



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 01:43 AM UTC

PDB ID : 1TLL / pdb_00001tll
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 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

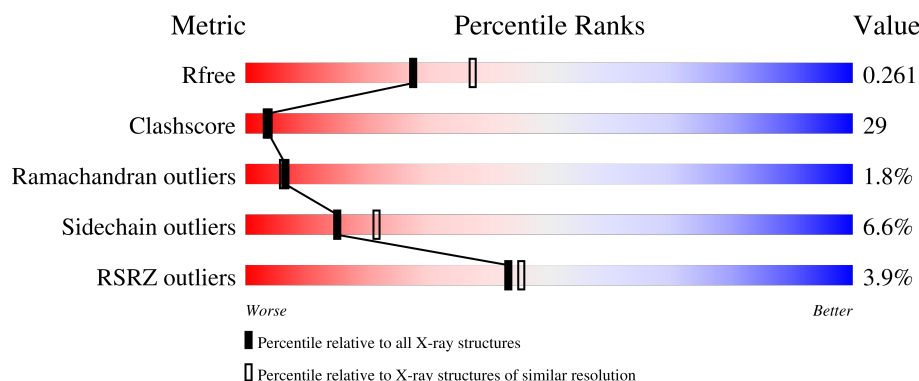
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 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	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.

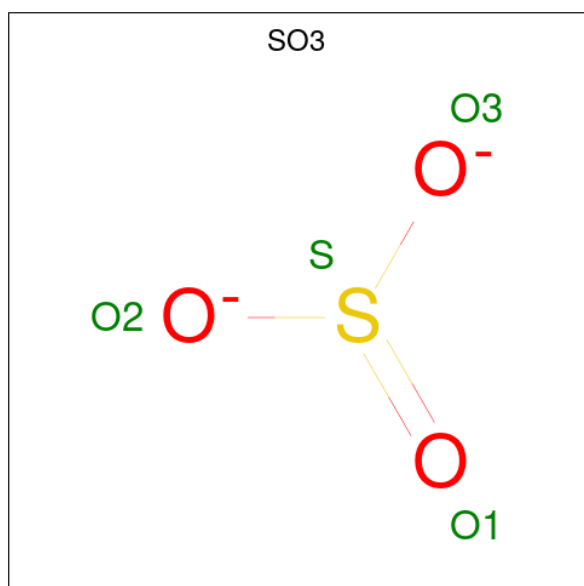
- Molecule 1 is a protein called Nitric-oxide synthase, brain.

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 (CCD ID: SO3) (formula: O₃S).



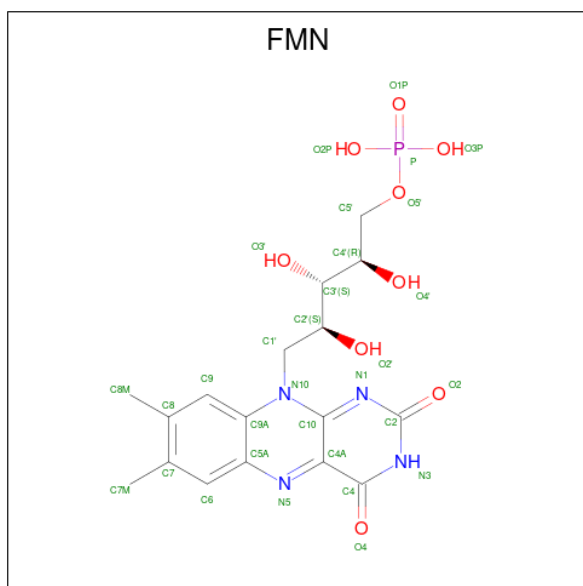
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			4	3	1		

