wwPDB X-ray Structure Validation Summary Report (i)

Dec 19, 2023 – 08:31 PM EST

PDB ID	:	1O5W
Title	:	The structure basis of specific recognitions for substrates and inhibitors of rat monoamine oxidase A
Authors	:	Ma, J.; Yoshimura, M.; Yamashita, E.; Nakagawa, A.; Ito, A.; Tsukihara, T.
Deposited on	:	2003-10-06
Resolution	:	3.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

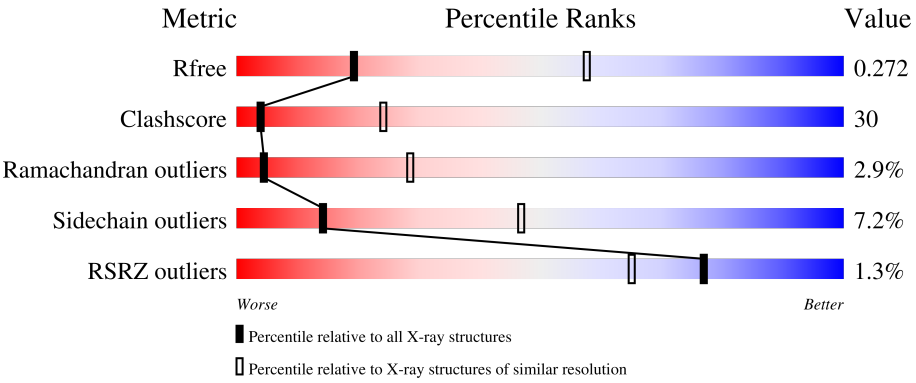
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	534	2% 51% 40% 5% •
1	B	534	47% 41% 5% • 6%
1	C	534	% 50% 40% 5% • •
1	D	534	% 50% 39% 5% 5%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 16456 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 Amine oxidase [flavin-containing] A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	511	Total	C	N	O	S	0	0	0
			4071	2620	691	738	22			
1	B	503	Total	C	N	O	S	0	0	0
			4002	2570	682	729	21			
1	C	512	Total	C	N	O	S	0	0	0
			4079	2626	692	739	22			
1	D	506	Total	C	N	O	S	0	0	0
			4024	2585	685	732	22			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	expression tag	UNP P21396
A	-6	GLY	-	expression tag	UNP P21396
A	-5	HIS	-	expression tag	UNP P21396
A	-4	HIS	-	expression tag	UNP P21396
A	-3	HIS	-	expression tag	UNP P21396
A	-2	HIS	-	expression tag	UNP P21396
A	-1	HIS	-	expression tag	UNP P21396
A	0	HIS	-	expression tag	UNP P21396
A	17	VAL	GLY	SEE REMARK 999	UNP P21396
A	18	VAL	LEU	SEE REMARK 999	UNP P21396
A	361	LEU	GLN	SEE REMARK 999	UNP P21396
B	993	MET	-	expression tag	UNP P21396
B	994	GLY	-	expression tag	UNP P21396
B	995	HIS	-	expression tag	UNP P21396
B	996	HIS	-	expression tag	UNP P21396
B	997	HIS	-	expression tag	UNP P21396
B	998	HIS	-	expression tag	UNP P21396
B	999	HIS	-	expression tag	UNP P21396
B	1000	HIS	-	expression tag	UNP P21396
B	1017	VAL	GLY	SEE REMARK 999	UNP P21396
B	1018	VAL	LEU	SEE REMARK 999	UNP P21396

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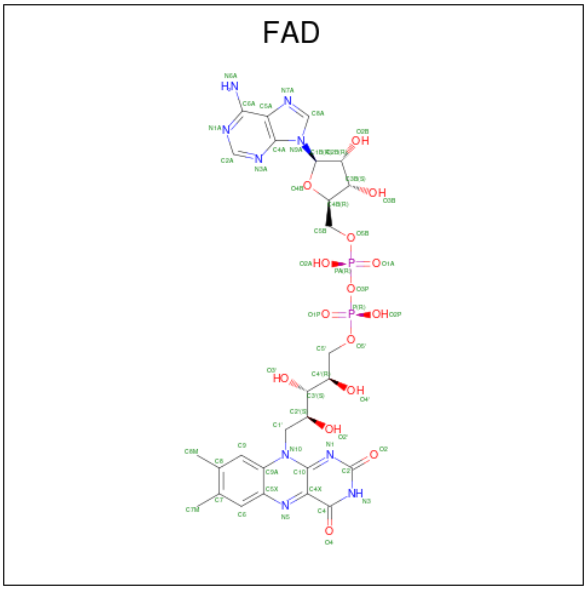
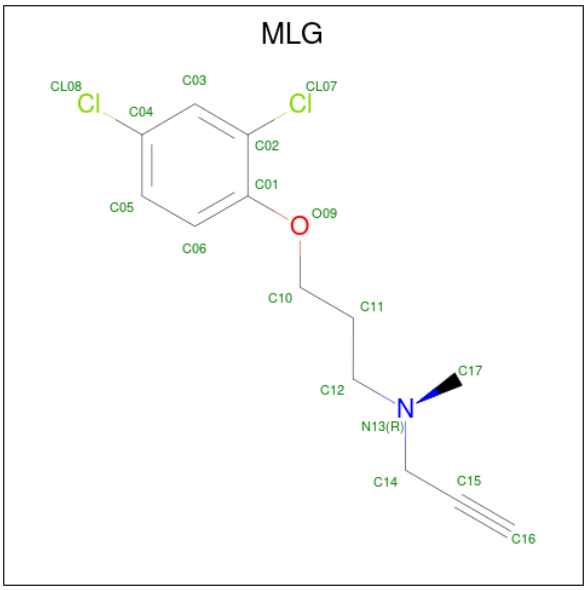
Chain	Residue	Modelled	Actual	Comment	Reference
B	1361	LEU	GLN	SEE REMARK 999	UNP P21396
C	1993	MET	-	expression tag	UNP P21396
C	1994	GLY	-	expression tag	UNP P21396
C	1995	HIS	-	expression tag	UNP P21396
C	1996	HIS	-	expression tag	UNP P21396
C	1997	HIS	-	expression tag	UNP P21396
C	1998	HIS	-	expression tag	UNP P21396
C	1999	HIS	-	expression tag	UNP P21396
C	2000	HIS	-	expression tag	UNP P21396
C	2017	VAL	GLY	SEE REMARK 999	UNP P21396
C	2018	VAL	LEU	SEE REMARK 999	UNP P21396
C	2361	LEU	GLN	SEE REMARK 999	UNP P21396
D	2993	MET	-	expression tag	UNP P21396
D	2994	GLY	-	expression tag	UNP P21396
D	2995	HIS	-	expression tag	UNP P21396
D	2996	HIS	-	expression tag	UNP P21396
D	2997	HIS	-	expression tag	UNP P21396
D	2998	HIS	-	expression tag	UNP P21396
D	2999	HIS	-	expression tag	UNP P21396
D	3000	HIS	-	expression tag	UNP P21396
D	3017	VAL	GLY	SEE REMARK 999	UNP P21396
D	3018	VAL	LEU	SEE REMARK 999	UNP P21396
D	3361	LEU	GLN	SEE REMARK 999	UNP P21396

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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 N-[3-(2,4-DICHLOROPHENOXY)PROPYL]-N-METHYL-N-PROP-2-YNYL AMINE (three-letter code: MLG) (formula: $C_{13}H_{15}Cl_2NO$).



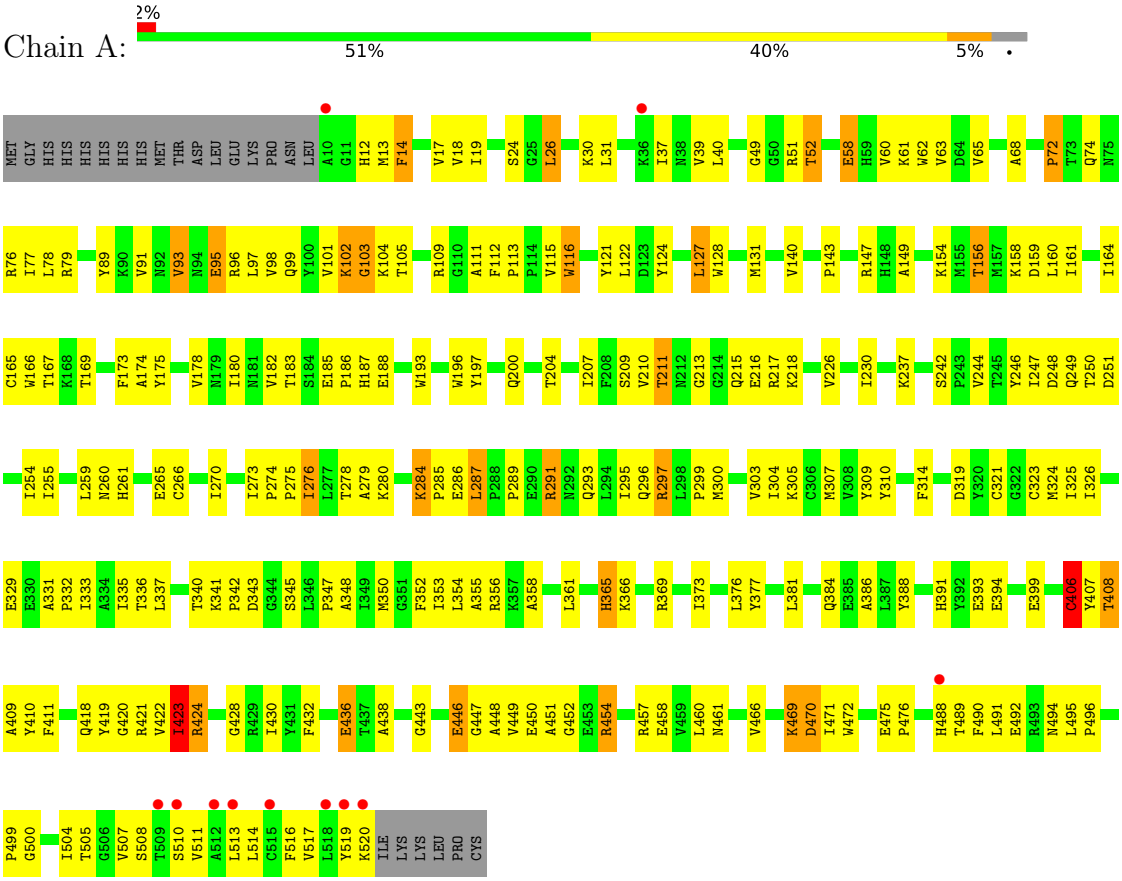
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			17	13	2	1	1		
3	B	1	Total	C	Cl	N	O	0	0
			17	13	2	1	1		
3	C	1	Total	C	Cl	N	O	0	0
			17	13	2	1	1		
3	D	1	Total	C	Cl	N	O	0	0
			17	13	2	1	1		

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.

