



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 16, 2023 – 12:04 AM JST

PDB ID : 6K8K
Title : Crystal structure of Arabidopsis thaliana BIC2-CRY2 complex
Authors : Wang, X.; Ma, L.; Guan, Z.; Yin, P.
Deposited on : 2019-06-12
Resolution : 2.50 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 : 4.02b-467
Mogul : 1.8.5 (274361), 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

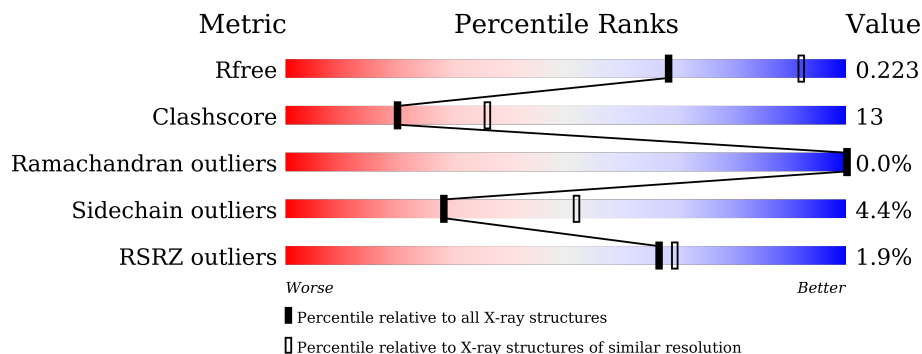
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	612	 2% 61% 18% • 21%
1	B	612	 2% 52% 24% • 21%
1	D	612	 1% 62% 17% • 21%
1	G	612	 2% 60% 18% • 20%
2	C	71	 3% 58% 13% • 28%
2	E	71	 3% 69% 7% • 23%

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Mol	Chain	Length	Quality of chain
2	F	71	 55% 23% 21%
2	H	71	 4% 62% 15% 20%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 17901 atoms, of which 10 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 Cryptochrome-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	484	3933	2540	671	705	17	0	0	0
1	B	481	3911	2527	667	700	17	0	0	0
1	D	486	3952	2555	673	705	19	0	0	0
1	G	490	3980	2571	678	712	19	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	78	GLN	LYS	See Sequence details	UNP Q96524
A	95	PRO	ALA	See Sequence details	UNP Q96524
A	366	GLY	ALA	See Sequence details	UNP Q96524
A	534	VAL	ALA	See Sequence details	UNP Q96524
B	78	GLN	LYS	See Sequence details	UNP Q96524
B	95	PRO	ALA	See Sequence details	UNP Q96524
B	366	GLY	ALA	See Sequence details	UNP Q96524
B	534	VAL	ALA	See Sequence details	UNP Q96524
D	78	GLN	LYS	See Sequence details	UNP Q96524
D	95	PRO	ALA	See Sequence details	UNP Q96524
D	366	GLY	ALA	See Sequence details	UNP Q96524
D	534	VAL	ALA	See Sequence details	UNP Q96524
G	78	GLN	LYS	See Sequence details	UNP Q96524
G	95	PRO	ALA	See Sequence details	UNP Q96524
G	366	GLY	ALA	See Sequence details	UNP Q96524
G	534	VAL	ALA	See Sequence details	UNP Q96524

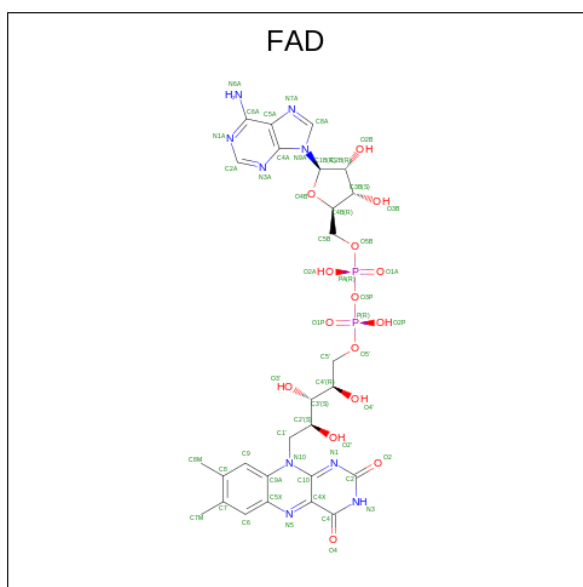
- Molecule 2 is a protein called Protein BIC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
2	E	55	Total	C	H	N	O	S	0	0	0
			424	265	2	78	77	2			
2	C	51	Total	C	H	N	O	S	0	0	0
			396	246	2	74	71	3			
2	F	56	Total	C	H	N	O	S	0	0	0
			432	269	2	79	79	3			
2	H	57	Total	C	H	N	O	S	0	1	0
			452	280	4	84	81	3			

There are 24 discrepancies between the modelled and reference sequences:

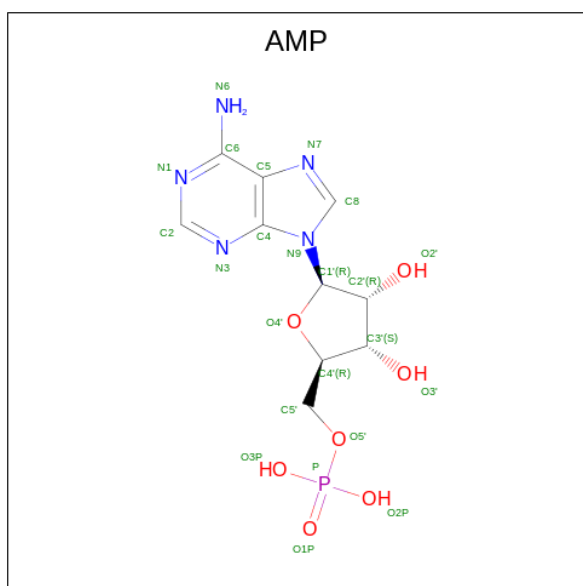
Chain	Residue	Modelled	Actual	Comment	Reference
E	98	HIS	-	expression tag	UNP Q9M280
E	99	HIS	-	expression tag	UNP Q9M280
E	100	HIS	-	expression tag	UNP Q9M280
E	101	HIS	-	expression tag	UNP Q9M280
E	102	HIS	-	expression tag	UNP Q9M280
E	103	HIS	-	expression tag	UNP Q9M280
C	98	HIS	-	expression tag	UNP Q9M280
C	99	HIS	-	expression tag	UNP Q9M280
C	100	HIS	-	expression tag	UNP Q9M280
C	101	HIS	-	expression tag	UNP Q9M280
C	102	HIS	-	expression tag	UNP Q9M280
C	103	HIS	-	expression tag	UNP Q9M280
F	98	HIS	-	expression tag	UNP Q9M280
F	99	HIS	-	expression tag	UNP Q9M280
F	100	HIS	-	expression tag	UNP Q9M280
F	101	HIS	-	expression tag	UNP Q9M280
F	102	HIS	-	expression tag	UNP Q9M280
F	103	HIS	-	expression tag	UNP Q9M280
H	98	HIS	-	expression tag	UNP Q9M280
H	99	HIS	-	expression tag	UNP Q9M280
H	100	HIS	-	expression tag	UNP Q9M280
H	101	HIS	-	expression tag	UNP Q9M280
H	102	HIS	-	expression tag	UNP Q9M280
H	103	HIS	-	expression tag	UNP Q9M280

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
			Total	C	N	O			P	
3	A	1	Total	53	27	9	15	2	0	0
3	B	1	Total	53	27	9	15	2	0	0
3	D	1	Total	53	27	9	15	2	0	0
3	G	1	Total	53	27	9	15	2	0	0

- Molecule 4 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	D	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	G	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

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

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

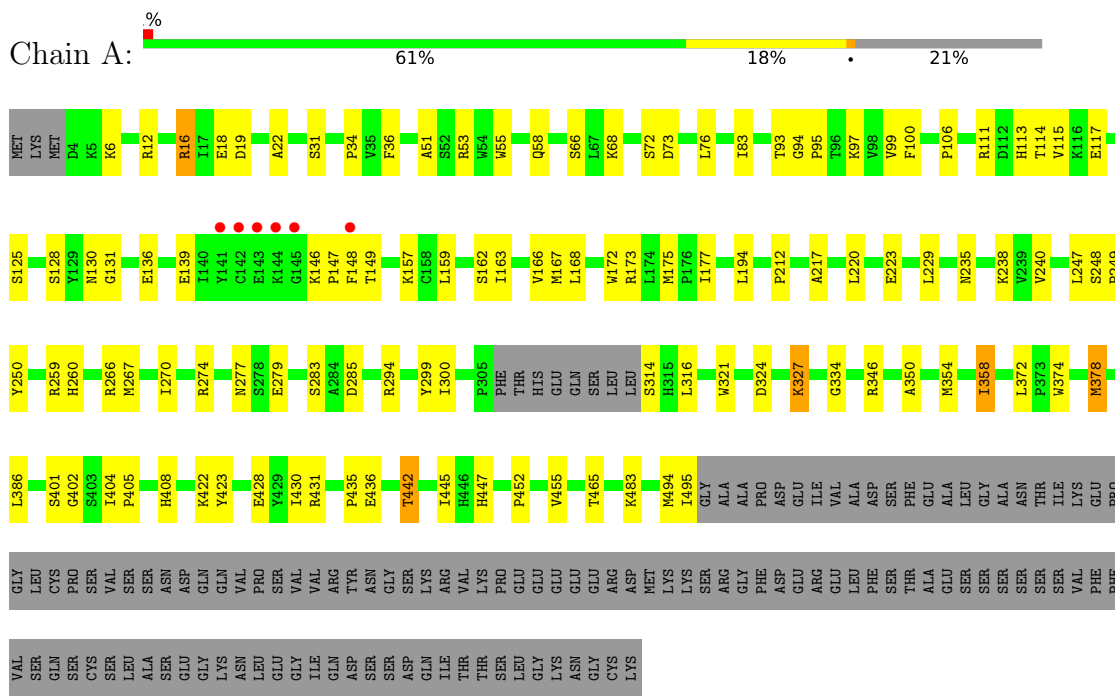
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	29	Total	O	0	0
			29	29		
6	E	3	Total	O	0	0
			3	3		
6	B	16	Total	O	0	0
			16	16		
6	C	2	Total	O	0	0
			2	2		
6	D	42	Total	O	0	0
			42	42		
6	F	2	Total	O	0	0
			2	2		
6	G	16	Total	O	0	0
			16	16		
6	H	3	Total	O	0	0
			3	3		

