



wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 09:17 pm BST

PDB ID : 1TLL
Title : CRYSTAL STRUCTURE OF RAT NEURONAL NITRIC-OXIDE SYNTHASE REDUCTASE MODULE AT 2.3 Å RESOLUTION.
Authors : Garcin, E.D.; Bruns, C.M.; Lloyd, S.J.; Hosfield, D.J.; Tiso, M.; Gachhui, R.; Stuehr, D.J.; Tainer, J.A.; Getzoff, E.D.
Deposited on : 2004-06-09
Resolution : 2.30 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

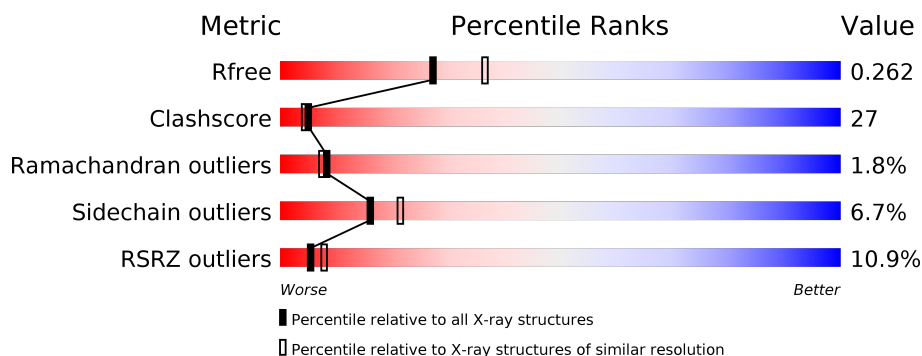
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 on 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	688	
1	B	688	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 10408 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.

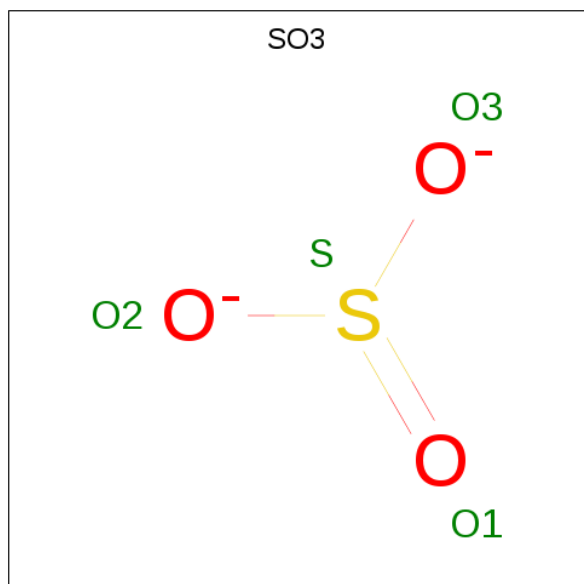
- Molecule 1 is a protein called Nitric-oxide synthase, brain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	630	Total	C	N	O	S	0	0	0
			5010	3170	882	932	26			
1	B	616	Total	C	N	O	S	0	0	0
			4903	3106	862	909	26			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1008	SER	PHE	SEE REMARK 999	UNP P29476
B	3008	SER	PHE	SEE REMARK 999	UNP P29476

- Molecule 2 is SULFITE ION (three-letter code: SO3) (formula: O₃S).



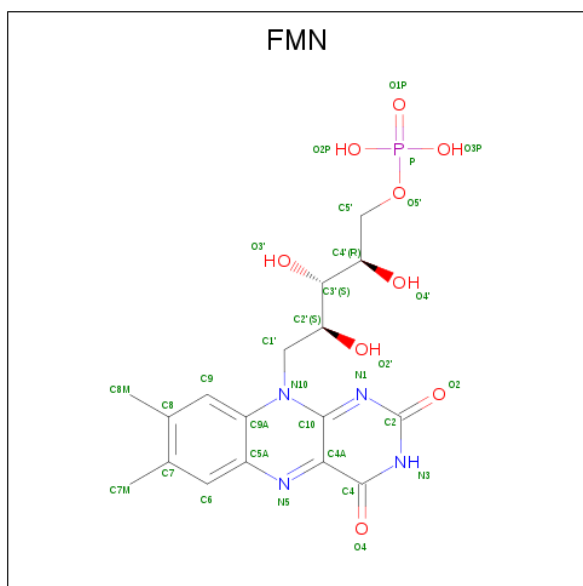
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			4	3	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			4	3	1		

- Molecule 3 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



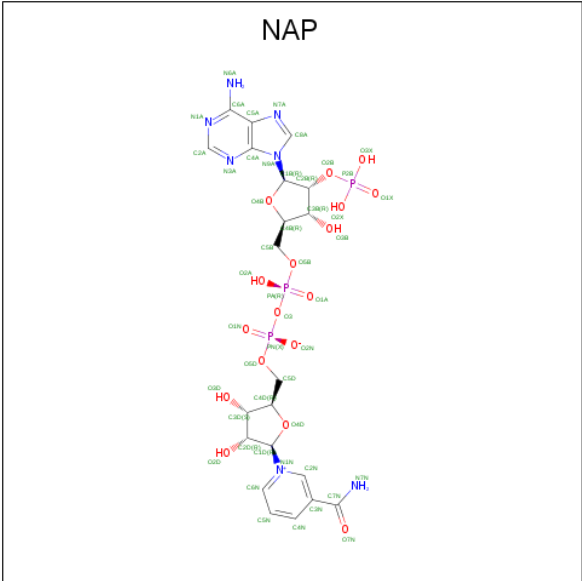
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 5 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	127	Total	O	0	0
			127	127		
6	B	96	Total	O	0	0
			96	96		

These plots are drawn for all protein, RNA and DNA 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.

