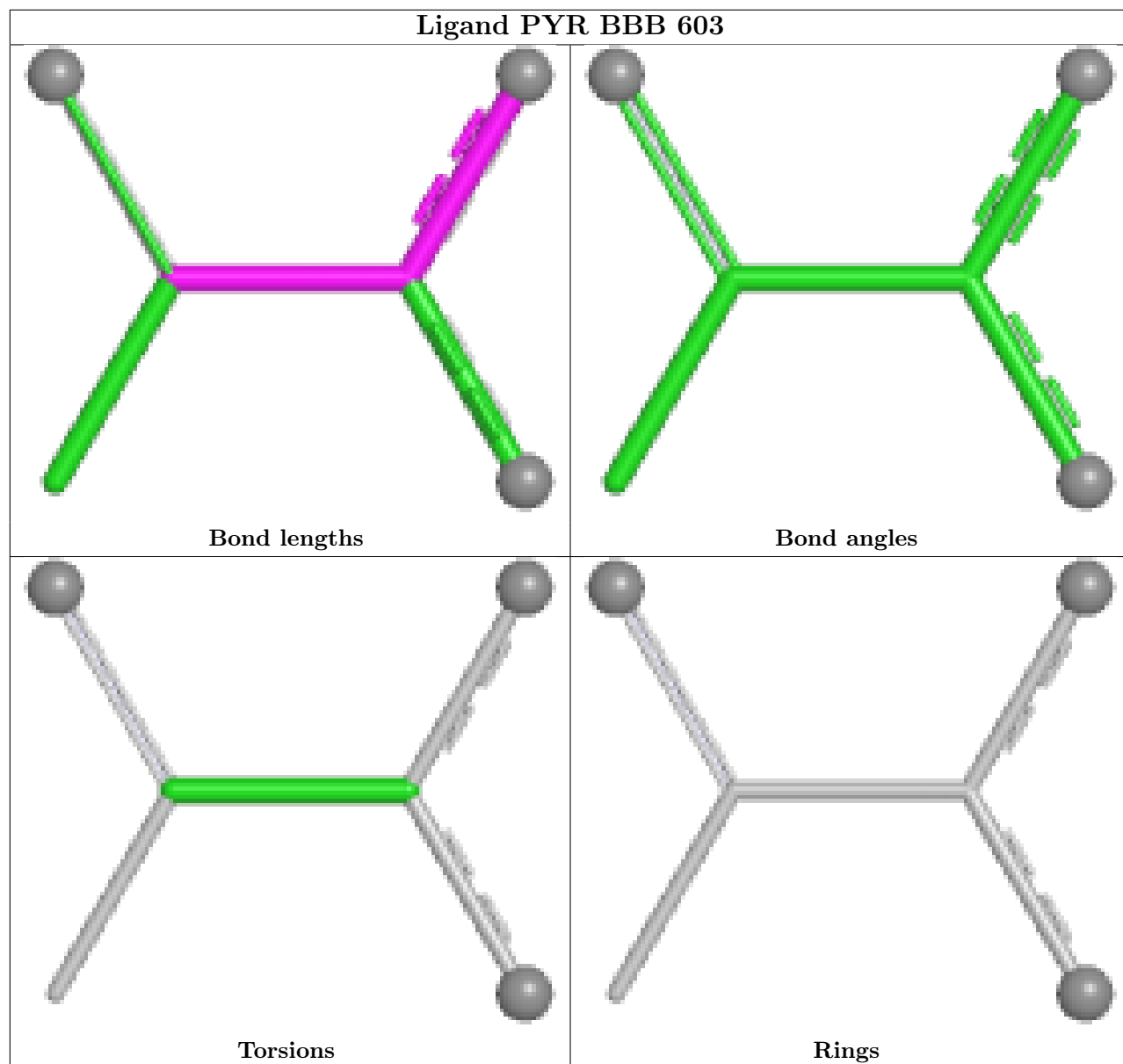
6 monomers are involved in 18 short contacts:

