



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 03:04 AM UTC

PDB ID : 1O5W / pdb_00001o5w
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 ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

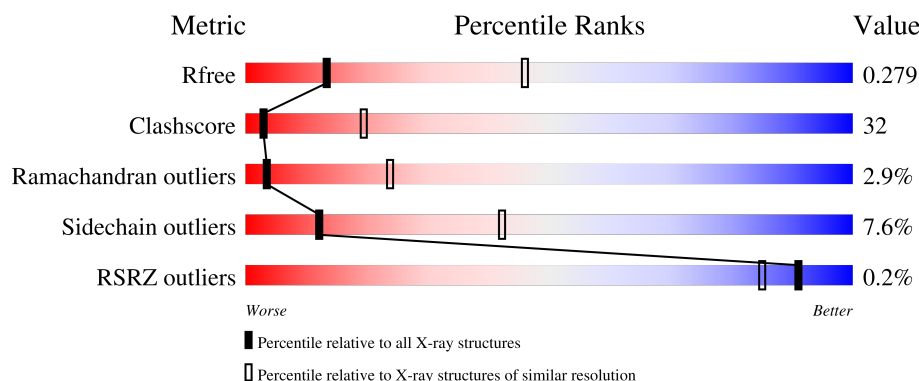
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (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 $\leq 5\%$. 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	534	
1	B	534	
1	C	534	
1	D	534	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MLG	C	2709	-	X	-	-

2 Entry composition

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:

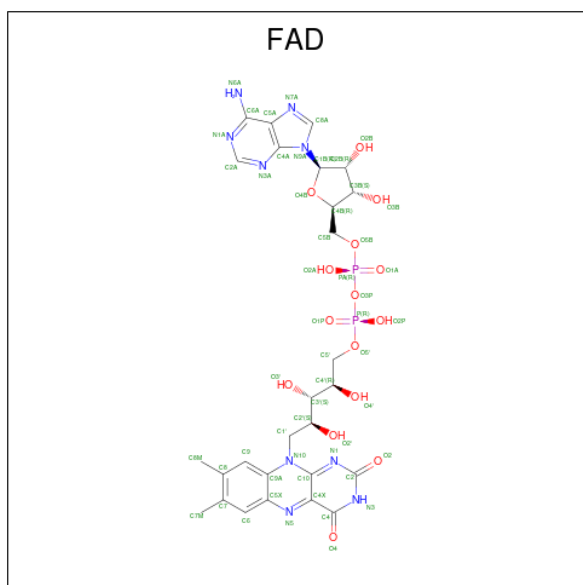
Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	expression tag	UNP P21396
A	-6	GLY	-	expression tag	UNP P21396
A	-5	HIS	-	expression tag	UNP P21396
A	-4	HIS	-	expression tag	UNP P21396
A	-3	HIS	-	expression tag	UNP P21396
A	-2	HIS	-	expression tag	UNP P21396
A	-1	HIS	-	expression tag	UNP P21396
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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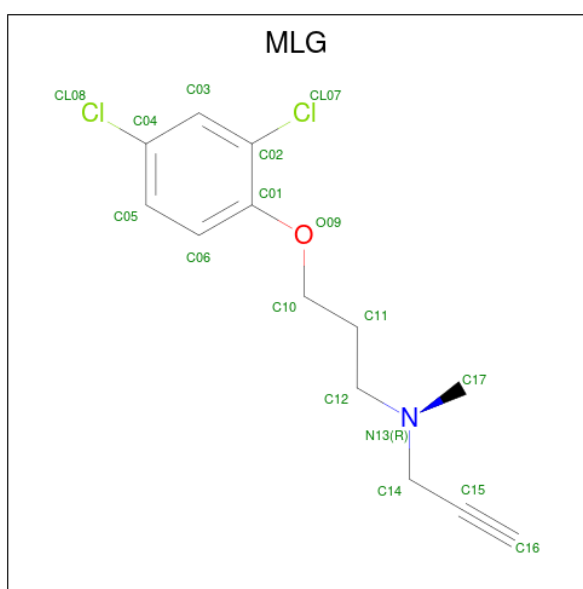
Chain	Residue	Modelled	Actual	Comment	Reference
B	1361	LEU	GLN	SEE REMARK 999	UNP P21396
C	1993	MET	-	expression tag	UNP P21396
C	1994	GLY	-	expression tag	UNP P21396
C	1995	HIS	-	expression tag	UNP P21396
C	1996	HIS	-	expression tag	UNP P21396
C	1997	HIS	-	expression tag	UNP P21396
C	1998	HIS	-	expression 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 (CCD ID: 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 (CCD ID: MLG) (formula: C₁₃H₁₅Cl₂NO).

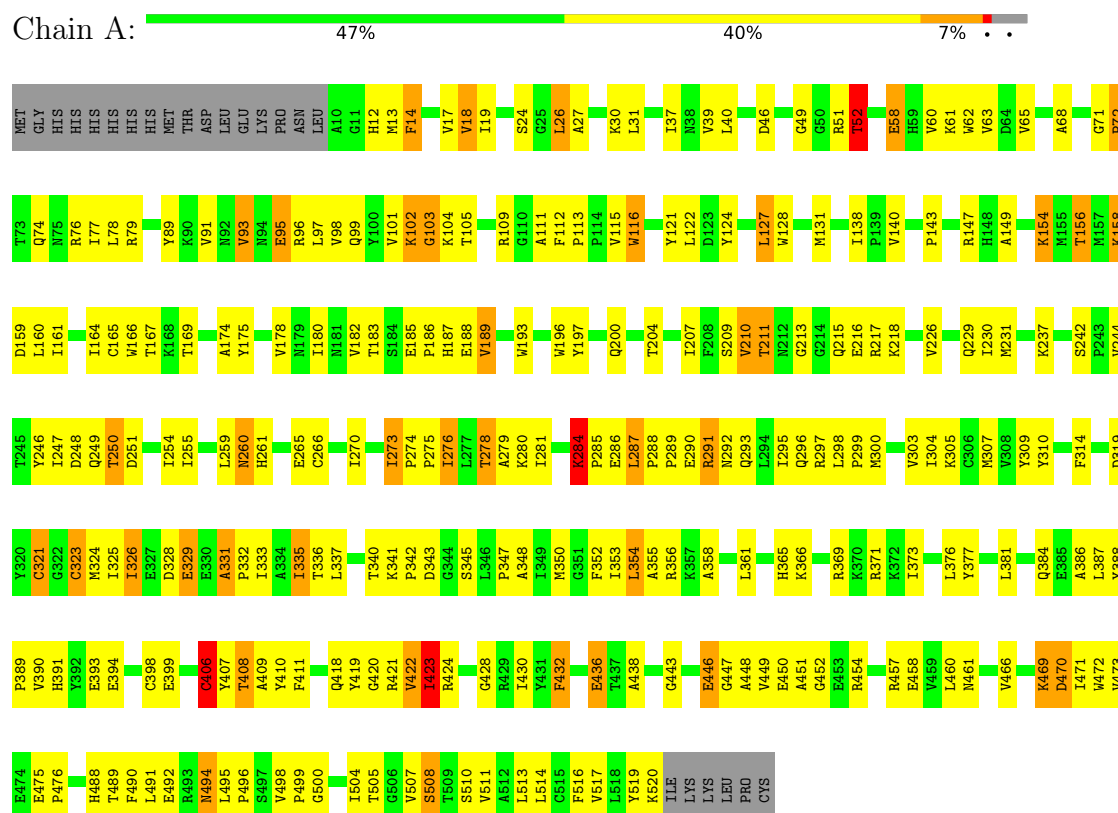


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			17	13	2	1	1		
3	B	1	Total	C	Cl	N	O	0	0
			17	13	2	1	1		
3	C	1	Total	C	Cl	N	O	0	0
			17	13	2	1	1		
3	D	1	Total	C	Cl	N	O	0	0
			17	13	2	1	1		