- [illegible]

- Chain B: 

R3385	D3386	R3389	R3390	R3391	G3396	T3397	R3398	L3399	R3400	T3401	R3402	R3403	R3404	R3405	R3406	R3407	L3408	R3409	R3410	S3411	S3412	R3413	ALA	PHE	ILE	GLU	SER	LYS	LYS	ASP	ALA	ASP	GLU	VAL	PHE	SER	SER																												
P3319	R3320	R3321	R3322	R3323	Q3324	D3325	R3326	R3327	R3328	N3329	P3330	Q3331	R3332	R3333	R3334	R3335	R3336	R3337	R3338	R3339	R3340	R3341	R3342	R3343	R3344	R3345	R3346	R3347	R3348	R3349	R3350	R3351	R3352	R3353	R3354	R3355	R3356	R3357	R3358	R3359	R3360	R3361	R3362	R3363	R3364	R3365	R3366	R3367	R3368	R3369	R3370	R3371	R3372	S3373	E3374	R3375	D3376	A3377	G3378	R3379	R3380	L3381	S3382	R3383	R3384
T3218	Q3219	A3220	D3221	G3226	R3238	N3239	P3240	Q3241	V3242	R3243	C3244	I3245	R3246	V3247	G3250	T3251	G3252	I3253	R3257	W3260	Q3261	Q3262	D3266	W3272	V3280	F3281	G3282	G3283	R3284	Q3285	S3286	K3287	I3288	D3289	A3299	V3304	R3305	R3306	E3307	I3308	Y3309	Y3312	S3313	R3314	E3315	P3316	R3317	R3318																	
E3121	K3122	Q3123	R3124	L3125	L3126	W3127	K3130	Q3131	L3132	Q3133	R3134	Y3135	E3136	E3137	W3140	P3144	T3145	N3146	V3147	E3148	V3149	Q3157	M3158	P3159	A3160	T3161	L3162	T3165	Q3166	L3167	Q3171	Y3174	Y3175	S3176	S3180	V3188	R3189	A3193	T3194	V3195	S3196	Y3197	R3198	D3201	G3202	W3214																			
L3033	G3034	R3040	V3044	E3049	R3050	L3051	I3052	N3053	A3054	P3055	R3056	A3057	R3058	R3059	K3062	V3063	E3064	N3065	L3066	E3067	R3068	R3069	R3070	T3071	A3072	L3073	T3076	S3077	R3078	W3079	K3080	D3081	T3089	I3090	F3091	Q3092	P3103	P3104	L3107	Q3108	L3109	Q3110	F3112	A3113	S3114	L3115	A3116	E3119	R3120																
N2949	I2950	K2951	K2952	PRO	ASN	ASN	SER	LEU	ILE	S2959	N2960	D2961	R2962	S2963	W2964	K2965	R2966	N2967	K2968	F2969	R2970	L2971	T2972	Y2973	Y2974	A2975	E2976	D2979	L2980	T2981	A2984	A2985	R2986	L2987	S2988	Q3000	Q3001	N3002	L3003	Q3004	S3008	R3010	F3014	V3015	T3019	N3020	G3021	N3022	L3025	Q3026															
L2815	E2816	N2817	G2818	E2819	K2820	F2821	G2822	C2823	A2824	L2825	K2826	E2827	R2828	HIS	PRO	ASN	SER	VAL	GLN	GLU	ARG	LYS	S2840	Y2841	K2842	V2843	R2844	F2845	N2846	SER	VAL	SER	SER	TYR	SER	ASP	SER	ARG	LYS	SER	GLY	ASP	GLY	PRO	ASP	LEU	ARG	ASN	A2800	L2801	PHE	GLU	SER	THR	GLY	PRO									
ALA	LYS	LEU	MET	GLY	GLN	ALA	MET	ALA	LYS	R2752	V2753	K2754	A2755	T2756	I2757	L2758	Y2759	A2760	T2761	E2762	K2765	S2766	Y2769	L2773	E2774	E2775	L2776	F2777	K2778	H2779	A2780	F2781	D2782	A2783	K2784	M2786	S2787	M2788	E2789	E2790	Y2791	D2792	L2793	V2794	H2795	L2796	E2799	A2800	L2801	L2802	L2803	V2804	V2805	T2806											

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	65.76Å 69.17Å 82.63Å 76.80° 72.07° 67.14°	Depositor
Resolution (Å)	35.21 – 2.30 35.21 – 2.17	Depositor EDS
% Data completeness (in resolution range)	97.8 (35.21-2.30) 95.5 (35.21-2.17)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 2.18Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.244 , 0.272 0.237 , 0.262	Depositor DCC
R_{free} test set	1909 reflections (2.98%)	wwPDB-VP
Wilson B-factor (Å ²)	37.4	Xtriage
Anisotropy	0.505	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 55.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10408	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, NAP, SO3, 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	0.43	2/5122 (0.0%)	0.71	2/6932 (0.0%)
1	B	0.40	0/5014	0.76	6/6788 (0.1%)
All	All	0.41	2/10136 (0.0%)	0.73	8/13720 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1133	GLN	CA-CB	-5.70	1.41	1.53
1	A	1133	GLN	CG-CD	-5.18	1.39	1.51

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	3364	ARG	NE-CZ-NH1	19.58	130.09	120.30
1	B	3364	ARG	NE-CZ-NH2	-16.65	111.97	120.30
1	B	2944	VAL	N-CA-C	-6.22	94.21	111.00
1	B	2966	ARG	N-CA-C	5.69	126.37	111.00
1	B	3364	ARG	CD-NE-CZ	5.38	131.14	123.60

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	5010	0	4925	260	1
1	B	4903	0	4814	287	1
2	A	4	0	0	0	0
2	B	4	0	0	0	0
3	A	31	0	18	0	0
3	B	31	0	18	0	0
4	A	53	0	28	0	0
4	B	53	0	28	0	0
5	A	48	0	24	9	0
5	B	48	0	24	13	0
6	A	127	0	0	2	0
6	B	96	0	0	6	0
All	All	10408	0	9879	545	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 27.

The worst 5 of 545 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)
5:A:1453:NAP:O3D	5:A:1453:NAP:O2A	1.55	1.21
1:B:3360:LYS:O	1:B:3364:ARG:CD	1.98	1.11
1:B:3196:SER:N	6:B:6093:HOH:O	1.59	1.10
1:A:991:ARG:HH11	1:A:991:ARG:HG3	1.12	1.08
1:B:3053:ASP:HB2	1:B:3160:ALA:H	1.11	1.06

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)
1:A:1133:GLN:OE1	1:B:3364:ARG:NE[1_654]	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	622/688 (90%)	569 (92%)	40 (6%)	13 (2%)	7	5
1	B	608/688 (88%)	548 (90%)	51 (8%)	9 (2%)	10	10
All	All	1230/1376 (89%)	1117 (91%)	91 (7%)	22 (2%)	8	7

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	839	LYS
1	A	848	VAL
1	A	960	ASN
1	A	963	SER
1	A	1411	GLU

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	543/601 (90%)	506 (93%)	37 (7%)	16	21
1	B	531/601 (88%)	496 (93%)	35 (7%)	16	22
All	All	1074/1202 (89%)	1002 (93%)	72 (7%)	16	21