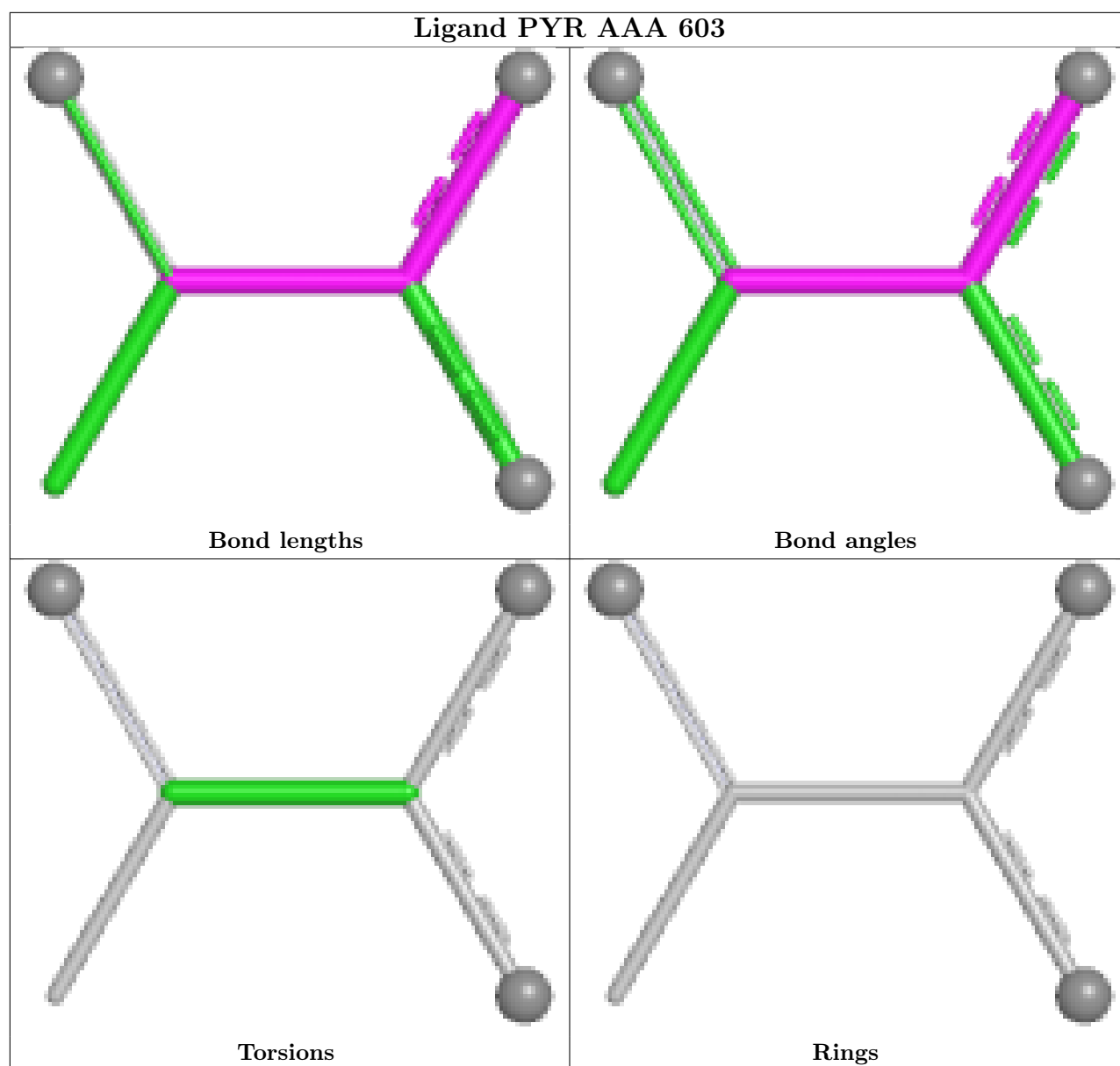
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	AAA	602	FMT	3	0
2	BBB	601	NAP	3	0
3	BBB	602	FMT	2	0
2	AAA	601	NAP	7	0
4	BBB	603	PYR	1	0
4	AAA	603	PYR	5	0

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 than 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.