3 Residue-property plots

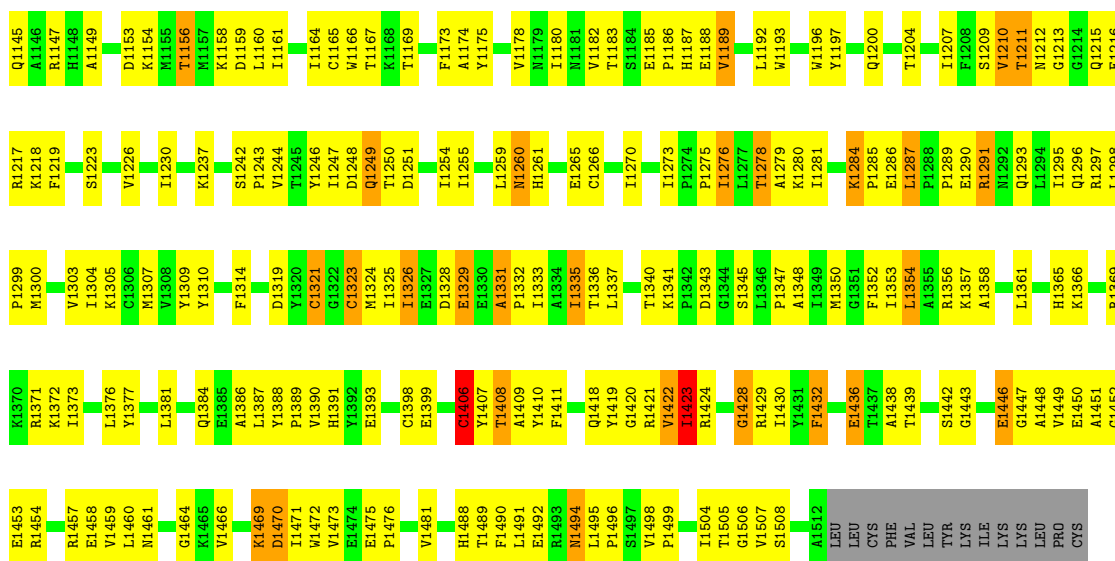
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



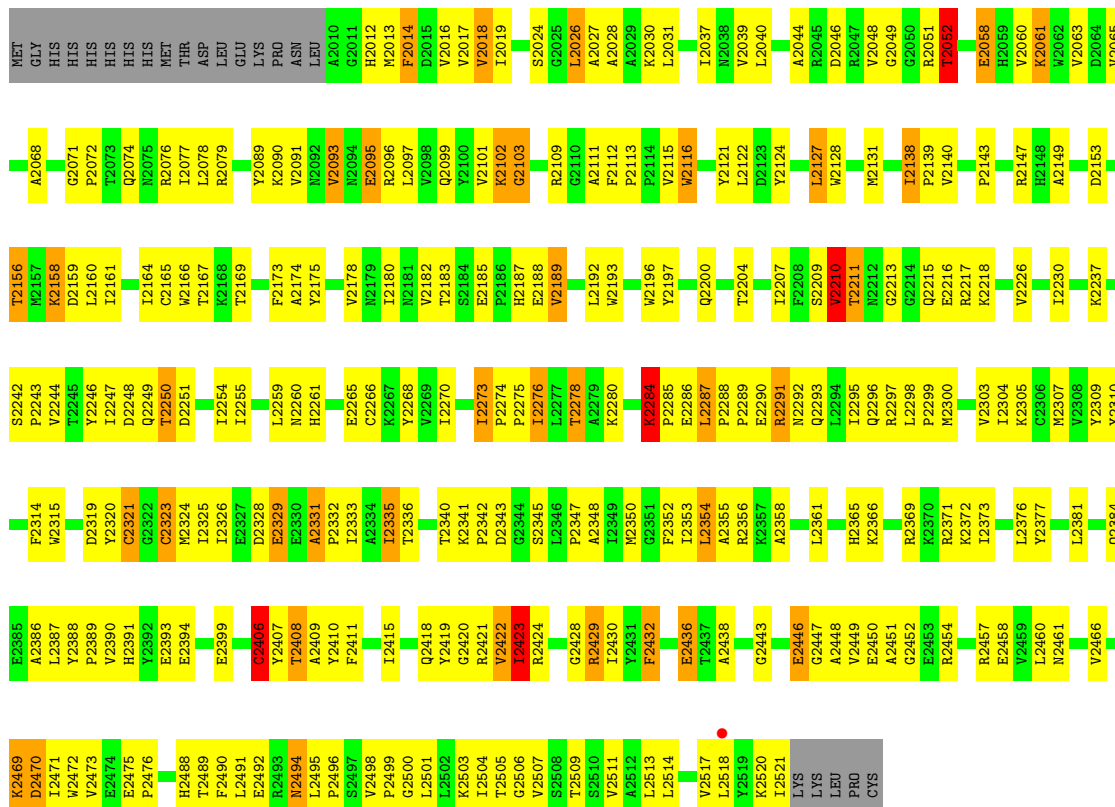
• Molecule 1: Amine oxidase [flavin-containing] A





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

Chain C: 46% 42% 7% . .



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

Chain D: 47% 40% 7% 5%

R3457	R3458	V3459	L3460	N3461	G3464	K3465	V3466	K3469	D3470	I3471	W3472	V3473	E3474	E3475	H3488	T3489	F3490	L3491	E3492	R3493	N3494	L3495	P3496	S3497	V3498	P3499	L3504	T3505	G3506	V3507	S3508	T3509	S3510	V3511	C3515	PHE	VAL	LEU	TYR	LYS	ILE	LYS	LYS	LEU	PRO	CYS										
L3381	Q3384	E3385	A3386	L3387	P3388	P3389	V3390	H3391	V3392	E3393	E3394	E3399	S3403	G3404	G3405	C3406	T3407	T3408	A3409	Y3410	F3411	T3415	Q3418	Y3419	G3420	R3421	V3422	R3423	R3424	G3428	R3429	T3430	F3431	F3432	E3436	T3439	S3442	G3443	E3446	G3447	A3448	V3449	E3450	A3451	G3452	R3454										
K3305	C3306	M3307	V3308	Y3309	Y3310	F3314	W3315	D3319	Y3320	C3321	G3322	C3323	M3324	I3325	I3326	F3327	D3328	E3329	E3330	A3331	P3332	I3333	A3334	I3335	T3336	T3340	K3341	P3342	D3343	G3344	S3345	L3346	P3347	A3348	I3349	M3350	F3351	F3352	I3353	L3354	A3355	R3356	K3357	A3358	L3361	H3365	K3366	R3369	T3373	L3376	Y3377					
V3226	T3230	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	K3280	I3281	K3284	P3285	E3286	L3287	P3288	P3289	E3290	R3291	R3292	Q3293	L3294	I3295	Q3296	R3297	L3298	P3299	M3300	V3303	I3304							
A3068	Y3069	V3070	T3156	M3157	K3158	D3159	L3160	L3161	I3164	C3165	W3166	T3167	K3168	A3170	F3173	A3174	Y3175	V3178	N3179	I3180	M3181	V3182	T3183	S3184	G3103	R3109	G3110	A3111	A3028	F3112	P3113	P3114	V3115	W3116	Y3121	L3122	D3123	Y3124	L3127	W3128	M3131	T3210	T3211	N3212	P3138	V3140	P3143	W3144	V3060	K3061	A3062	R3147	V3063	D3064	A3149	
MET	GLY	HIS	HIS	HIS	HIS	HIS	MET	THR	ASP	LEU	GLU	LYS	PRO	ASN	LEU	N3091	N3092	V3093	N3094	E3095	R3096	L3097	V3098	V3017	V3018	L3019	G3020	S3024	G3025	L3026	A3027	A3028	A3029	K3030	L3031	I3037	R3038	L3040	A3044	R3045	D3046	R3047	V3048	G3049	G3050	R3051	T3052	E3058	W3059	V3060	K3061	A3062	R3147	V3063	D3064	A3149

4 Data and refinement statistics

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 16.19 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.2 (16.19-3.20) 98.2 (16.19-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 3.07Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.220 , 0.282 0.221 , 0.279	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 , 78.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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.*

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, 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	0.49	0/4171	1.04	29/5657 (0.5%)
1	B	0.46	0/4100	1.02	25/5561 (0.4%)
1	C	0.47	0/4179	1.04	28/5668 (0.5%)
1	D	0.46	0/4122	1.03	26/5591 (0.5%)
All	All	0.47	0/16572	1.03	108/22477 (0.5%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	406	CYS	N-CA-C	13.22	129.84	112.12
1	C	2406	CYS	N-CA-C	13.09	129.66	112.12
1	B	1406	CYS	N-CA-C	12.94	129.46	112.12
1	D	3406	CYS	N-CA-C	12.86	129.35	112.12
1	B	1298	LEU	CA-C-N	8.55	128.49	119.85

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	4071	0	4085	275	0
1	B	4002	0	4007	285	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	4079	0	4096	274	0
1	D	4024	0	4034	268	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	1054	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 32.

