Full wwPDB X-ray Structure Validation Report ⓘ

Aug 1, 2024 – 10:30 am BST

PDB ID	:	9EV6
Title	:	Corynebacterium glutamicum pyruvate:quinone oxidoreductase (PQO), C-terminal truncated construct
Authors	:	Da Silva Lameira, C.; Muenssinger, S.; Yang, L.; Eikmanns, B.J.; Bellinzoni, M.
Deposited on	:	2024-03-28
Resolution	:	1.89 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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:

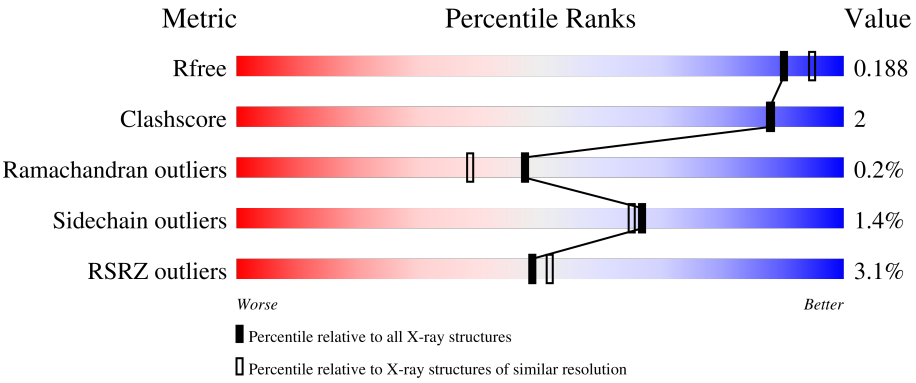
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 1.89 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	564	3% 90% 5% 5%
1	B	564	% 91% · 5%
1	C	564	2% 90% 5% 5%
1	D	564	5% 90% 5% 5%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 17270 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.

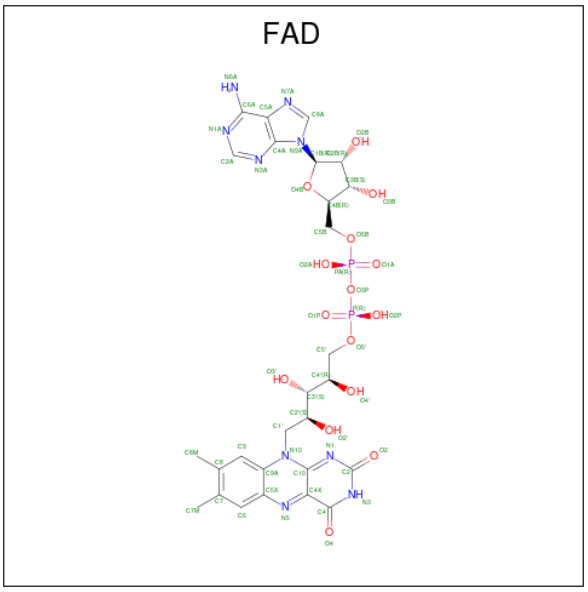
- Molecule 1 is a protein called Thiamine pyrophosphate-requiring enzymes [acetolactate synthase, pyruvate dehydrogenase (Cytochrome), glyoxylate carboligase, phosphonopyruvate decarboxylase].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	535	Total	C	N	O	S	0	0	0
			3974	2496	690	770	18			
1	B	536	Total	C	N	O	S	0	0	0
			3997	2510	693	776	18			
1	C	535	Total	C	N	O	S	0	0	0
			4000	2512	693	777	18			
1	D	537	Total	C	N	O	S	0	0	0
			3974	2498	690	768	18			

There are 8 discrepancies between the modelled and reference sequences:

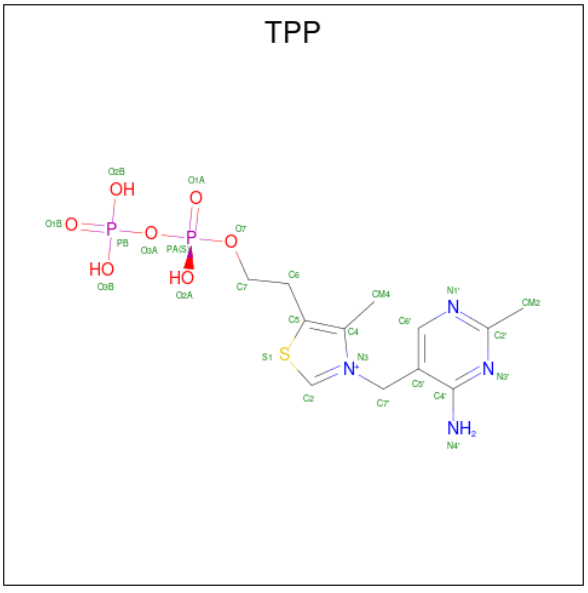
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q8NMG5
A	0	HIS	-	expression tag	UNP Q8NMG5
B	-1	GLY	-	expression tag	UNP Q8NMG5
B	0	HIS	-	expression tag	UNP Q8NMG5
C	-1	GLY	-	expression tag	UNP Q8NMG5
C	0	HIS	-	expression tag	UNP Q8NMG5
D	-1	GLY	-	expression tag	UNP Q8NMG5
D	0	HIS	-	expression tag	UNP Q8NMG5

- Molecule 2 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
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 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
3	A	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	B	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	C	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	D	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		

- Molecule 5 is water.

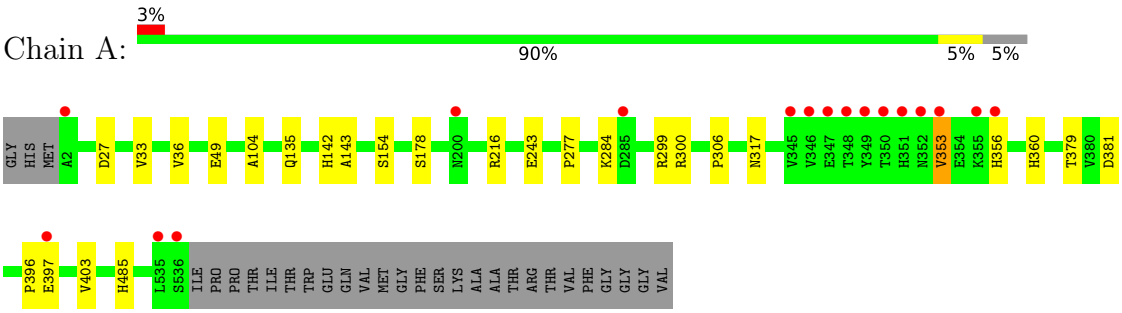
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	262	Total	O	0	0
			262	262		
5	B	276	Total	O	0	0
			276	276		
5	C	238	Total	O	0	0
			238	238		
5	D	229	Total	O	0	0
			229	229		

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.

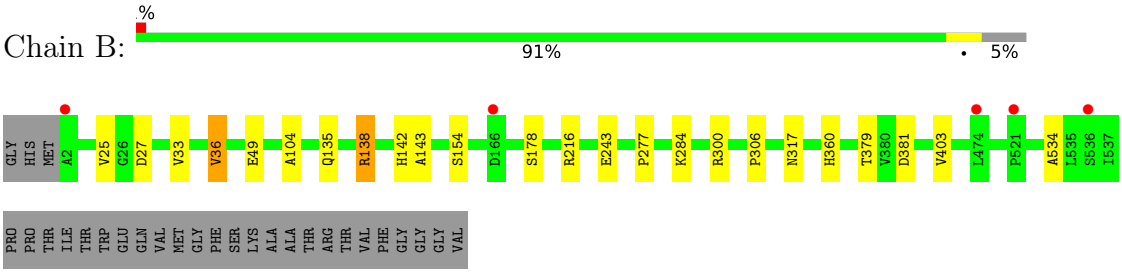
• Molecule 1: Thiamine pyrophosphate-requiring enzymes [acetolactate synthase, pyruvate dehydrogenase (Cytochrome), glyoxylate carboligase, phosphonopyruvate decarboxylase]

Chain A:



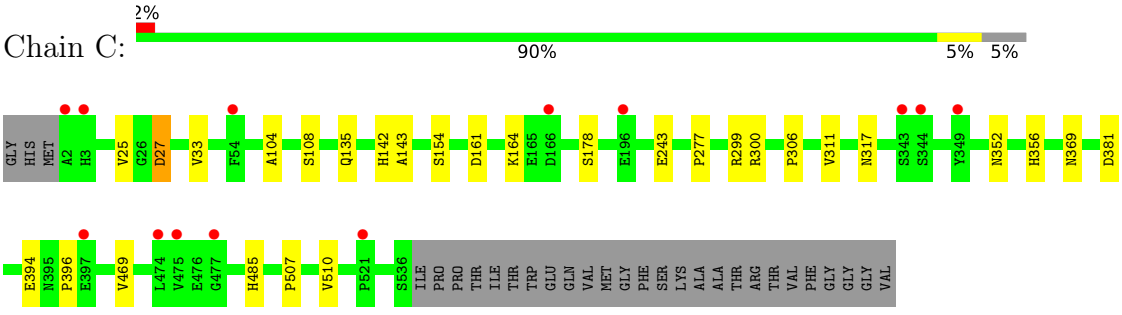
• Molecule 1: Thiamine pyrophosphate-requiring enzymes [acetolactate synthase, pyruvate dehydrogenase (Cytochrome), glyoxylate carboligase, phosphonopyruvate decarboxylase]

Chain B:



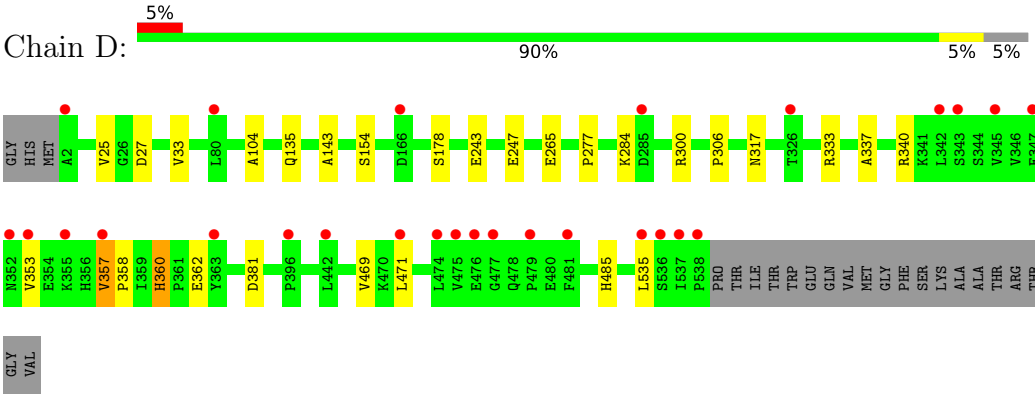
• Molecule 1: Thiamine pyrophosphate-requiring enzymes [acetolactate synthase, pyruvate dehydrogenase (Cytochrome), glyoxylate carboligase, phosphonopyruvate decarboxylase]

Chain C:



• Molecule 1: Thiamine pyrophosphate-requiring enzymes [acetolactate synthase, pyruvate dehydrogenase (Cytochrome), glyoxylate carboligase, phosphonopyruvate decarboxylase]

Chain D:


5%
90%
5%
5%
GLY HIS MET A2 V25 G26 D27 V33 L50 A104 Q135 A143 S154 D166 S178 E243 E247 E265 P277 K284 D285 R300 P306 N317 T326 R333 A337 R340 K341 L342 S343 S344 V345 V346 E347 T348 Y349 T350 H351
N352 V353 E354 K355 H356 V357 P358 I359 H360 P361 E362 Y363 D381 P396 L442 V469 K470 L471 L474 V475 E476 G477 Q478 P479 E480 F481 H485 L535 S536 I537 P538 PRO THR ILE THR TRP GLU GLN VAL MET GLY PHE SER LYS ALA ALA THR ARG THR VAL PHE GLY GLY
GLY VAL

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	100.55Å 98.48Å 110.52Å 90.00° 90.84° 90.00°	Depositor
Resolution (Å)	37.46 – 1.89 37.46 – 1.89	Depositor EDS
% Data completeness (in resolution range)	77.8 (37.46-1.89) 77.7 (37.46-1.89)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.59 (at 1.89Å)	Xtriage
Refinement program	BUSTER 2.10.4	Depositor
R, R_{free}	0.168 , 0.197 0.162 , 0.188	Depositor DCC
R_{free} test set	6391 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å^2)	30.0	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 56.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l 0.000 for -k,-h,-l 0.019 for h,-k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	17270	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% 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: MG, TPP, FAD

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	0.44	0/4050	0.56	0/5512
1	B	0.44	0/4073	0.57	0/5541
1	C	0.41	0/4076	0.55	0/5543
1	D	0.41	0/4050	0.55	0/5514
All	All	0.42	0/16249	0.56	0/22110

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	A	3974	0	3883	16	0
1	B	3997	0	3917	15	0
1	C	4000	0	3930	21	0
1	D	3974	0	3881	18	0
2	A	53	0	31	0	0
2	B	53	0	31	1	0
2	C	53	0	31	1	0
2	D	53	0	31	0	0
3	A	26	0	16	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	26	0	16	3	0
3	C	26	0	16	2	0
3	D	26	0	16	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	262	0	0	1	1
5	B	276	0	0	0	0
5	C	238	0	0	2	0
5	D	229	0	0	4	0
All	All	17270	0	15799	65	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 2.

All (65) 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:C:394:GLU:HG3	1:C:396:PRO:HD3	1.68	0.73
1:D:277:PRO:HA	1:D:300:ARG:HD2	1.72	0.71
1:A:277:PRO:HA	1:A:300:ARG:HD2	1.73	0.71
1:B:277:PRO:HA	1:B:300:ARG:HD2	1.73	0.71
1:B:138:ARG:NH1	1:C:108:SER:OG	2.24	0.70
1:D:300:ARG:HA	5:D:801:HOH:O	1.89	0.70
1:D:265:GLU:OE2	1:D:333:ARG:NH2	2.25	0.69
1:C:277:PRO:HA	1:C:300:ARG:HD2	1.76	0.68
1:A:178:SER:HB2	1:C:306:PRO:HB2	1.77	0.67
1:A:306:PRO:HB2	1:C:178:SER:HB2	1.78	0.66
1:D:360:HIS:ND1	1:D:362:GLU:OE2	2.29	0.65
1:B:138:ARG:NH1	1:B:142:HIS:NE2	2.45	0.65
1:A:485:HIS:HD2	5:A:1028:HOH:O	1.82	0.61
1:B:138:ARG:NH2	5:D:801:HOH:O	2.34	0.61
1:D:471:LEU:HD13	1:D:535:LEU:HB3	1.85	0.59
1:C:485:HIS:HD2	5:C:981:HOH:O	1.86	0.58
1:B:138:ARG:NH1	1:C:108:SER:HG	2.01	0.57
3:C:702:TPP:HN42	3:C:702:TPP:H2	1.70	0.56
1:B:306:PRO:HB2	1:D:178:SER:HB2	1.88	0.56
1:B:178:SER:HB2	1:D:306:PRO:HB2	1.88	0.56
1:B:104:ALA:HA	1:C:135:GLN:HB2	1.88	0.56
1:D:485:HIS:HD2	5:D:984:HOH:O	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:353:VAL:HA	1:D:360:HIS:CD2	2.40	0.55
1:D:337:ALA:HA	1:D:340:ARG:HE	1.72	0.54
1:B:33:VAL:HA	1:B:36:VAL:HG13	1.90	0.53
1:D:25:VAL:HG21	1:D:33:VAL:HG21	1.89	0.53
3:A:702:TPP:HN42	3:A:702:TPP:H2	1.75	0.52
1:A:356:HIS:CD2	1:A:360:HIS:CE1	2.98	0.52
1:B:25:VAL:HG21	1:B:33:VAL:HG21	1.91	0.52
1:C:369:ASN:OD1	1:C:394:GLU:HG2	2.11	0.51
1:D:485:HIS:HE1	5:D:1016:HOH:O	1.92	0.51
1:C:25:VAL:HG21	1:C:33:VAL:HG21	1.92	0.51
1:A:33:VAL:HA	1:A:36:VAL:HG13	1.92	0.51
3:B:702:TPP:HN42	3:B:702:TPP:H2	1.75	0.51
1:B:360:HIS:CE1	1:B:534:ALA:HB1	2.46	0.50
1:A:104:ALA:HA	1:D:135:GLN:HB2	1.94	0.50
1:C:507:PRO:HA	1:C:510:VAL:HG23	1.94	0.50
3:D:702:TPP:H2	3:D:702:TPP:HN42	1.77	0.50
3:C:702:TPP:HN42	3:C:702:TPP:C2	2.25	0.48
1:A:396:PRO:O	1:A:397:GLU:HB2	2.13	0.48
1:C:352:ASN:O	1:C:356:HIS:HB2	2.13	0.47
1:C:143:ALA:HB1	1:C:154:SER:HB3	1.97	0.47
1:C:485:HIS:HE1	5:C:1024:HOH:O	1.97	0.46
1:B:135:GLN:HB2	1:C:104:ALA:HA	1.98	0.46
1:C:161:ASP:HA	1:C:164:LYS:NZ	2.30	0.46
1:D:357:VAL:CB	1:D:358:PRO:HD3	2.45	0.46
1:C:469:VAL:HG11	1:D:25:VAL:HG13	1.99	0.45
3:A:702:TPP:HN42	3:A:702:TPP:C2	2.30	0.44
1:A:143:ALA:HB1	1:A:154:SER:HB3	1.99	0.44
1:D:143:ALA:HB1	1:D:154:SER:HB3	2.00	0.44
1:A:356:HIS:CD2	1:A:360:HIS:NE2	2.86	0.44
1:C:25:VAL:HG13	1:D:469:VAL:HG11	1.99	0.43
3:D:702:TPP:HN42	3:D:702:TPP:C2	2.31	0.43
1:A:49:GLU:OE2	3:B:702:TPP:N1'	2.52	0.43
1:B:143:ALA:HB1	1:B:154:SER:HB3	2.01	0.43
1:B:379:THR:HA	1:B:403:VAL:O	2.20	0.42
1:A:135:GLN:HB2	1:D:104:ALA:HA	2.02	0.41
1:A:353:VAL:HG12	1:A:360:HIS:CD2	2.55	0.41
1:A:379:THR:HA	1:A:403:VAL:O	2.21	0.41
1:A:299:ARG:HA	1:C:142:HIS:CE1	2.56	0.41
3:B:702:TPP:HN42	3:B:702:TPP:C2	2.32	0.41
1:A:142:HIS:CE1	1:C:299:ARG:HA	2.56	0.40
3:A:702:TPP:N1'	1:B:49:GLU:OE2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:701:FAD:H9	2:B:701:FAD:H1'1	1.91	0.40
1:C:311:VAL:HG23	2:C:701:FAD:C2A	2.51	0.40

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)
5:A:847:HOH:O	5:A:911:HOH:O[2_655]	2.08	0.12

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	533/564 (94%)	526 (99%)	6 (1%)	1 (0%)	47	38
1	B	534/564 (95%)	528 (99%)	5 (1%)	1 (0%)	47	38
1	C	533/564 (94%)	526 (99%)	6 (1%)	1 (0%)	47	38
1	D	535/564 (95%)	526 (98%)	7 (1%)	2 (0%)	34	24
All	All	2135/2256 (95%)	2106 (99%)	24 (1%)	5 (0%)	47	38

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	357	VAL
1	A	27	ASP
1	B	27	ASP
1	C	27	ASP
1	D	27	ASP

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	416/451 (92%)	410 (99%)	6 (1%)	67	65
1	B	421/451 (93%)	414 (98%)	7 (2%)	60	57
1	C	423/451 (94%)	419 (99%)	4 (1%)	78	79
1	D	414/451 (92%)	408 (99%)	6 (1%)	67	65
All	All	1674/1804 (93%)	1651 (99%)	23 (1%)	67	65