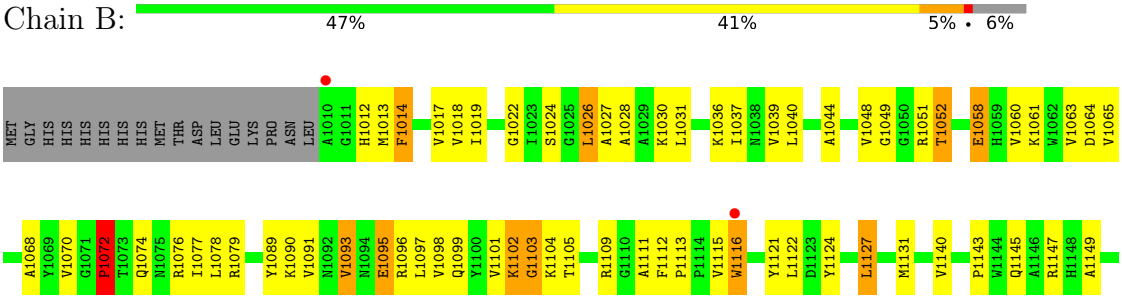
• Molecule 1: Amine oxidase [flavin-containing] A

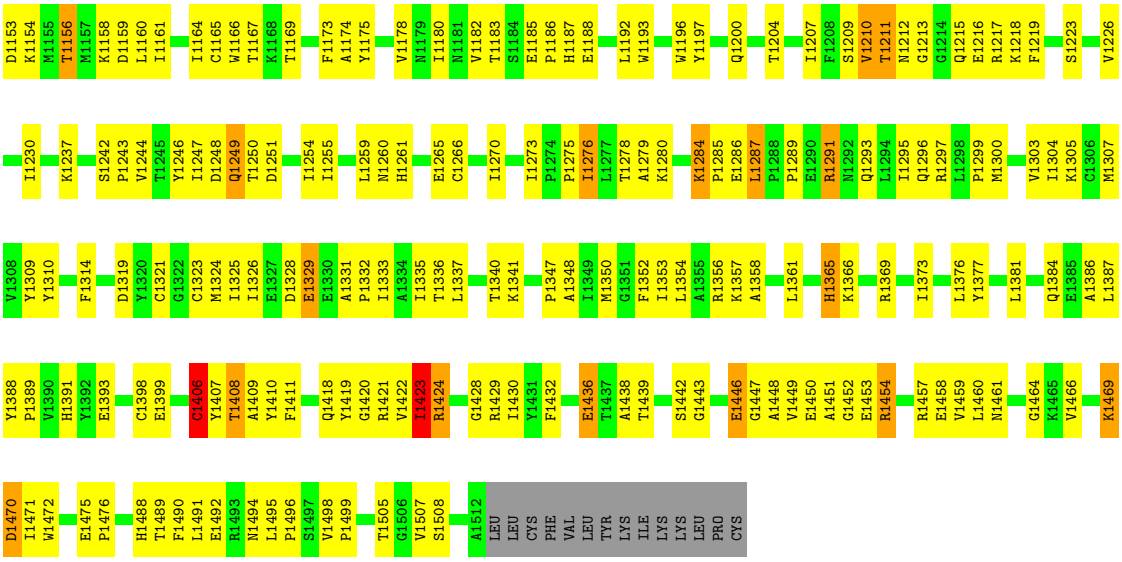
Chain A:



• Molecule 1: Amine oxidase [flavin-containing] A

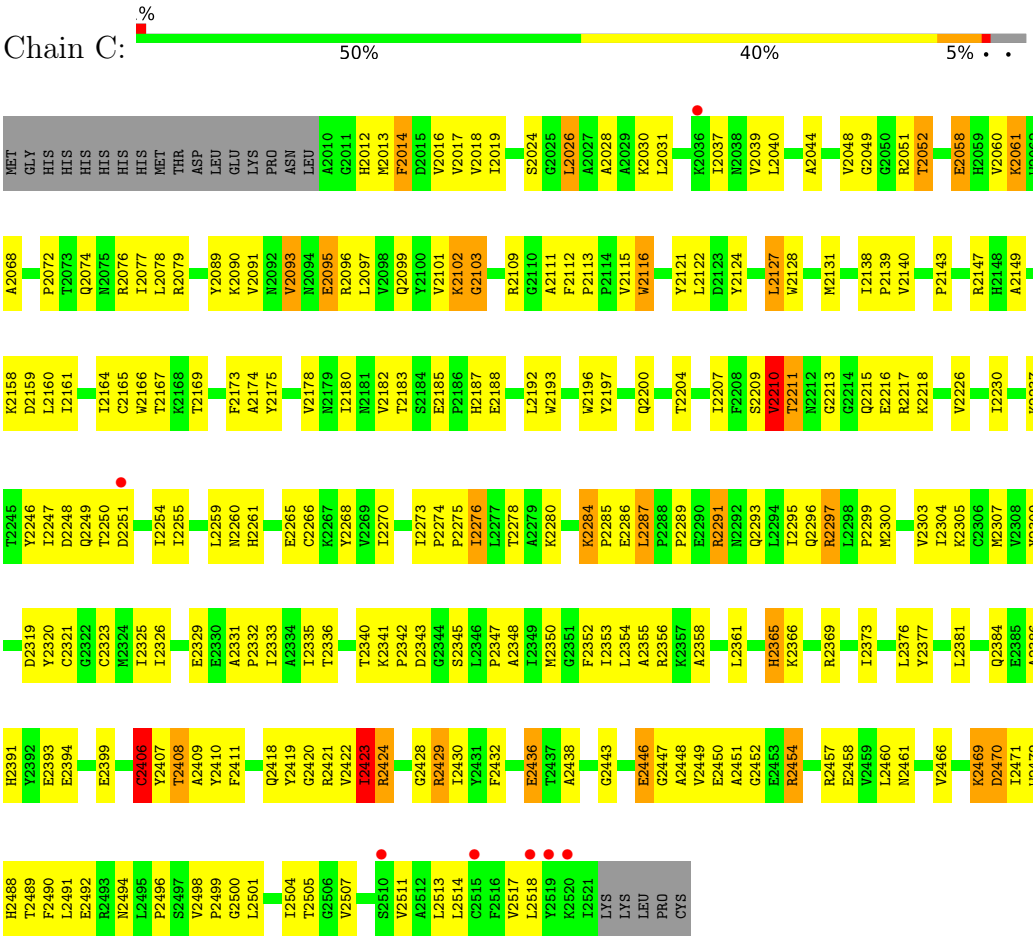
Chain B:





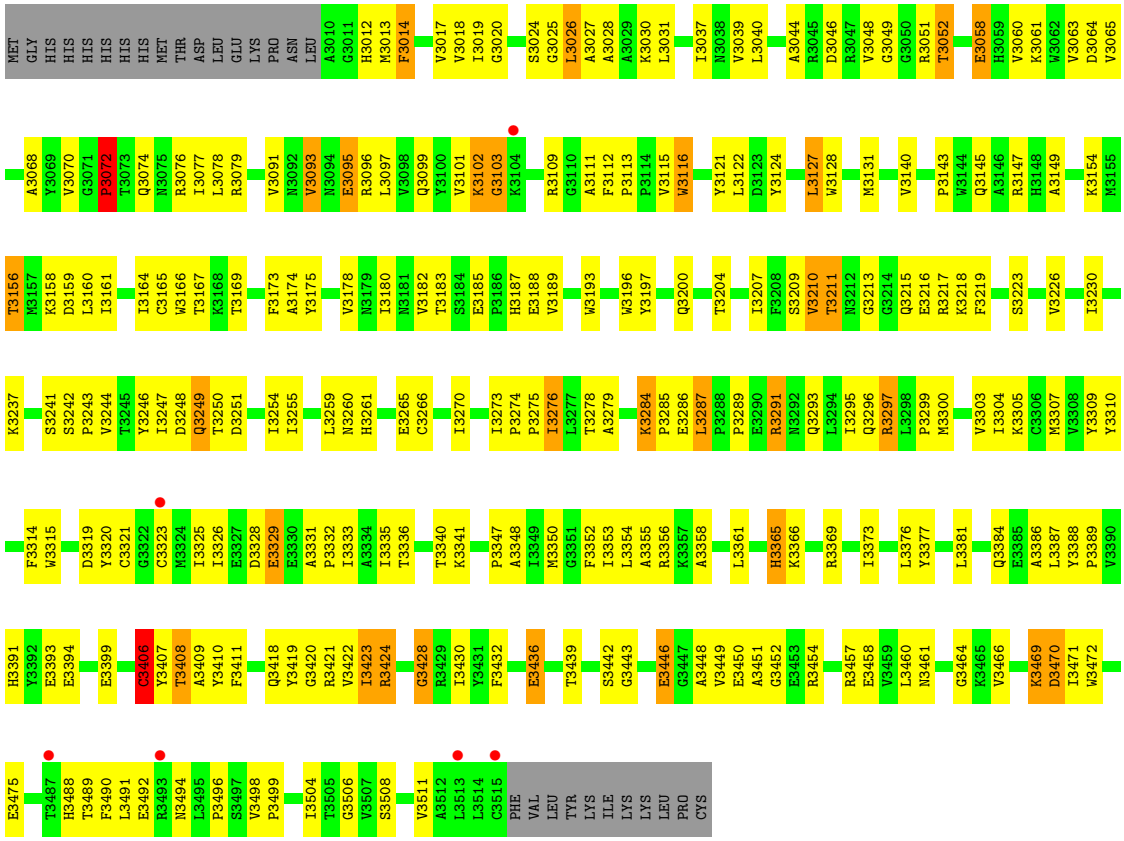
• Molecule 1: Amine oxidase [flavin-containing] A

Chain C:



• Molecule 1: Amine oxidase [flavin-containing] A

Chain D:


MET GLY HIS HIS HIS HIS HIS MET THR ASP LEU GLU LYS PRO ASN LEU A3010 G3011 H3012 M3013 F3014 V3017 V3018 I3019 G3020 S3024 G3025 L3026 A3027 A3028 A3029 K3030 L3031 I3037 N3038 V3039 L3040 A3044 R3045 D3046 R3047 V3048 G3049 G3050 R3051 T3052 E3058 H3059 V3060 K3061 W3062 V3063 D3064 V3065
A3068 Y3069 V3070 G3071 P3072 T3073 Q3074 N3075 R3076 I3077 L3078 R3079 V3091 N3092 V3093 N3094 E3095 R3096 L3097 V3098 Q3099 Y3100 V3101 K3102 G3103 K3104 R3109 G3110 A3111 F3112 P3113 P3114 V3115 W3116 Y3121 L3122 D3123 Y3124 L3127 W3128 M3131 V3140 P3143 W3144 Q3145 A3146 R3147 H3148 A3149 K3154 M3155
T3156 M3157 K3158 D3159 L3160 I3161 I3164 C3165 W3166 T3167 K3168 T3169 F3173 A3174 Y3175 V3178 N3179 I3180 M3181 V3182 T3183 S3184 E3185 P3186 H3187 E3188 V3189 W3193 W3196 Y3197 Q3200 T3204 I3207 F3208 S3209 V3210 T3211 N3212 G3213 G3214 Q3215 E3216 R3217 K3218 F3219 S3223 V3226 I3230
K3237 S3241 S3242 P3243 V3244 T3245 Y3246 I3247 D3248 Q3249 T3250 D3251 I3254 I3255 L3259 N3260 H3261 E3265 C3266 I3270 I3273 P3274 P3275 I3276 L3277 T3278 A3279 K3284 P3285 E3286 L3287 P3288 P3289 E3290 R3291 N3292 Q3293 L3294 I3295 Q3296 R3297 L3298 P3299 M3300 V3303 I3304 K3305 C3306 M3307 V3308 Y3309 Y3310
F3314 W3315 D3319 Y3320 C3321 G3322 C3323 M3324 I3325 I3326 E3327 D3328 E3329 E3330 A3331 P3332 I3333 A3334 I3335 T3336 T3340 K3341 P3347 A3348 I3349 M3350 G3351 F3352 I3353 L3354 A3355 R3356 K3357 A3358 L3361 H3365 K3366 R3369 I3373 L3376 Y3377 L3381 Q3384 E3385 A3386 L3387 Y3388 P3389 V3390
H3391 Y3392 E3393 E3394 E3399 C3406 Y3407 T3408 A3409 Y3410 F3411 Q3418 Y3419 G3420 R3421 V3422 I3423 R3424 G3428 R3429 I3430 Y3431 F3432 E3436 T3439 S3442 G3443 E3446 G3447 A3448 V3449 E3450 A3451 G3452 E3453 R3454 R3457 E3458 V3459 L3460 N3461 G3464 K3465 V3466 K3469 D3470 I3471 W3472
E3475 T3487 H3488 T3489 F3490 L3491 E3492 R3493 N3494 L3495 P3496 S3497 V3498 P3499 I3504 T3505 G3506 V3507 S3508 V3511 A3512 L3513 L3514 C3515 PHE VAL LEU TYR LYS ILE LYS LYS LEU PRO CYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	157.56Å 157.56Å 257.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	16.19 – 3.20 16.18 – 3.08	Depositor EDS
% Data completeness (in resolution range)	99.2 (16.19-3.20) 98.9 (16.18-3.08)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.59 (at 3.07Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.220 , 0.282 0.210 , 0.272	Depositor DCC
R_{free} test set	2988 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	106.5	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 74.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	16456	wwPDB-VP
Average B, all atoms (Å^2)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% 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: FAD, MLG

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	0.41	0/4171	0.65	1/5657 (0.0%)
1	B	0.39	1/4100 (0.0%)	0.64	2/5561 (0.0%)
1	C	0.39	1/4179 (0.0%)	0.65	2/5668 (0.0%)
1	D	0.39	1/4122 (0.0%)	0.65	1/5591 (0.0%)
All	All	0.40	3/16572 (0.0%)	0.65	6/22477 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	3210	VAL	CB-CG1	-5.23	1.41	1.52
1	C	2210	VAL	CB-CG2	-5.17	1.42	1.52
1	B	1210	VAL	CB-CG1	-5.06	1.42	1.52

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	406	CYS	N-CA-C	6.98	129.84	111.00
1	C	2406	CYS	N-CA-C	6.91	129.66	111.00
1	B	1406	CYS	N-CA-C	6.83	129.46	111.00
1	D	3406	CYS	N-CA-C	6.79	129.35	111.00
1	B	1406	CYS	CA-CB-SG	-5.38	104.31	114.00

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	4071	0	4085	256	0
1	B	4002	0	4007	270	0
1	C	4079	0	4096	260	0
1	D	4024	0	4034	257	0
2	A	53	0	29	0	0
2	B	53	0	29	0	0
2	C	53	0	29	0	0
2	D	53	0	29	0	0
3	A	17	0	15	4	0
3	B	17	0	15	3	0
3	C	17	0	15	2	0
3	D	17	0	15	2	0
All	All	16456	0	16398	997	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 30.

The worst 5 of 997 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:B:1464:GLY:HA3	1:D:3145:GLN:HG2	1.18	1.15
1:A:458:GLU:HA	1:A:471:ILE:HD11	1.33	1.10
1:C:2458:GLU:HA	1:C:2471:ILE:HD11	1.33	1.10
1:D:3458:GLU:HA	1:D:3471:ILE:HD11	1.34	1.06
1:B:1458:GLU:HA	1:B:1471:ILE:HD11	1.34	1.03

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	509/534 (95%)	428 (84%)	67 (13%)	14 (3%)	5	29
1	B	501/534 (94%)	416 (83%)	70 (14%)	15 (3%)	4	28
1	C	510/534 (96%)	422 (83%)	73 (14%)	15 (3%)	4	28
1	D	504/534 (94%)	418 (83%)	71 (14%)	15 (3%)	4	28
All	All	2024/2136 (95%)	1684 (83%)	281 (14%)	59 (3%)	4	28

5 of 59 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	102	LYS
1	A	408	THR
1	A	423	ILE
1	B	1102	LYS
1	B	1127	LEU

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	433/455 (95%)	402 (93%)	31 (7%)	14	47
1	B	425/455 (93%)	395 (93%)	30 (7%)	14	47
1	C	434/455 (95%)	401 (92%)	33 (8%)	13	45
1	D	428/455 (94%)	398 (93%)	30 (7%)	15	48
All	All	1720/1820 (94%)	1596 (93%)	124 (7%)	14	47

5 of 124 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1454	ARG
1	D	3249	GLN
1	C	2116	TRP
1	D	3211	THR
1	D	3424	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	2293	GLN
1	C	2401	GLN
1	D	3494	ASN
1	C	2391	HIS
1	C	2418	GLN

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)

8 ligands are modelled in this entry.

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	MLG	A	709	2	16,17,17	3.46	9 (56%)	20,21,21	7.48	5 (25%)
3	MLG	D	3709	2	16,17,17	3.50	10 (62%)	20,21,21	7.55	5 (25%)
2	FAD	B	1652	1,3	53,58,58	2.20	12 (22%)	68,89,89	1.38	10 (14%)
3	MLG	C	2709	2	16,17,17	3.47	9 (56%)	20,21,21	7.50	5 (25%)
3	MLG	B	1709	2	16,17,17	3.48	9 (56%)	20,21,21	7.61	5 (25%)
2	FAD	A	652	1,3	53,58,58	2.16	13 (24%)	68,89,89	1.40	9 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	FAD	C	2652	1,3	53,58,58	2.20	14 (26%)	68,89,89	1.42	11 (16%)
2	FAD	D	3652	1,3	53,58,58	2.22	10 (18%)	68,89,89	1.39	10 (14%)

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	MLG	A	709	2	-	4/9/10/10	0/1/1/1
3	MLG	D	3709	2	-	4/9/10/10	0/1/1/1
2	FAD	B	1652	1,3	-	2/30/50/50	0/6/6/6
3	MLG	C	2709	2	-	5/9/10/10	0/1/1/1
3	MLG	B	1709	2	-	4/9/10/10	0/1/1/1
2	FAD	A	652	1,3	-	2/30/50/50	0/6/6/6
2	FAD	C	2652	1,3	-	2/30/50/50	0/6/6/6
2	FAD	D	3652	1,3	-	2/30/50/50	0/6/6/6

The worst 5 of 86 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	709	MLG	C15-C16	8.12	1.42	1.18
3	C	2709	MLG	C15-C16	7.93	1.41	1.18
3	D	3709	MLG	C15-C16	7.63	1.41	1.18
3	B	1709	MLG	C15-C16	7.49	1.40	1.18
2	C	2652	FAD	C4X-N5	7.40	1.45	1.30

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1709	MLG	C14-C15-C16	-33.38	121.67	177.67
3	D	3709	MLG	C14-C15-C16	-33.17	122.02	177.67
3	C	2709	MLG	C14-C15-C16	-32.94	122.40	177.67
3	A	709	MLG	C14-C15-C16	-32.84	122.58	177.67
2	C	2652	FAD	N3A-C2A-N1A	-3.77	122.79	128.68

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	709	MLG	C02-C01-O09-C10
3	B	1709	MLG	C02-C01-O09-C10
3	C	2709	MLG	C02-C01-O09-C10
3	D	3709	MLG	C02-C01-O09-C10
3	A	709	MLG	C10-C11-C12-N13

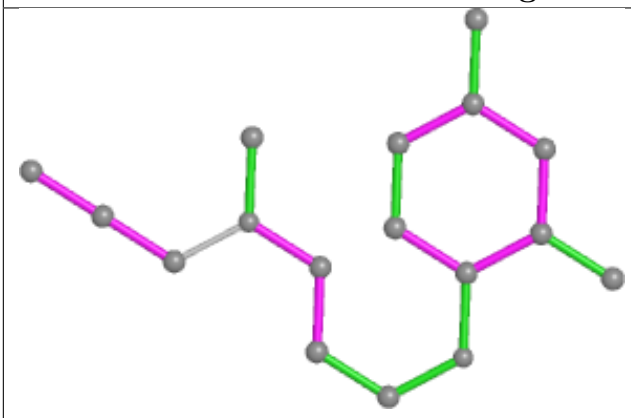
There are no ring outliers.

4 monomers are involved in 11 short contacts:

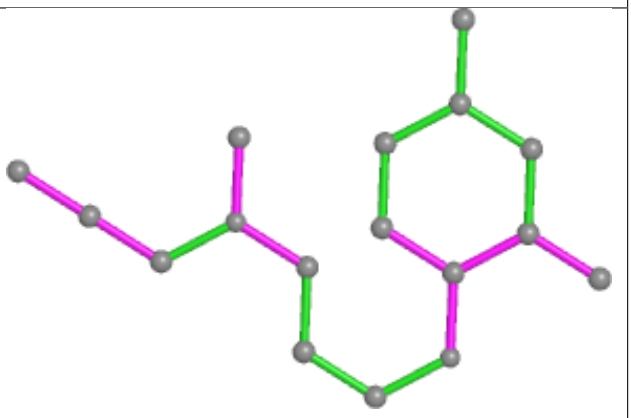
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	709	MLG	4	0
3	D	3709	MLG	2	0
3	C	2709	MLG	2	0
3	B	1709	MLG	3	0

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.