The worst 5 of 1054 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%)	4	25
1	B	501/534 (94%)	416 (83%)	70 (14%)	15 (3%)	3	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	510/534 (96%)	422 (83%)	73 (14%)	15 (3%)	3	24
1	D	504/534 (94%)	418 (83%)	71 (14%)	15 (3%)	3	23
All	All	2024/2136 (95%)	1684 (83%)	281 (14%)	59 (3%)	3	24

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 ⓘ

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%)	401 (93%)	32 (7%)	13	43
1	B	425/455 (93%)	394 (93%)	31 (7%)	13	43
1	C	434/455 (95%)	400 (92%)	34 (8%)	11	41
1	D	428/455 (94%)	395 (92%)	33 (8%)	12	41
All	All	1720/1820 (94%)	1590 (92%)	130 (8%)	12	42

5 of 130 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	3251	ASP
1	D	3287	LEU
1	B	1249	GLN
1	B	1211	THR
1	D	3335	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	3249	GLN
1	D	3260	ASN
1	D	3418	GLN
1	B	1260	ASN
1	B	1249	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	D	3709	2	16,17,17	3.43	10 (62%)	20,21,21	7.80	5 (25%)
3	MLG	A	709	2	16,17,17	3.40	10 (62%)	20,21,21	7.73	5 (25%)
2	FAD	D	3652	1,3	58,58,58	2.05	12 (20%)	85,89,89	1.64	14 (16%)
2	FAD	A	652	1,3	58,58,58	2.02	14 (24%)	85,89,89	1.62	14 (16%)
3	MLG	C	2709	2	16,17,17	3.41	10 (62%)	20,21,21	7.75	5 (25%)
2	FAD	B	1652	1,3	58,58,58	2.06	13 (22%)	85,89,89	1.63	14 (16%)
2	FAD	C	2652	1,3	58,58,58	2.03	14 (24%)	85,89,89	1.63	14 (16%)
3	MLG	B	1709	2	16,17,17	3.41	10 (62%)	20,21,21	7.86	5 (25%)

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	D	3709	2	-	4/9/10/10	0/1/1/1
3	MLG	A	709	2	-	4/9/10/10	0/1/1/1
2	FAD	D	3652	1,3	-	3/34/50/50	0/6/6/6
2	FAD	A	652	1,3	-	3/34/50/50	0/6/6/6
3	MLG	C	2709	2	-	5/9/10/10	0/1/1/1
2	FAD	B	1652	1,3	-	3/34/50/50	0/6/6/6
2	FAD	C	2652	1,3	-	3/34/50/50	0/6/6/6
3	MLG	B	1709	2	-	4/9/10/10	0/1/1/1

The worst 5 of 93 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	709	MLG	C15-C16	8.28	1.42	1.18
3	C	2709	MLG	C15-C16	8.09	1.41	1.18
3	D	3709	MLG	C15-C16	7.77	1.41	1.18
3	B	1709	MLG	C15-C16	7.64	1.40	1.18
2	C	2652	FAD	C4X-N5	6.67	1.45	1.30

The worst 5 of 76 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1709	MLG	C14-C15-C16	-34.50	121.67	177.63
3	D	3709	MLG	C14-C15-C16	-34.29	122.02	177.63
3	C	2709	MLG	C14-C15-C16	-34.05	122.40	177.63
3	A	709	MLG	C14-C15-C16	-33.94	122.58	177.63
2	B	1652	FAD	C4A-N9A-C8A	-6.54	98.88	105.74

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

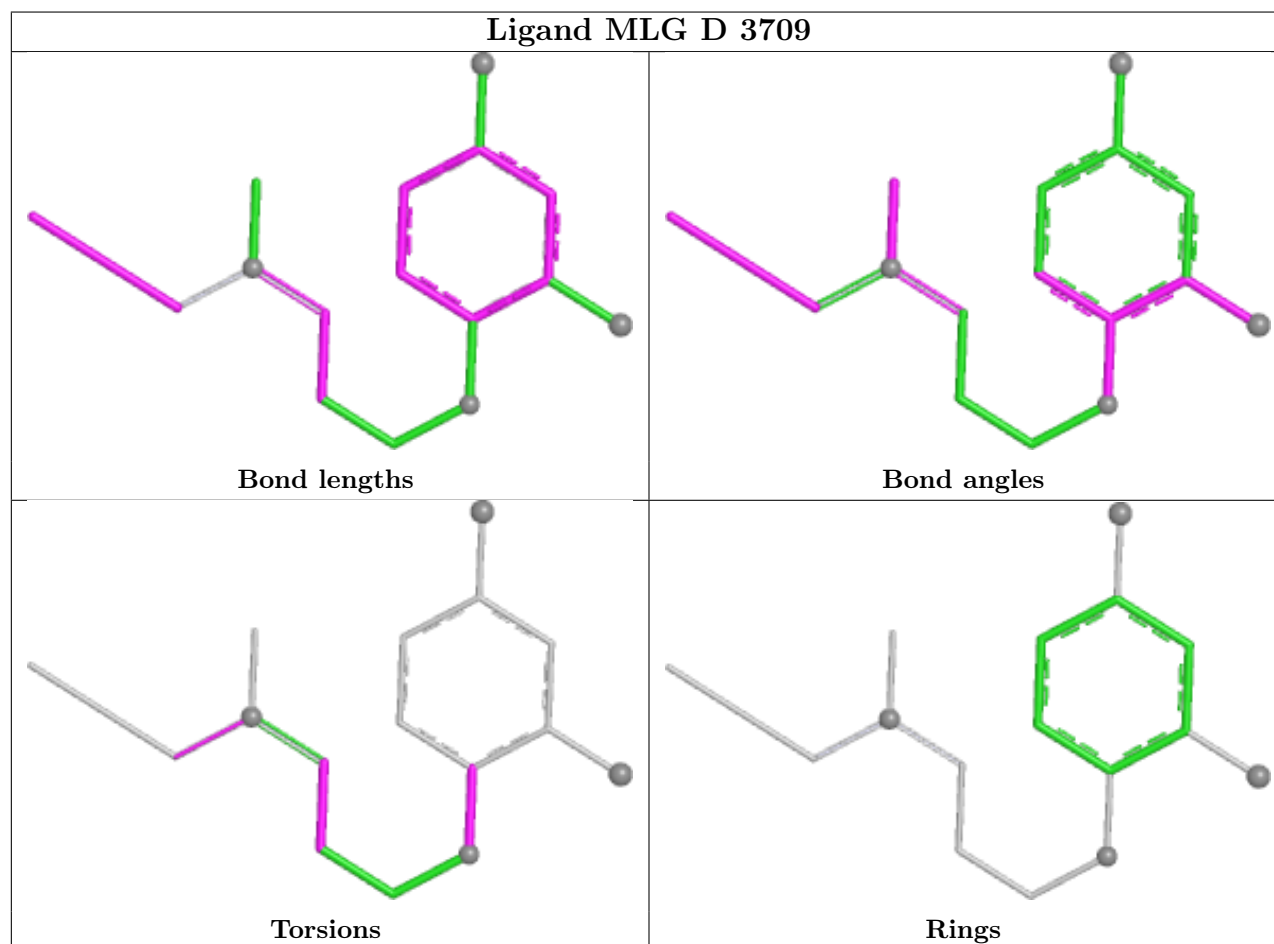
Mol	Chain	Res	Type	Atoms
3	A	709	MLG	C02-C01-O09-C10
3	B	1709	MLG	C02-C01-O09-C10
3	C	2709	MLG	C02-C01-O09-C10
3	D	3709	MLG	C02-C01-O09-C10
3	A	709	MLG	C10-C11-C12-N13