5 of 72 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1324	GLN
1	B	2840	SER
1	B	3324	GLN
1	A	1333	GLU
1	A	1405	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1262	GLN
1	A	1324	GLN
1	B	3262	GLN
1	A	1264	GLN
1	A	1268	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 carbohydrates 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	$\# Z > 2$
2	SO3	A	1500	-	1,3,3	2.51	1 (100%)	0,3,3	0.00	-
3	FMN	B	2451	-	31,33,33	5.97	19 (61%)	40,50,50	3.27	12 (30%)
4	FAD	B	2452	-	51,58,58	5.56	35 (68%)	60,89,89	3.01	27 (45%)
5	NAP	B	2453	-	45,52,52	2.90	10 (22%)	56,80,80	1.77	15 (26%)
5	NAP	A	1453	-	45,52,52	2.01	9 (20%)	56,80,80	1.55	12 (21%)
3	FMN	A	1451	-	31,33,33	5.57	21 (67%)	40,50,50	3.35	15 (37%)
4	FAD	A	1452	-	51,58,58	5.64	36 (70%)	60,89,89	2.97	29 (48%)
2	SO3	B	2500	-	1,3,3	2.48	1 (100%)	0,3,3	0.00	-

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	FMN	B	2451	-	-	0/18/18/18	0/3/3/3
4	FAD	B	2452	-	-	4/30/50/50	0/6/6/6
5	NAP	B	2453	-	-	12/31/67/67	0/5/5/5
5	NAP	A	1453	-	-	14/31/67/67	0/5/5/5
3	FMN	A	1451	-	-	0/18/18/18	0/3/3/3
4	FAD	A	1452	-	-	4/30/50/50	0/6/6/6

The worst 5 of 132 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2451	FMN	C4A-C10	23.12	1.61	1.38
3	A	1451	FMN	C4A-C10	20.39	1.59	1.38
4	B	2452	FAD	C4A-N3A	15.31	1.56	1.35
4	B	2452	FAD	C2B-C1B	-14.79	1.31	1.53
4	A	1452	FAD	C2B-C1B	-14.43	1.31	1.53

The worst 5 of 110 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1451	FMN	C4-N3-C2	11.19	124.59	115.14
3	B	2451	FMN	C4-N3-C2	10.42	123.94	115.14
4	A	1452	FAD	C5X-C9A-N10	-8.86	111.29	117.72
4	B	2452	FAD	C5X-C9A-N10	-8.66	111.44	117.72
4	B	2452	FAD	C4-N3-C2	8.28	122.13	115.14

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	2453	NAP	C5B-O5B-PA-O1A
5	B	2453	NAP	C5B-O5B-PA-O2A
5	B	2453	NAP	C5B-O5B-PA-O3
5	B	2453	NAP	C5D-O5D-PN-O3
5	B	2453	NAP	O4D-C4D-C5D-O5D

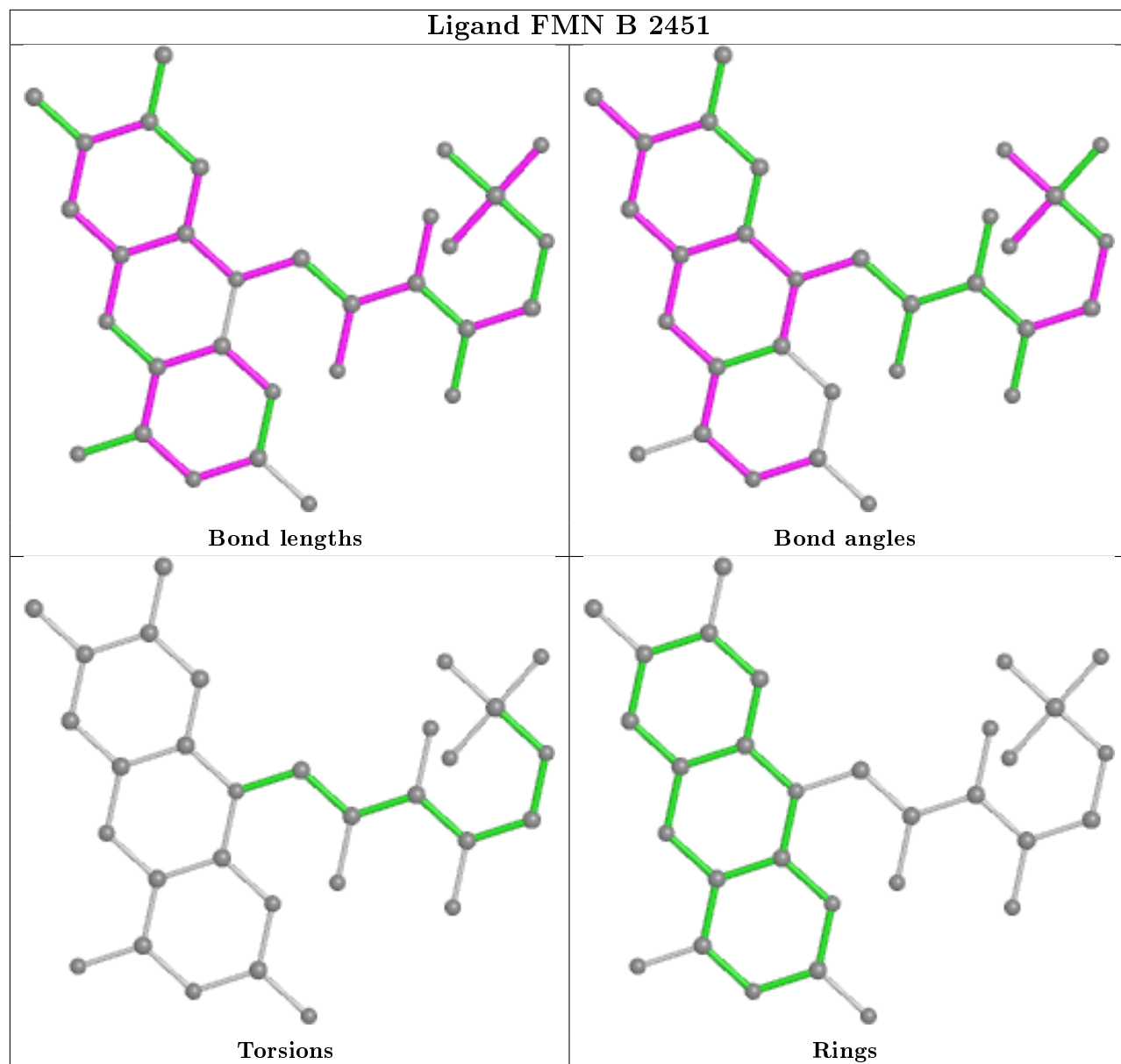
There are no ring outliers.