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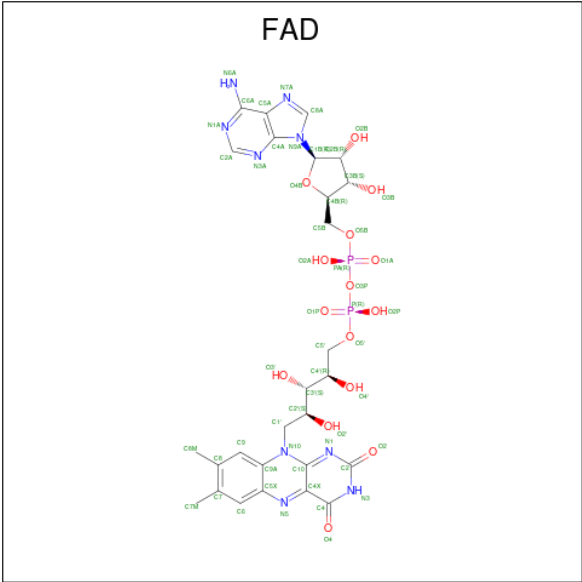
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			4	3	1		

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



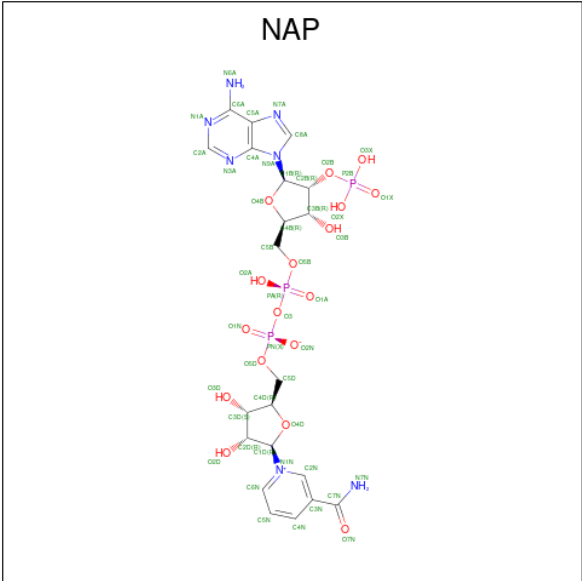
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: 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 (CCD ID: 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		