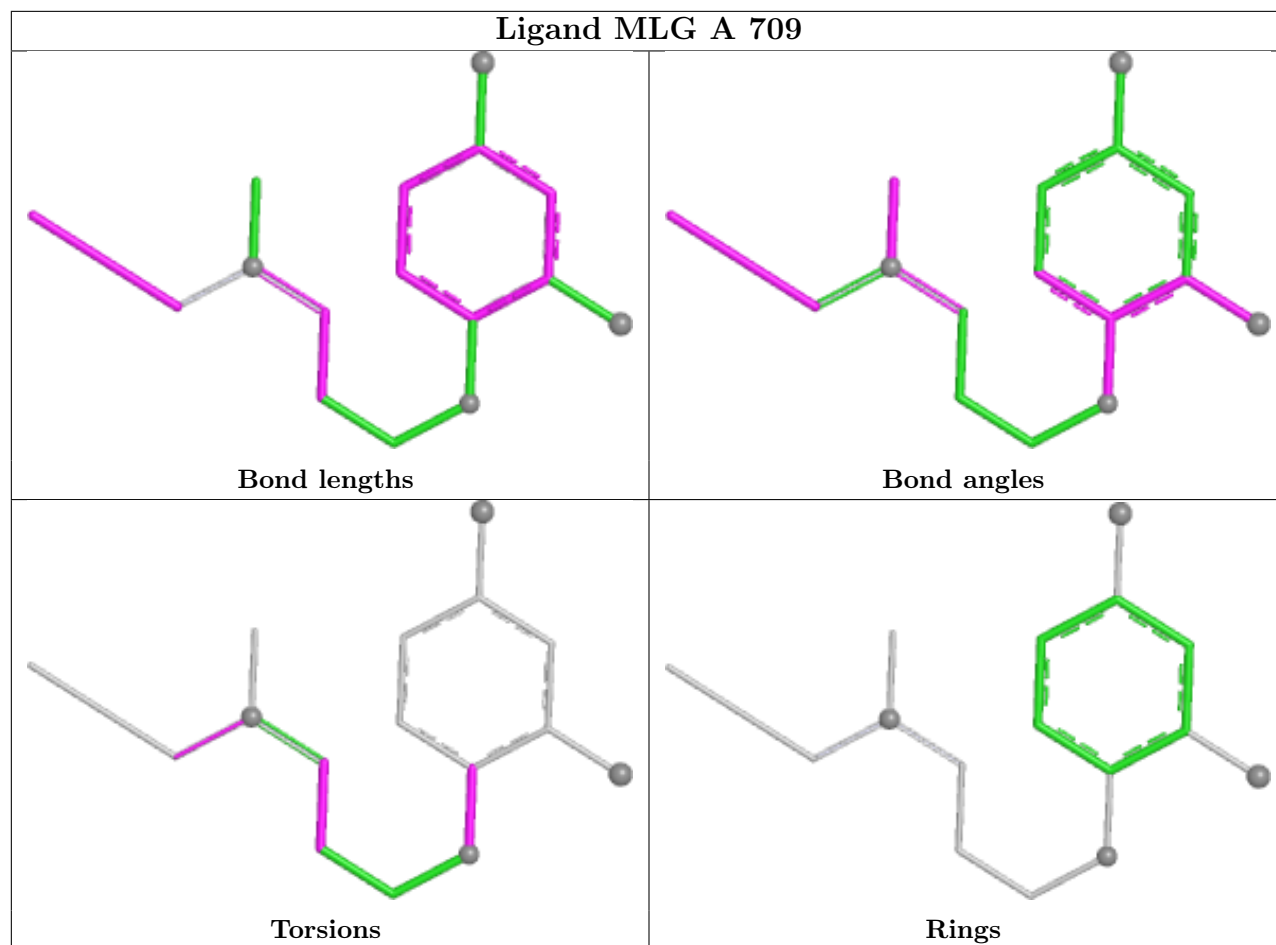
There are no ring outliers.

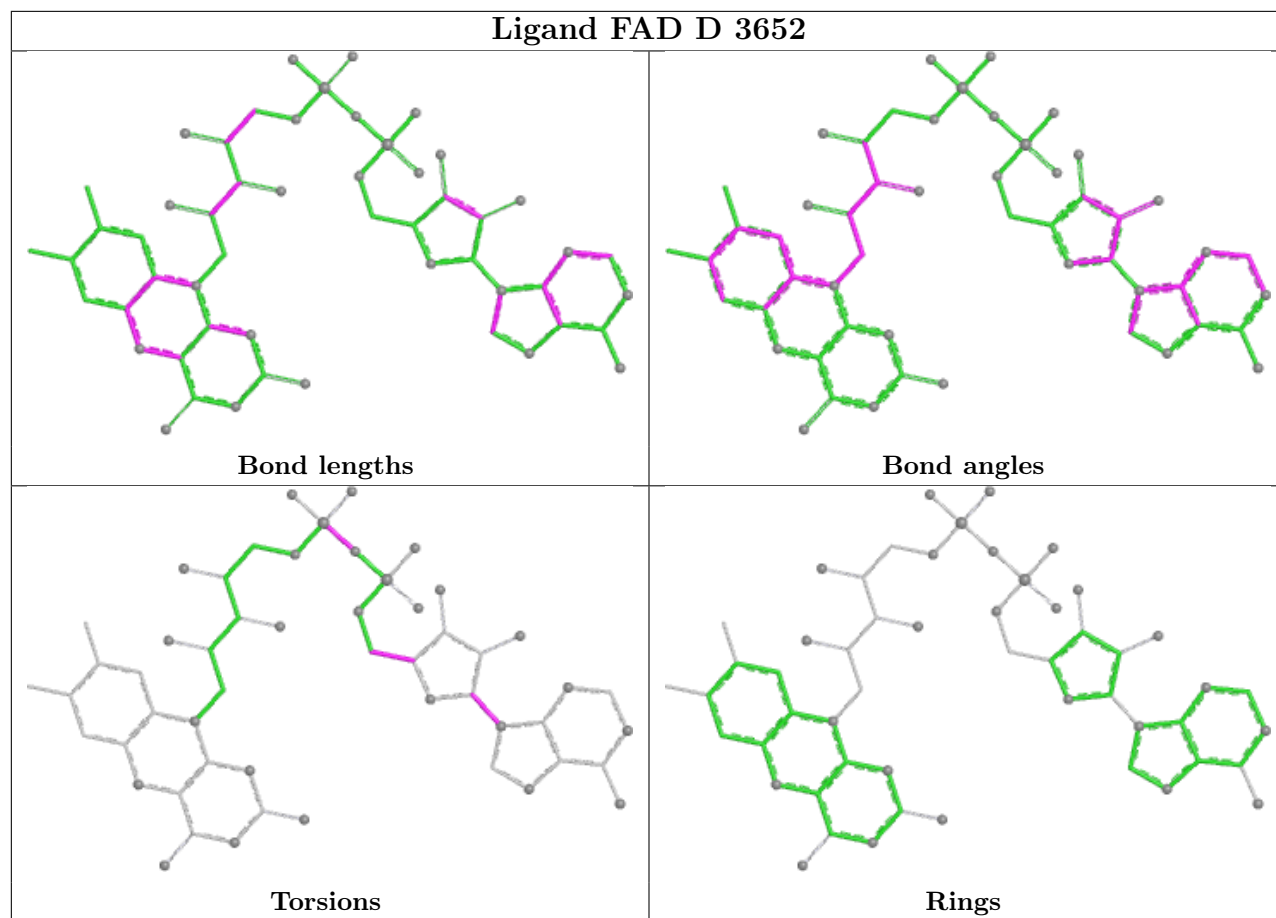
4 monomers are involved in 11 short contacts:

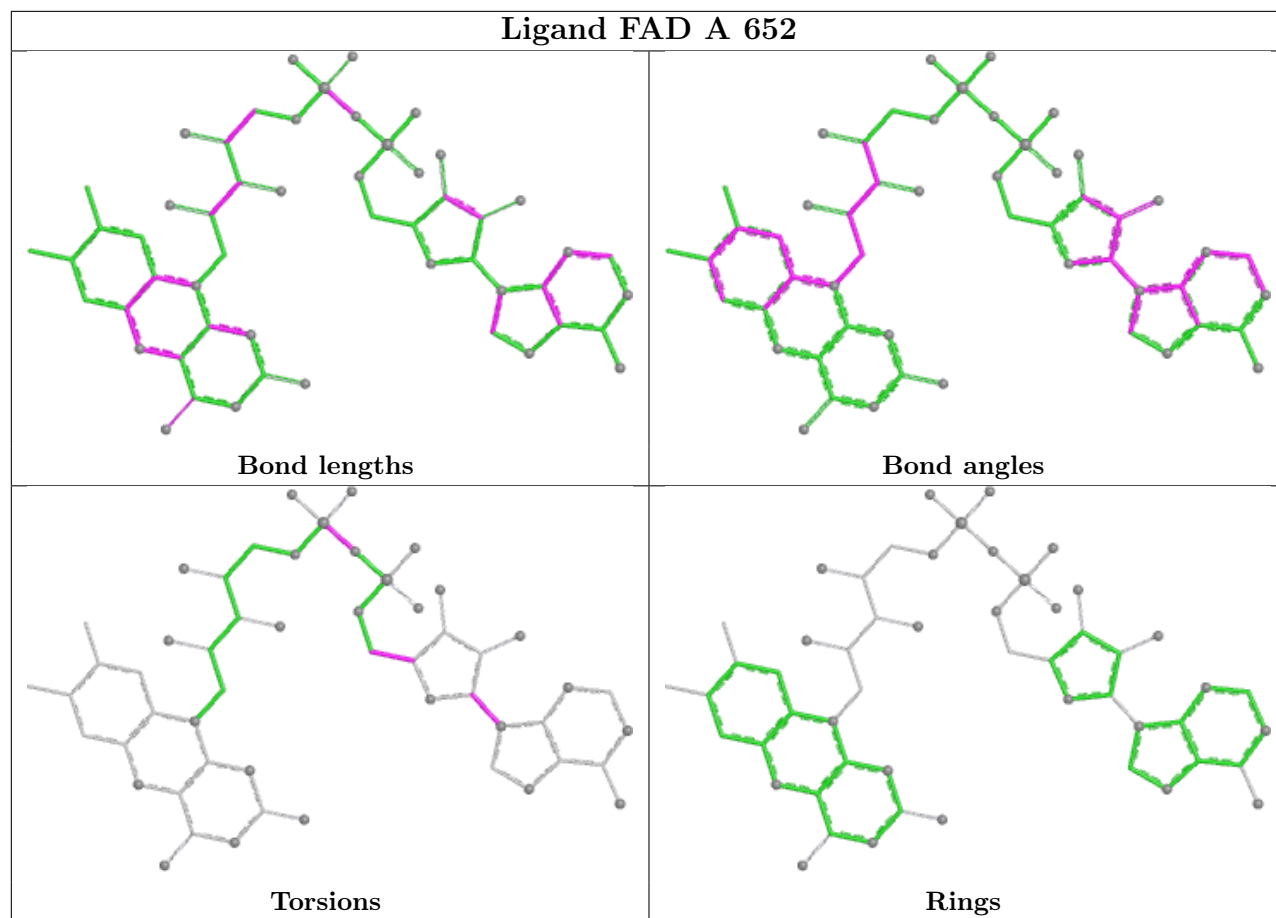
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	3709	MLG	2	0
3	A	709	MLG	4	0
3	C	2709	MLG	2	0
3	B	1709	MLG	3	0