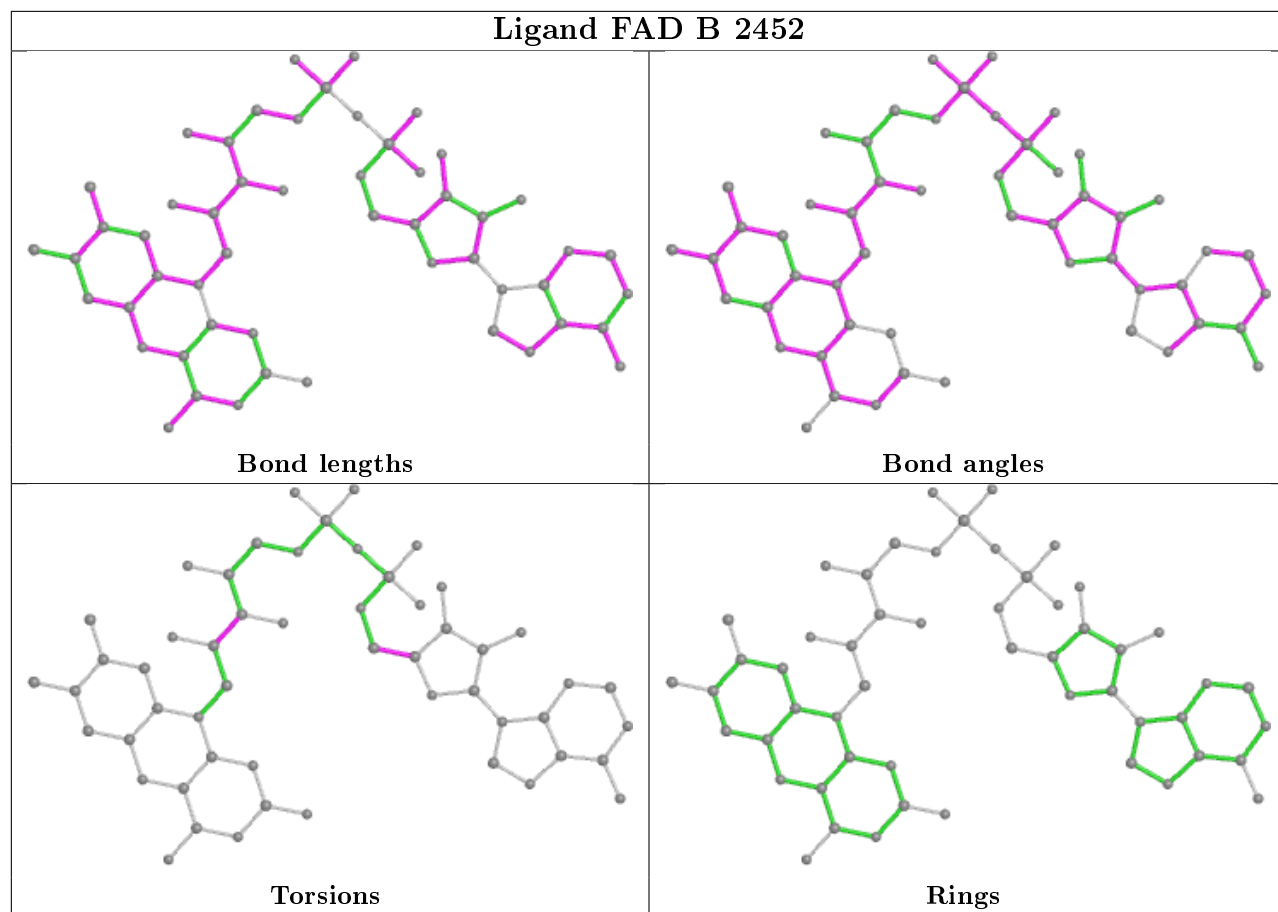
2 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	2453	NAP	13	0
5	A	1453	NAP	9	0

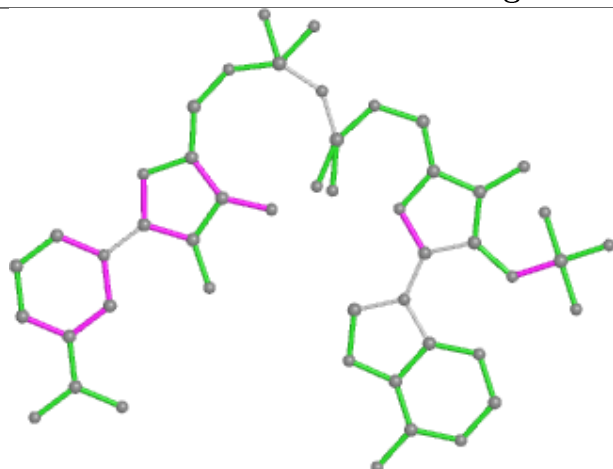
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand FMN B 2451