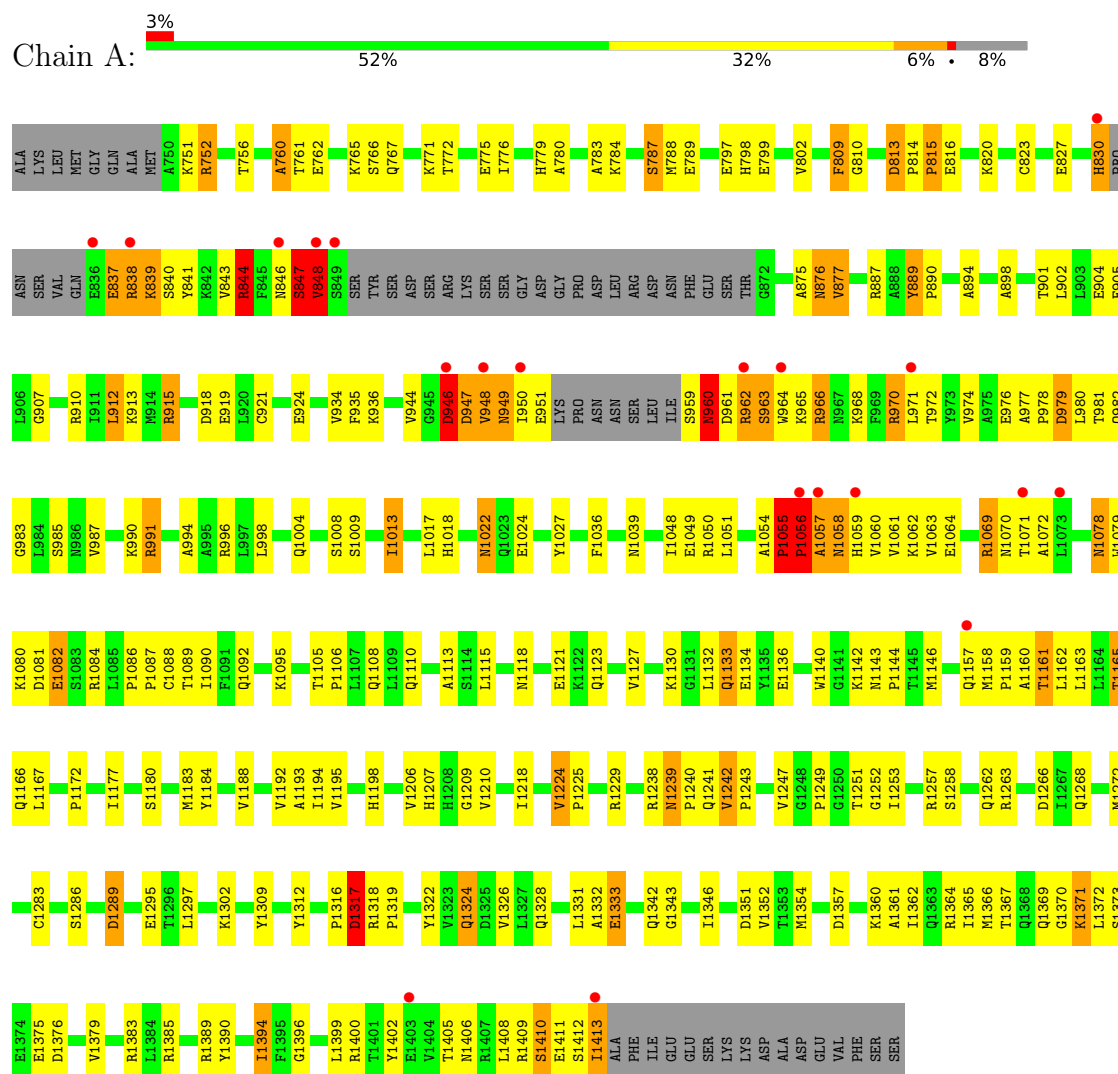
- Molecule 6 is water.

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

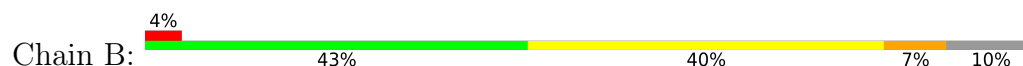
3 Residue-property plots

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: Nitric-oxide synthase, brain