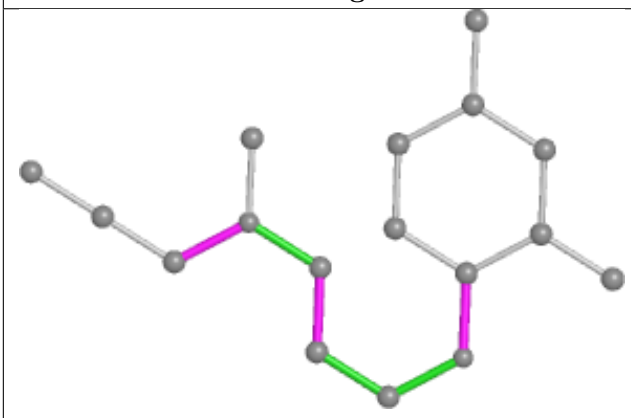
Ligand MLG A 709



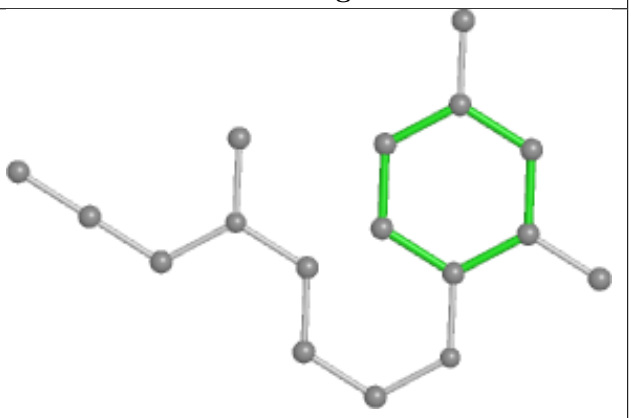
Bond lengths



Bond angles

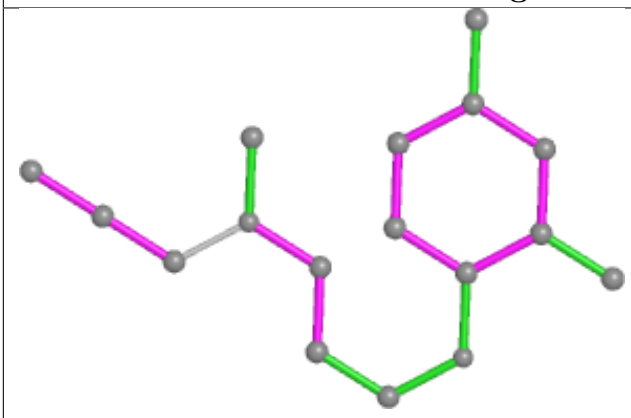


Torsions

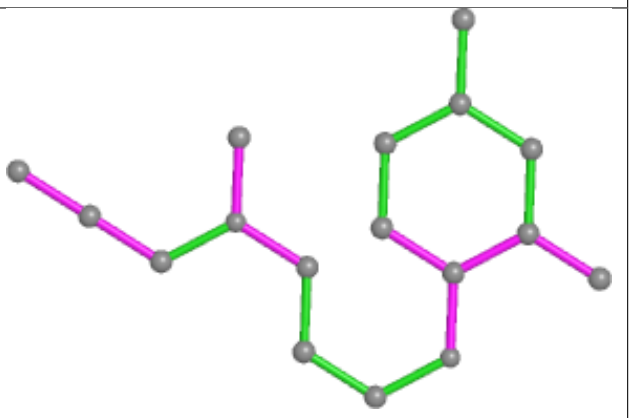


Rings

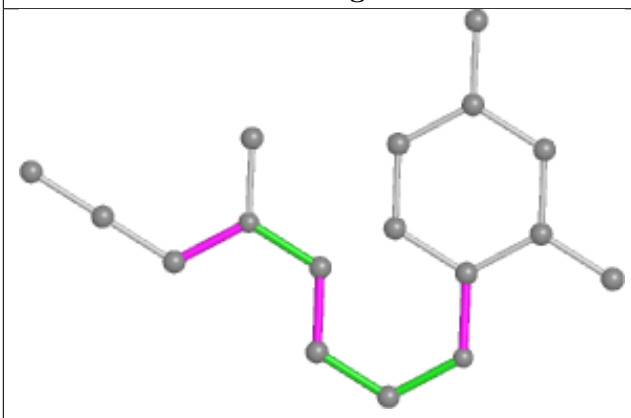
Ligand MLG D 3709



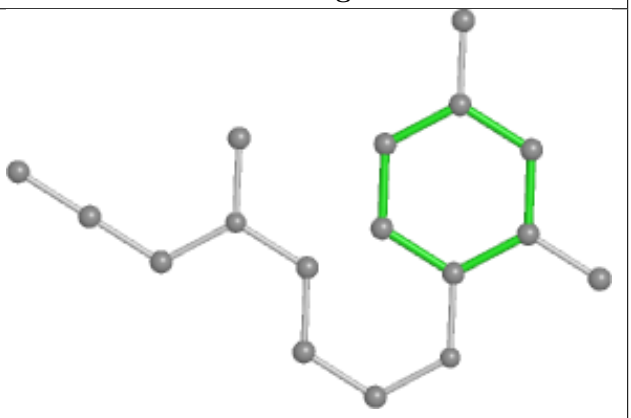
Bond lengths



Bond angles

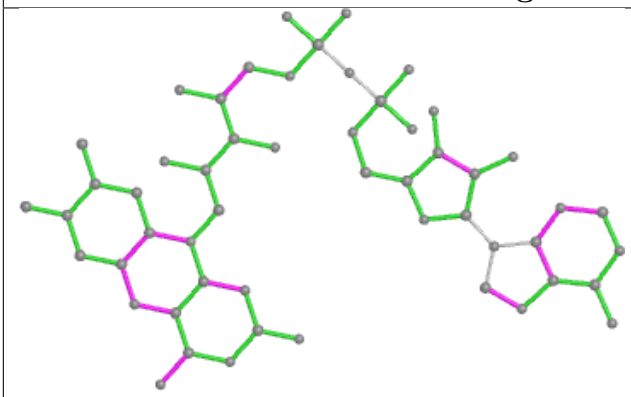


Torsions

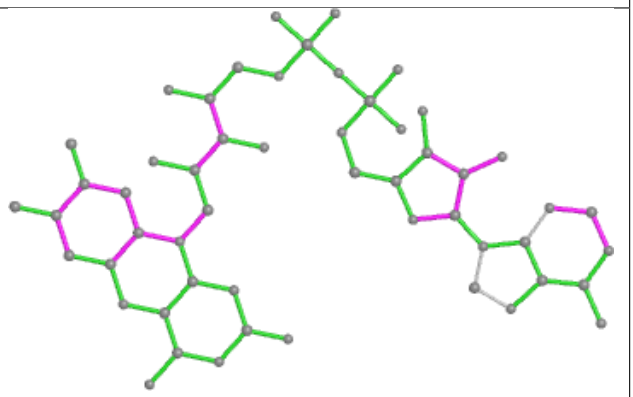


Rings

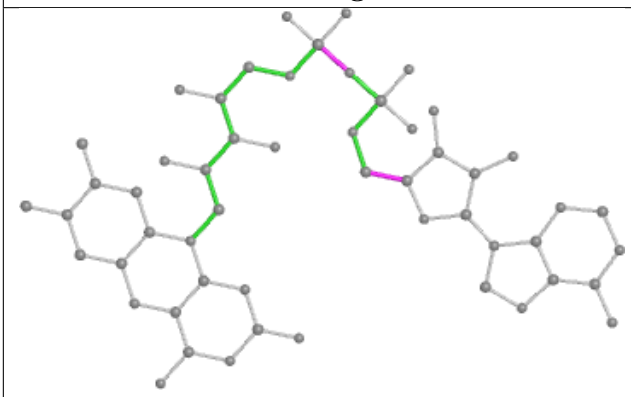
Ligand FAD B 1652



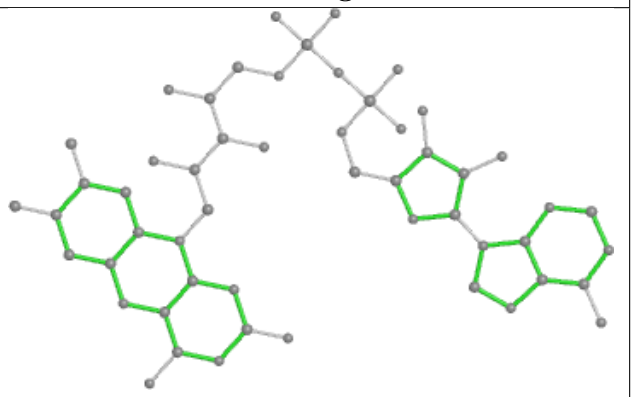
Bond lengths



Bond angles

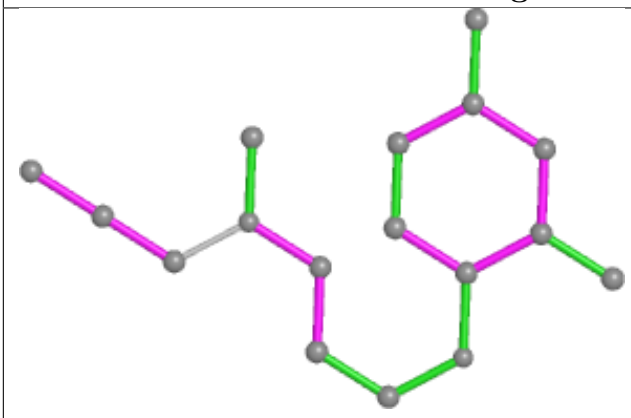