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	216	ARG
1	A	243	GLU
1	A	284	LYS
1	A	317	ASN
1	A	353	VAL
1	A	381	ASP
1	B	36	VAL
1	B	138	ARG
1	B	216	ARG
1	B	243	GLU
1	B	284	LYS
1	B	317	ASN
1	B	381	ASP
1	C	27	ASP
1	C	243	GLU
1	C	317	ASN
1	C	381	ASP
1	D	243	GLU
1	D	247	GLU
1	D	284	LYS
1	D	317	ASN
1	D	360	HIS
1	D	381	ASP

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

Mol	Chain	Res	Type
1	C	485	HIS
1	D	485	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	$\#\|Z\| > 2$
3	TPP	B	702	4	22,27,27	0.61	0	29,40,40	0.67	0
2	FAD	C	701	-	53,58,58	0.55	0	68,89,89	0.58	1 (1%)
2	FAD	A	701	-	53,58,58	0.54	0	68,89,89	0.61	1 (1%)
3	TPP	A	702	4	22,27,27	0.76	1 (4%)	29,40,40	0.79	0
2	FAD	D	701	-	53,58,58	0.52	0	68,89,89	0.60	1 (1%)
3	TPP	D	702	4	22,27,27	0.63	0	29,40,40	0.76	1 (3%)
3	TPP	C	702	4	22,27,27	0.62	0	29,40,40	0.76	0
2	FAD	B	701	-	53,58,58	0.52	0	68,89,89	0.62	1 (1%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TPP	B	702	4	-	1/16/17/17	0/2/2/2
2	FAD	C	701	-	-	4/30/50/50	0/6/6/6
2	FAD	A	701	-	-	4/30/50/50	0/6/6/6
3	TPP	A	702	4	-	2/16/17/17	0/2/2/2
2	FAD	D	701	-	-	4/30/50/50	0/6/6/6
3	TPP	D	702	4	-	2/16/17/17	0/2/2/2
3	TPP	C	702	4	-	2/16/17/17	0/2/2/2
2	FAD	B	701	-	-	3/30/50/50	0/6/6/6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	TPP	C6-C5	-2.39	1.49	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	701	FAD	C5A-C6A-N6A	2.31	123.86	120.35
2	B	701	FAD	C5A-C6A-N6A	2.28	123.81	120.35
2	D	701	FAD	C5A-C6A-N6A	2.22	123.73	120.35
2	A	701	FAD	C5A-C6A-N6A	2.15	123.63	120.35
3	D	702	TPP	C5-C4-N3	2.05	111.67	107.57

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	702	TPP	PA-O3A-PB-O3B
3	C	702	TPP	PA-O3A-PB-O3B
3	D	702	TPP	PA-O3A-PB-O3B
2	A	701	FAD	C2'-C1'-N10-C10
2	B	701	FAD	C2'-C1'-N10-C10
2	C	701	FAD	C2'-C1'-N10-C10
2	D	701	FAD	C2'-C1'-N10-C10
3	B	702	TPP	PA-O3A-PB-O3B
2	D	701	FAD	PA-O3P-P-O1P

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Mol	Chain	Res	Type	Atoms
3	C	702	TPP	PA-O3A-PB-O1B
3	D	702	TPP	PA-O3A-PB-O1B
2	A	701	FAD	PA-O3P-P-O1P
2	A	701	FAD	PA-O3P-P-O2P
2	C	701	FAD	PA-O3P-P-O1P
2	C	701	FAD	PA-O3P-P-O2P
2	D	701	FAD	PA-O3P-P-O2P
3	A	702	TPP	PA-O3A-PB-O1B
2	A	701	FAD	O4B-C4B-C5B-O5B
2	B	701	FAD	PA-O3P-P-O2P
2	B	701	FAD	O4B-C4B-C5B-O5B
2	C	701	FAD	O4B-C4B-C5B-O5B
2	D	701	FAD	O4B-C4B-C5B-O5B

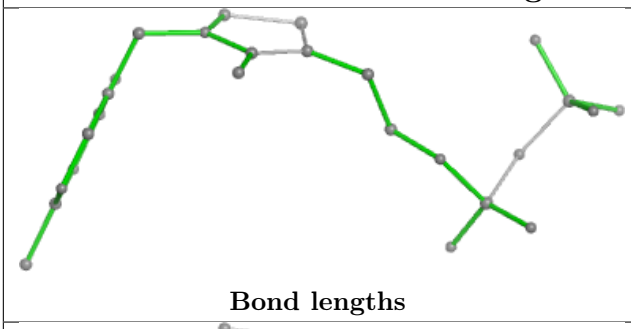
There are no ring outliers.

6 monomers are involved in 12 short contacts:

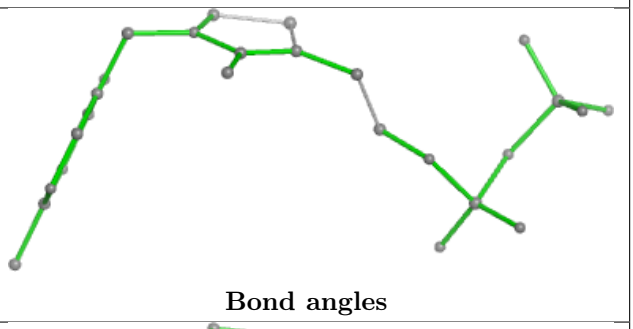
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	702	TPP	3	0
2	C	701	FAD	1	0
3	A	702	TPP	3	0
3	D	702	TPP	2	0
3	C	702	TPP	2	0
2	B	701	FAD	1	0

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.

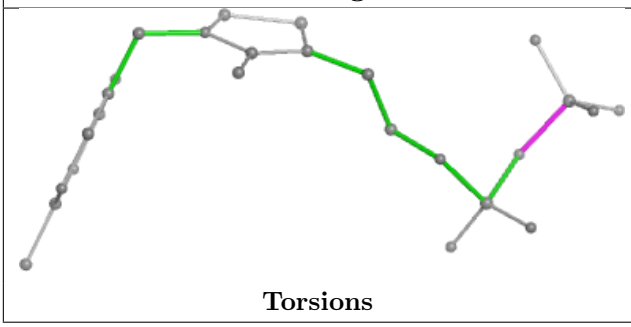
Ligand TPP B 702



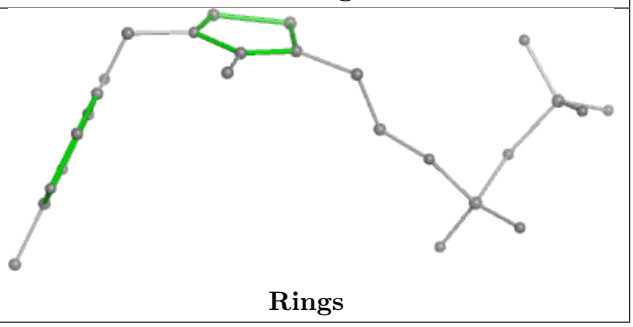
Bond lengths



Bond angles

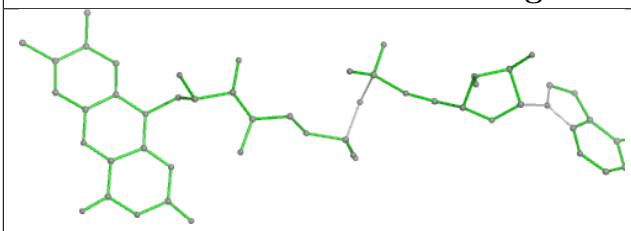


Torsions

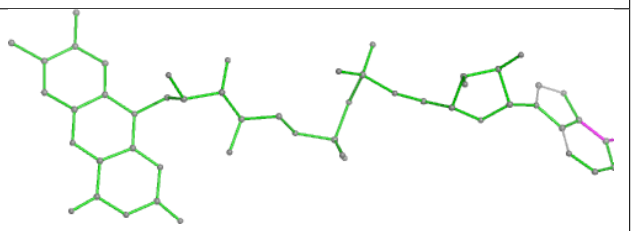


Rings

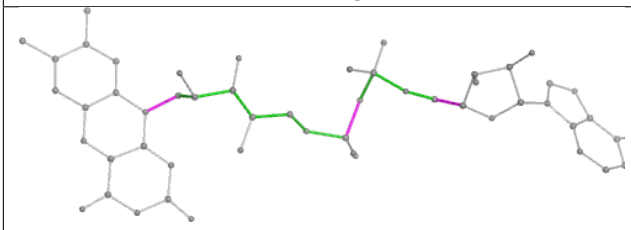
Ligand FAD C 701



Bond lengths



Bond angles



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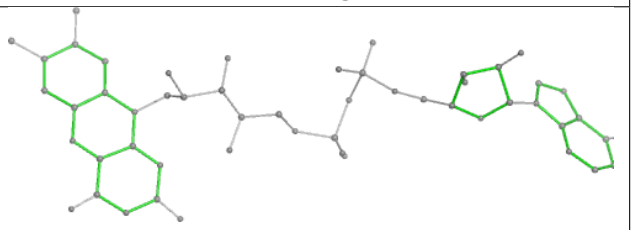
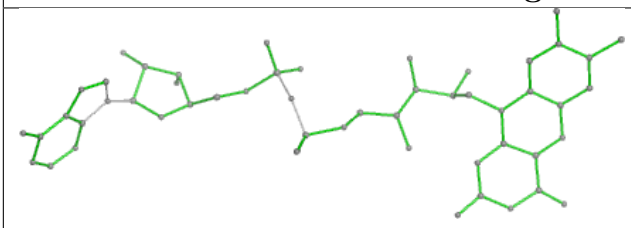


Rings

Ligand FAD A 701



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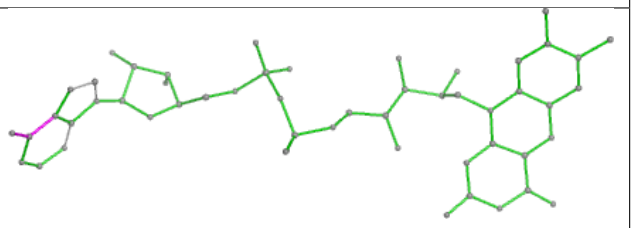
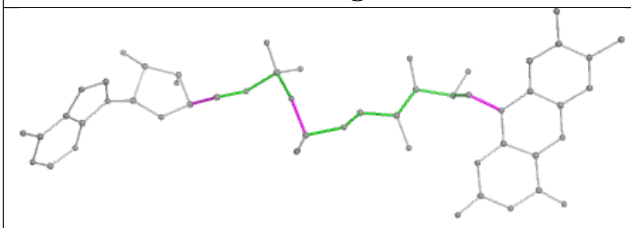