• Molecule 1: Nitric-oxide synthase, brain



F3380	R3385	D3386	D3387	K3388	R3389	V3390	H3391	G3396	V3397	T3397	L3398	R3399	R3400	T3401	Y3402	E3403	V3404	T3405	N3406	L3407	L3408	R3409	S3410	E3411	S3412	I3413	ALA	PHE	ILE	GLU	GLU	SER	LYS	LYS	ASP	ALA	ASP	GLU	VAL	PHE	SER	SER	S3313	R3314	E3315	F3316	D3317	K3320	K3321	D3322	V3323	Q3324	Q3325	V3326	L3327	G3328	E3329	Q3330	Q3331	L3332	A3332	V3335	Y3336	R3337	A3338	E3341	Q3342	Q3343	F3344	H3345	I3346	Y3347	V3348	D3351	V3352	T3353	H3354	L3359	K3360	A3361	I3362	Q3363	R3364	I3365	H3366	T3367	Q3368	Q3369	G3370	K3371	L3372	S3373	E3374	E3375	H3376	A3377	G3378	V3379	V3218	Q3219	A3220	D3221	D3222	G3226	R3238	N3239	P3240	Q3241	V3242	P3243	G3244	I3245	L3246	V3247	G3248	P3249	G3250	T3251	G3252	I3253	A3254	R3257	S3258	F3259	V3260	Q3261	Q3262	D3266	M3272	V3280	F3281	G3282	C3283	R3284	Q3285	S3286	K3287	I3288	D3289	T3296	A3299	V3304	F3305	R3306	E3307	L3308	V3309	V3312	R3124	L3125	L3126	K3130	K3131	L3132	Q3133	E3134	Y3135	E3136	E3137	V3140	N3143	T3144	T3145	M3146	V3147	E3148	V3149	E3152	F3153	Q3157	M3158	P3159	A3160	T3161	L3162	L3163	L3164	T3165	Q3166	L3167	Q3171	S3180	F3091	Q3092	P3103	P3104	L3107	Q3108	L3109	Q3110	Q3111	N3022	A3113	S3114	L3115	E3121	K3122	Q3123	K2962	ASN	SER	LEU	ILE	S2959	D2960	D2961	R2962	S2963	W2964	R2965	R2966	K2967	R2968	F2969	R2970	L2971	Y2972	Y2973	V2974	A2975	E2976	A2977	D2978	D2979	L2980	T2981	A2994	L2998	S2999	R3000	Q3001	N3002	L3003	Q3004	S3008	S3009	R3010	F3014	V3015	T3019	N3020	G3021	F2942	C2943	V2944	G2945	D2946	D2947	V2948	N2949	L2812	F2815	E2816	N2817	G2818	F2821	G2822	C2823	A2824	L2825	W2826	E2827	M2828	R2829	HIS	PRO	ASN	SER	VAL	GLN	GLU	GLU	ARG	LYS	S2840	Y2841	F2842	R2843	R2844	F2845	N2846	SER	VAL	SER	SER	TYR	SER	ASP	SER	ARG	LYS	SER	SER	GLY	ASP	GLY	PRO	ASP	LEU	ARG	ASP	ASN	PHE	GLU	SER	V2805	V2806	V2769	Y2773	C2774	E2775	I2776	F2777	K2778	H2779	D2782	A2783	K2784	M2786	S2787	M2788	E2789	E2790	Y2791	D2792	I2793	V2794	H2795	E2799	A2800	L2801	V2802	L2803	V2804	V2805	GLY	PRO
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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 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.8 (35.21-2.30) 97.8 (35.21-2.30)	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 0.236 , 0.261	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 , 51.9	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	0.53	2/5122 (0.0%)	1.11	43/6932 (0.6%)
1	B	0.49	0/5014	1.10	46/6788 (0.7%)
All	All	0.51	2/10136 (0.0%)	1.11	89/13720 (0.6%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1133	GLN	CA-CB	-7.70	1.41	1.53
1	A	1133	GLN	CG-CD	-5.17	1.39	1.52

The worst 5 of 89 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2966	ARG	N-CA-C	11.98	126.37	112.72
1	A	946	ASP	N-CA-C	-9.76	98.97	113.61
1	B	2943	CYS	N-CA-C	9.73	124.67	111.24
1	B	2944	VAL	N-CA-C	-9.66	94.21	108.89
1	A	877	VAL	N-CA-C	9.53	122.17	109.21

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	275	1
1	B	4903	0	4814	302	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	576	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 29.

The worst 5 of 576 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:O2A	5:A:1453:NAP:O3D	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:HG3	1:A:991:ARG:HH11	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%)	5	4
1	B	608/688 (88%)	548 (90%)	51 (8%)	9 (2%)	8	8
All	All	1230/1376 (89%)	1117 (91%)	91 (7%)	22 (2%)	6	6

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%)	509 (94%)	34 (6%)	16	23
1	B	531/601 (88%)	494 (93%)	37 (7%)	14	19
All	All	1074/1202 (89%)	1003 (93%)	71 (7%)	15	21