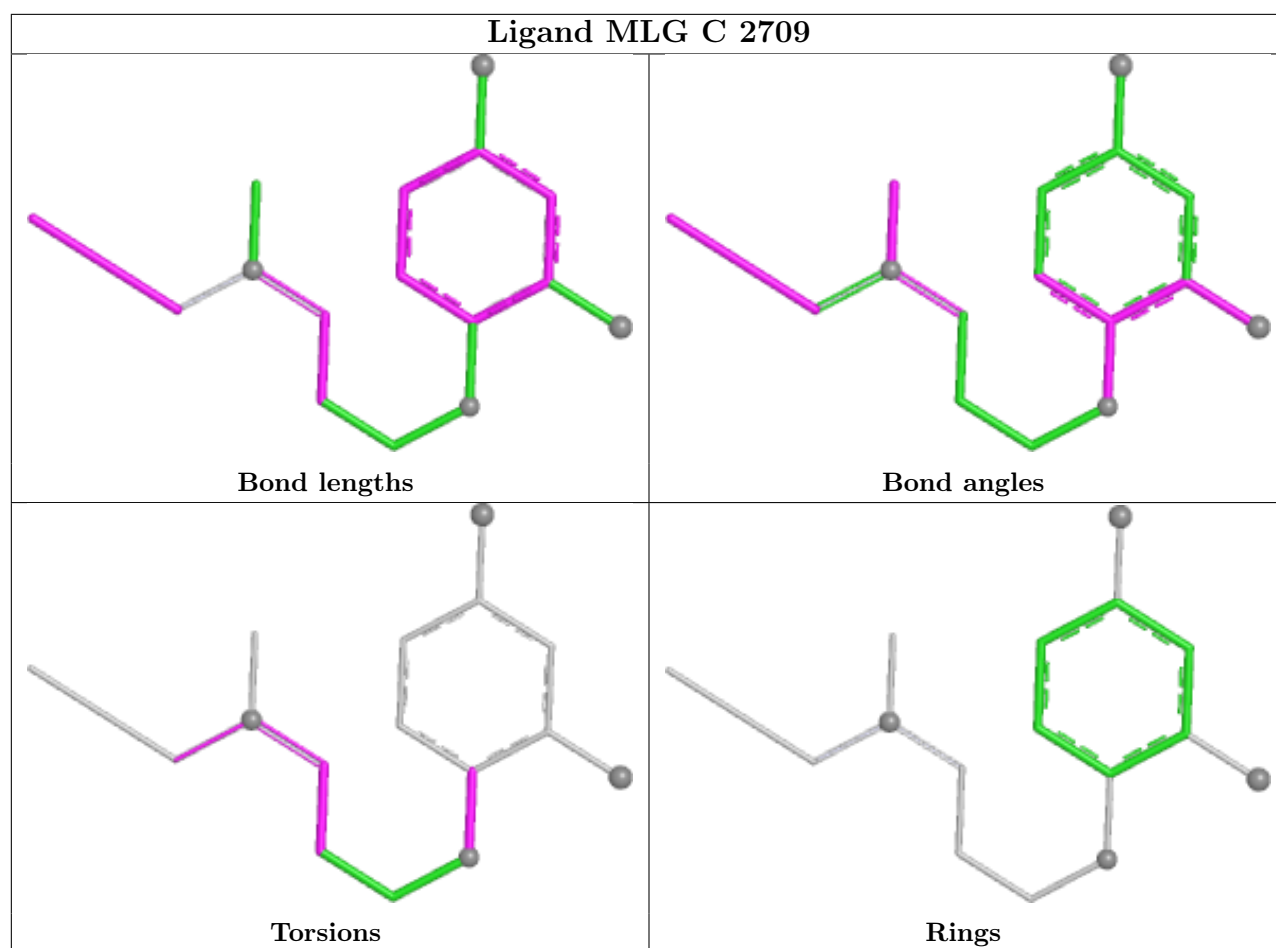
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