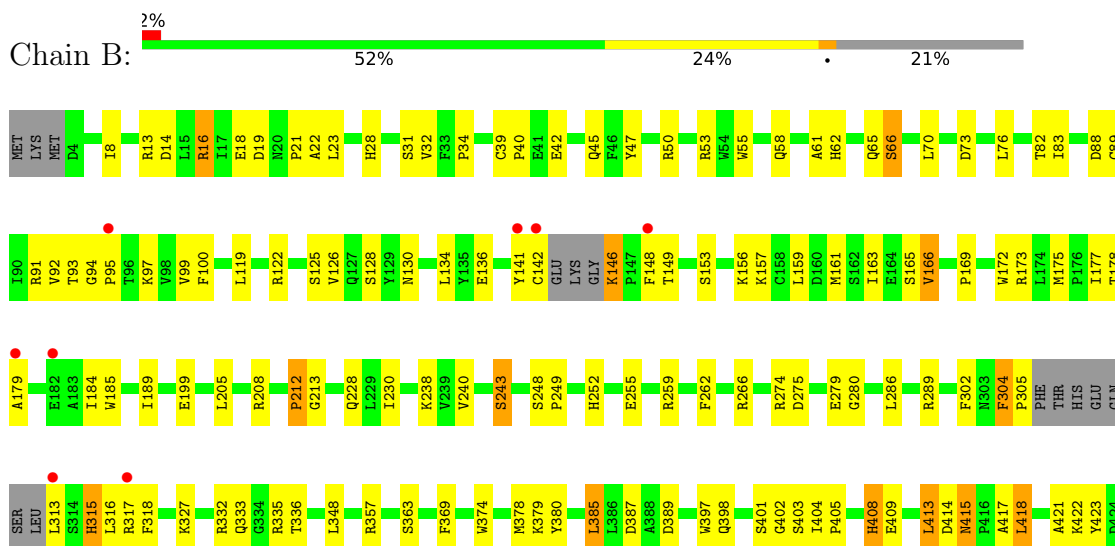
3 Residue-property plots

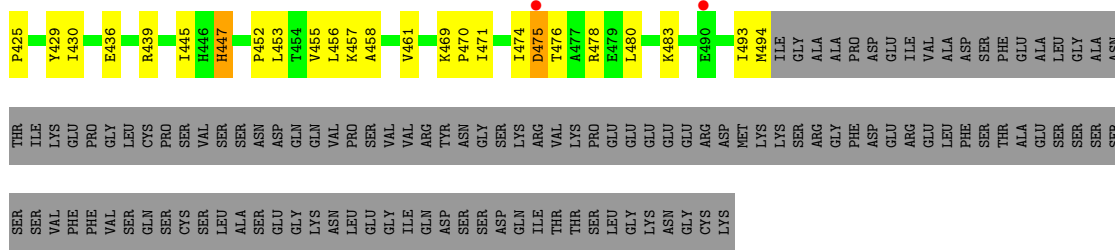
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Cryptochrome-2

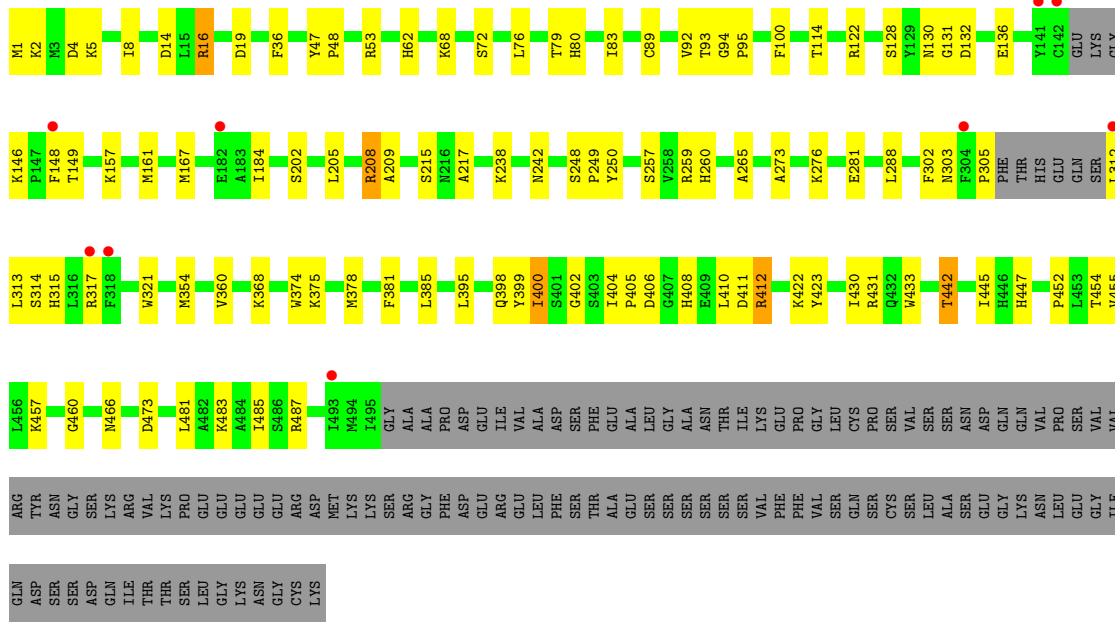


• Molecule 1: Cryptochrome-2

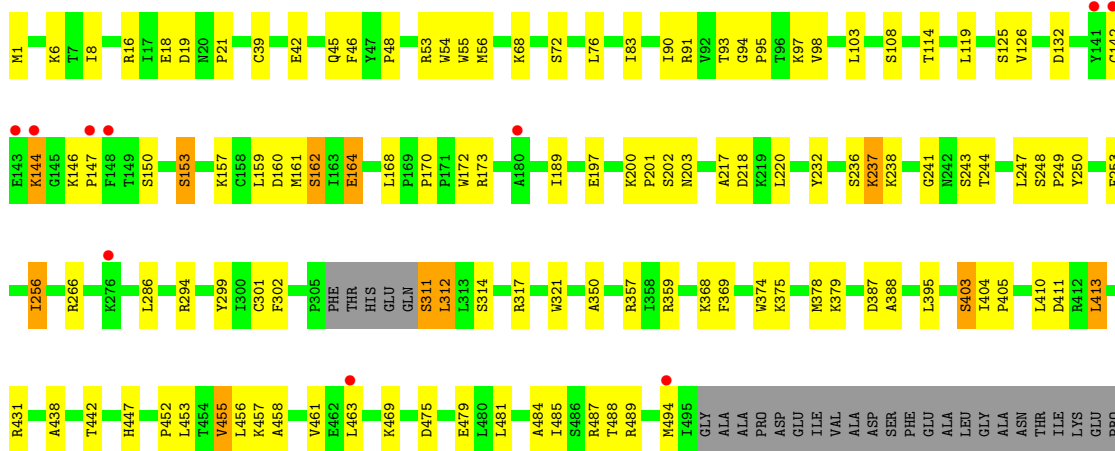




• Molecule 1: Cryptochrome-2



• Molecule 1: Cryptochrome-2



GLY LEU SER CYS PRO SER VAL SER ASN ASP GLN GLN VAL PRO VAL VAL VAL ARG TYR ASN GLY SER ASP LYS ARG VAL LYS PRO GLU GLU GLU GLU ARG ASP MET LYS LYS SER ARG GLY PHE ASP GLU ARG GLU LEU PHE SER THR THR ALA GLU SER SER SER SER VAL PHE

VAL SER GLN SER CYS SER LEU ALA SER GLY ASN VAL LEU GLY ILE THR ASP SER ASP LYS ILE THR THR SER LEU LYS ASN GLY CYS LYS

• Molecule 2: Protein BIC2



PRO GLU THR THR VAL V37 L38 R41 V55 W70 MET ASP PHE SER THR F76 D77 I85 S96 GLY HIS HIS HIS HIS HIS HIS

• Molecule 2: Protein BIC2



PRO GLU THR THR VAL L38 R46 E49 D59 S60 W61 G62 K63 W70 M71 ASP PHE SER THR PHE ASP ALA ALA F80 T81 R89 S96 GLY HIS HIS HIS HIS HIS HIS

• Molecule 2: Protein BIC2



PRO GLU THR THR VAL L38 R41 L44 R47 E50 V51 A52 V55 W70 M71 ASP PHE SER THR T75 F76 F80 T81 S82 I85 R89 L92 M93 S96 GLY HIS HIS HIS HIS HIS HIS

• Molecule 2: Protein BIC2



PRO GLU THR THR VAL V37 L44 K45 R46 R48 E49 E50 V55 W70 M71 ASP PHE SER T75 F76 D77 A78 A79 R89 L92 S96 GLY HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	142.55Å 142.55Å 526.43Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.42 – 2.50 48.42 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.0 (48.42-2.50) 99.0 (48.42-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.09 (at 2.51Å)	Xtrriage
Refinement program	PHENIX (1.15.2_3472: ???)	Depositor
R, R_{free}	0.171 , 0.223 0.171 , 0.223	Depositor DCC
R_{free} test set	5437 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	50.6	Xtrriage
Anisotropy	0.522	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 39.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17901	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.19% 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: FAD, MG, AMP

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	0.42	0/4049	0.57	0/5504
1	B	0.40	0/4026	0.55	1/5473 (0.0%)
1	D	0.45	0/4067	0.59	0/5526
1	G	0.44	0/4096	0.58	0/5565
2	C	0.39	0/400	0.51	0/534
2	E	0.41	0/429	0.55	0/575
2	F	0.41	0/437	0.52	0/585
2	H	0.42	0/455	0.54	0/609
All	All	0.43	0/17959	0.57	1/24371 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	385	LEU	CA-CB-CG	5.32	127.54	115.30

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	3933	0	3867	94	0
1	B	3911	0	3844	148	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3952	0	3900	78	0
1	G	3980	0	3928	99	0
2	C	394	2	398	8	0
2	E	422	2	421	6	0
2	F	430	2	428	19	0
2	H	448	4	449	13	0
3	A	53	0	31	7	0
3	B	53	0	30	4	0
3	D	53	0	30	1	0
3	G	53	0	30	12	0
4	A	23	0	12	0	0
4	B	23	0	12	0	0
4	D	23	0	12	1	0
4	G	23	0	12	1	0
5	A	1	0	0	0	0
5	D	2	0	0	0	0
5	G	1	0	0	0	0
6	A	29	0	0	1	0
6	B	16	0	0	1	0
6	C	2	0	0	0	0
6	D	42	0	0	1	0
6	E	3	0	0	0	0
6	F	2	0	0	0	0
6	G	16	0	0	1	0
6	H	3	0	0	0	0
All	All	17891	10	17404	442	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 13.