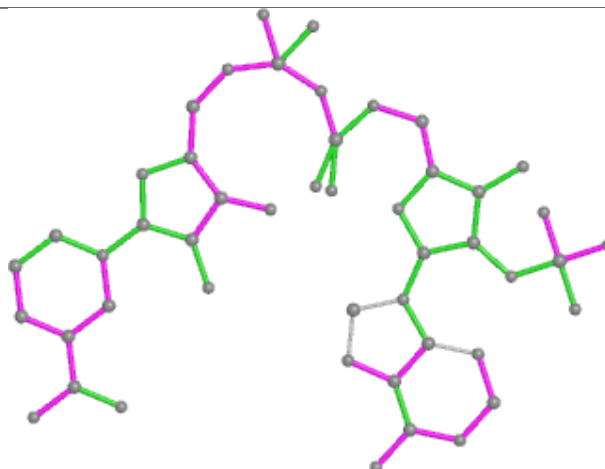




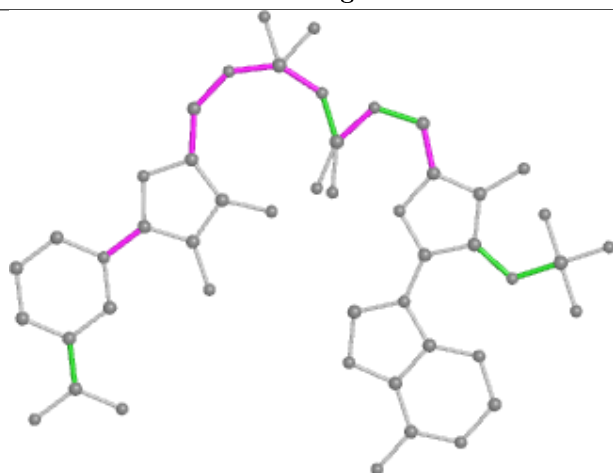
Ligand NAP B 2453



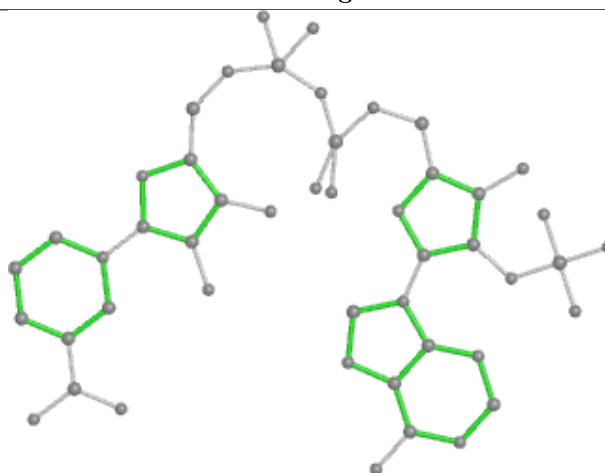
Bond lengths



Bond angles

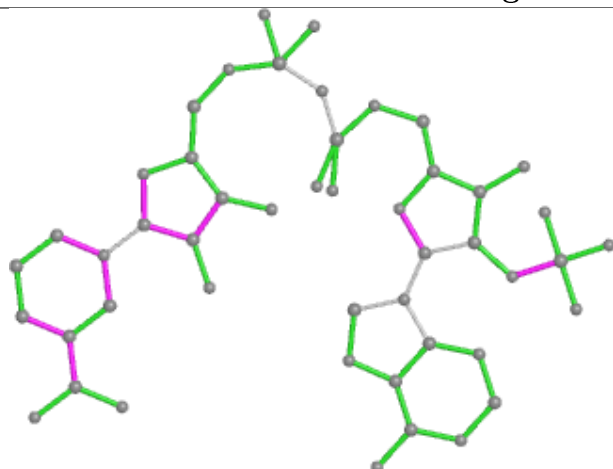


Torsions

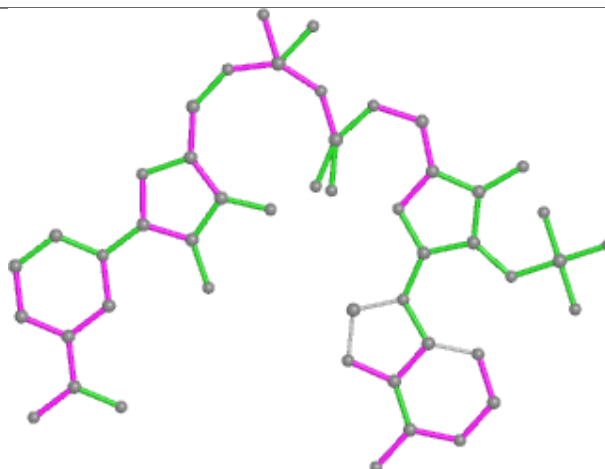


Rings

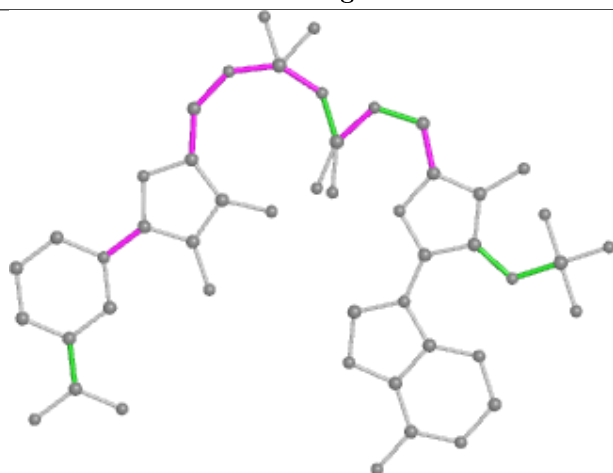
Ligand NAP A 1453



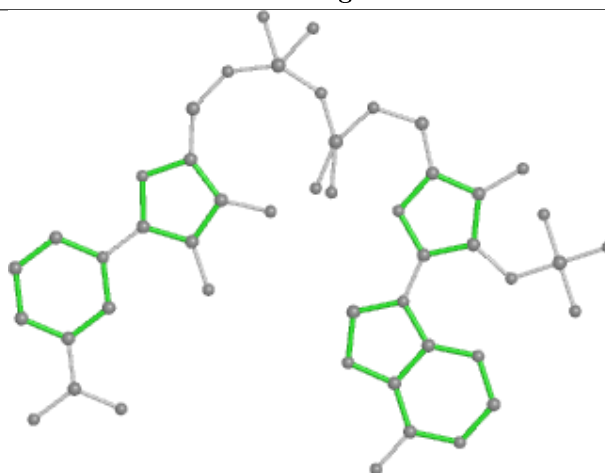
Bond lengths



Bond angles

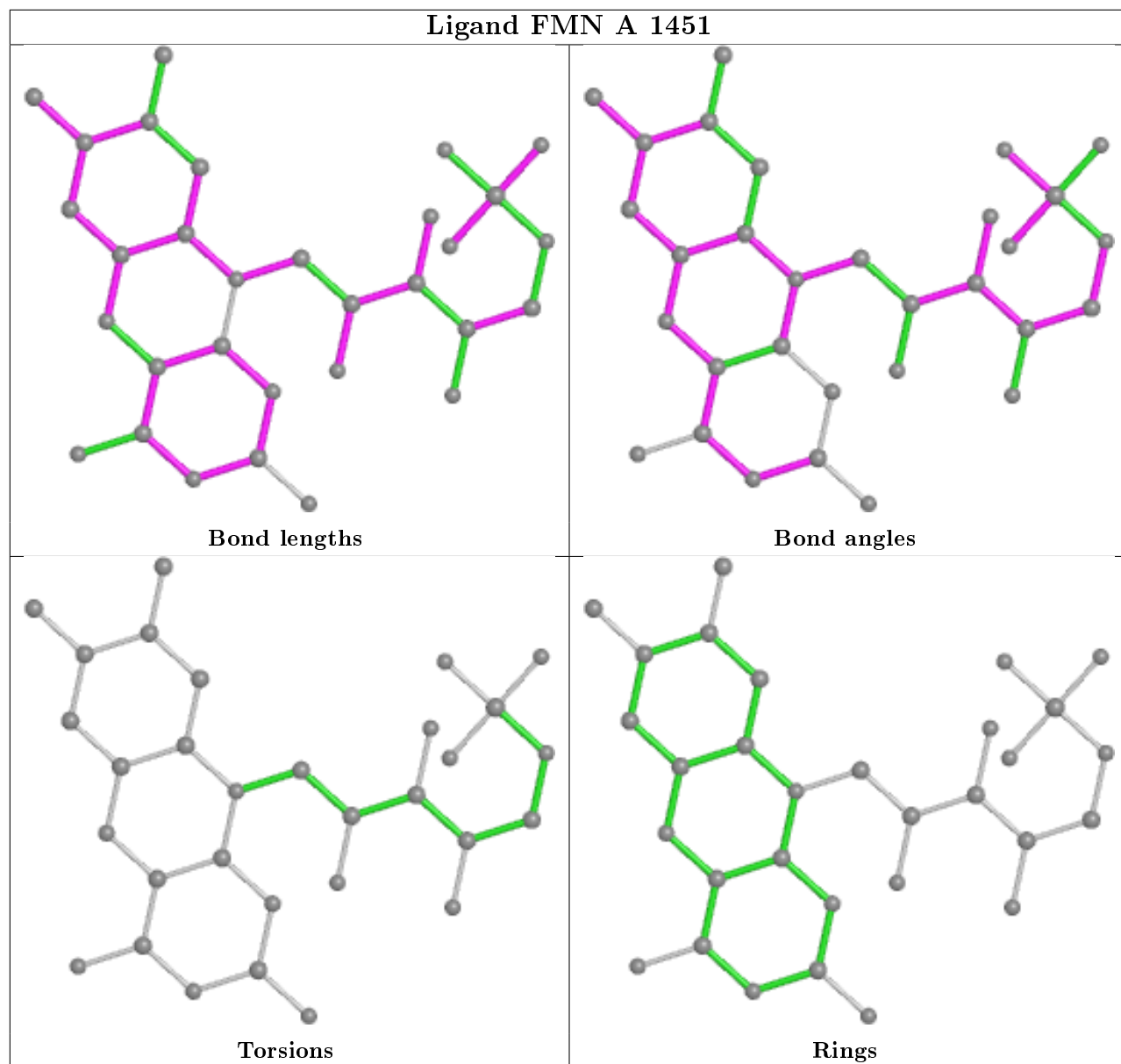


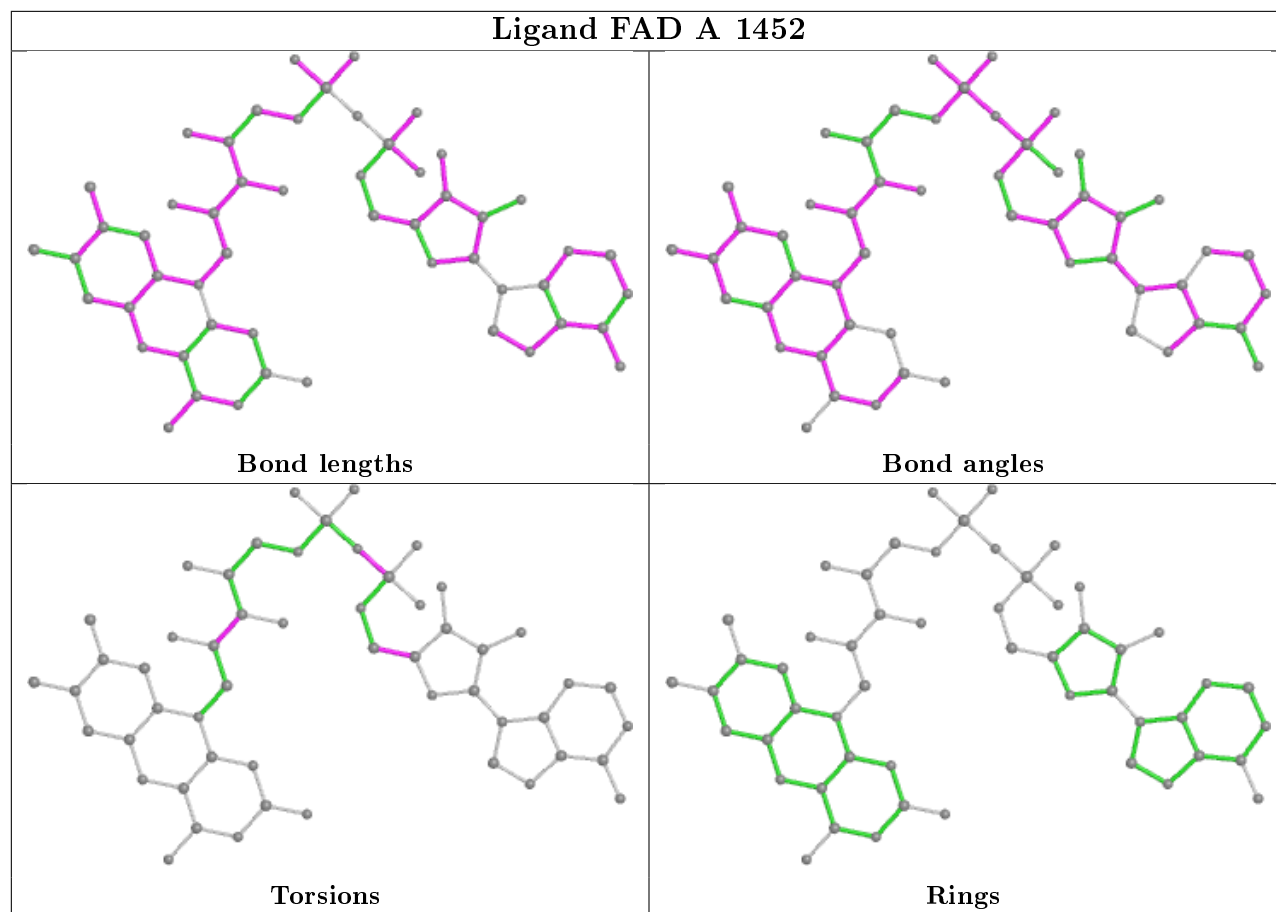
Torsions



Rings

Ligand FMN A 1451





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	630/688 (91%)	0.61	52 (8%) 11 15	28, 52, 88, 99	0
1	B	616/688 (89%)	0.84	84 (13%) 3 4	24, 61, 93, 100	0
All	All	1246/1376 (90%)	0.73	136 (10%) 5 8	24, 56, 92, 100	0

The worst 5 of 136 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	830	HIS	9.8
1	B	2902	LEU	8.7
1	B	3316	PRO	8.0
1	B	2845	PHE	7.5
1	A	950	ILE	7.2

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 carbohydrates in this entry.