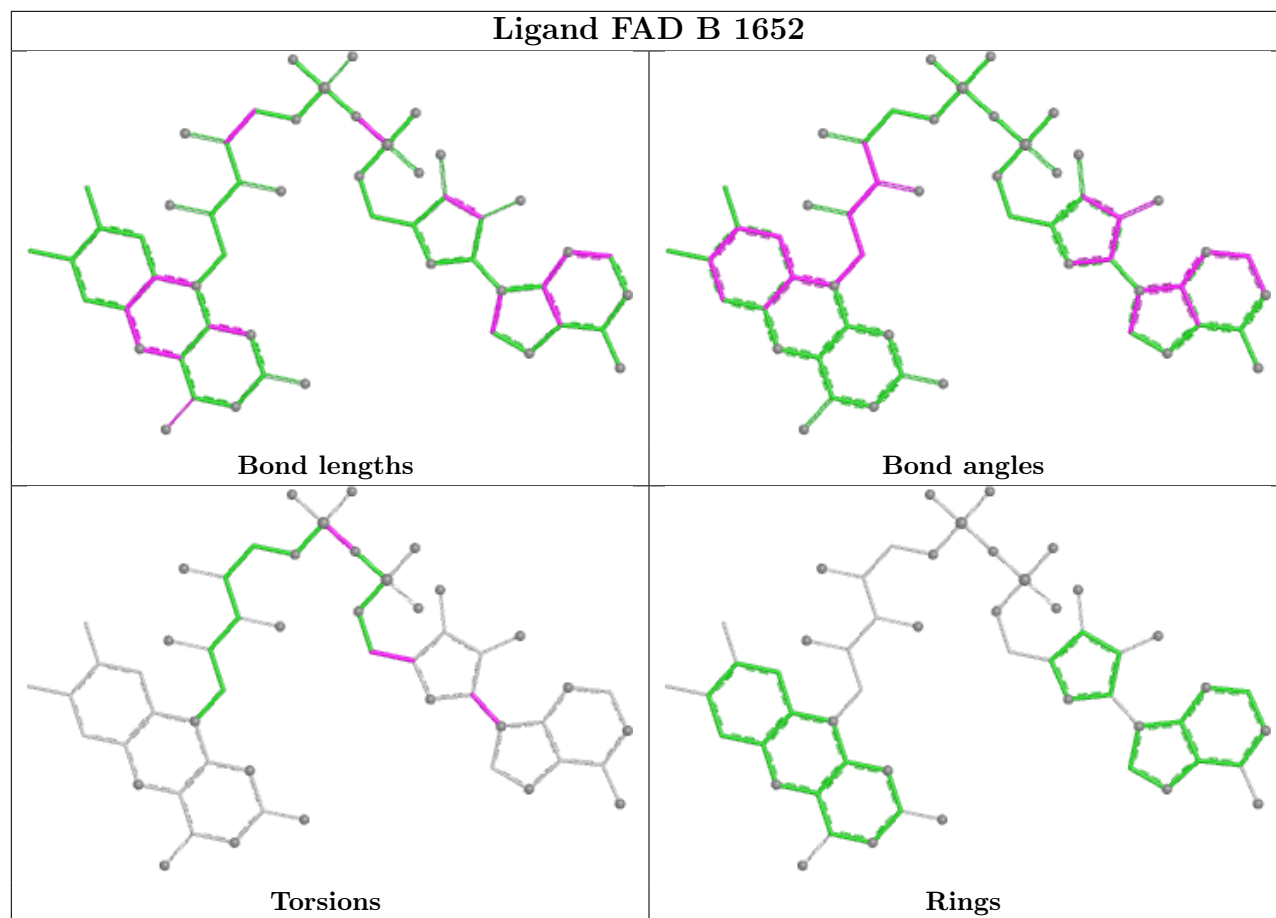


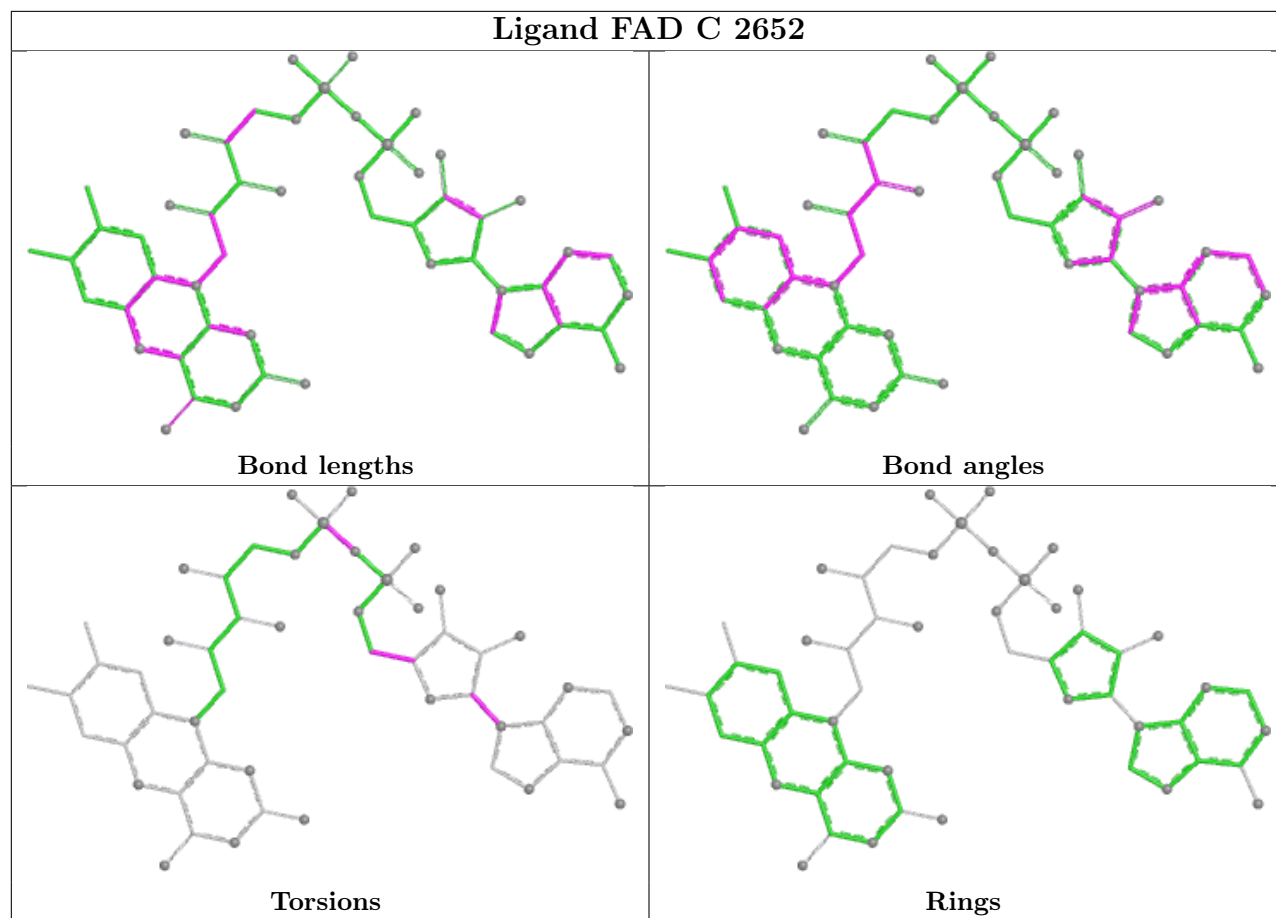


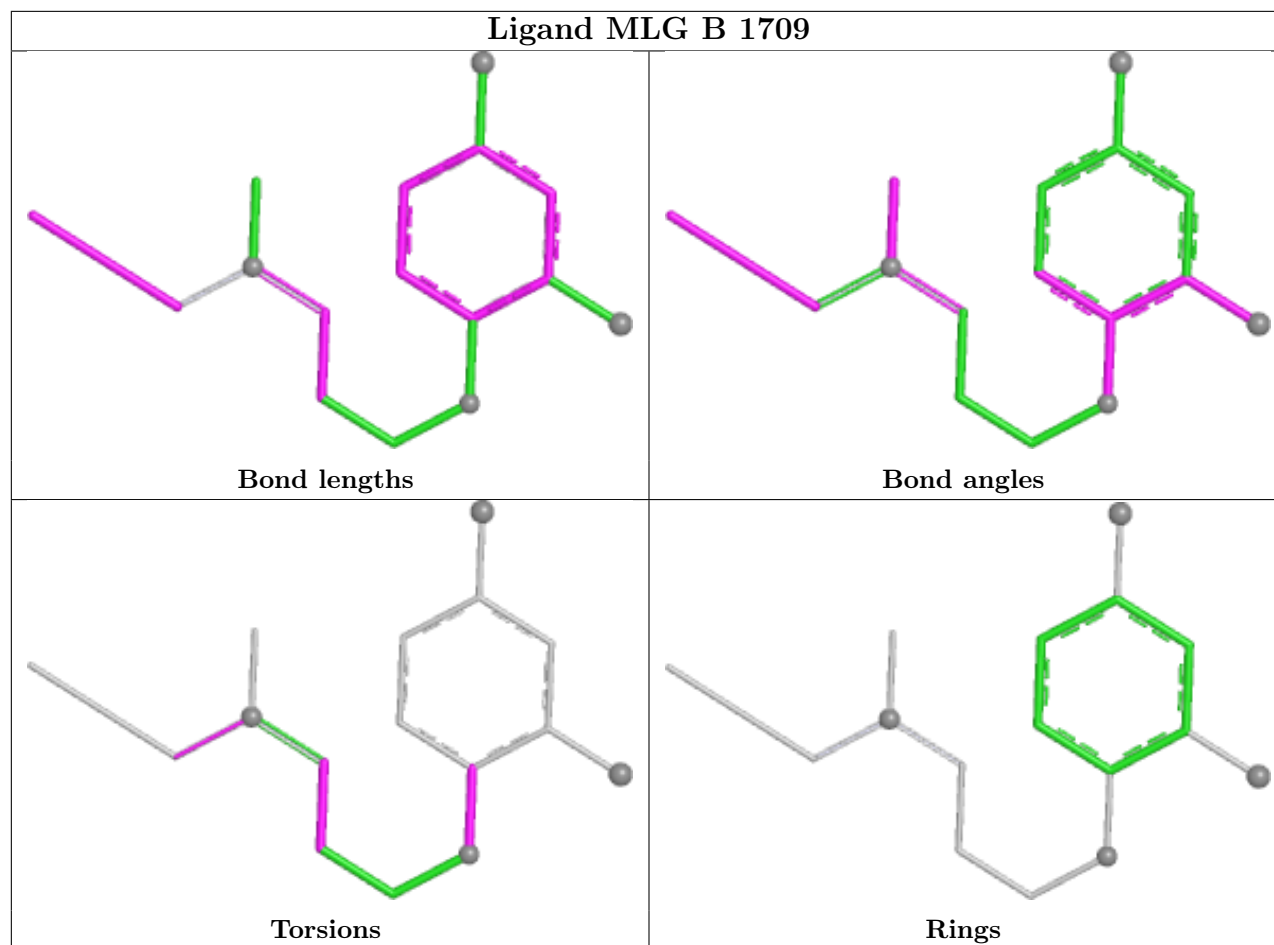












5.7 Other polymers [i](#)

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	511/534 (95%)	-0.44	0	100 100	41, 78, 146, 201	0
1	B	503/534 (94%)	-0.30	1 (0%)	91 85	43, 93, 152, 188	0
1	C	512/534 (95%)	-0.40	1 (0%)	91 85	41, 87, 151, 201	0
1	D	506/534 (94%)	-0.29	3 (0%)	85 73	48, 89, 150, 201	0
All	All	2032/2136 (95%)	-0.36	5 (0%)	91 85	41, 86, 150, 201	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	3403	SER	2.1
1	D	3510	SER	2.1
1	C	2518	LEU	2.1
1	D	3170	ALA	2.0
1	B	1120	ALA	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 oligosaccharides in this entry.