The worst 5 of 442 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:A:701:FAD:H51A	3:A:701:FAD:H8A	1.20	1.11
3:G:701:FAD:H51A	3:G:701:FAD:H8A	1.12	1.09
1:A:83:ILE:HD11	1:A:114:THR:HG22	1.40	1.03
1:A:465:THR:HG22	1:D:457:LYS:HE3	1.42	0.97
3:G:701:FAD:H8A	3:G:701:FAD:C5B	1.95	0.97

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	A	480/612 (78%)	468 (98%)	12 (2%)	0	100	100
1	B	475/612 (78%)	458 (96%)	17 (4%)	0	100	100
1	D	480/612 (78%)	464 (97%)	16 (3%)	0	100	100
1	G	486/612 (79%)	470 (97%)	15 (3%)	1 (0%)	47	68
2	C	47/71 (66%)	44 (94%)	3 (6%)	0	100	100
2	E	51/71 (72%)	51 (100%)	0	0	100	100
2	F	52/71 (73%)	51 (98%)	1 (2%)	0	100	100
2	H	54/71 (76%)	52 (96%)	2 (4%)	0	100	100
All	All	2125/2732 (78%)	2058 (97%)	66 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	403	SER

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	A	419/531 (79%)	403 (96%)	16 (4%)	33	58
1	B	417/531 (78%)	392 (94%)	25 (6%)	19	37
1	D	422/531 (80%)	408 (97%)	14 (3%)	38	64
1	G	425/531 (80%)	408 (96%)	17 (4%)	31	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	41/58 (71%)	39 (95%)	2 (5%)	25	47
2	E	43/58 (74%)	41 (95%)	2 (5%)	26	49
2	F	44/58 (76%)	42 (96%)	2 (4%)	27	51
2	H	46/58 (79%)	43 (94%)	3 (6%)	17	33
All	All	1857/2356 (79%)	1776 (96%)	81 (4%)	28	52

5 of 81 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	447	HIS
1	G	311	SER
2	F	51	VAL
1	G	162	SER
1	G	447	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	228	GLN
1	A	242	ASN
1	B	45	GLN
1	B	252	HIS

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 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	AMP	D	702	5	22,25,25	1.17	3 (13%)	25,38,38	3.10	4 (16%)
3	FAD	A	701	-	53,58,58	3.80	20 (37%)	68,89,89	2.61	23 (33%)
4	AMP	A	702	-	22,25,25	1.16	3 (13%)	25,38,38	3.31	4 (16%)
3	FAD	G	701	-	53,58,58	3.94	25 (47%)	68,89,89	2.49	24 (35%)
3	FAD	D	701	-	53,58,58	3.80	20 (37%)	68,89,89	2.24	20 (29%)
3	FAD	B	701	-	53,58,58	3.91	21 (39%)	68,89,89	2.23	23 (33%)
4	AMP	B	702	-	22,25,25	1.19	2 (9%)	25,38,38	3.33	5 (20%)
4	AMP	G	702	-	22,25,25	1.16	3 (13%)	25,38,38	3.30	5 (20%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AMP	D	702	5	-	2/6/26/26	0/3/3/3
3	FAD	A	701	-	-	13/30/50/50	0/6/6/6
4	AMP	A	702	-	-	0/6/26/26	0/3/3/3
3	FAD	G	701	-	-	11/30/50/50	0/6/6/6
3	FAD	D	701	-	-	3/30/50/50	0/6/6/6
3	FAD	B	701	-	-	11/30/50/50	0/6/6/6
4	AMP	B	702	-	-	2/6/26/26	0/3/3/3
4	AMP	G	702	-	-	5/6/26/26	0/3/3/3

The worst 5 of 97 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	701	FAD	O4B-C1B	15.41	1.62	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	FAD	O4B-C1B	14.66	1.61	1.41
3	D	701	FAD	O4B-C1B	14.14	1.60	1.41
3	G	701	FAD	C2B-C1B	-14.10	1.32	1.53
3	A	701	FAD	C2B-C1B	-13.93	1.32	1.53

The worst 5 of 108 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	702	AMP	C1'-N9-C4	10.45	145.00	126.64
4	A	702	AMP	C1'-N9-C4	10.30	144.74	126.64
4	G	702	AMP	C1'-N9-C4	9.66	143.61	126.64
4	G	702	AMP	C5-C6-N6	9.47	134.74	120.35
4	A	702	AMP	C5-C6-N6	9.26	134.43	120.35

There are no chirality outliers.

5 of 47 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	701	FAD	C2'-C1'-N10-C10
3	A	701	FAD	N10-C1'-C2'-O2'
3	A	701	FAD	N10-C1'-C2'-C3'
3	A	701	FAD	C2'-C3'-C4'-C5'
3	A	701	FAD	O3'-C3'-C4'-O4'

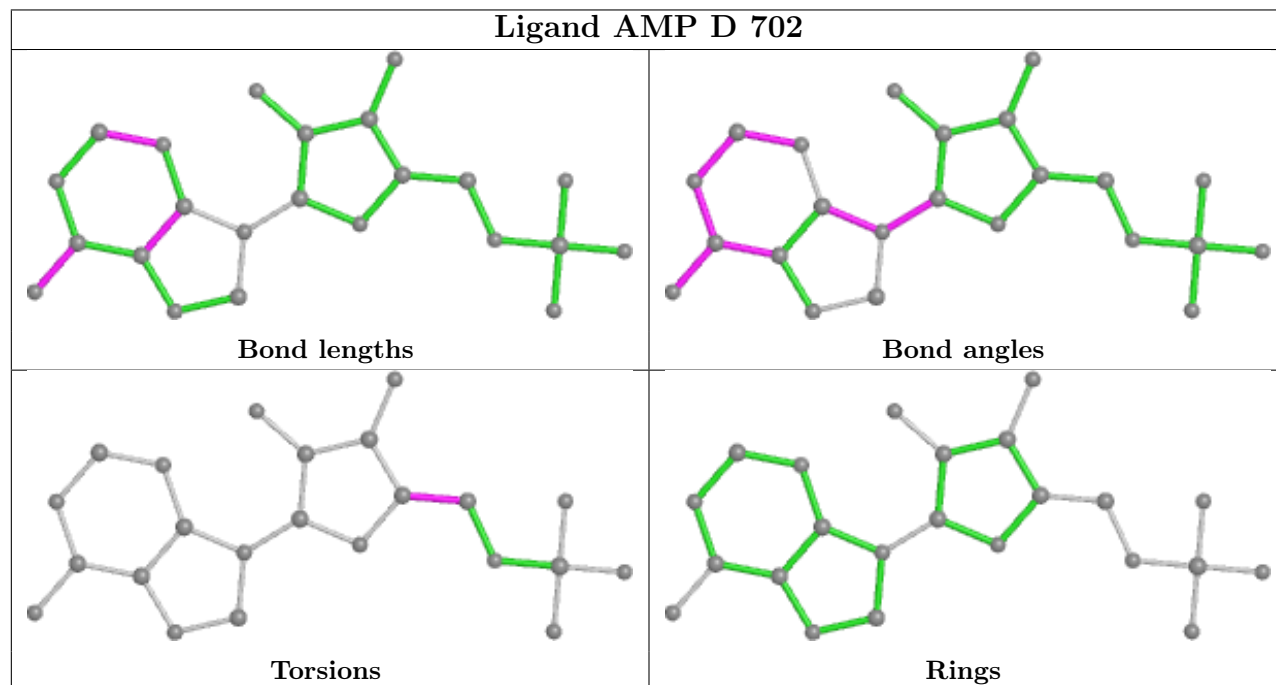
There are no ring outliers.