Bond angles



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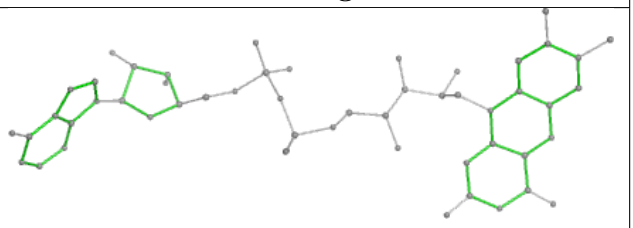
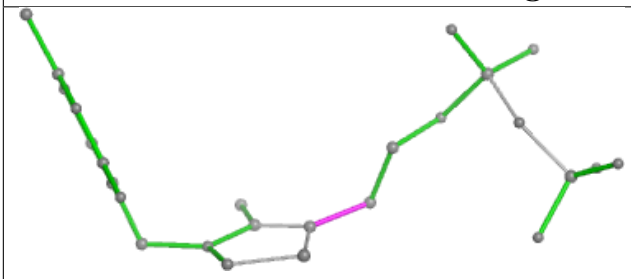


Rings

Ligand TPP A 702



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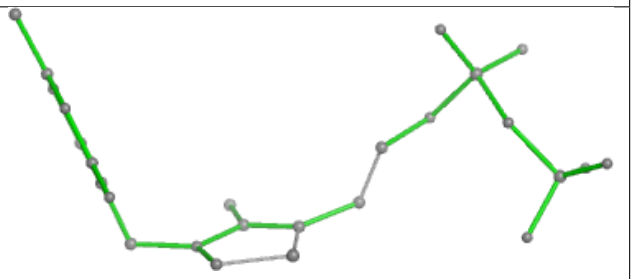
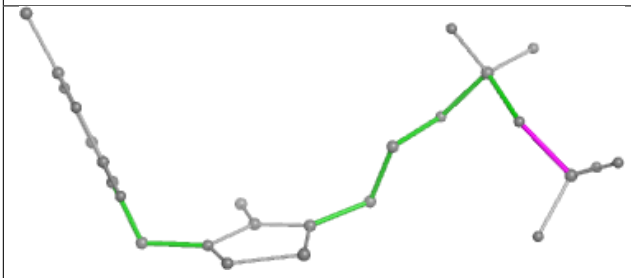
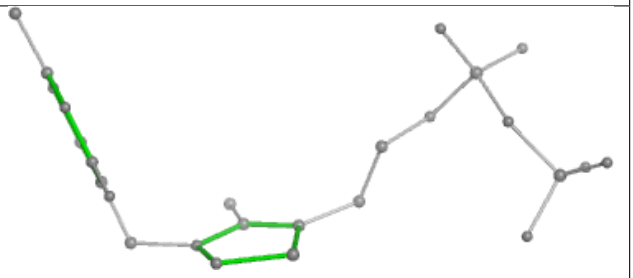