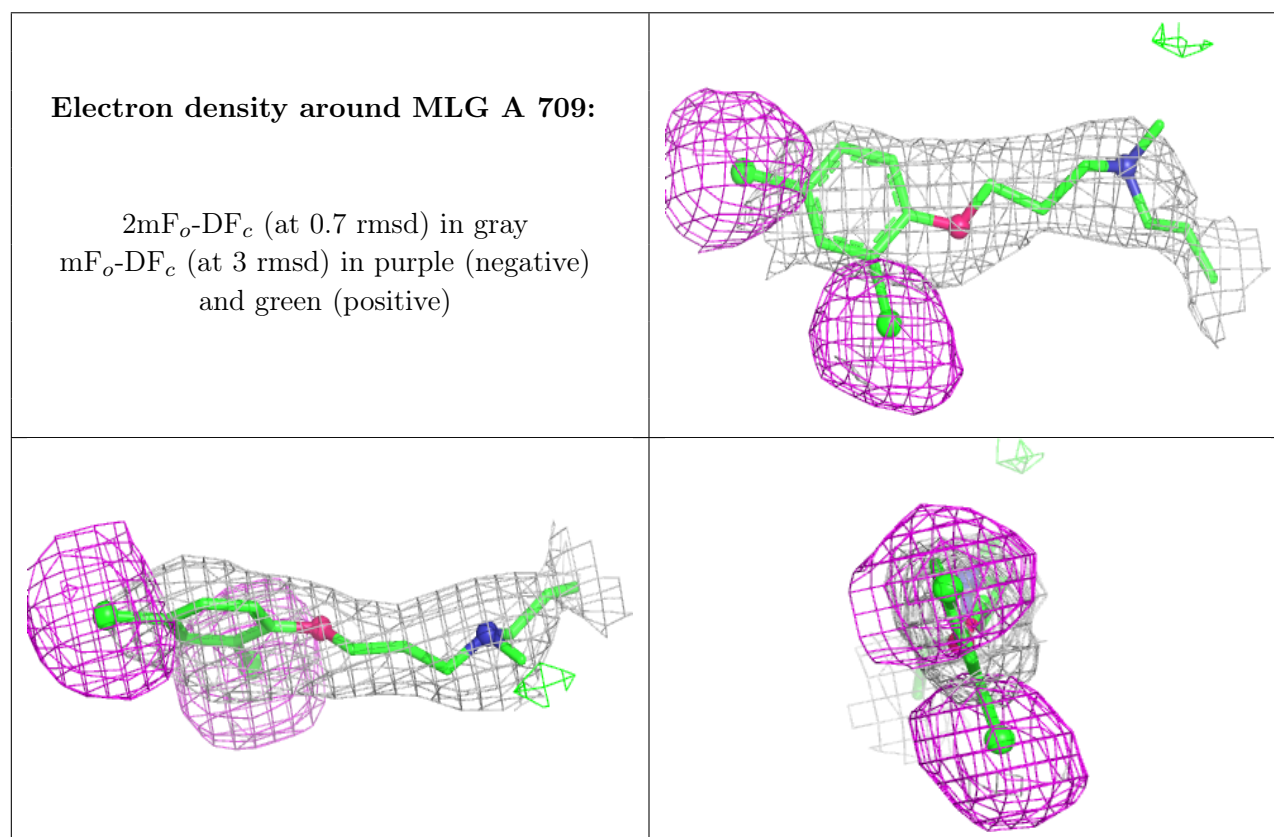
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

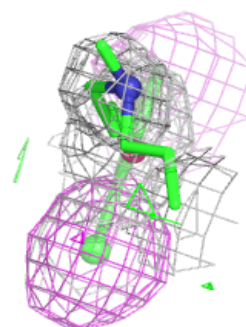
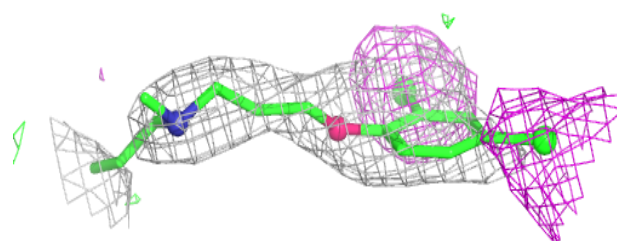
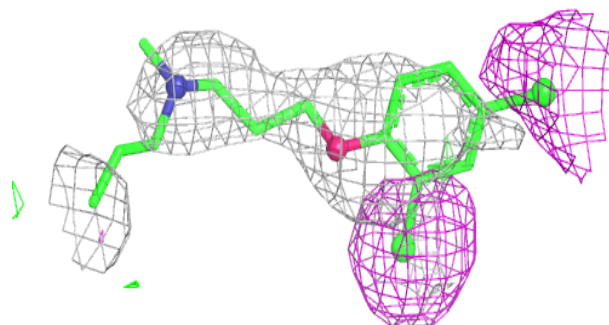
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MLG	A	709	17/17	0.66	0.18	48,67,114,126	0
3	MLG	C	2709	17/17	0.67	0.21	62,91,140,149	0
3	MLG	B	1709	17/17	0.71	0.18	46,121,168,184	0
3	MLG	D	3709	17/17	0.73	0.16	61,111,159,175	0
2	FAD	B	1652	53/53	0.93	0.09	34,72,138,153	0
2	FAD	C	2652	53/53	0.95	0.08	33,67,98,126	0
2	FAD	D	3652	53/53	0.95	0.09	35,75,119,148	0
2	FAD	A	652	53/53	0.96	0.07	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.

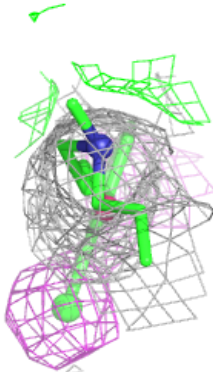
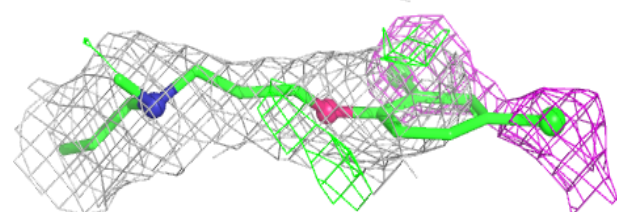
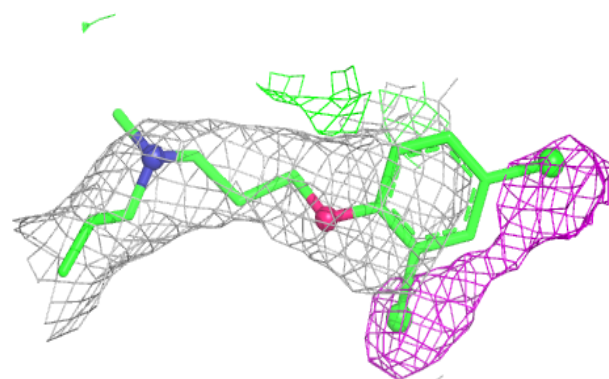


Electron density around MLG C 2709:

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

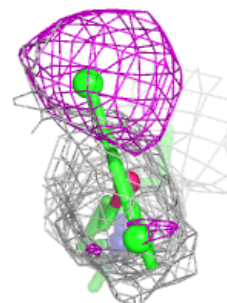
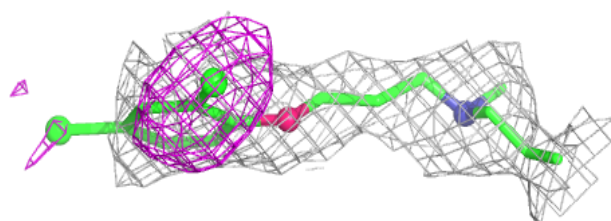
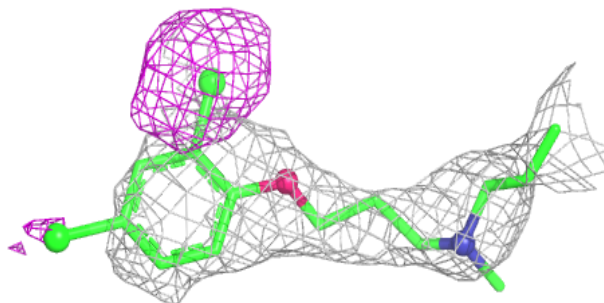
**Electron density around MLG B 1709:**