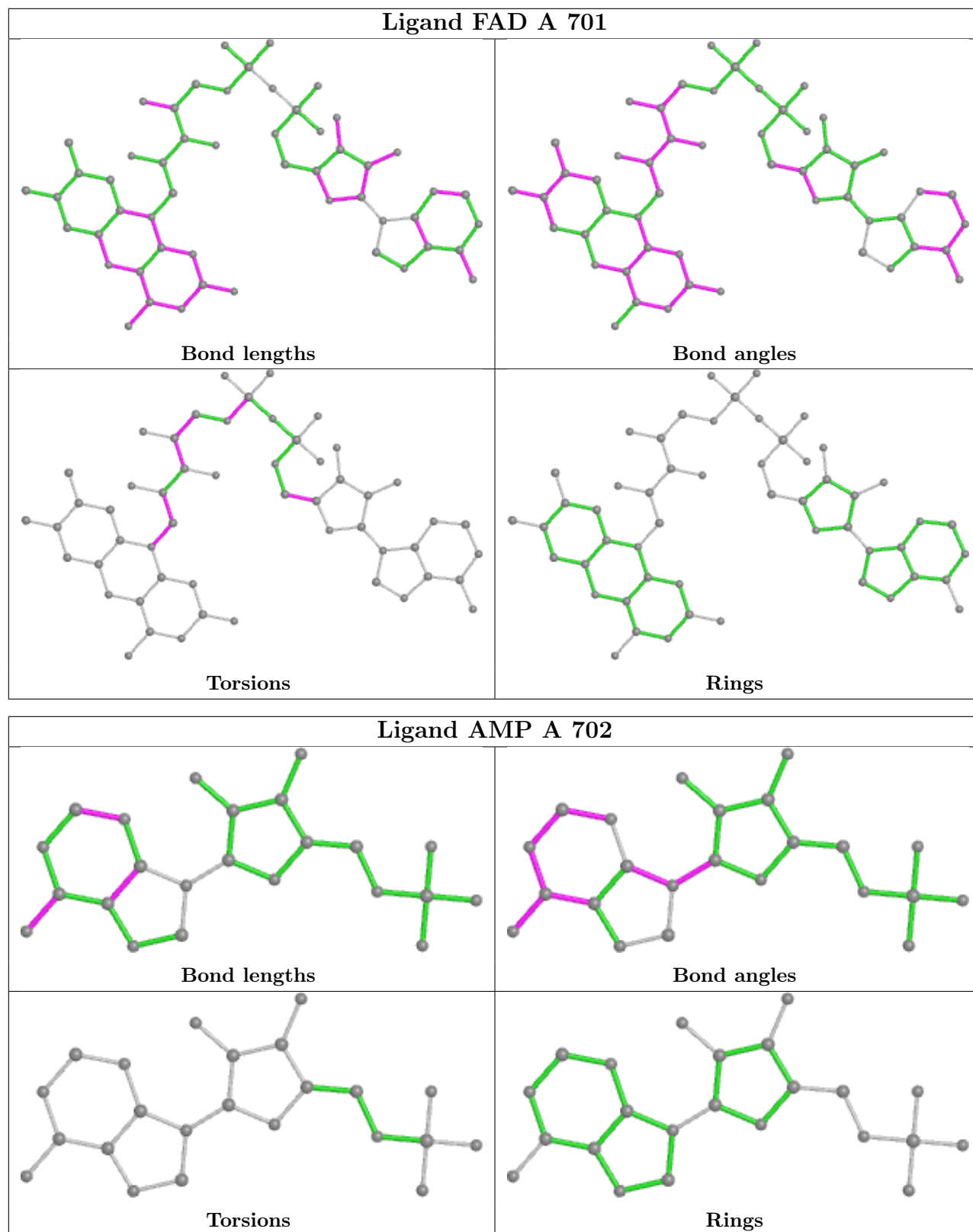
6 monomers are involved in 26 short contacts:

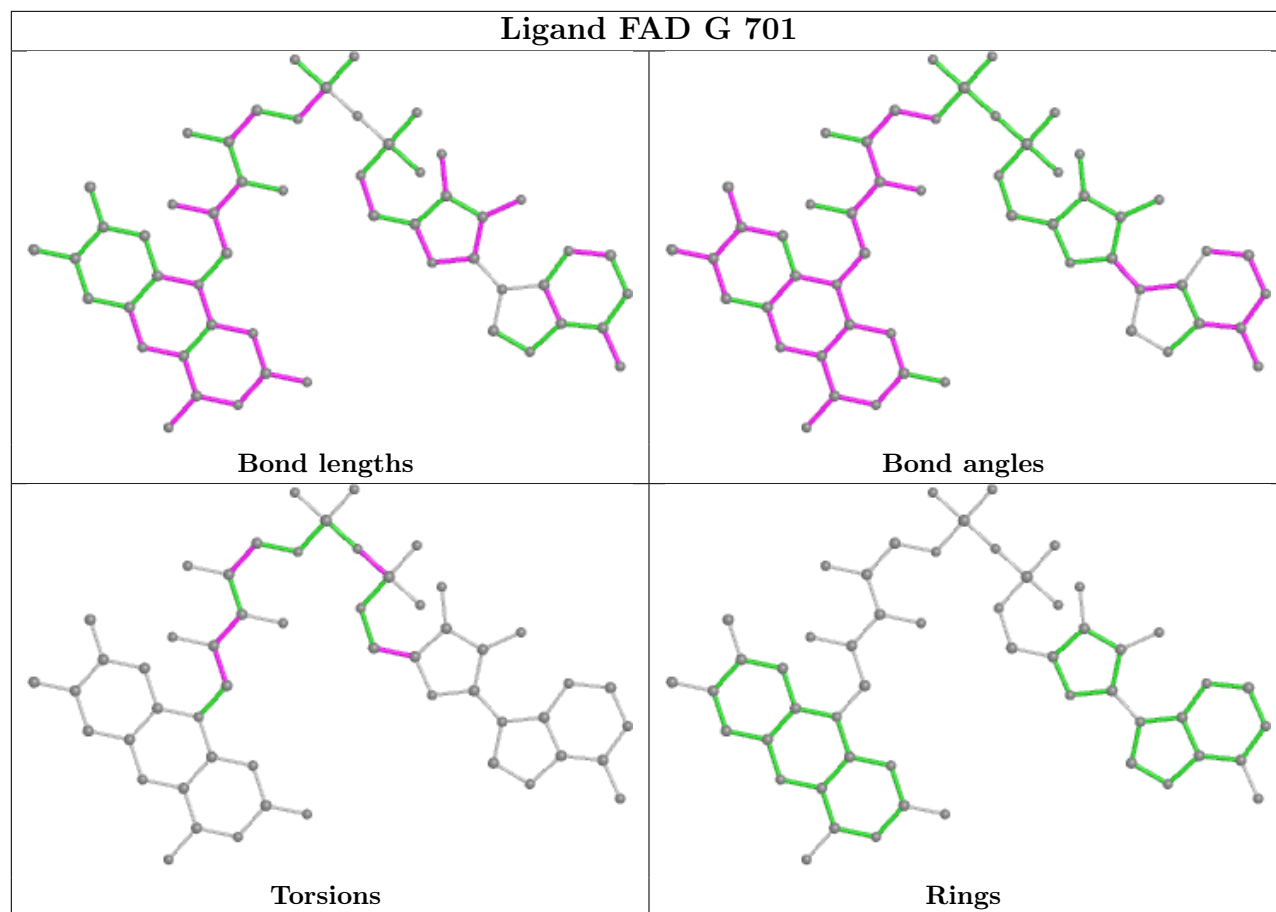
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	702	AMP	1	0
3	A	701	FAD	7	0
3	G	701	FAD	12	0
3	D	701	FAD	1	0
3	B	701	FAD	4	0
4	G	702	AMP	1	0

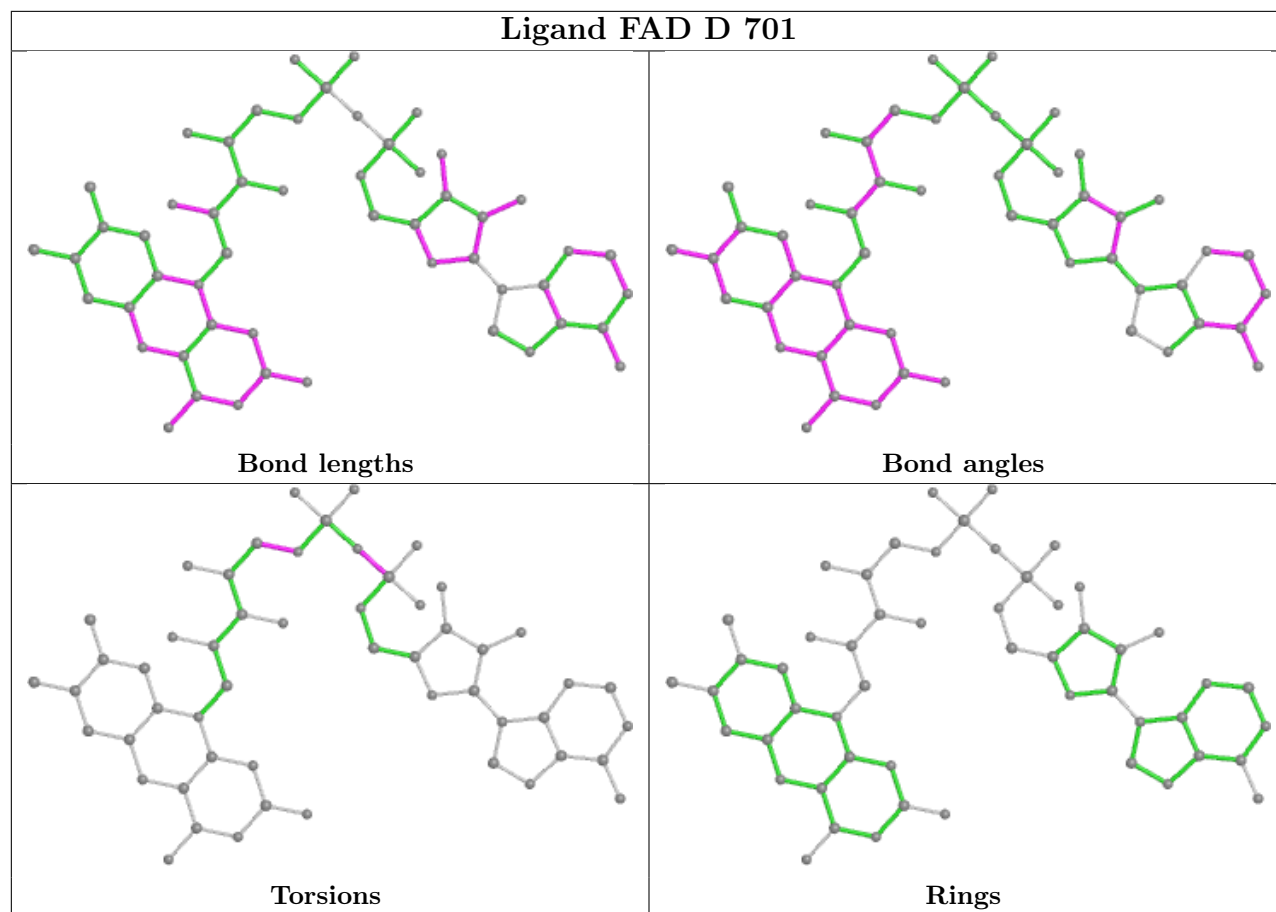
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