Torsions

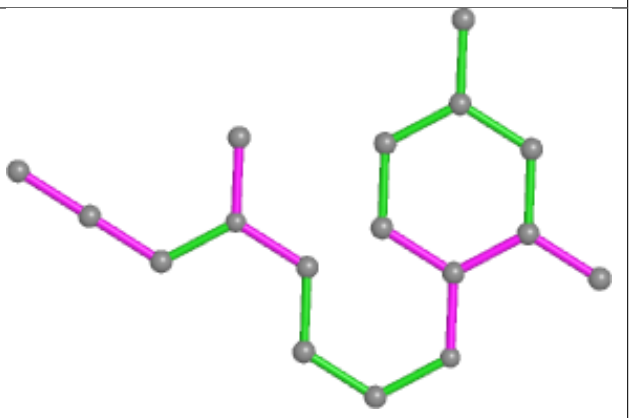


Rings

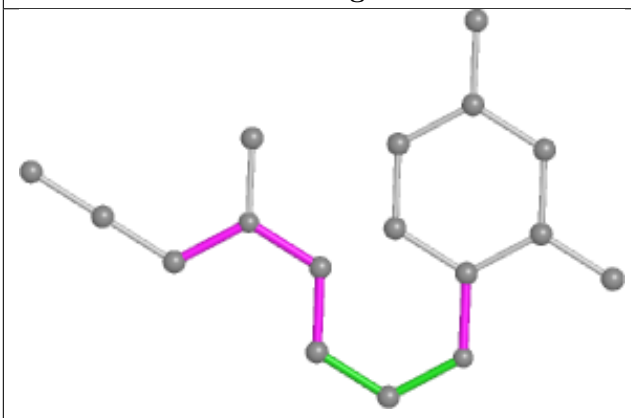
Ligand MLG C 2709



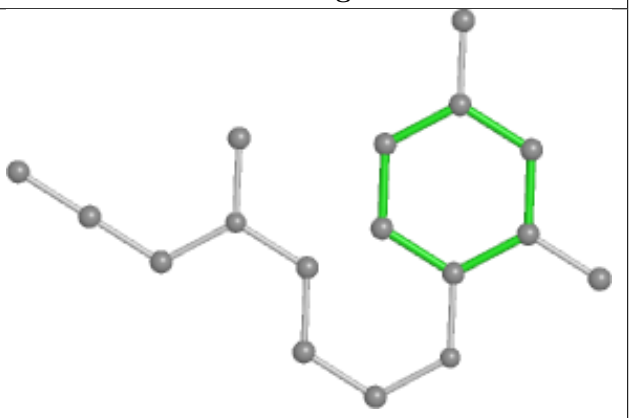
Bond lengths



Bond angles

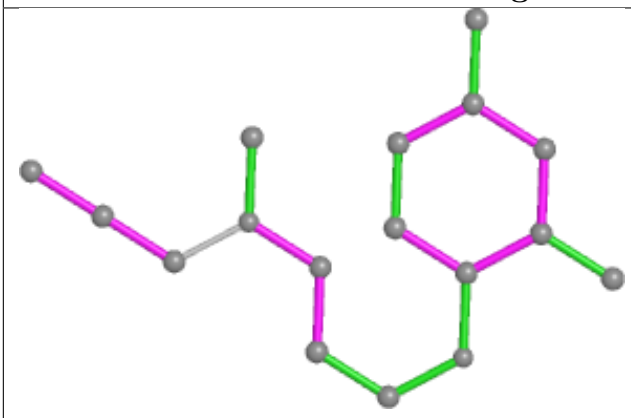


Torsions



Rings

Ligand MLG B 1709



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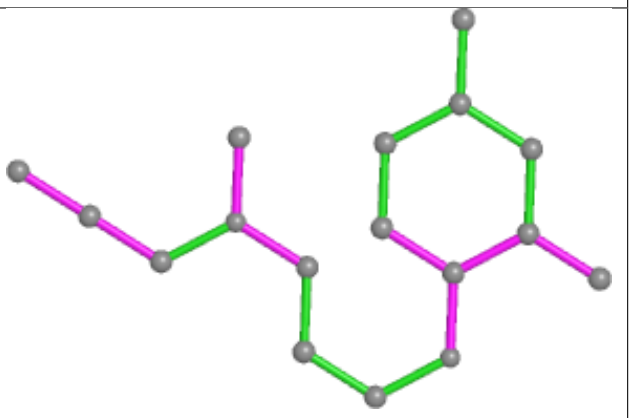
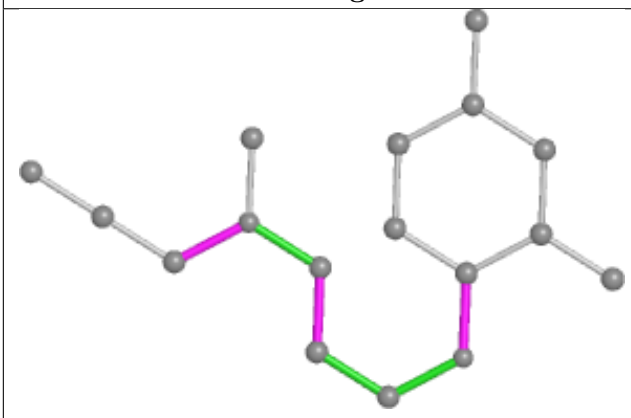


Bond angles



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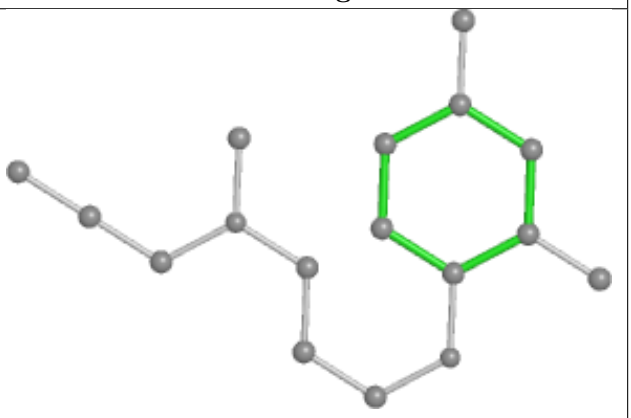
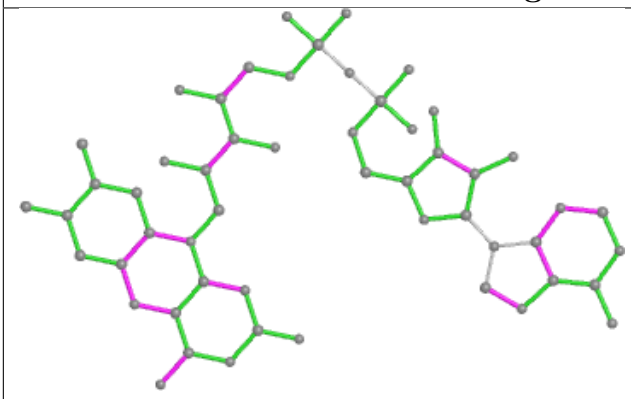
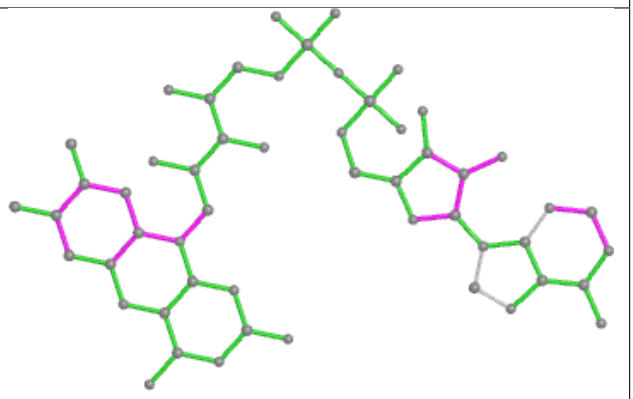