6.4 Ligands [i](#)

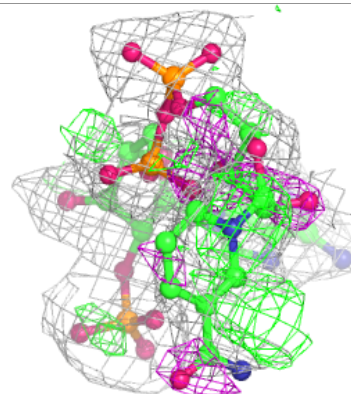
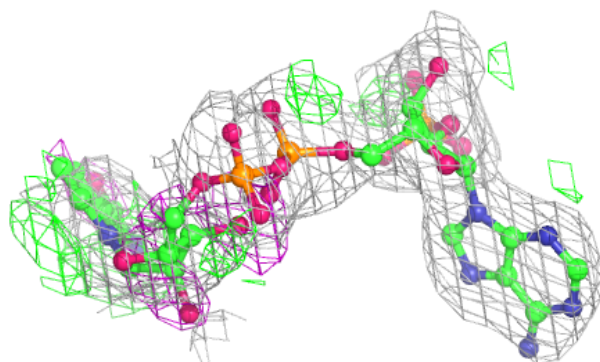
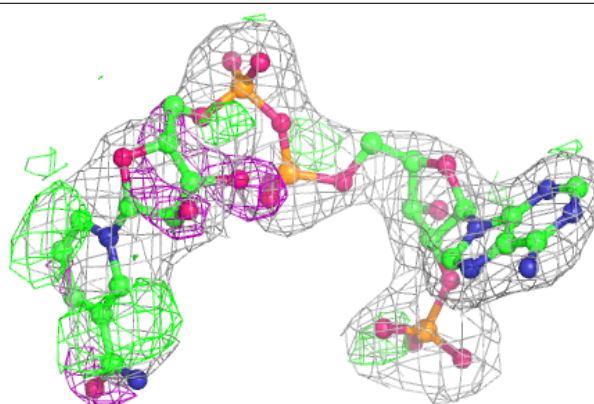
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SO3	A	1500	4/4	0.83	0.22	67,68,68,68	4
5	NAP	B	2453	48/48	0.87	0.18	40,47,59,61	0
5	NAP	A	1453	48/48	0.92	0.17	27,44,54,56	0
2	SO3	B	2500	4/4	0.92	0.13	79,80,81,82	0
4	FAD	B	2452	53/53	0.96	0.16	17,29,59,59	0
3	FMN	A	1451	31/31	0.96	0.17	32,35,38,41	0
3	FMN	B	2451	31/31	0.96	0.18	45,49,53,54	0
4	FAD	A	1452	53/53	0.97	0.17	17,30,51,53	0

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

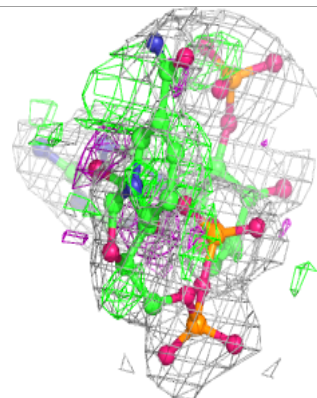
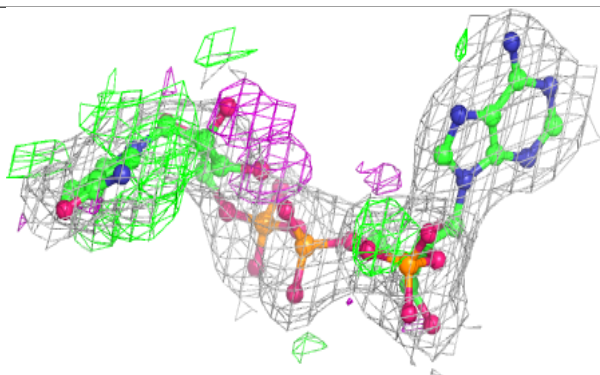
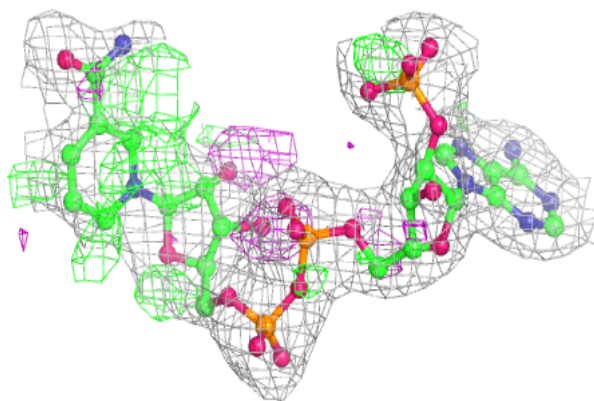
Electron density around NAP B 2453:

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

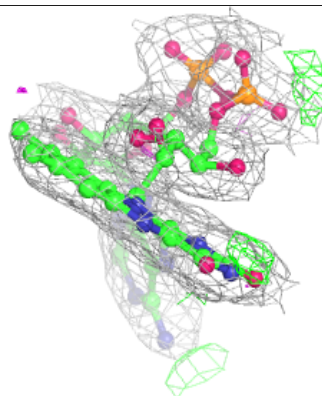
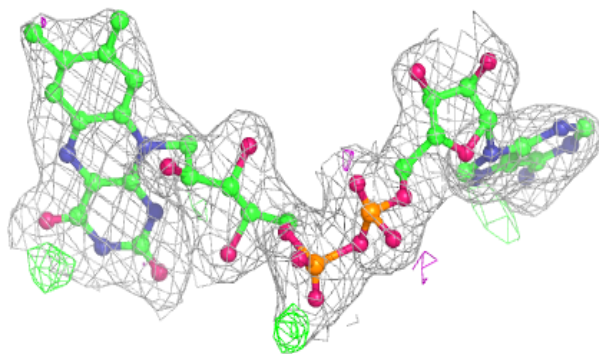
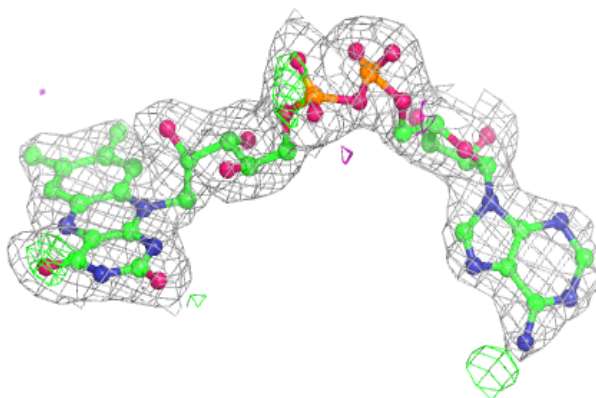