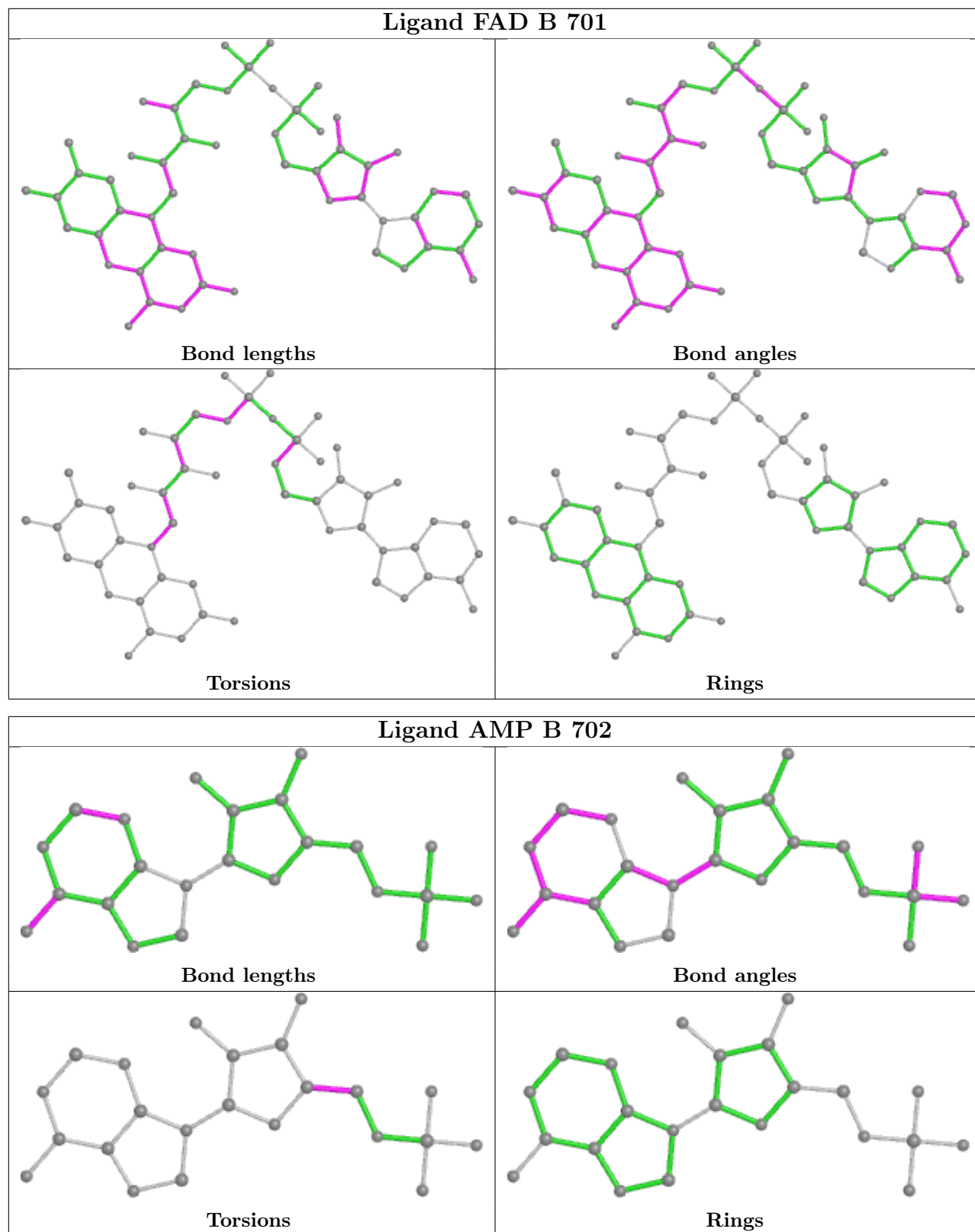
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

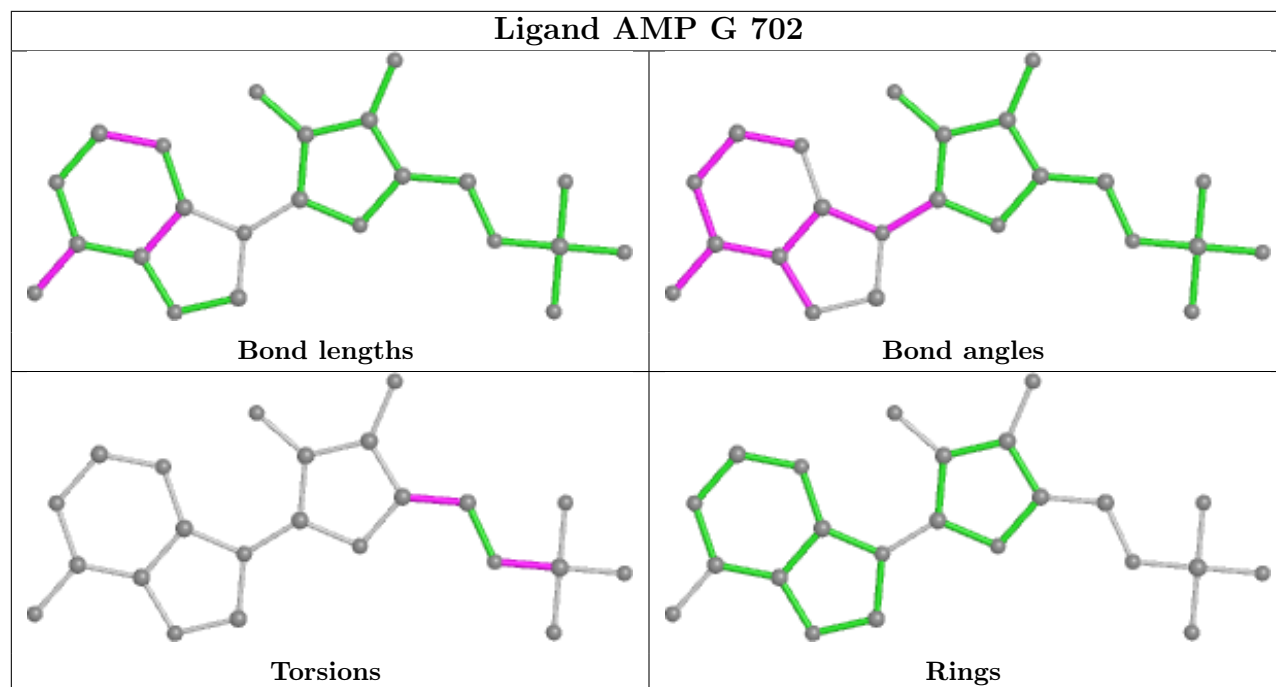












5.7 Other polymers [i](#)

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	A	484/612 (79%)	-0.24	6 (1%) 79 80	35, 54, 89, 143	0
1	B	481/612 (78%)	0.01	10 (2%) 63 66	41, 64, 101, 138	0
1	D	486/612 (79%)	-0.19	9 (1%) 66 69	35, 51, 93, 127	0
1	G	490/612 (80%)	-0.11	10 (2%) 65 68	36, 57, 92, 126	0
2	C	51/71 (71%)	0.10	2 (3%) 39 42	58, 75, 107, 111	0
2	E	55/71 (77%)	-0.04	2 (3%) 42 46	49, 68, 102, 141	0
2	F	56/71 (78%)	-0.02	0 100 100	45, 69, 112, 117	0
2	H	57/71 (80%)	0.31	3 (5%) 26 28	53, 74, 112, 132	0
All	All	2160/2732 (79%)	-0.11	42 (1%) 66 69	35, 58, 99, 143	0

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	143	GLU	6.8
1	A	142	CYS	6.4
1	G	142	CYS	5.6
1	D	493	ILE	5.1
1	A	144	LYS	5.0

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

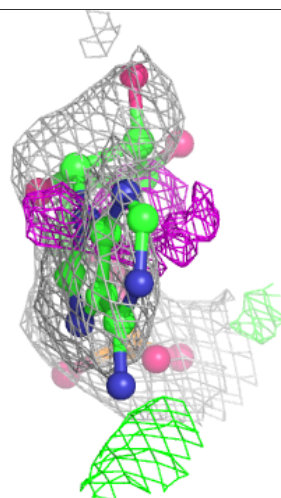
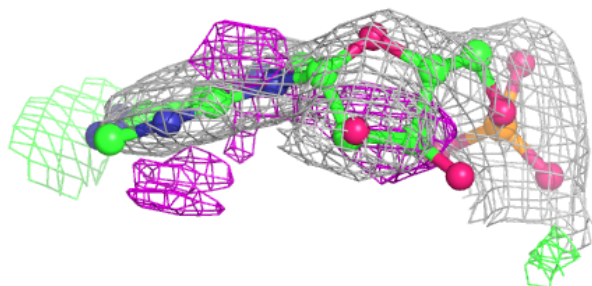
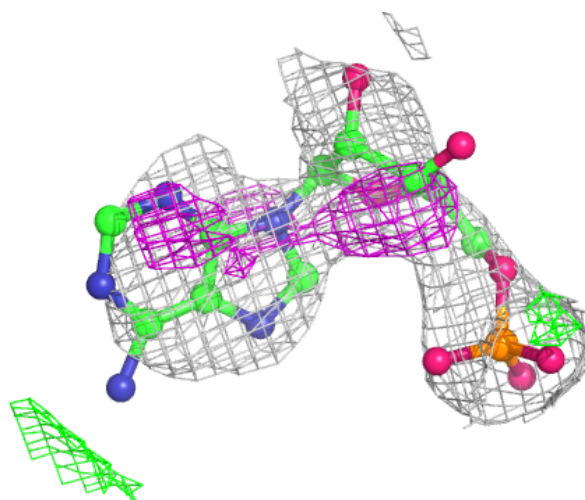
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	AMP	B	702	23/23	0.79	0.28	86,105,143,148	0
4	AMP	G	702	23/23	0.87	0.17	58,70,107,108	0
5	MG	A	703	1/1	0.87	0.25	64,64,64,64	0
4	AMP	A	702	23/23	0.88	0.25	70,84,129,134	0
5	MG	G	703	1/1	0.89	0.29	65,65,65,65	0
4	AMP	D	702	23/23	0.91	0.18	65,81,108,114	0
5	MG	D	704	1/1	0.95	0.17	71,71,71,71	0
3	FAD	G	701	53/53	0.98	0.19	33,43,52,60	0
3	FAD	A	701	53/53	0.98	0.15	31,40,50,57	0
3	FAD	B	701	53/53	0.98	0.20	35,48,60,69	0
3	FAD	D	701	53/53	0.98	0.17	31,39,46,56	0
5	MG	D	703	1/1	0.99	0.42	62,62,62,62	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.