Rings

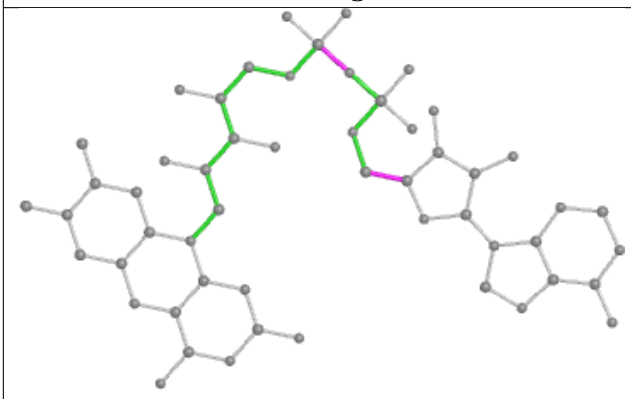
Ligand FAD A 652



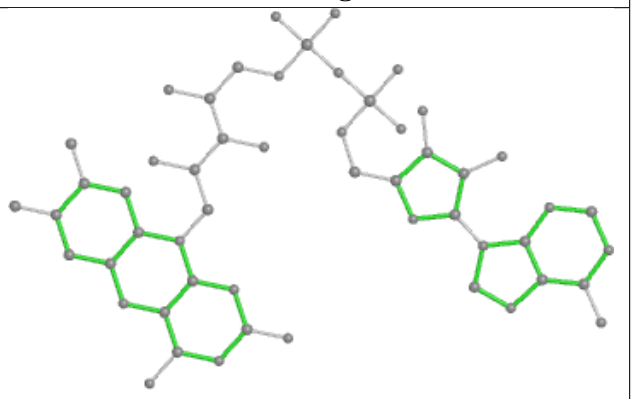
Bond lengths



Bond angles

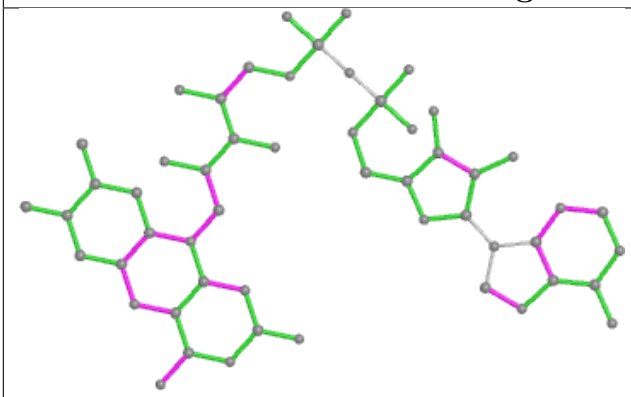


Torsions

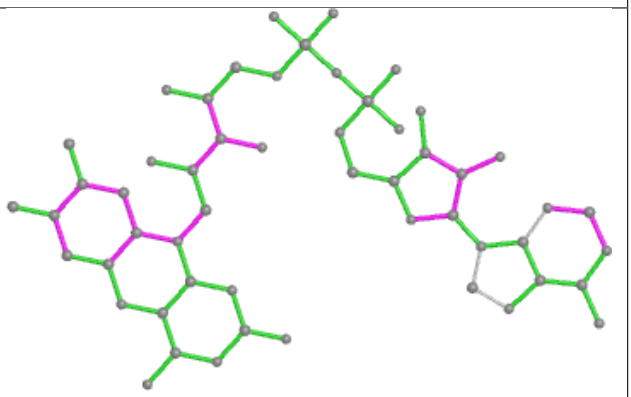


Rings

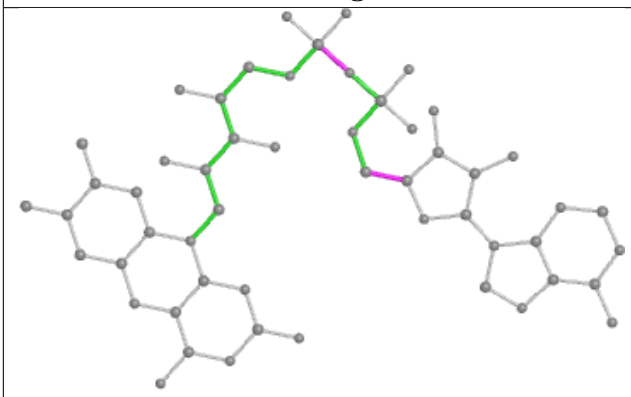
Ligand FAD C 2652



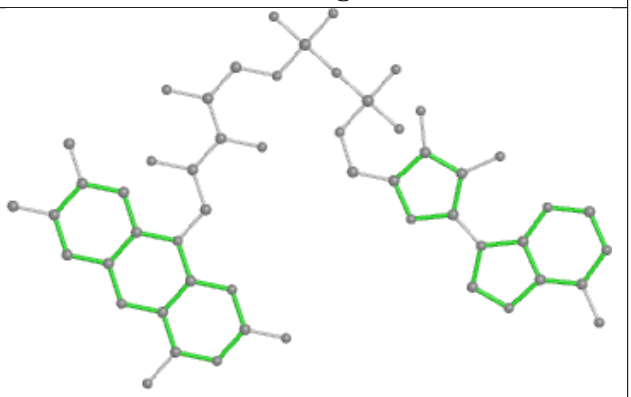
Bond lengths



Bond angles

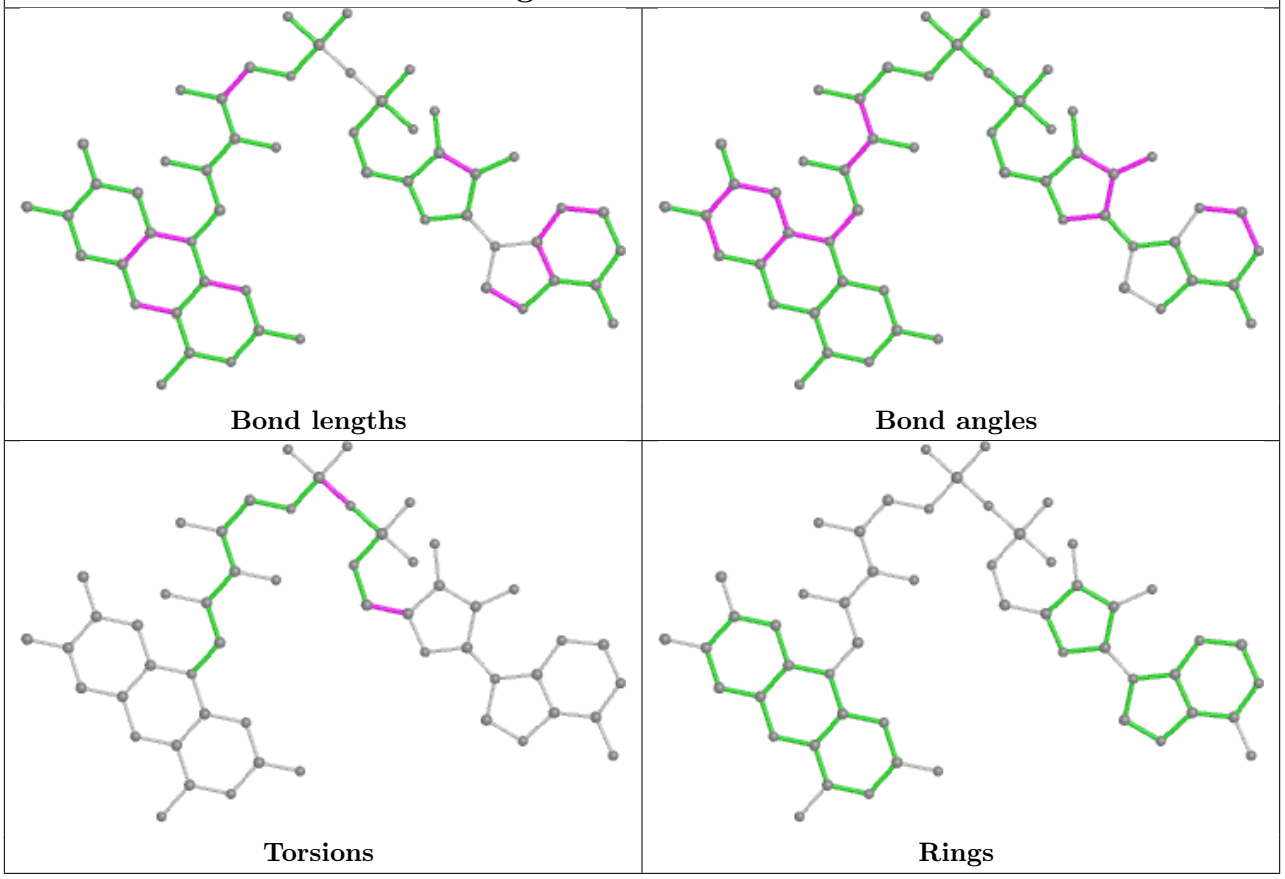


Torsions



Rings

Ligand FAD D 3652



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	511/534 (95%)	-0.50	11 (2%)	62	48	41, 78, 146, 201	0
1	B	503/534 (94%)	-0.45	2 (0%)	92	89	43, 93, 152, 188	0
1	C	512/534 (95%)	-0.50	7 (1%)	75	63	41, 87, 151, 201	0
1	D	506/534 (94%)	-0.48	6 (1%)	79	67	48, 89, 150, 201	0
All	All	2032/2136 (95%)	-0.48	26 (1%)	77	65	41, 86, 150, 201	0

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	3515	CYS	6.9
1	C	2519	TYR	6.6
1	C	2518	LEU	5.8
1	A	10	ALA	4.9
1	A	519	TYR	4.6

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

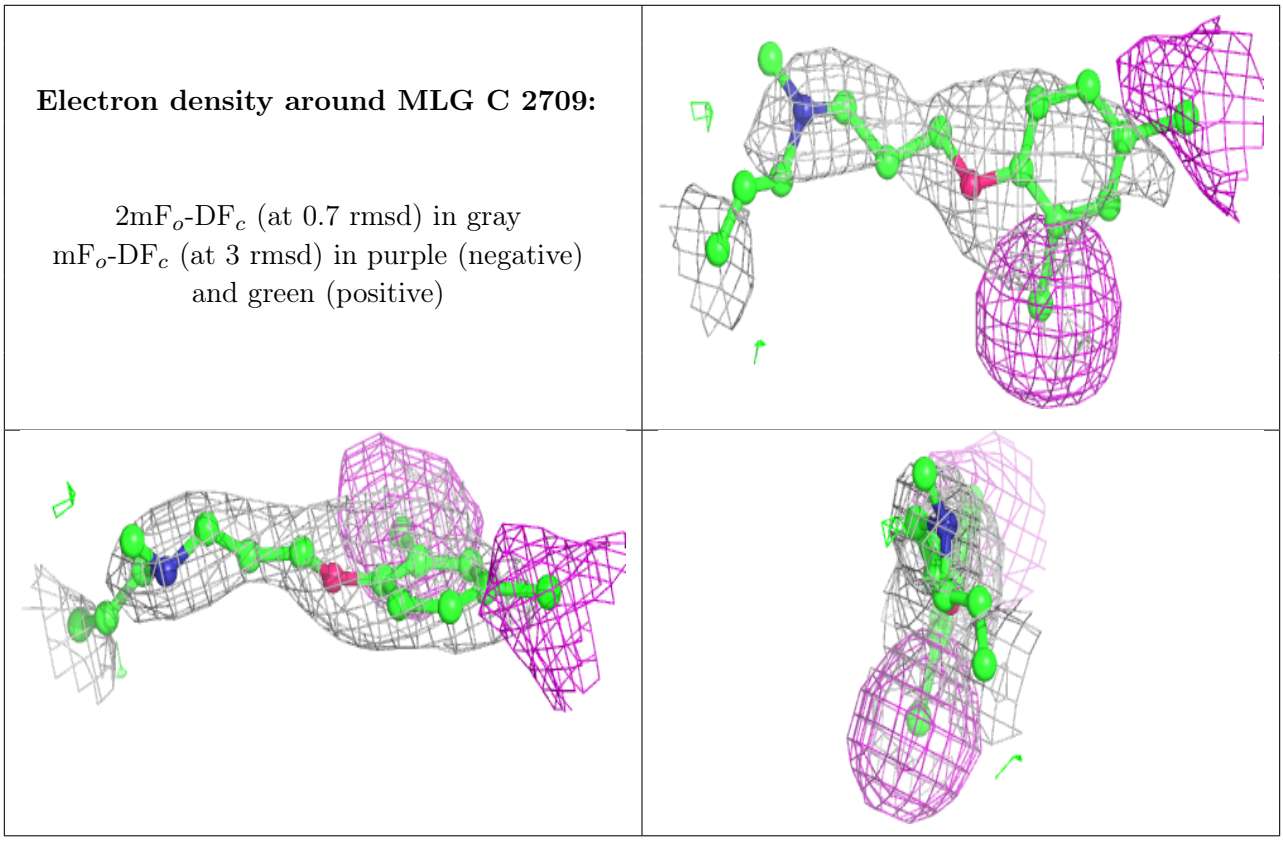
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MLG	C	2709	17/17	0.73	0.35	62,91,140,149	0
3	MLG	D	3709	17/17	0.74	0.31	61,111,159,175	0
3	MLG	B	1709	17/17	0.76	0.34	46,121,168,184	0
3	MLG	A	709	17/17	0.79	0.28	48,67,114,126	0
2	FAD	B	1652	53/53	0.95	0.17	34,72,138,153	0
2	FAD	C	2652	53/53	0.96	0.15	33,67,98,126	0
2	FAD	D	3652	53/53	0.96	0.16	35,75,119,148	0
2	FAD	A	652	53/53	0.97	0.16	32,62,102,113	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.

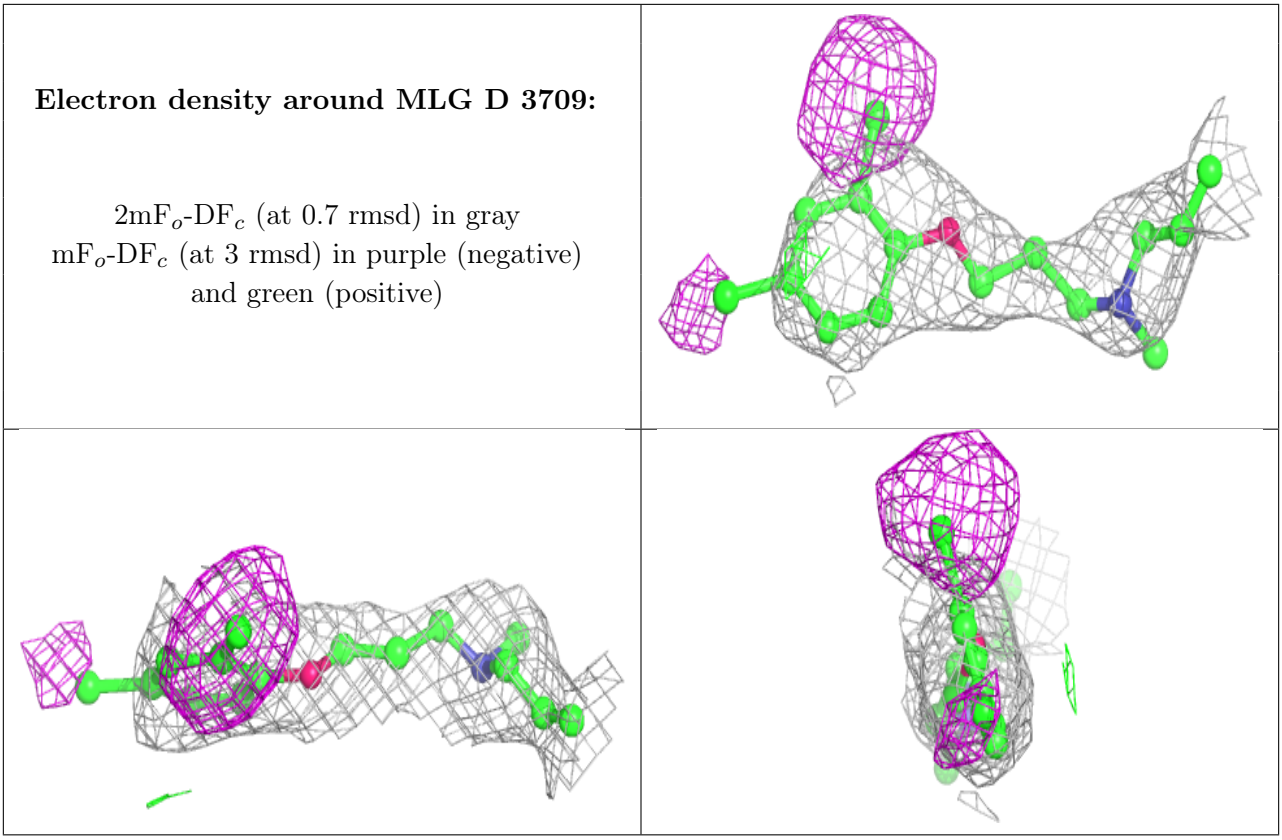
Electron density around MLG C 2709:

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



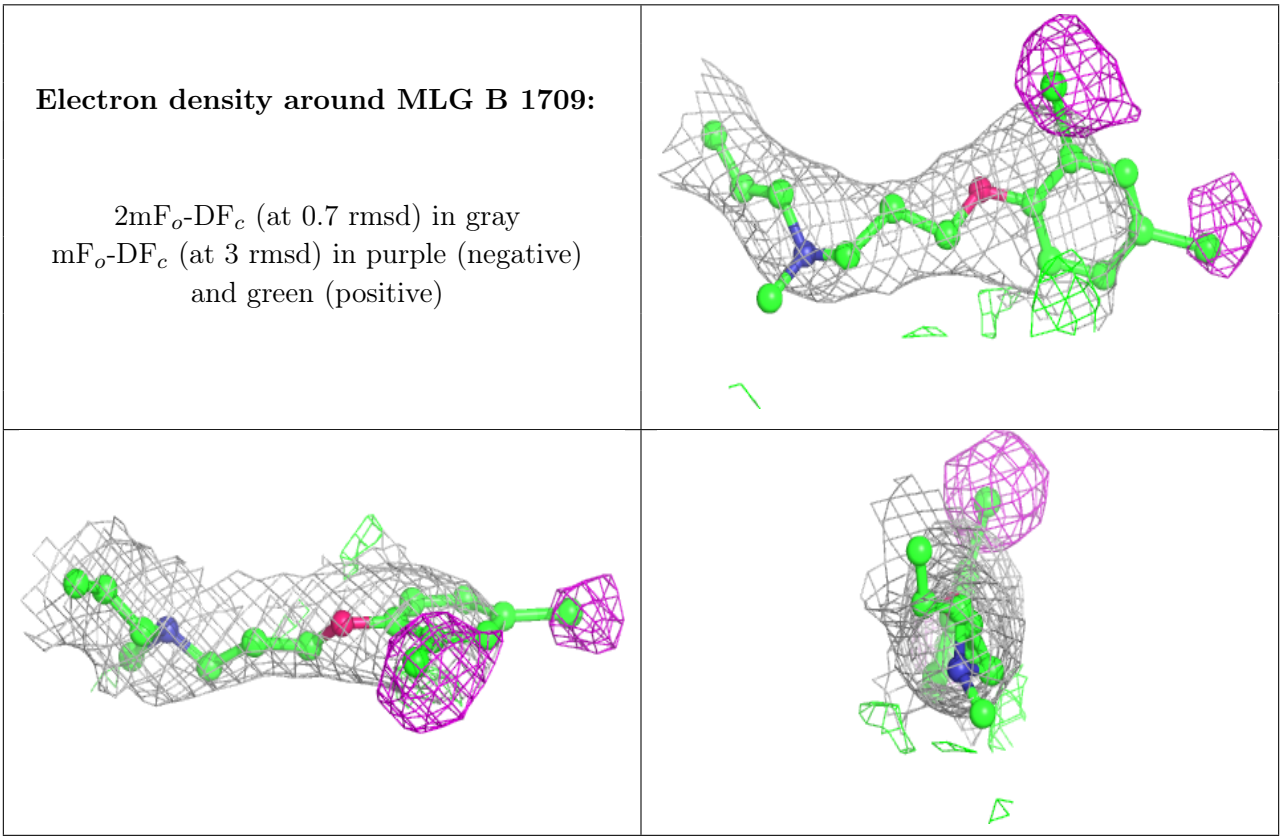
Electron density around MLG D 3709:

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



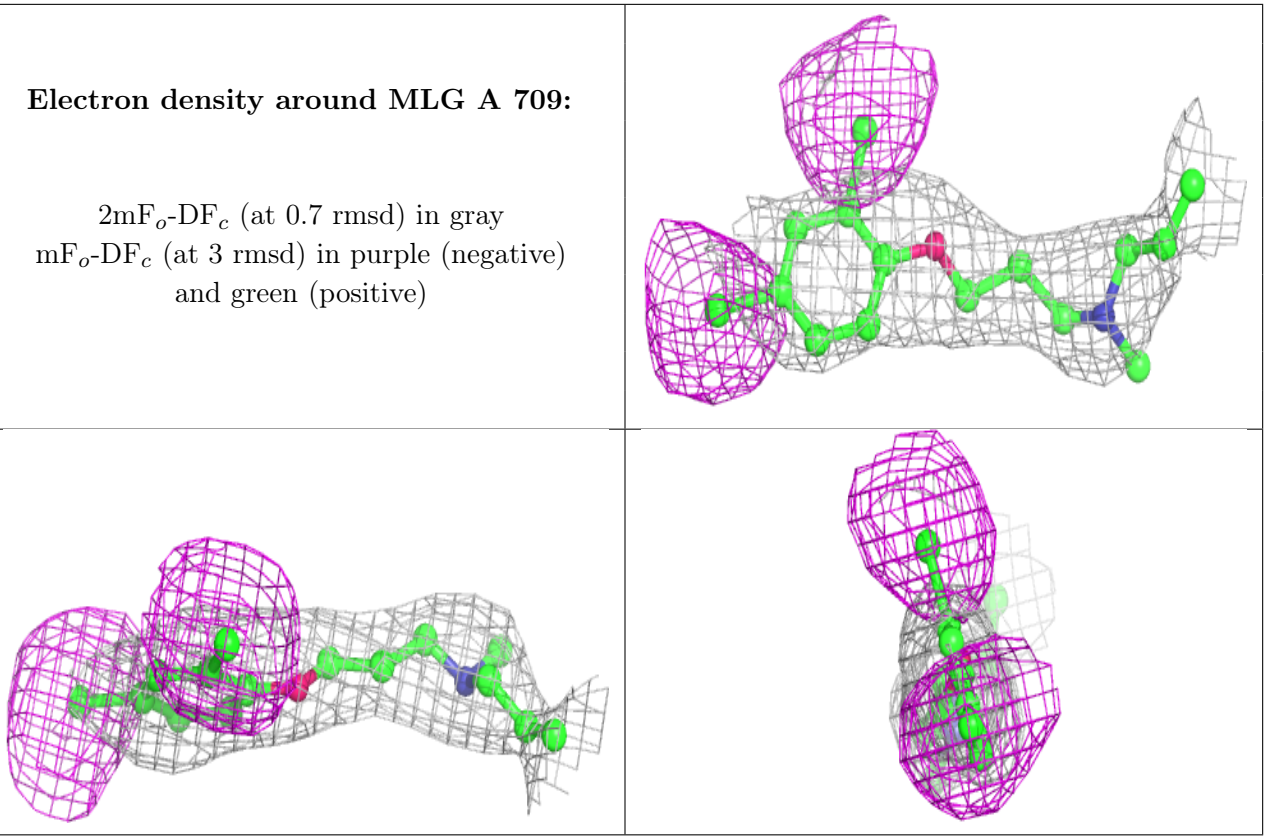
Electron density around MLG B 1709:

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



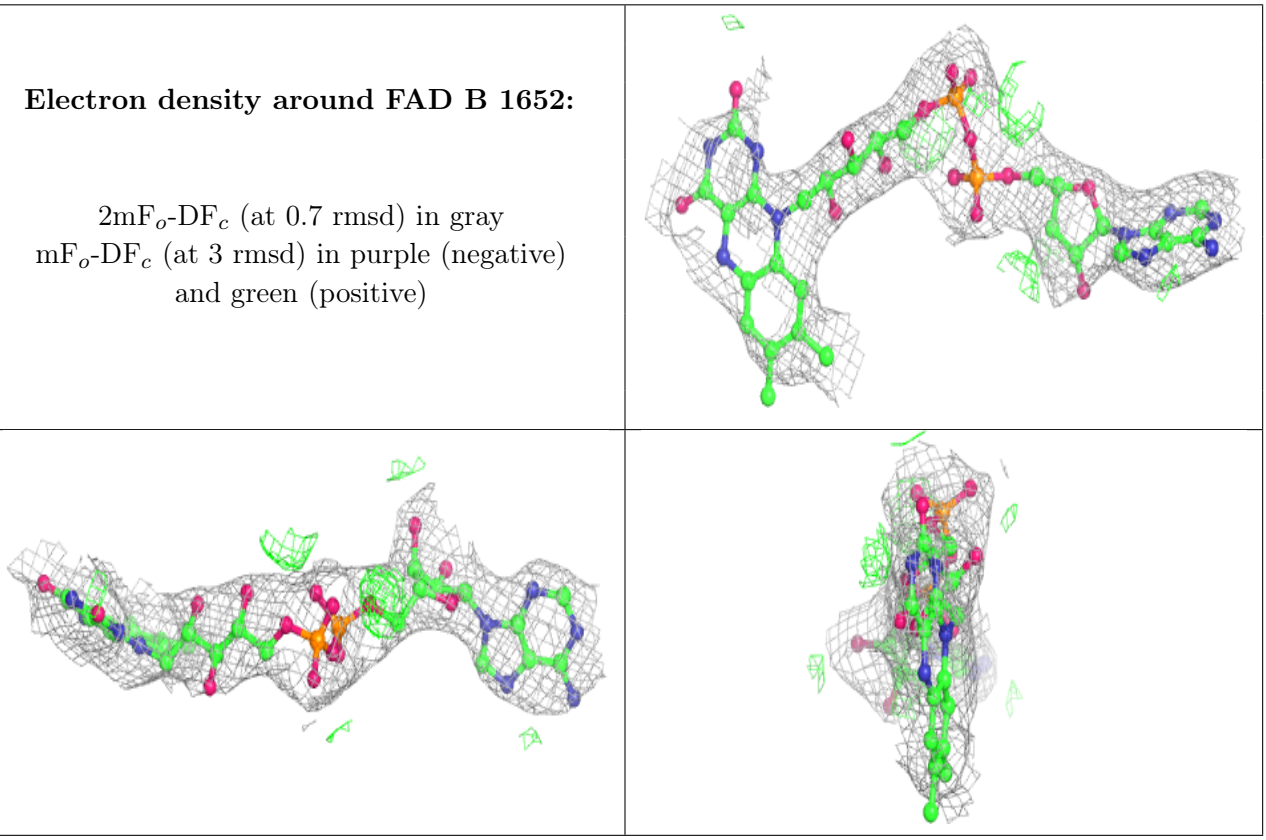
Electron density around MLG A 709:

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



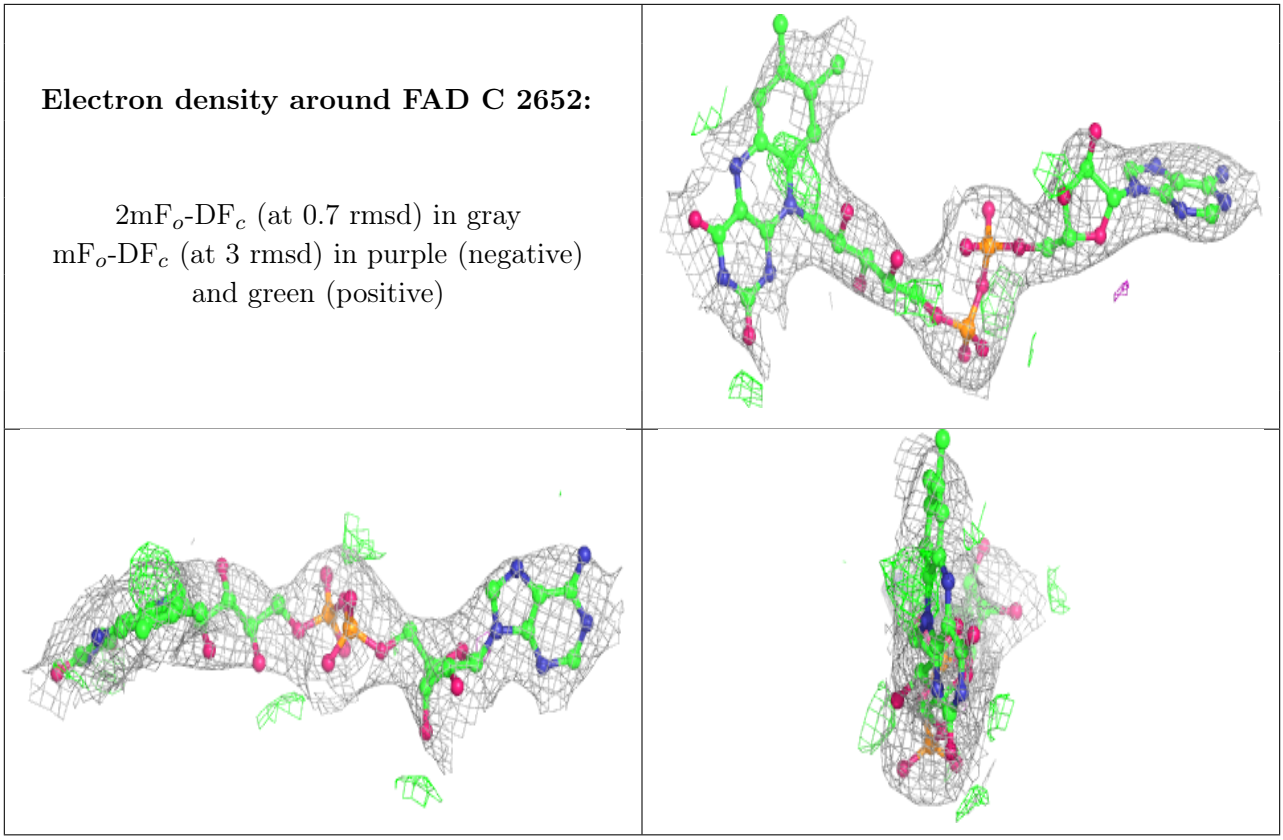
Electron density around FAD B 1652:

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



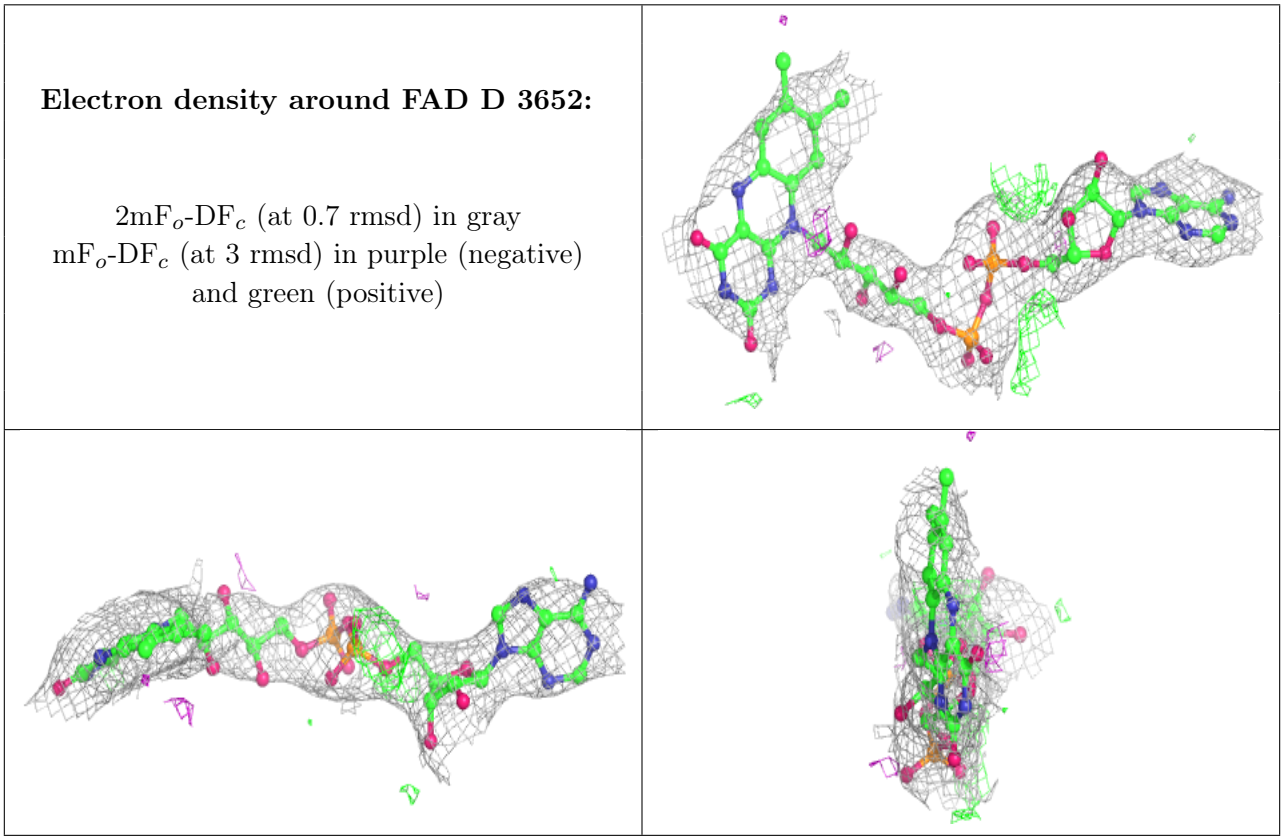
Electron density around FAD C 2652:

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



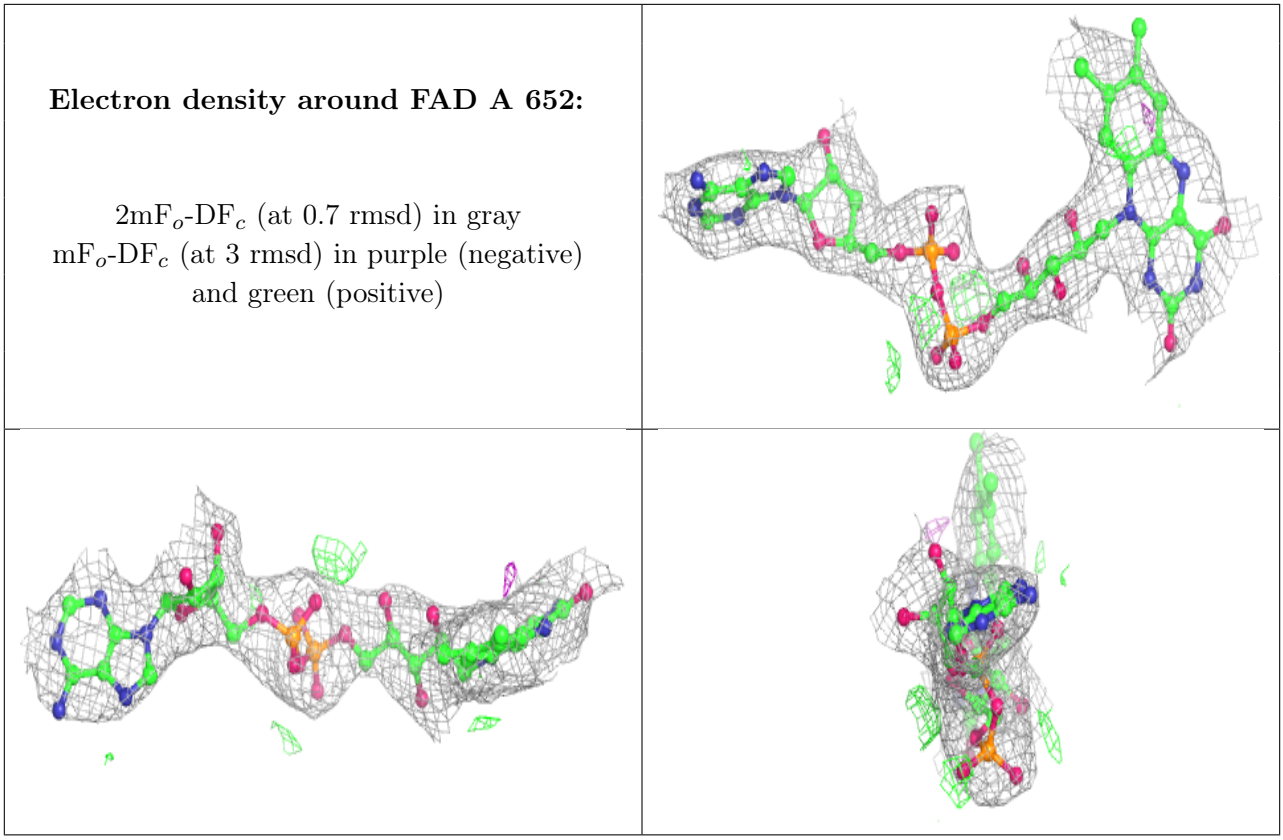
Electron density around FAD D 3652:

$2mF_o$-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 652:

$2mF_o$-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.