Bond angles

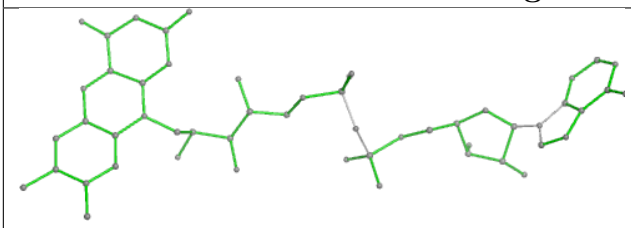


Torsions

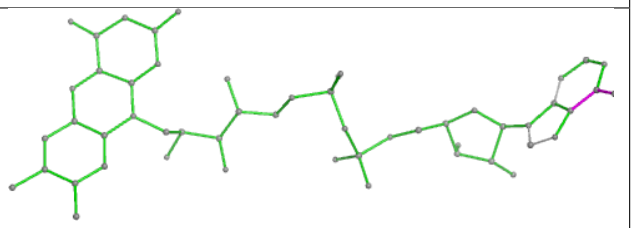


Rings

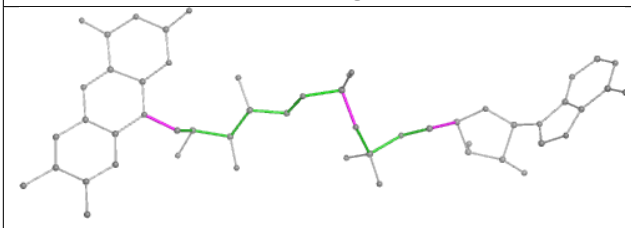
Ligand FAD D 701



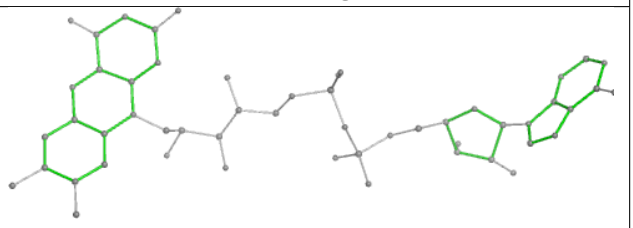
Bond lengths



Bond angles

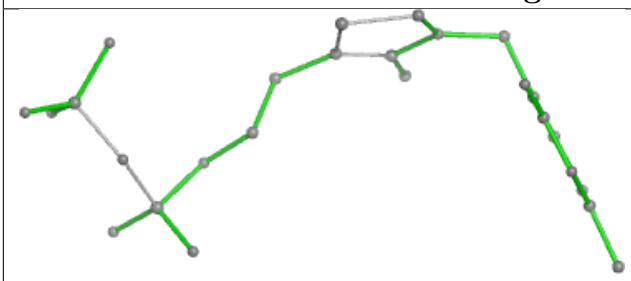


Torsions

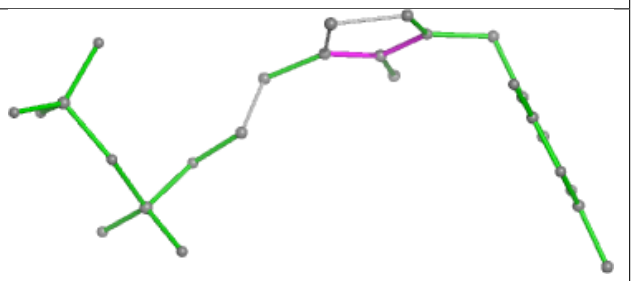


Rings

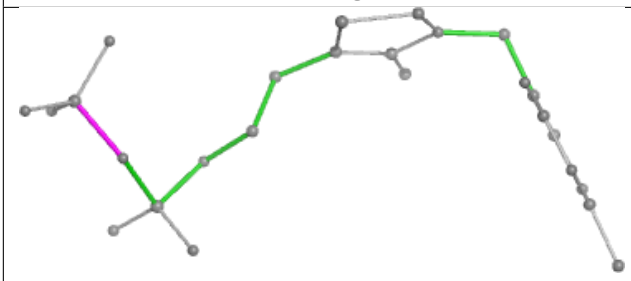
Ligand TPP D 702



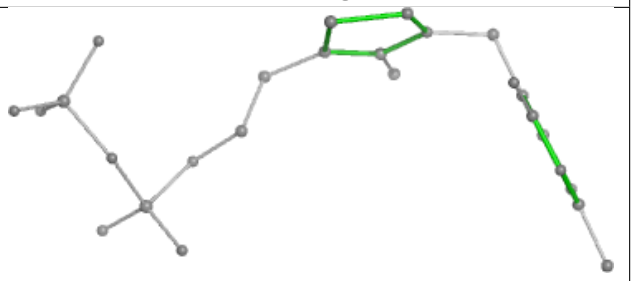
Bond lengths



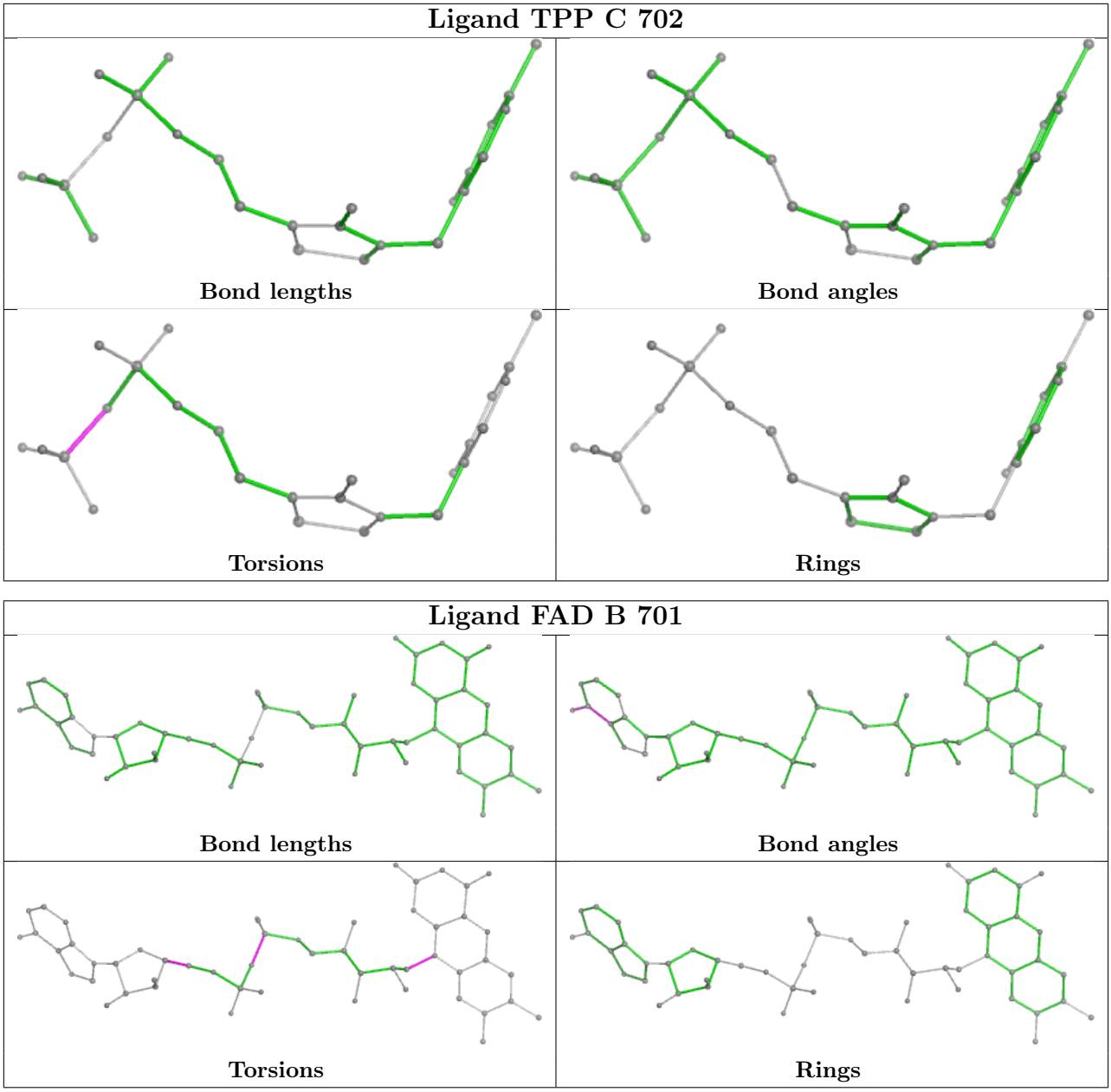
Bond angles



Torsions



Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	535/564 (94%)	-0.22	17 (3%) 47 50	19, 33, 54, 86	0
1	B	536/564 (95%)	-0.29	5 (0%) 84 85	22, 33, 53, 65	0
1	C	535/564 (94%)	-0.11	13 (2%) 59 62	23, 37, 57, 70	0
1	D	537/564 (95%)	0.13	31 (5%) 23 25	19, 41, 77, 110	0
All	All	2143/2256 (94%)	-0.12	66 (3%) 49 51	19, 35, 63, 110	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	353	VAL	8.0
1	D	349	TYR	7.7
1	D	2	ALA	6.4
1	B	2	ALA	6.3
1	D	351	HIS	6.2
1	D	535	LEU	6.1
1	D	350	THR	5.9
1	D	348	THR	5.2
1	A	351	HIS	5.1
1	C	2	ALA	4.8
1	D	355	LYS	4.7
1	D	474	LEU	4.6
1	D	347	GLU	4.6
1	D	345	VAL	4.5
1	A	350	THR	4.3
1	D	537	ILE	4.2
1	D	475	VAL	4.2
1	D	352	ASN	4.0
1	A	536	SER	3.8
1	A	2	ALA	3.7
1	A	349	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	397	GLU	3.4
1	A	535	LEU	3.3
1	D	342	LEU	3.3
1	D	326	THR	3.2
1	A	355	LYS	3.2
1	A	353	VAL	3.2
1	D	357	VAL	3.2
1	C	475	VAL	3.2
1	B	166	ASP	3.1
1	D	538	PRO	3.0
1	C	343	SER	3.0
1	C	344	SER	3.0
1	D	536	SER	3.0
1	A	346	VAL	2.9
1	C	474	LEU	2.9
1	B	474	LEU	2.8
1	C	521	PRO	2.8
1	C	166	ASP	2.8
1	A	348	THR	2.7
1	D	477	GLY	2.7
1	A	347	GLU	2.7
1	D	363	TYR	2.6
1	B	521	PRO	2.6
1	D	396	PRO	2.6
1	A	200	ASN	2.6
1	C	349	TYR	2.5
1	B	536	SER	2.5
1	A	345	VAL	2.5
1	A	285	ASP	2.4
1	D	481	PHE	2.4
1	D	285	ASP	2.3
1	D	343	SER	2.3
1	A	352	ASN	2.2
1	C	3	HIS	2.2
1	C	196	GLU	2.2
1	C	477	GLY	2.2
1	D	479	PRO	2.1
1	D	471	LEU	2.1
1	D	166	ASP	2.1
1	A	397	GLU	2.1
1	D	442	LEU	2.1
1	D	80	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	476	GLU	2.0
1	C	54	PHE	2.0
1	A	356	HIS	2.0

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 (i)

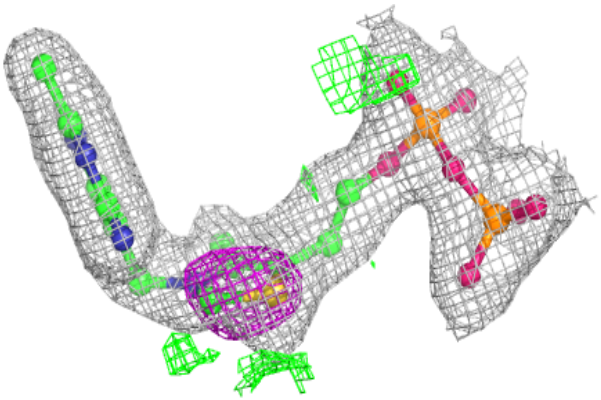
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

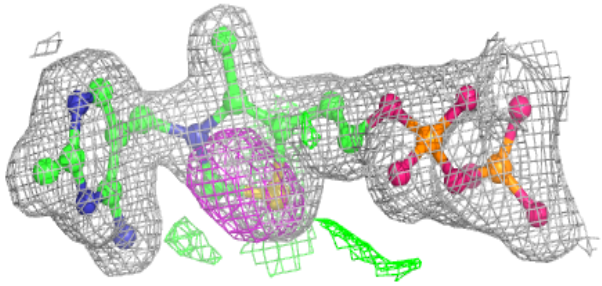
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	TPP	A	702	26/26	0.96	0.13	25,32,36,38	0
3	TPP	B	702	26/26	0.96	0.09	22,29,34,37	0
3	TPP	C	702	26/26	0.96	0.12	22,29,34,37	0
3	TPP	D	702	26/26	0.96	0.11	31,42,44,44	0
4	MG	C	703	1/1	0.96	0.07	30,30,30,30	0
2	FAD	B	701	53/53	0.98	0.08	22,24,26,28	0
2	FAD	C	701	53/53	0.98	0.08	24,27,30,32	0
2	FAD	D	701	53/53	0.98	0.10	29,32,35,38	0
2	FAD	A	701	53/53	0.98	0.09	24,27,30,31	0
4	MG	D	703	1/1	0.98	0.03	49,49,49,49	0
4	MG	A	703	1/1	0.99	0.05	27,27,27,27	0
4	MG	B	703	1/1	0.99	0.03	28,28,28,28	0

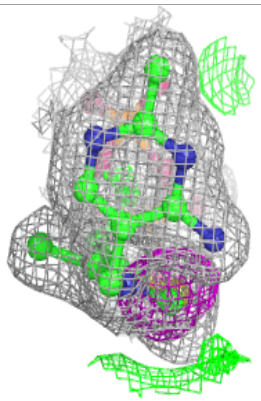
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TPP A 702:

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

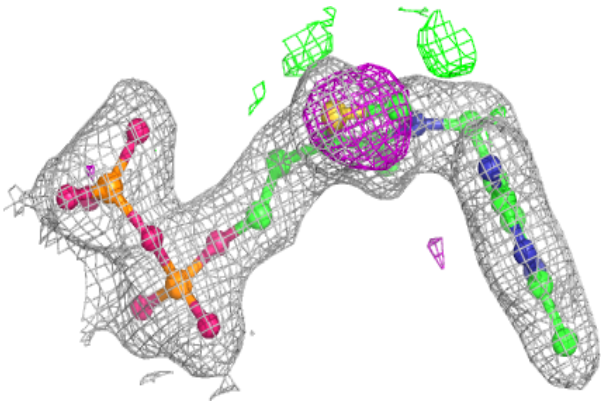


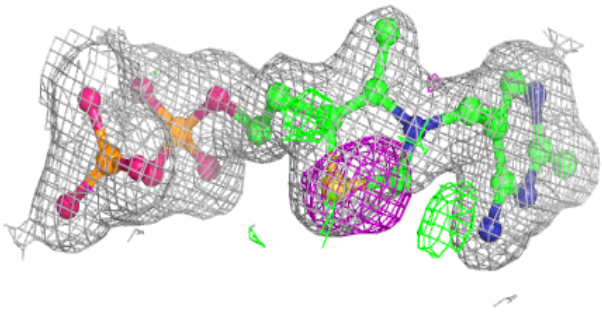


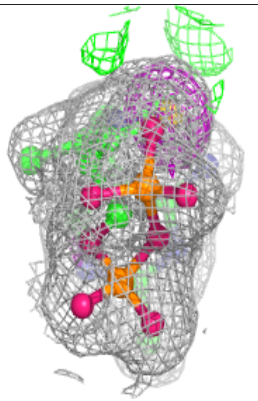


Electron density around TPP B 702:

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

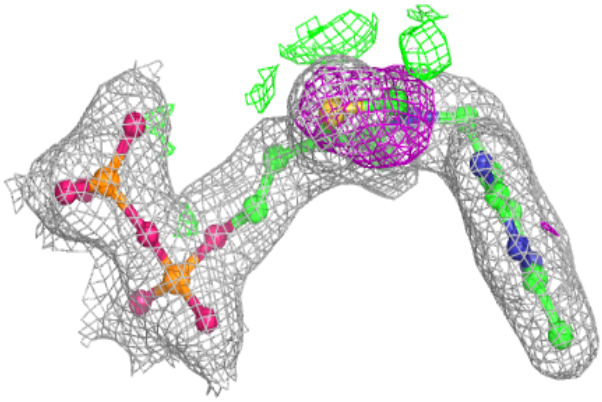


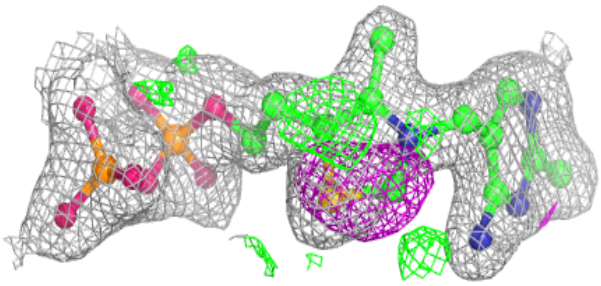


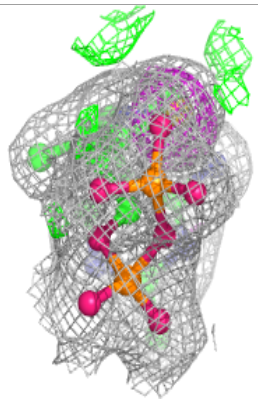


Electron density around TPP C 702:

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

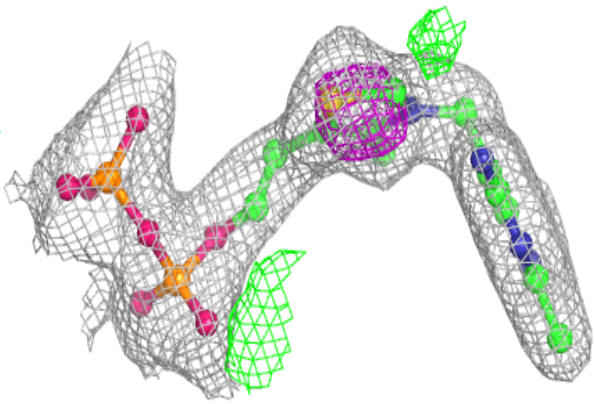


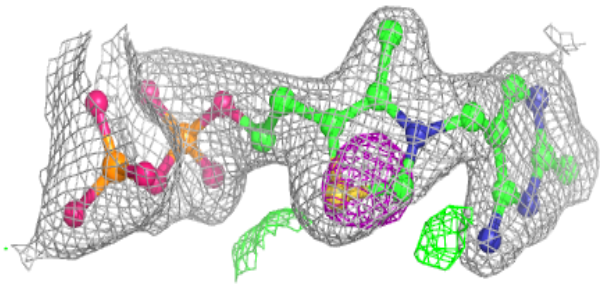


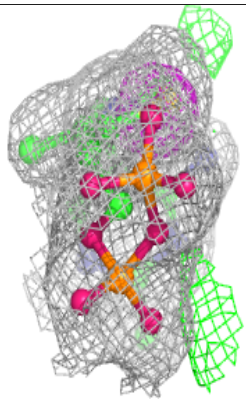


Electron density around TPP D 702:

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

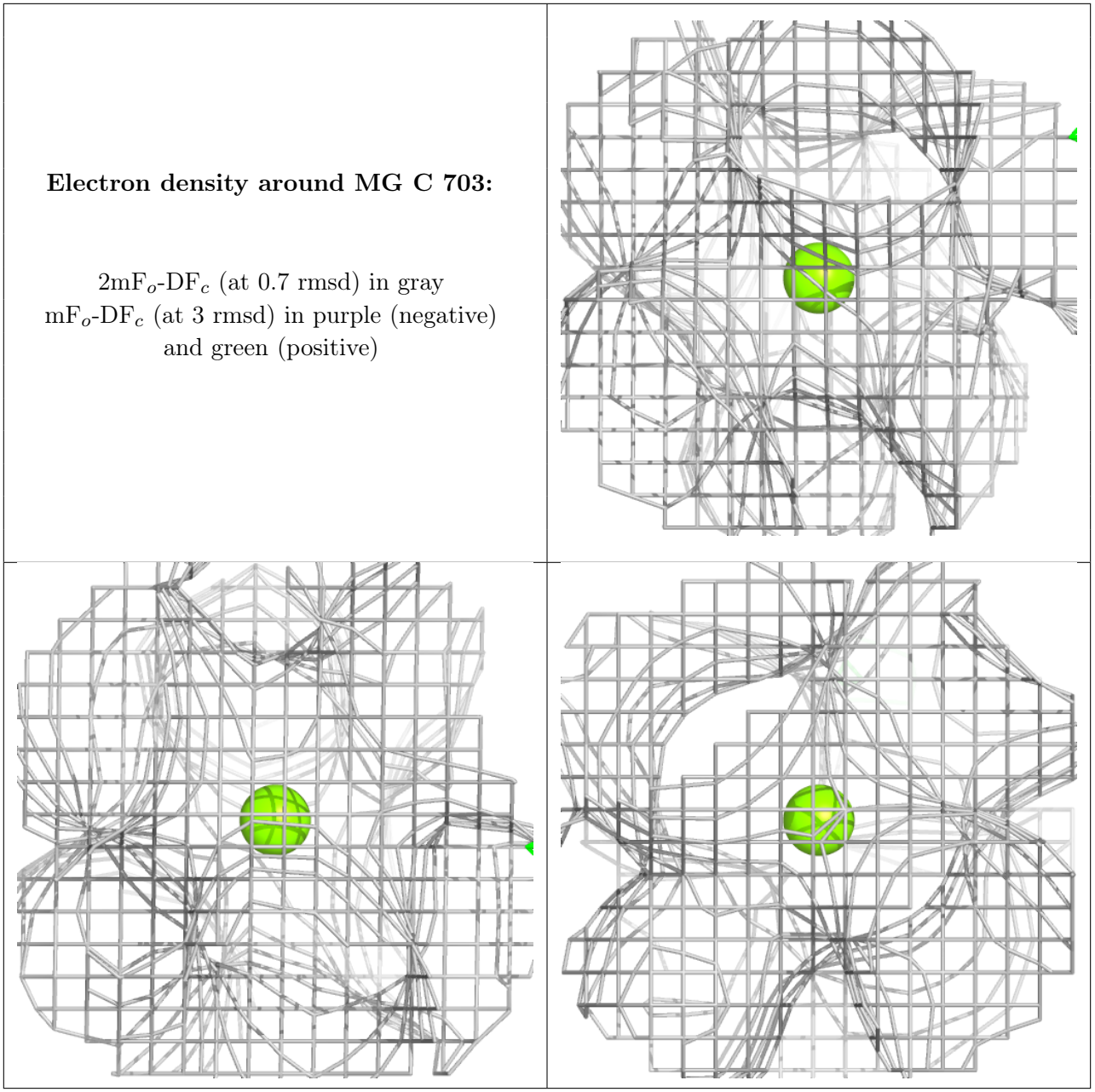






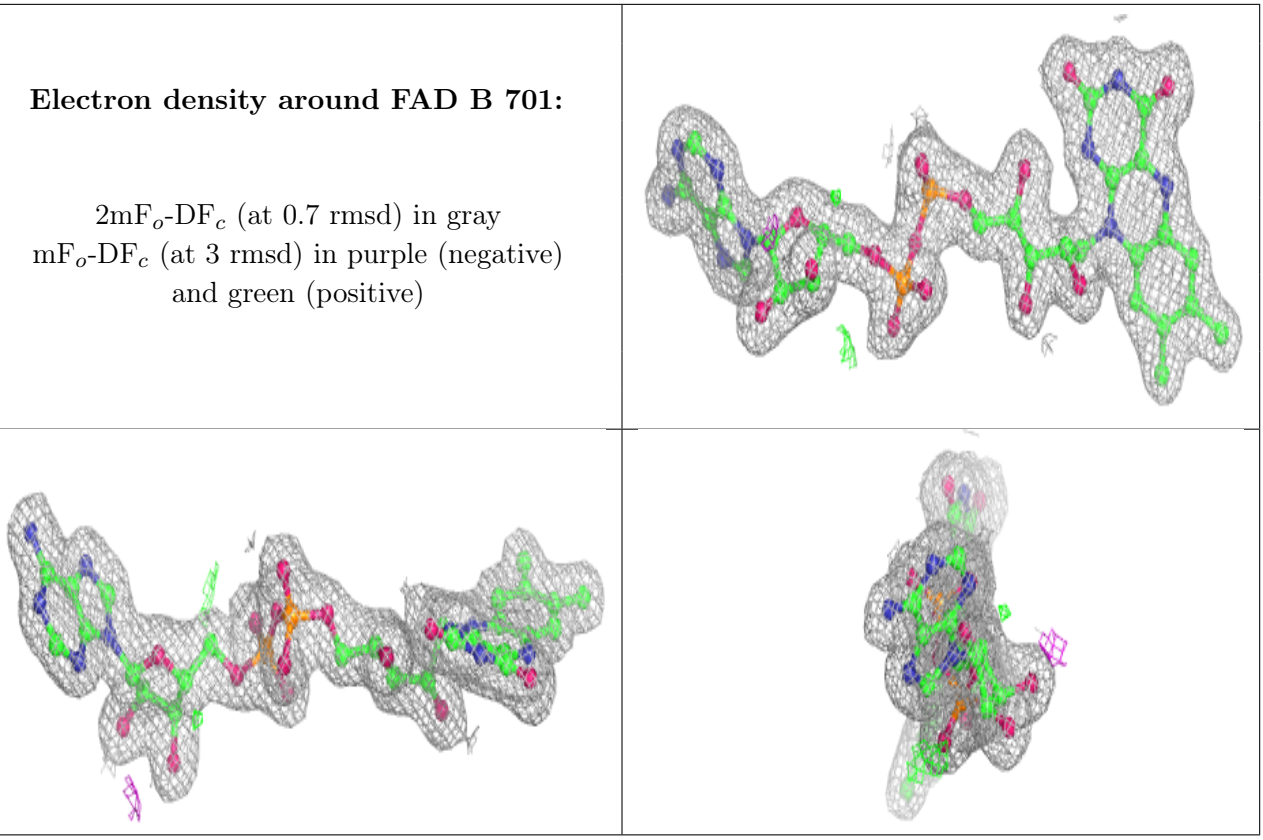
Electron density around MG C 703:

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



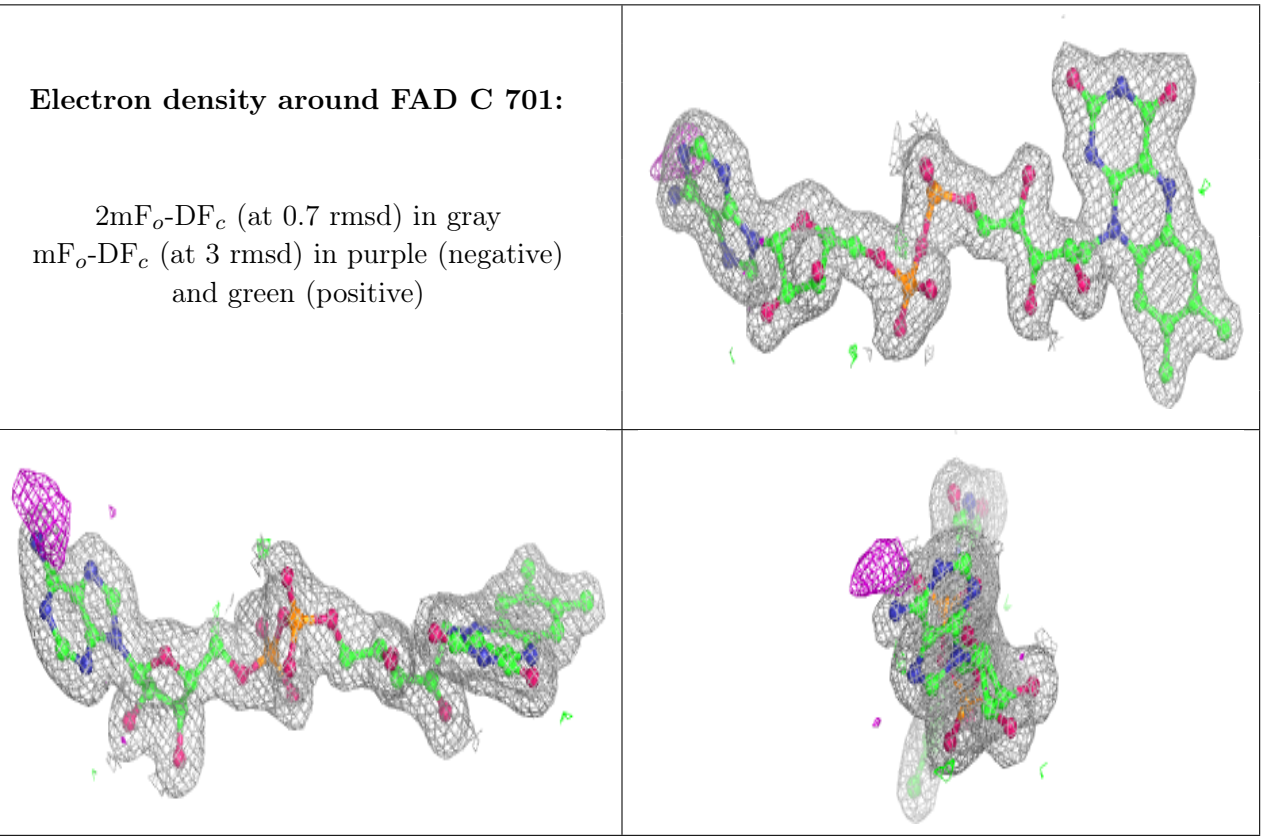
Electron density around FAD B 701:

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



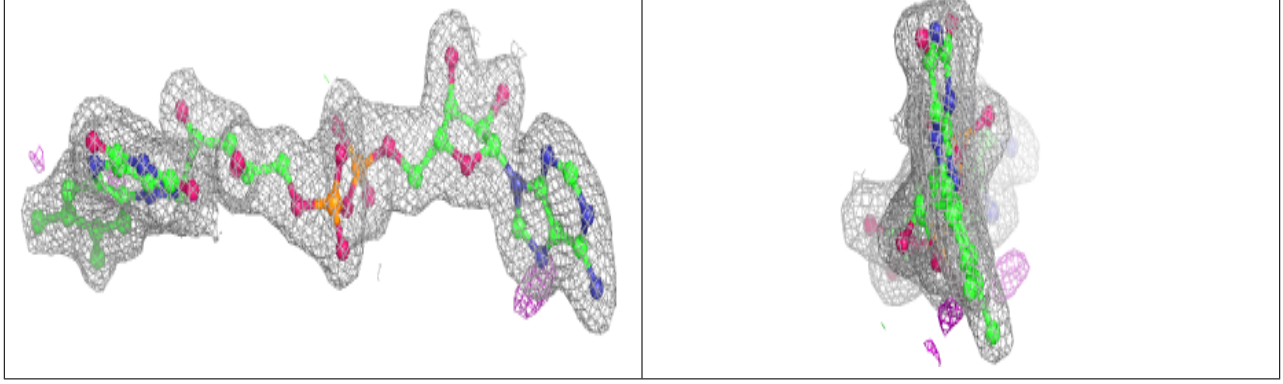
Electron density around FAD C 701:

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



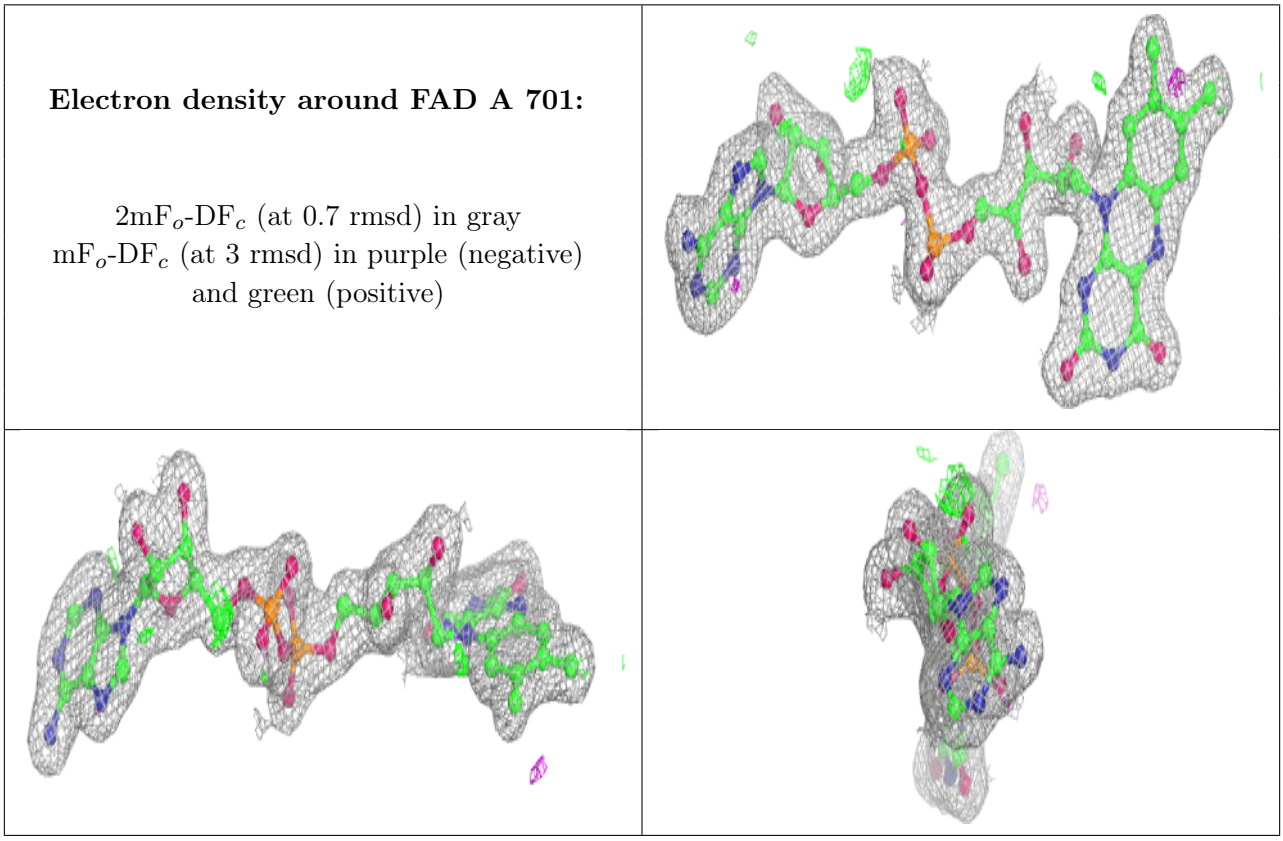
Electron density around FAD D 701:

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



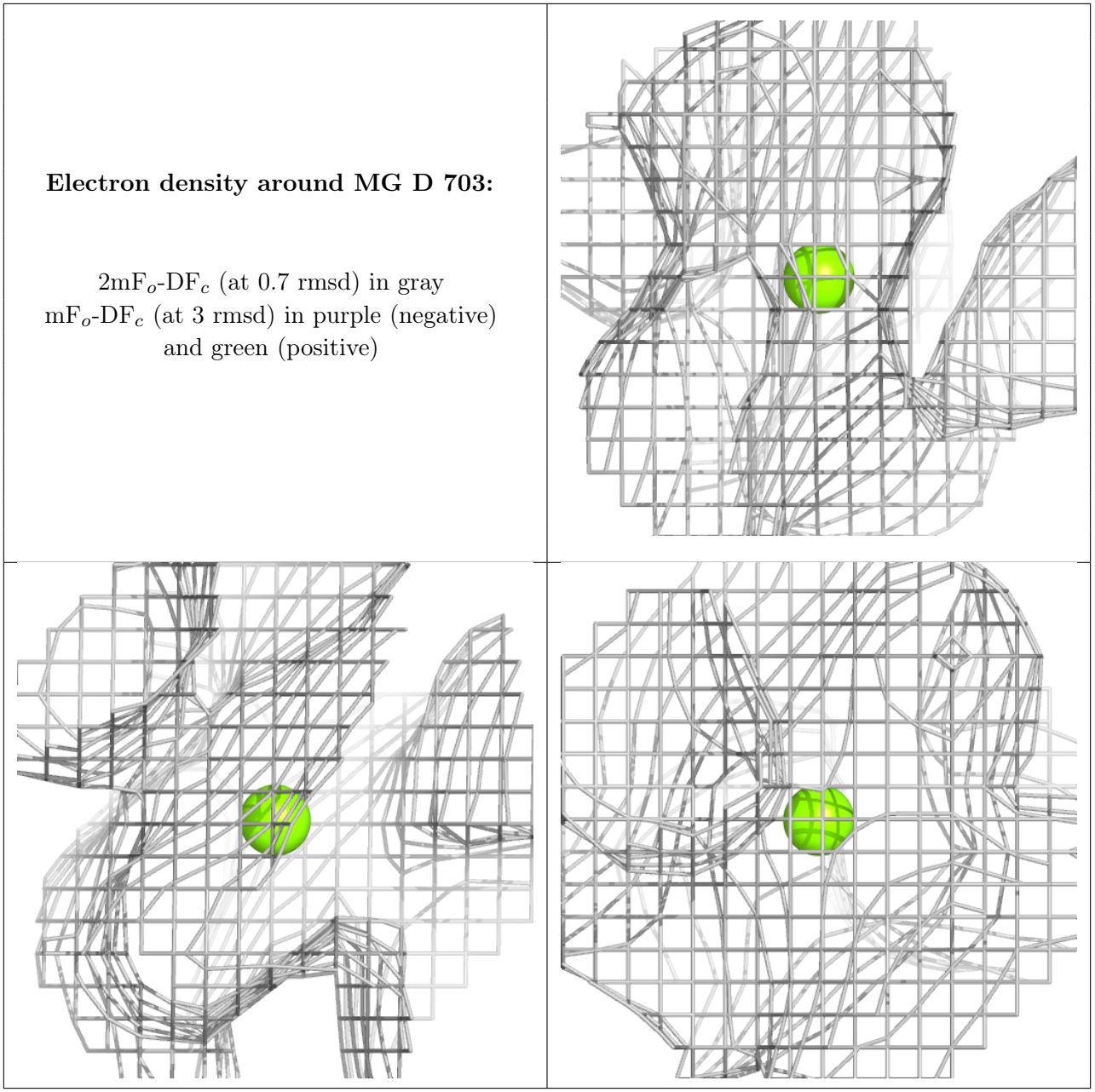
Electron density around FAD A 701:

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



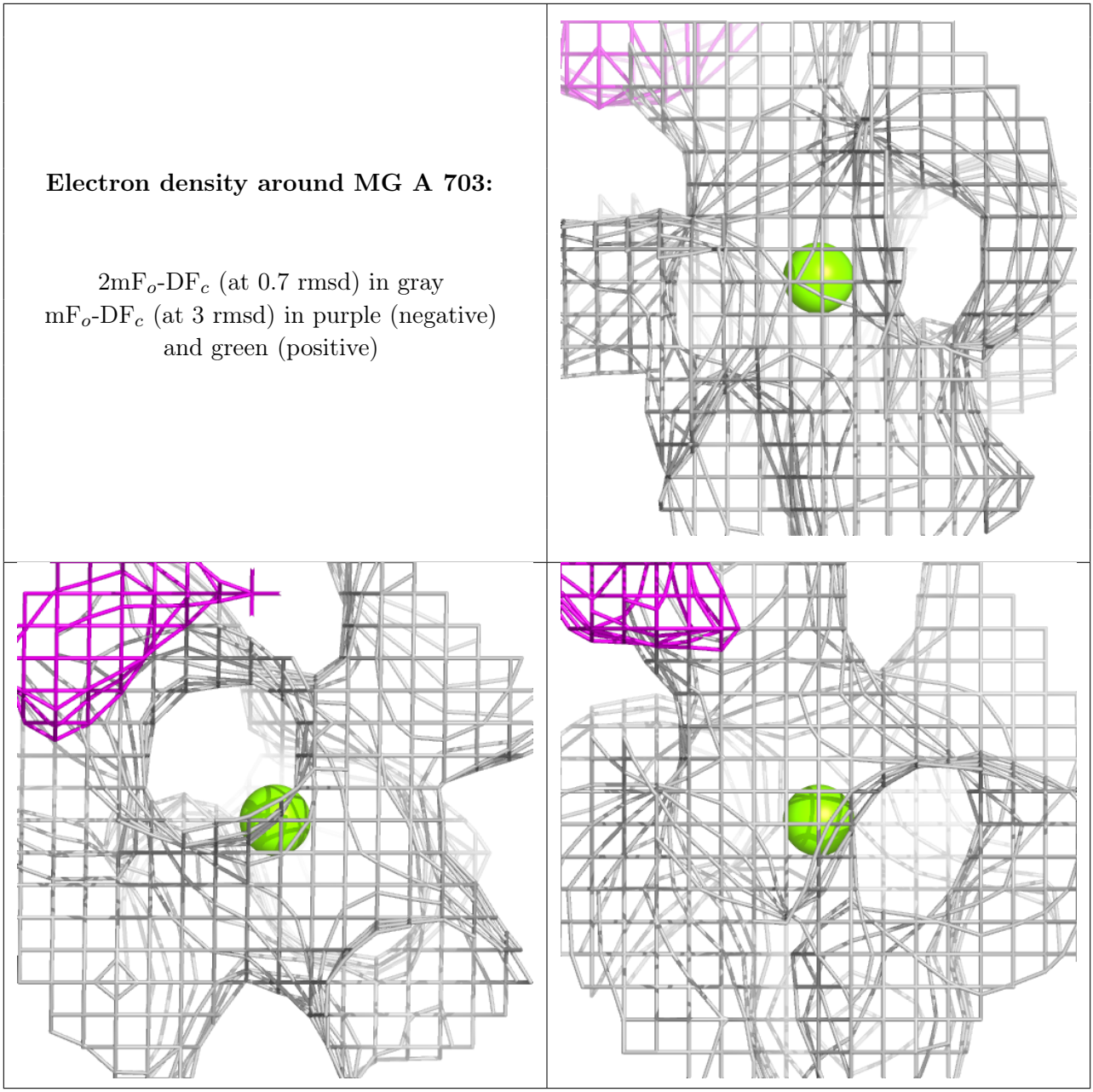
Electron density around MG D 703:

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



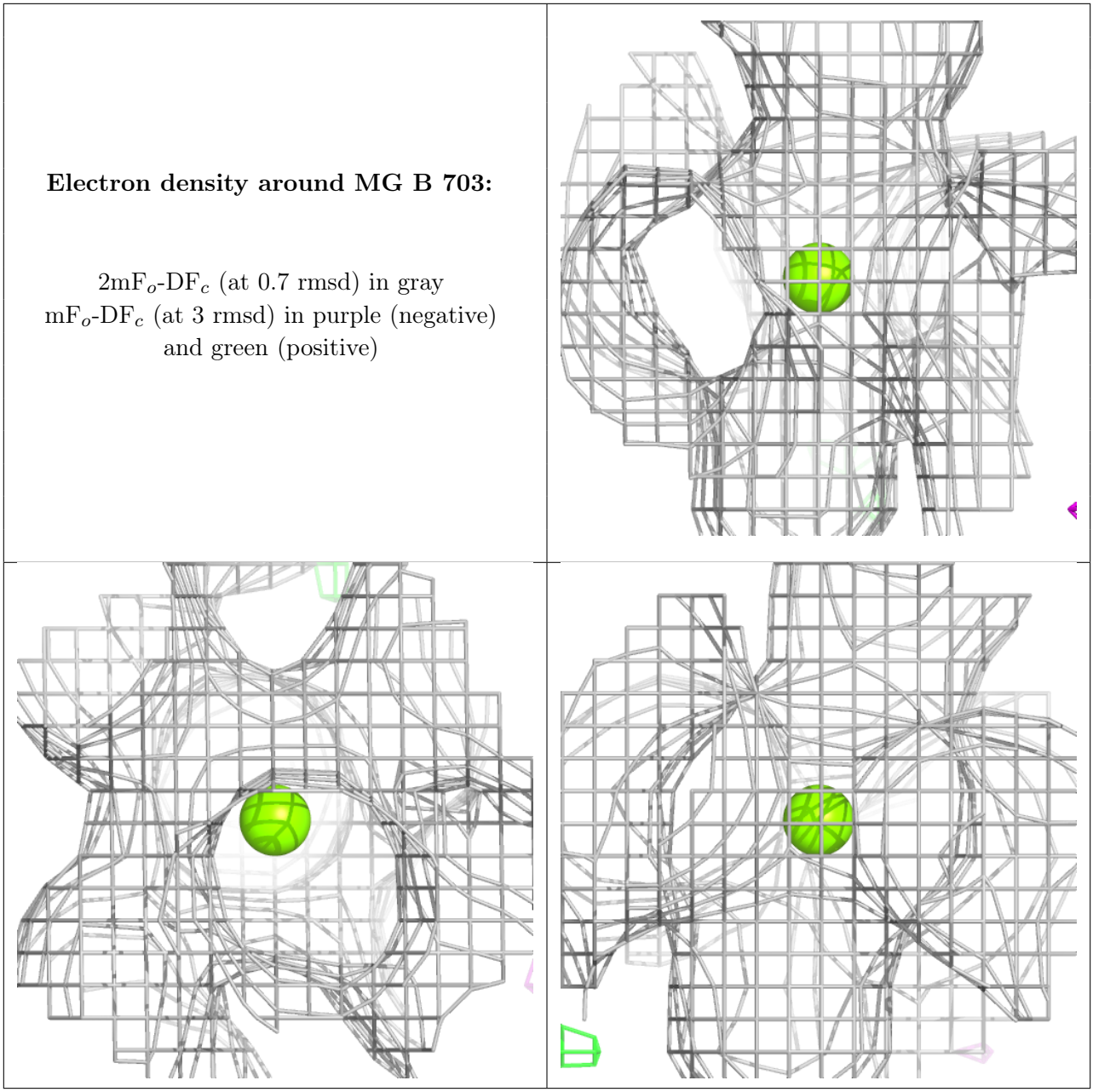
Electron density around MG A 703:

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



Electron density around MG B 703:

$2mF_o$-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.