Electron density around NAP A 1453:

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

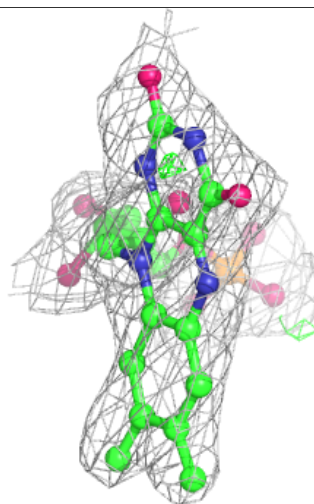
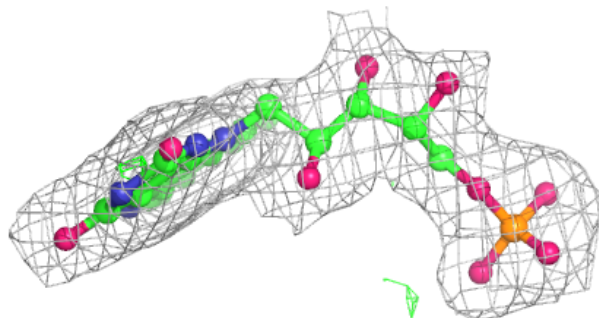
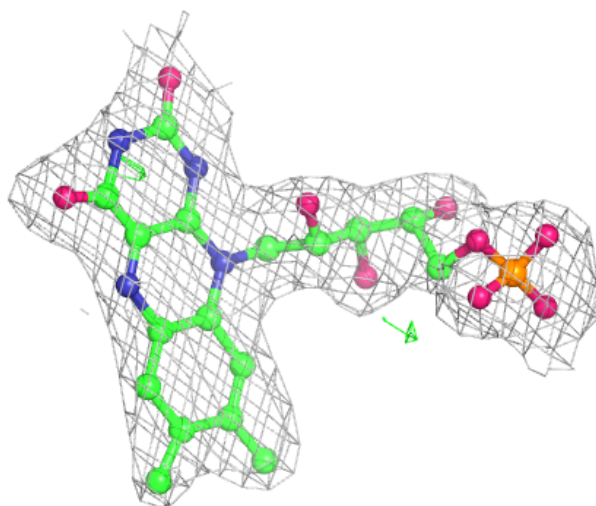
**Electron density around FAD B 2452:**

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



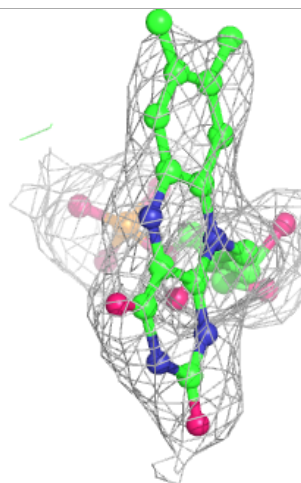
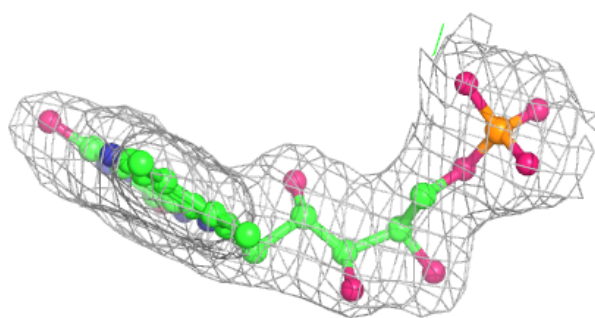
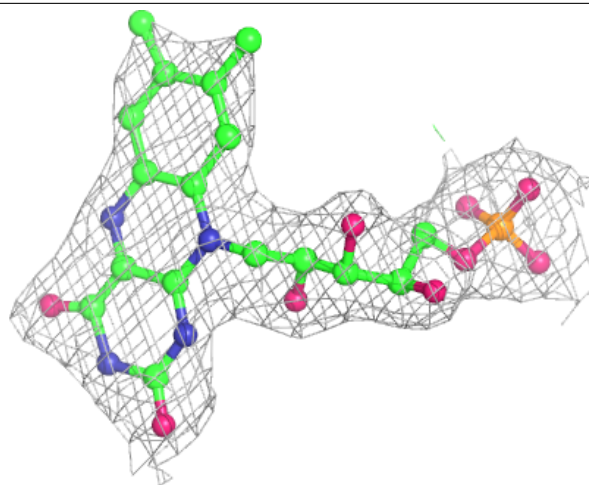
Electron density around FMN A 1451:

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



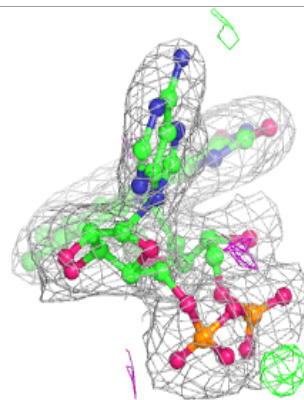
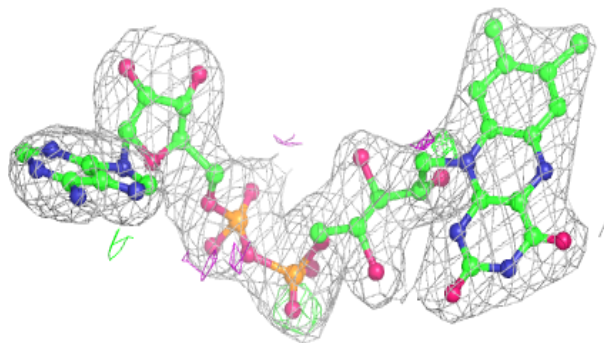
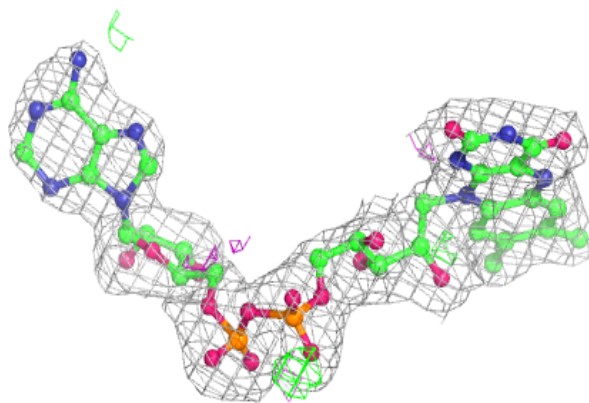
Electron density around FMN B 2451:

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



Electron density around FAD A 1452:

$2mF_o - DF_c$ (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.