5 of 71 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	3221	ASP
1	B	3266	ASP
1	B	3369	GLN
1	A	1165	THR
1	A	1161	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	2967	ASN
1	B	3110	GLN
1	B	2982	GLN
1	B	3004	GLN
1	B	3123	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	$\# Z > 2$
4	FAD	A	1452	-	58,58,58	5.98	44 (75%)	85,89,89	3.46	31 (36%)
4	FAD	B	2452	-	58,58,58	5.81	40 (68%)	85,89,89	3.47	31 (36%)
5	NAP	A	1453	-	50,52,52	2.02	10 (20%)	71,80,80	2.26	17 (23%)
5	NAP	B	2453	-	50,52,52	2.60	11 (22%)	71,80,80	2.51	24 (33%)
2	SO3	A	1500	-	1,3,3	2.49	1 (100%)	0,3,3	-	-
2	SO3	B	2500	-	1,3,3	2.46	1 (100%)	0,3,3	-	-
3	FMN	A	1451	-	33,33,33	4.06	19 (57%)	48,50,50	2.54	19 (39%)
3	FMN	B	2451	-	33,33,33	4.17	19 (57%)	48,50,50	2.46	17 (35%)

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
4	FAD	A	1452	-	-	5/34/50/50	0/6/6/6
4	FAD	B	2452	-	-	5/34/50/50	0/6/6/6
5	NAP	A	1453	-	-	18/35/67/67	0/5/5/5
5	NAP	B	2453	-	-	16/35/67/67	0/5/5/5
3	FMN	A	1451	-	-	0/18/18/18	0/3/3/3
3	FMN	B	2451	-	-	0/18/18/18	0/3/3/3

The worst 5 of 145 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1452	FAD	P-O3P	17.75	1.78	1.59
4	B	2452	FAD	P-O3P	16.14	1.76	1.59
4	A	1452	FAD	PA-O3P	-12.78	1.45	1.59
5	B	2453	NAP	C2N-N1N	12.30	1.48	1.35
4	B	2452	FAD	C2A-N1A	12.20	1.55	1.33

The worst 5 of 139 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2452	FAD	O4B-C1B-N9A	-15.40	78.51	108.09
4	A	1452	FAD	O4B-C1B-N9A	-15.20	78.90	108.09
4	A	1452	FAD	O2A-PA-O3P	13.52	143.82	107.27
4	B	2452	FAD	O2A-PA-O3P	13.24	143.06	107.27
5	B	2453	NAP	C4D-O4D-C1D	-9.73	101.02	109.92

There are no chirality outliers.

5 of 44 torsion outliers are listed below:

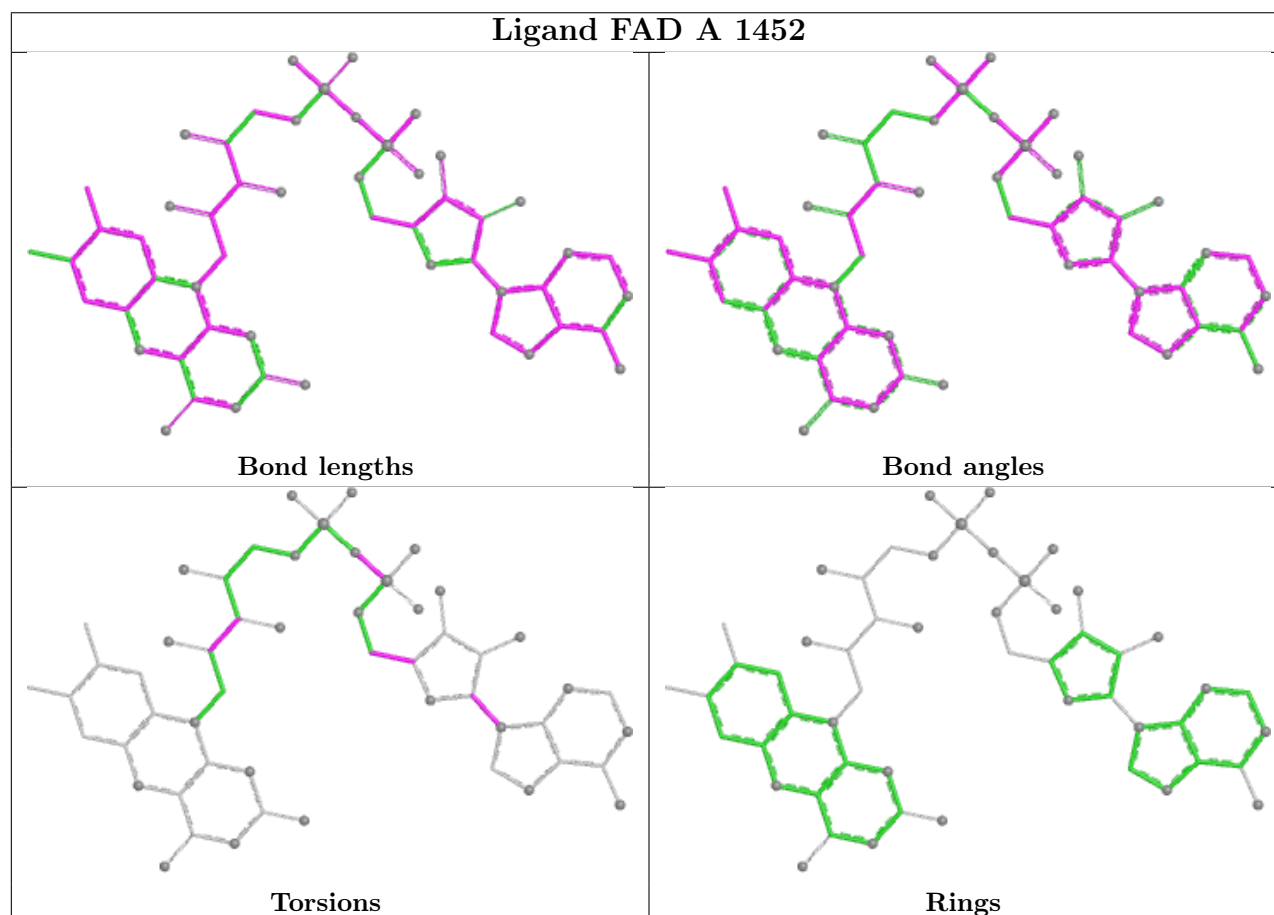
Mol	Chain	Res	Type	Atoms
5	A	1453	NAP	C5D-O5D-PN-O3
5	A	1453	NAP	C5D-O5D-PN-O1N
5	A	1453	NAP	C5D-O5D-PN-O2N
5	A	1453	NAP	O4D-C1D-N1N-C6N
5	B	2453	NAP	C5B-O5B-PA-O1A