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

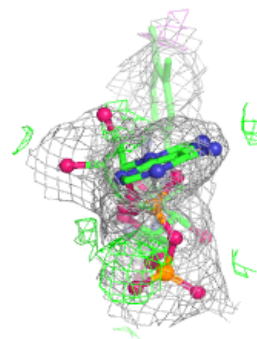
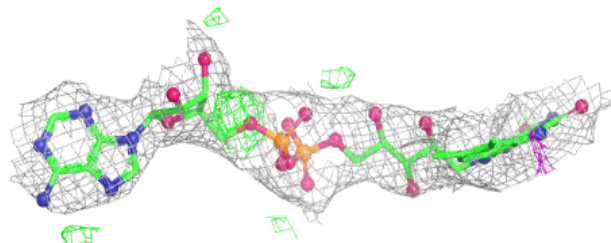
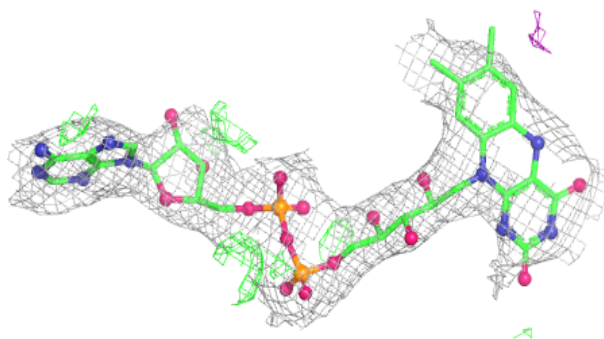


Electron density around MLG D 3709:

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

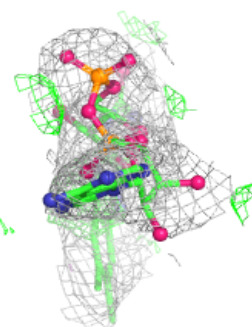
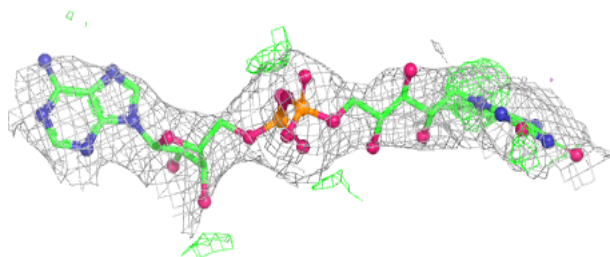
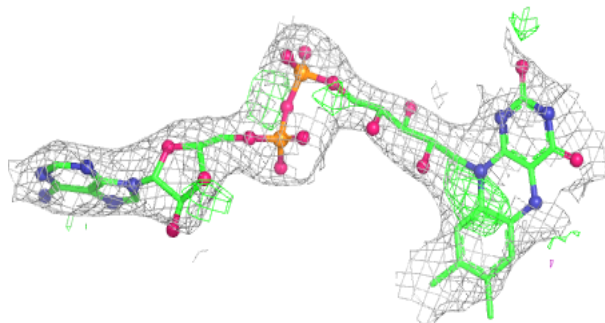
**Electron density around FAD B 1652:**

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

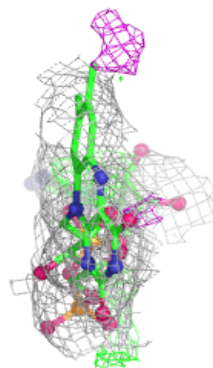
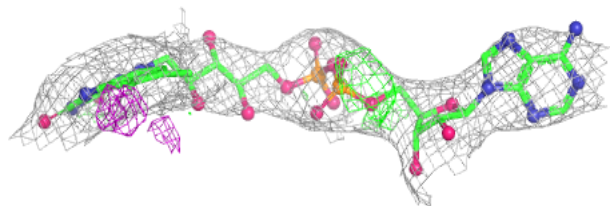
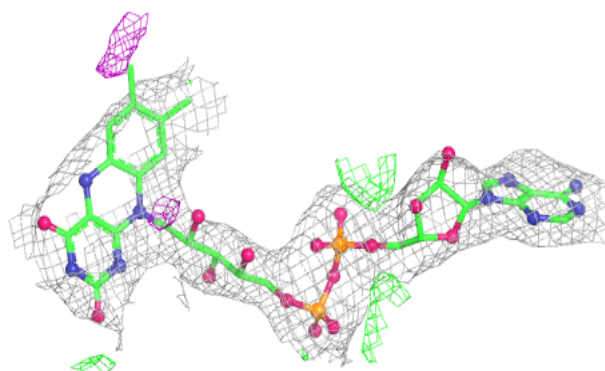


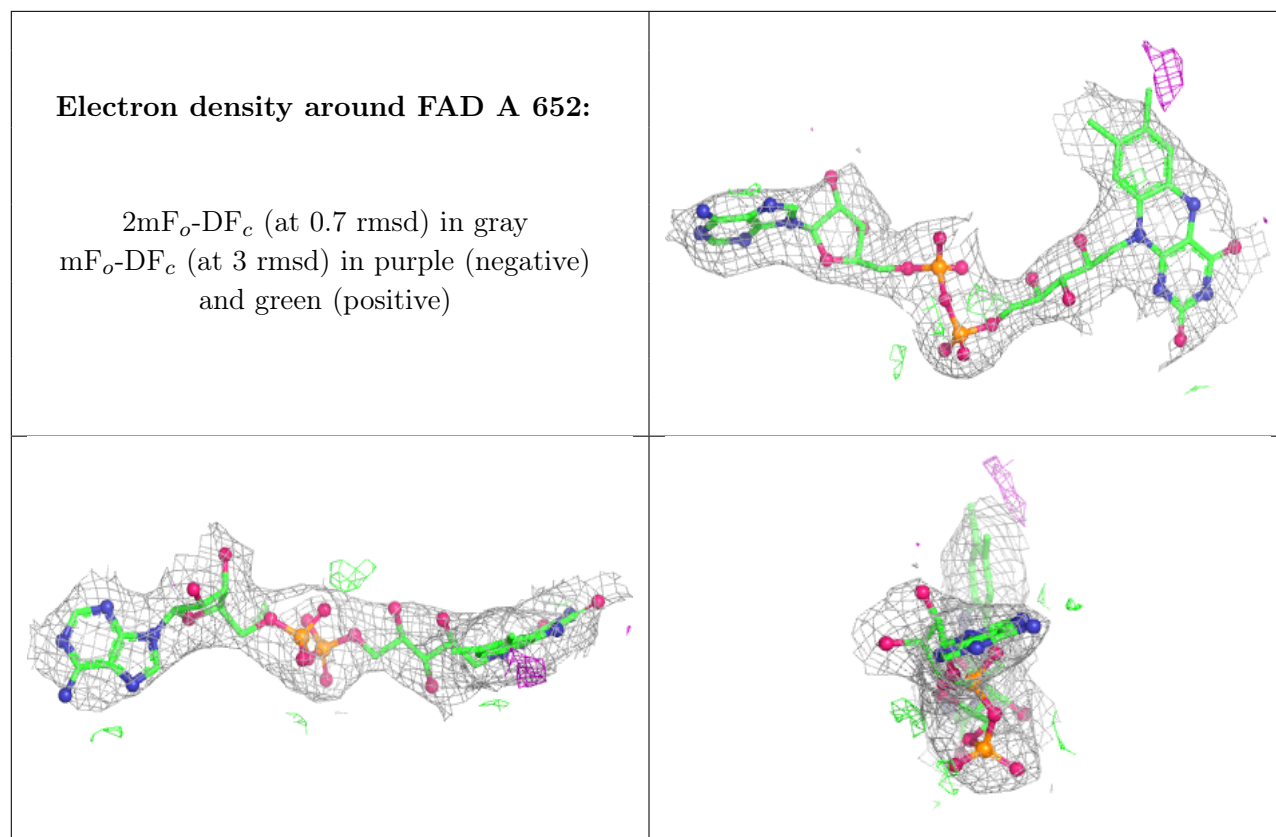
Electron density around FAD C 2652:

$2mF_o - DF_c$ (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)





6.5 Other polymers [i](#)

There are no such residues in this entry.