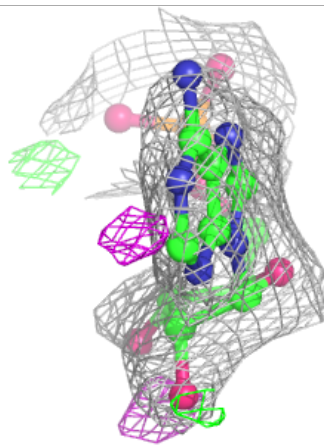
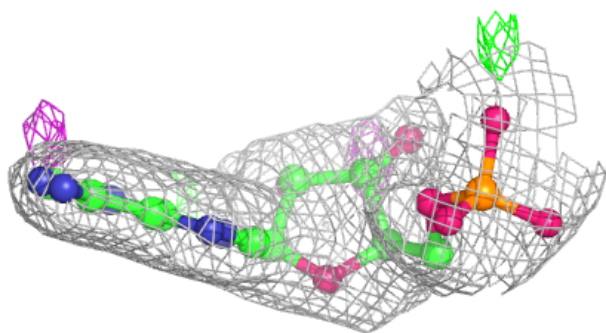
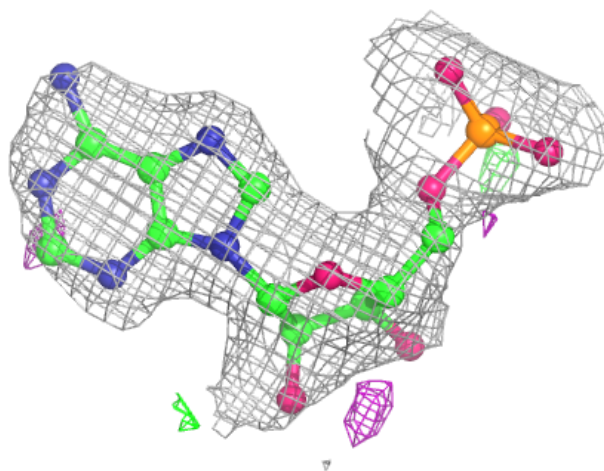
Electron density around AMP B 702:

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



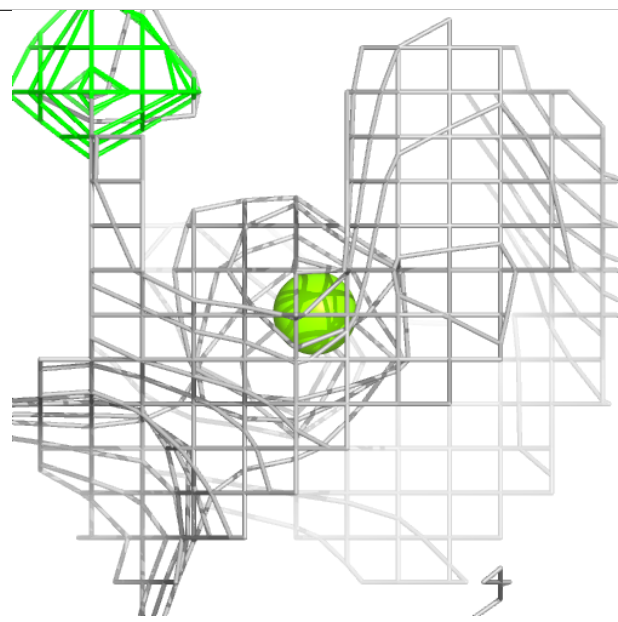
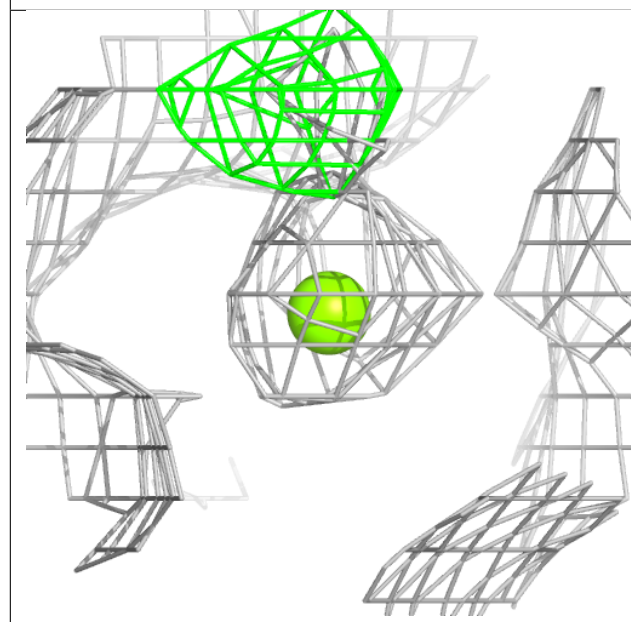
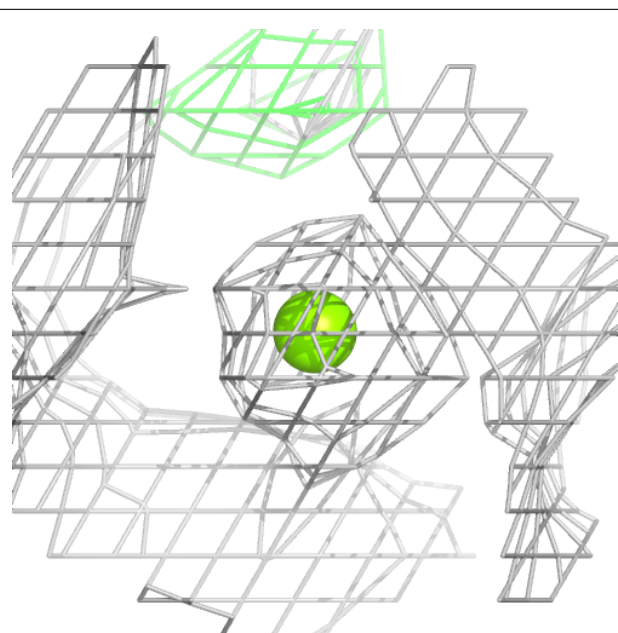
Electron density around AMP G 702:

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



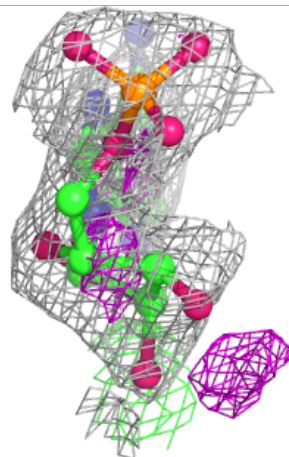
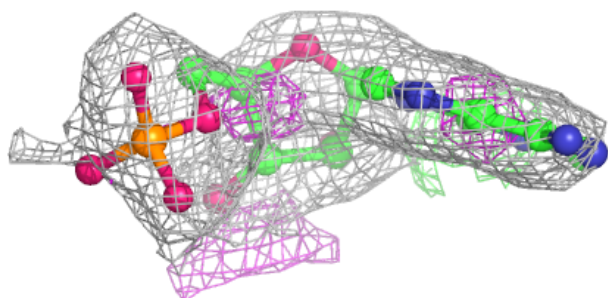
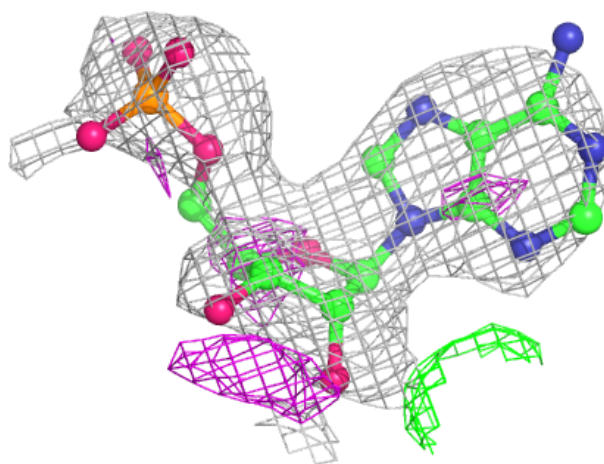
Electron density around MG A 703:

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



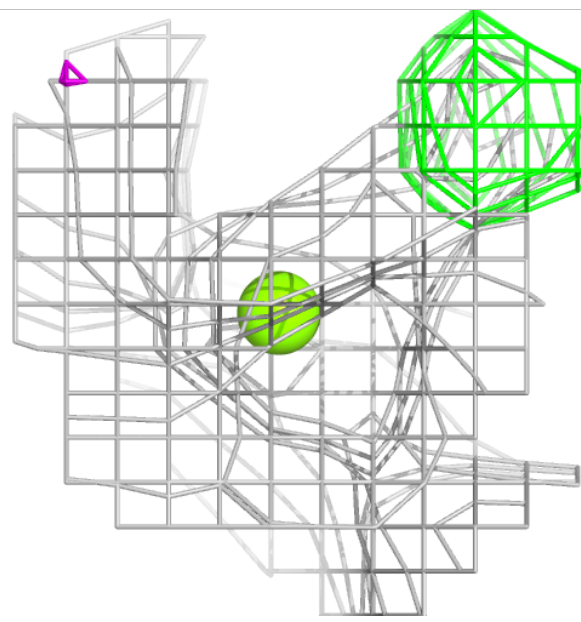
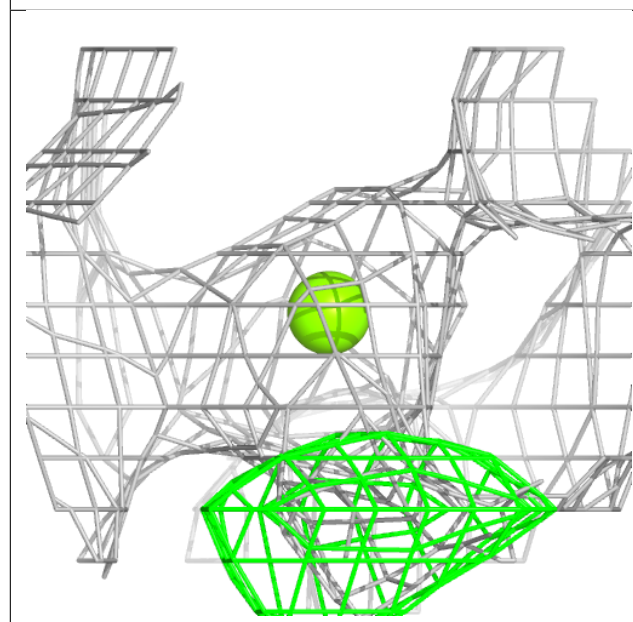
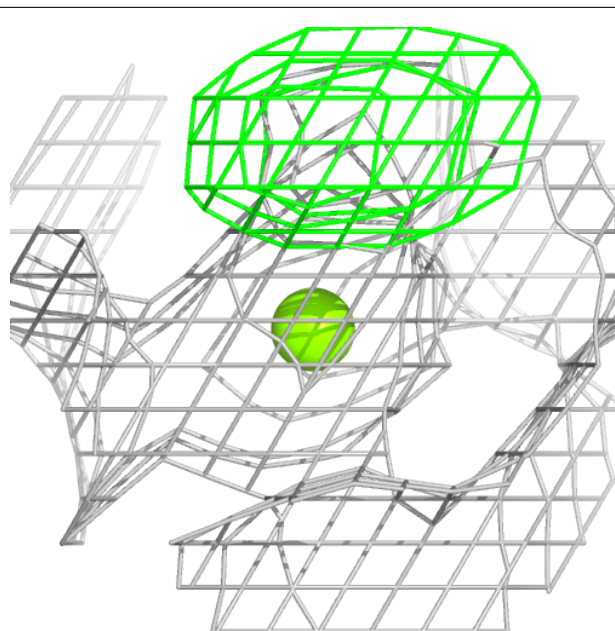
Electron density around AMP A 702:

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



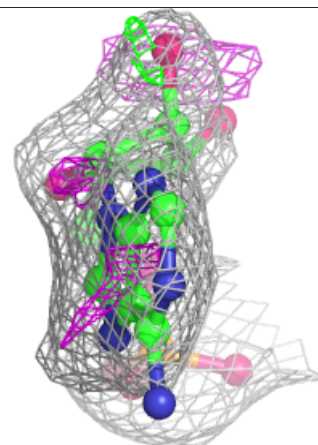
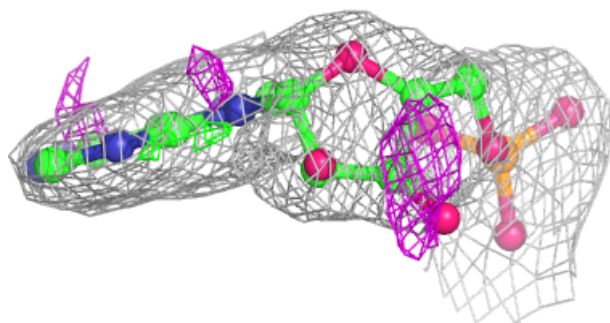
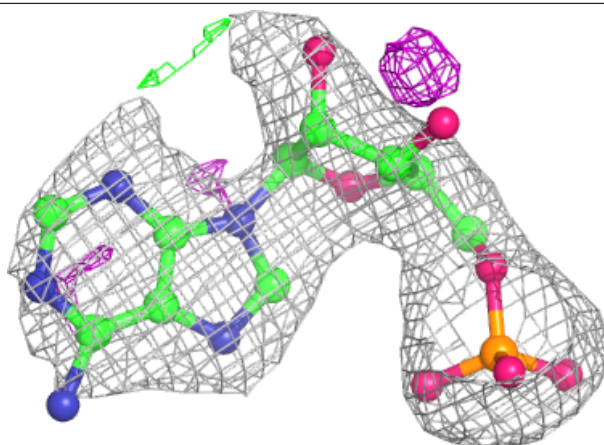
Electron density around MG G 703:

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



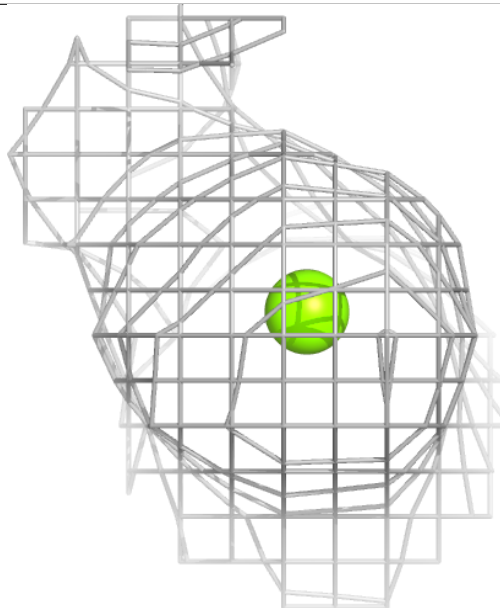
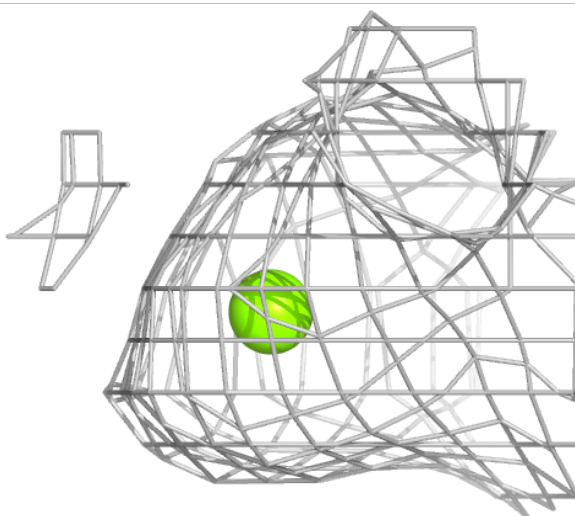
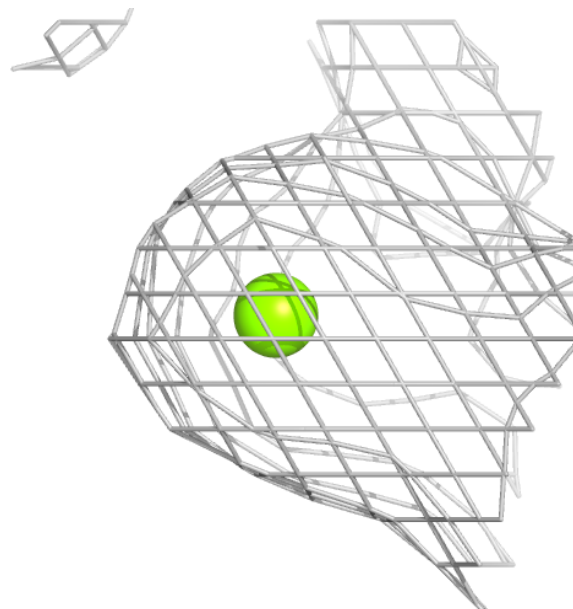
Electron density around AMP D 702:

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



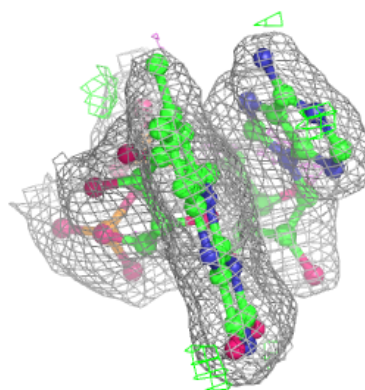
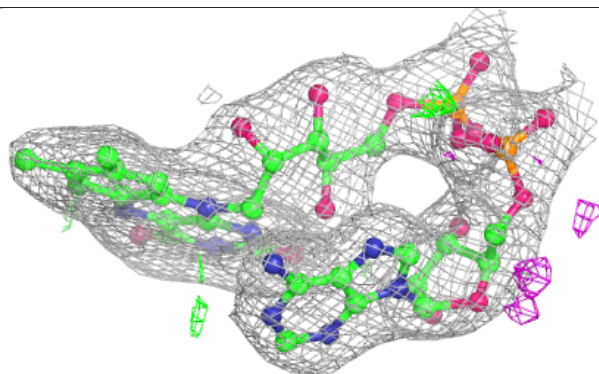
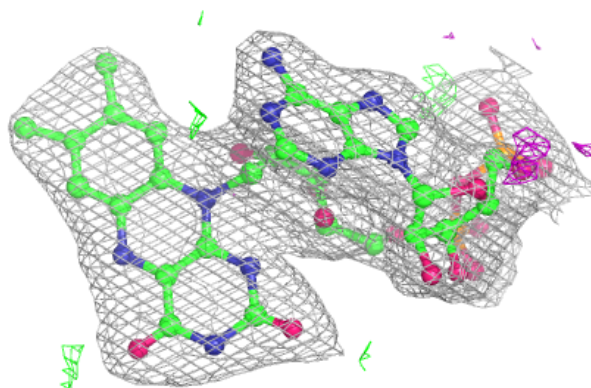
Electron density around MG D 704:

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and green (positive)

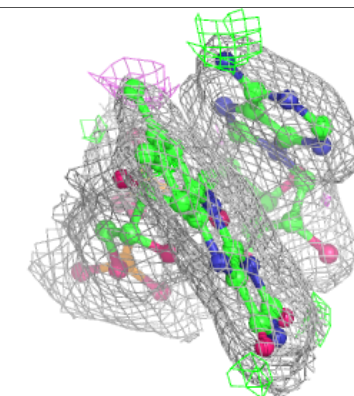
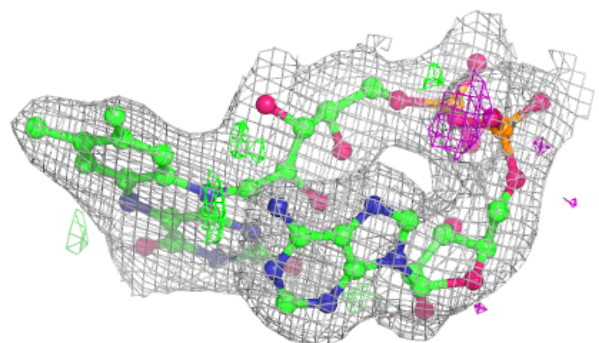
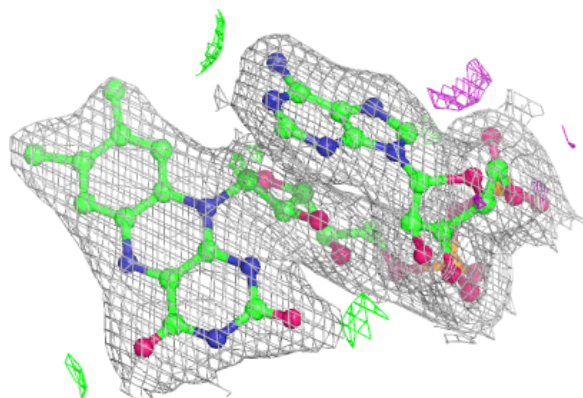


Electron density around FAD G 701:

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

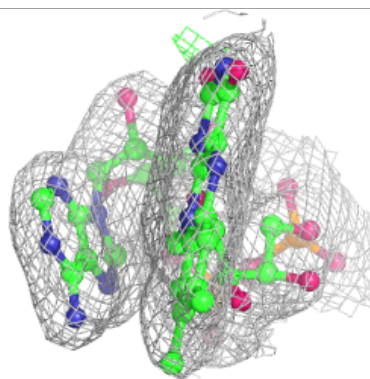
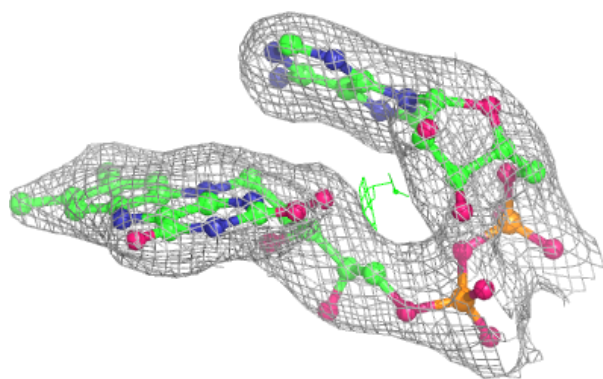
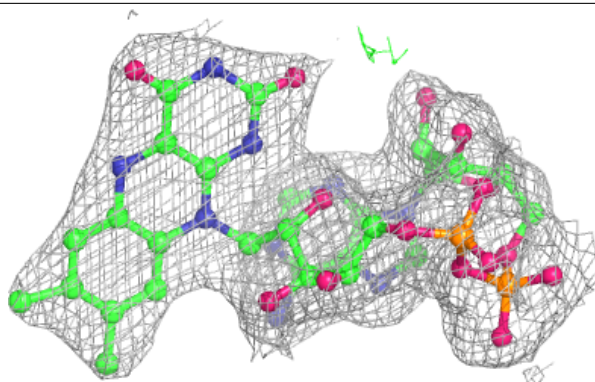
**Electron density around FAD A 701:**

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

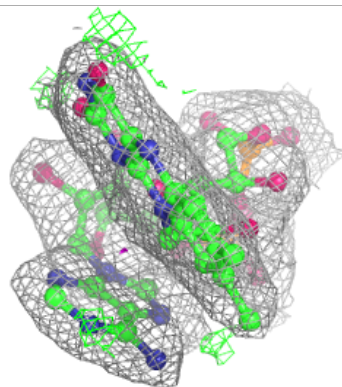
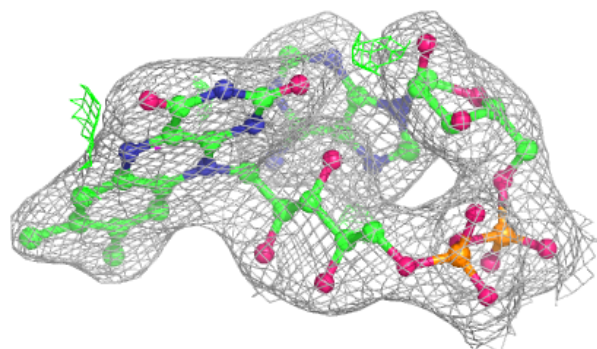
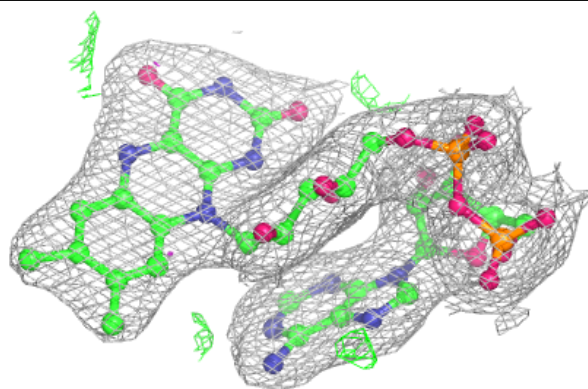


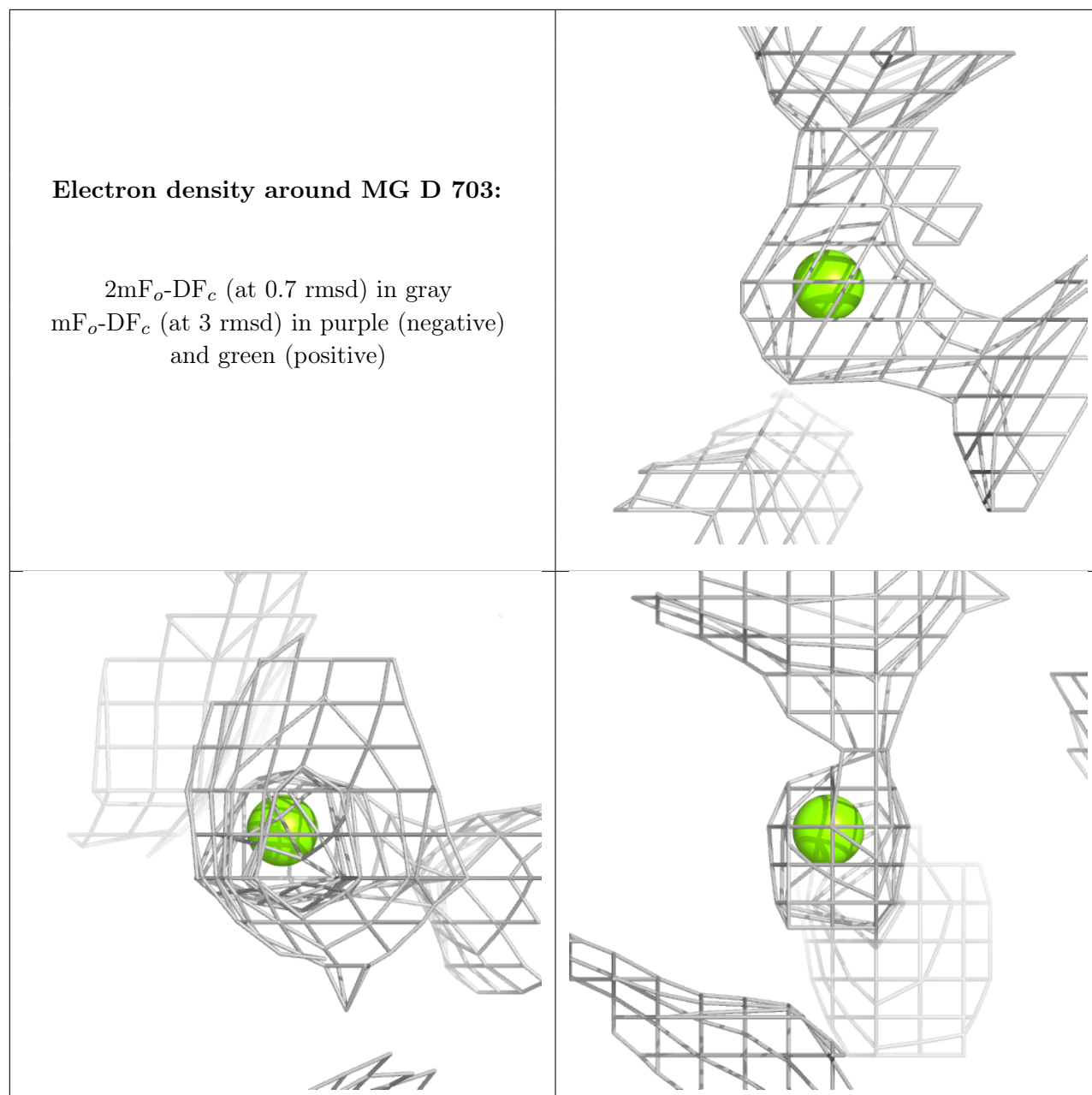
Electron density around FAD B 701:

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

**Electron density around FAD D 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.