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 [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	AAA	553/586 (94%)	0.38	11 (1%) 65 65	45, 72, 102, 138	0
1	BBB	509/586 (86%)	1.31	115 (22%) 2 2	58, 133, 179, 220	0
All	All	1062/1172 (90%)	0.83	126 (11%) 9 8	45, 92, 172, 220	0

The worst 5 of 126 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	194	LEU	5.9
1	BBB	470	PHE	4.1
1	BBB	415	GLY	4.0
1	BBB	464	PHE	3.9
1	BBB	191	LEU	3.9

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

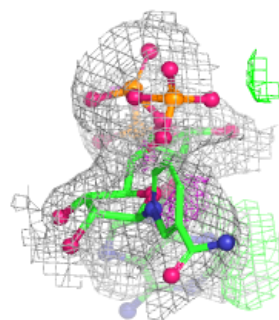
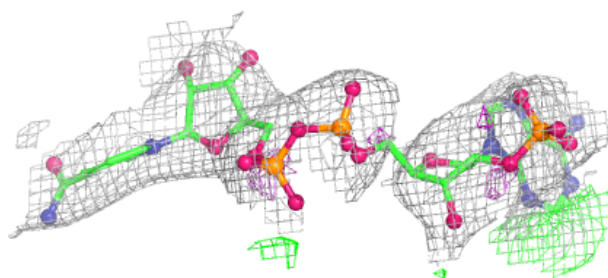
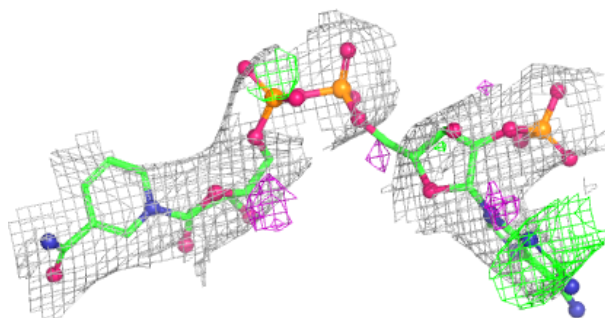
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAP	BBB	601	48/48	0.77	0.12	92,126,183,190	0
3	FMT	AAA	602	3/3	0.89	0.23	70,70,72,82	0
3	FMT	BBB	602	3/3	0.92	0.17	81,81,82,93	0
2	NAP	AAA	601	48/48	0.95	0.09	41,62,78,83	0
4	PYR	AAA	603	6/6	0.96	0.10	63,74,77,80	0
4	PYR	BBB	603	6/6	0.96	0.06	129,136,140,140	0
5	MG	BBB	604	1/1	0.98	0.10	108,108,108,108	0
5	MG	AAA	604	1/1	0.99	0.07	49,49,49,49	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.

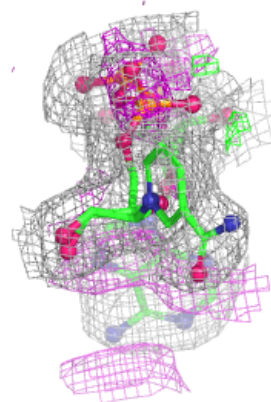
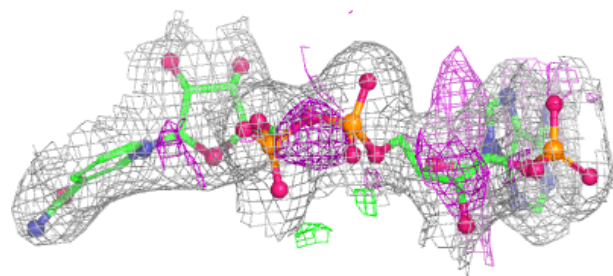
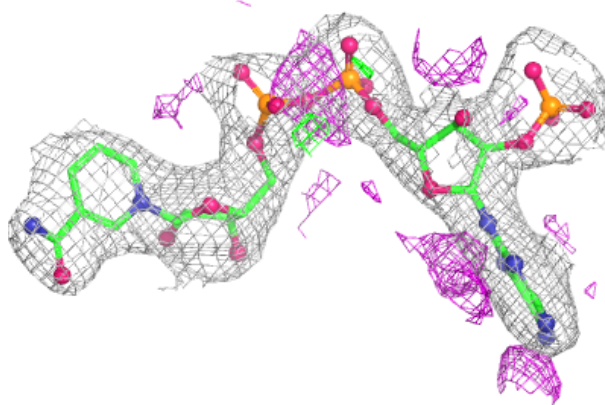
Electron density around NAP BBB 601:

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



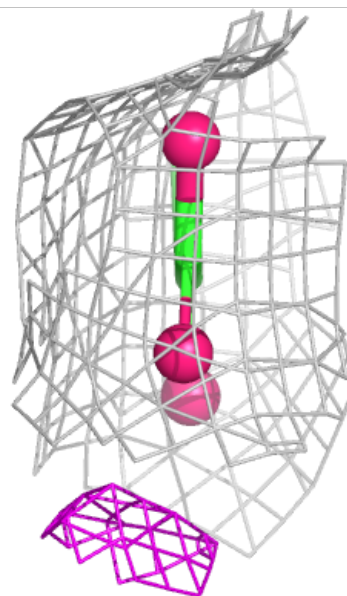
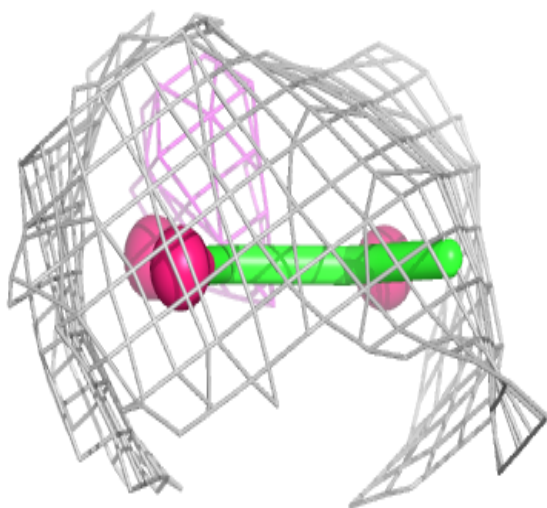
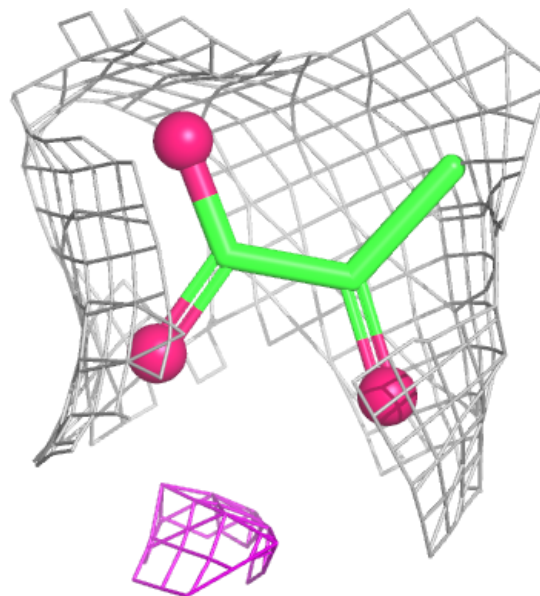
Electron density around NAP AAA 601:

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



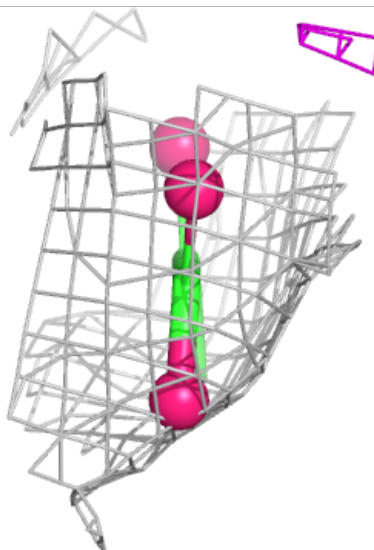
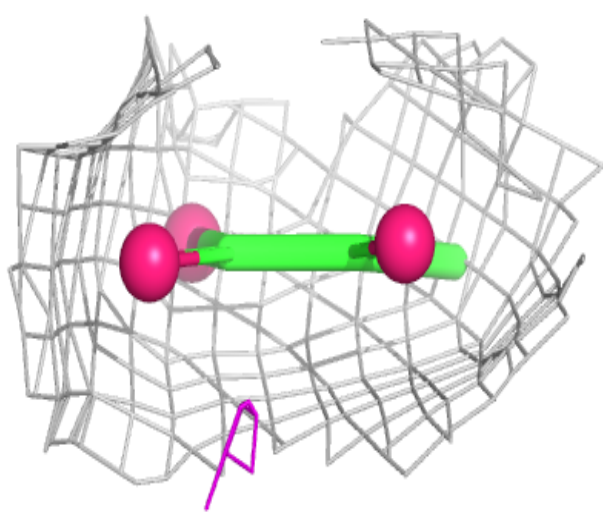
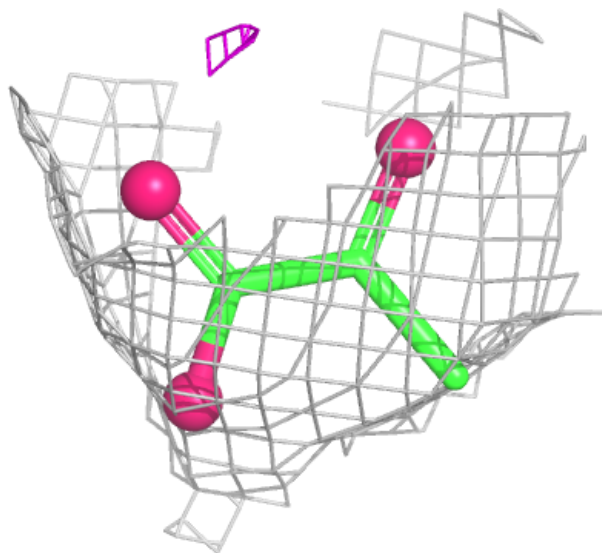
Electron density around PYR AAA 603:

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



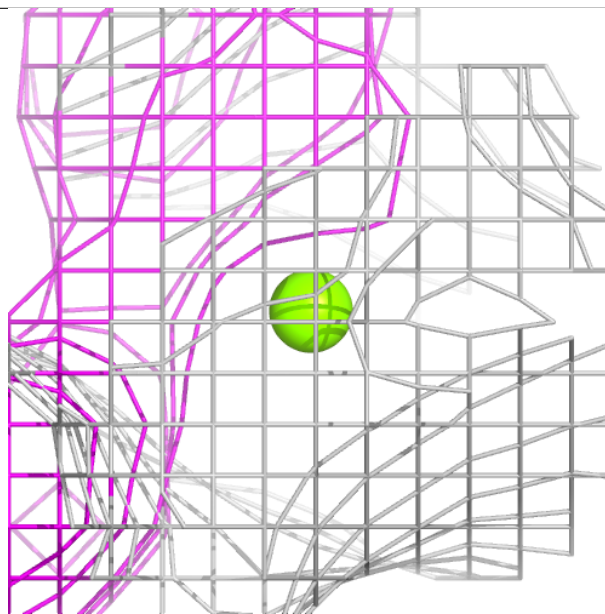
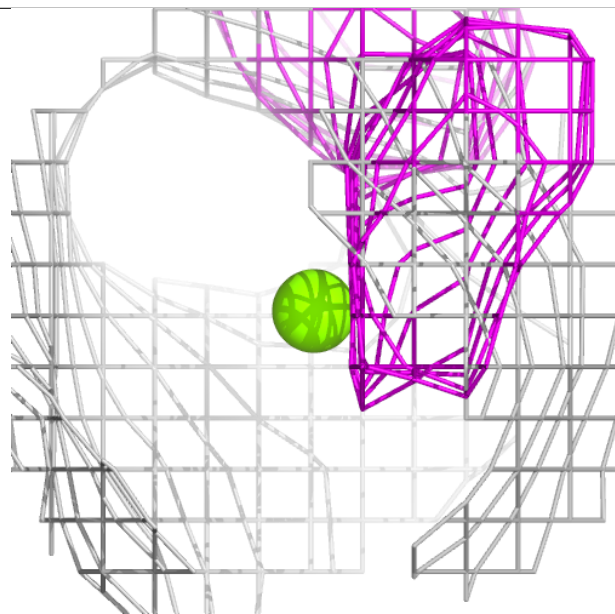
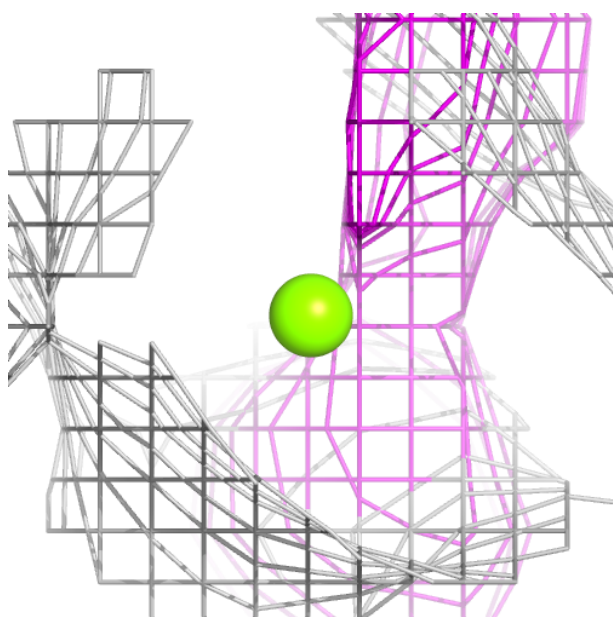
Electron density around PYR BBB 603:

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



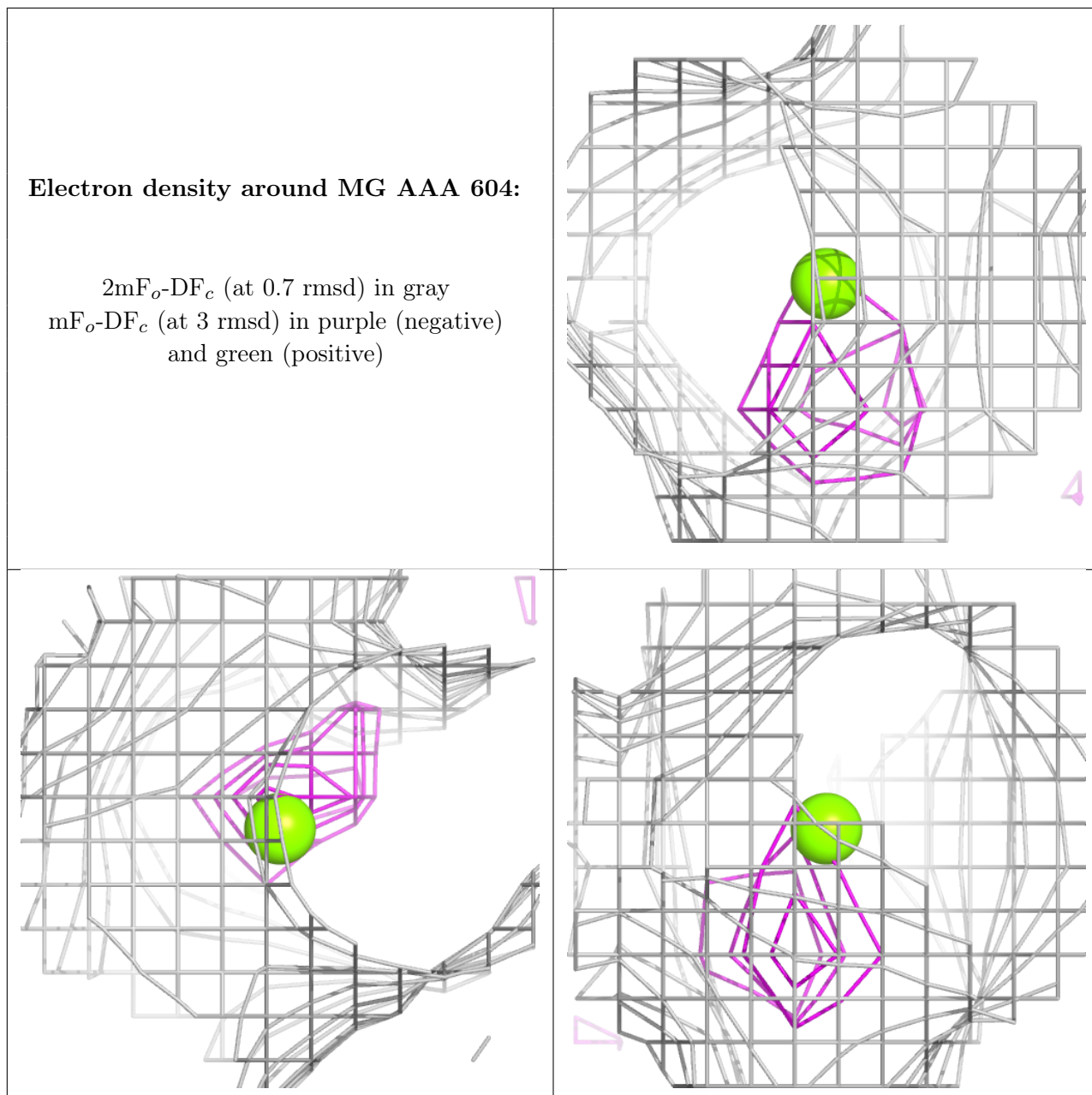
Electron density around MG BBB 604:

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



Electron density around MG AAA 604:

$2mF_o-DF_c$ (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.