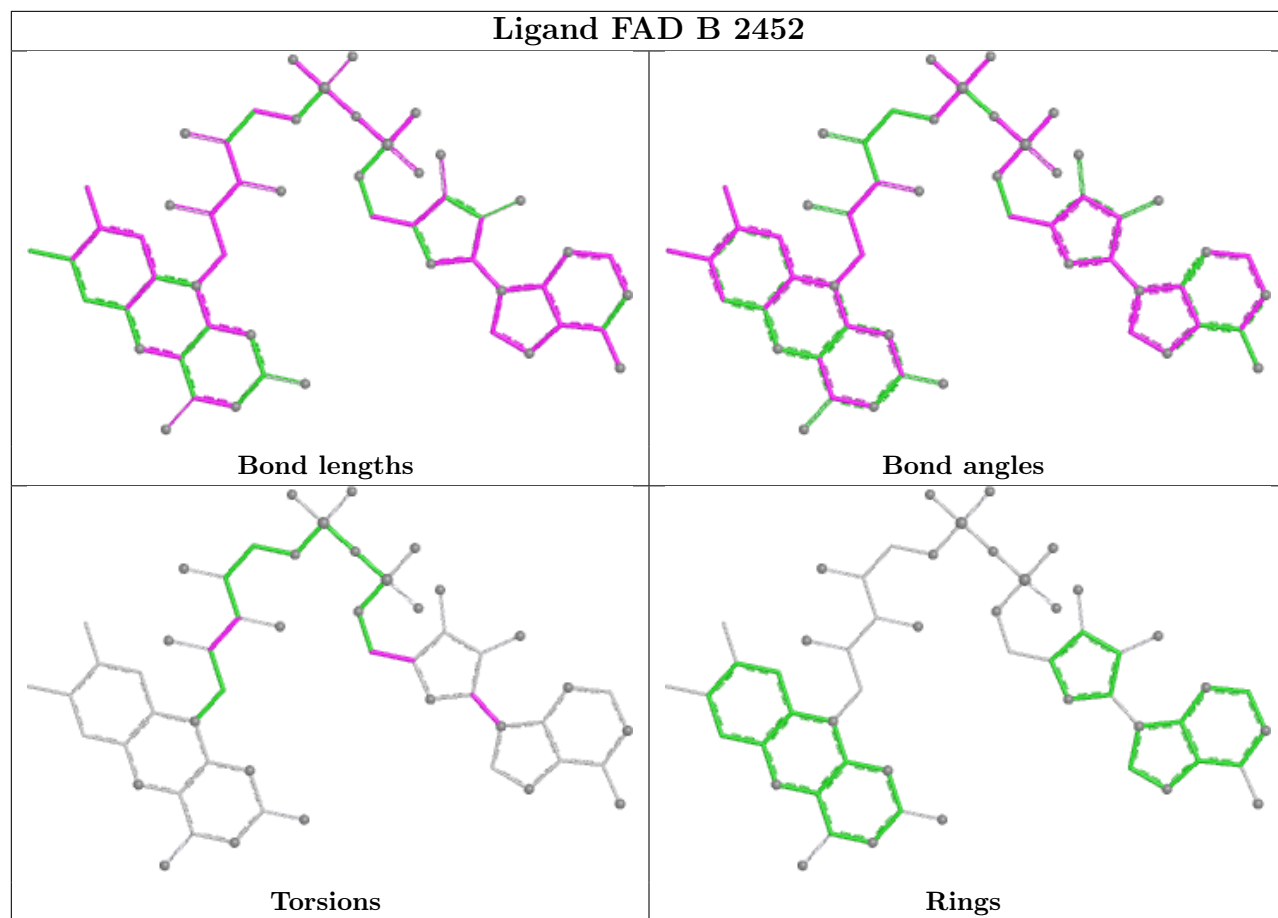
There are no ring outliers.

2 monomers are involved in 22 short contacts:

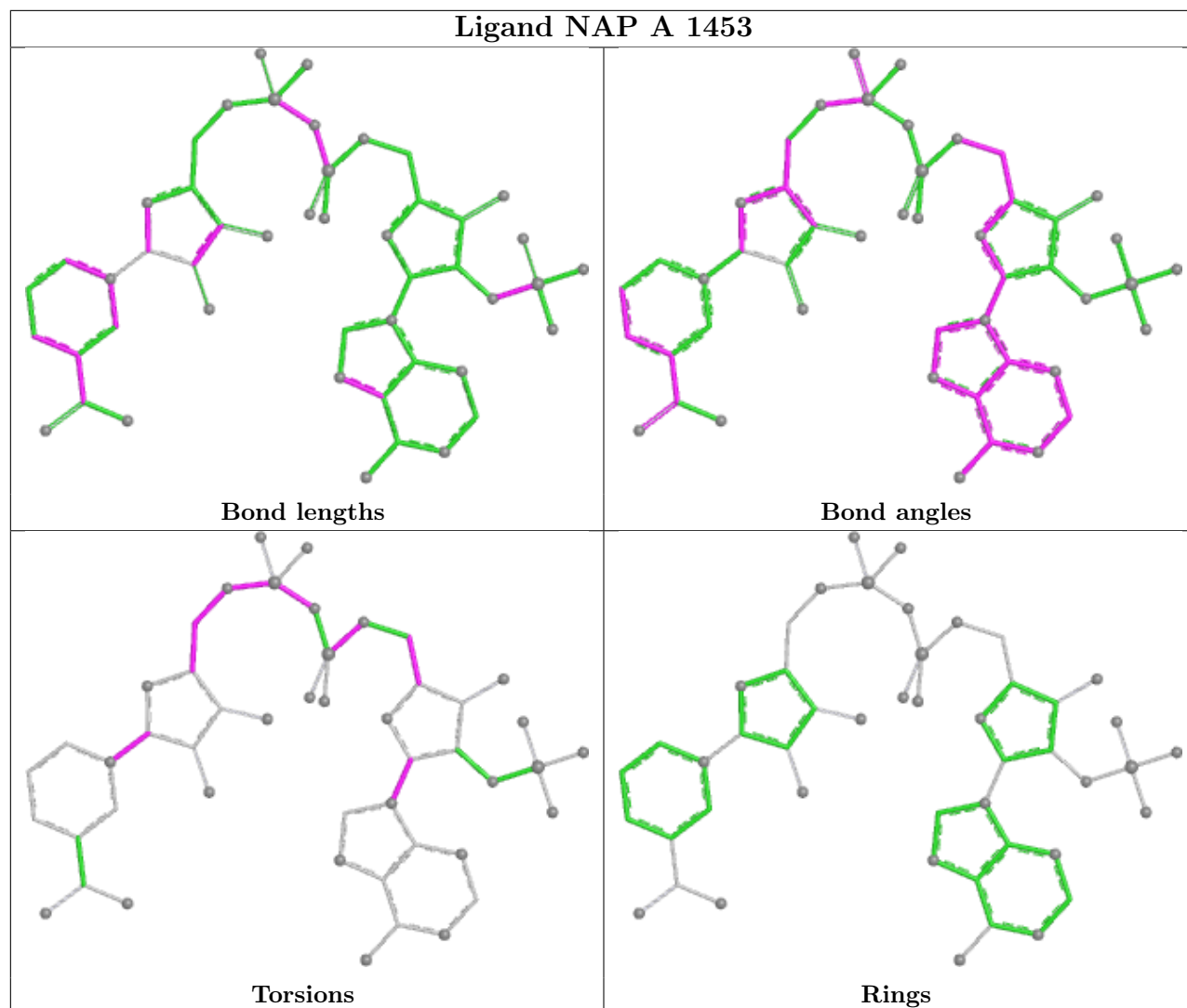
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1453	NAP	9	0
5	B	2453	NAP	13	0

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.

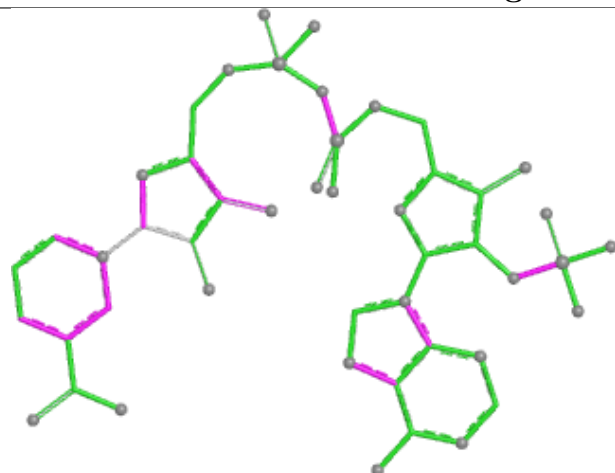




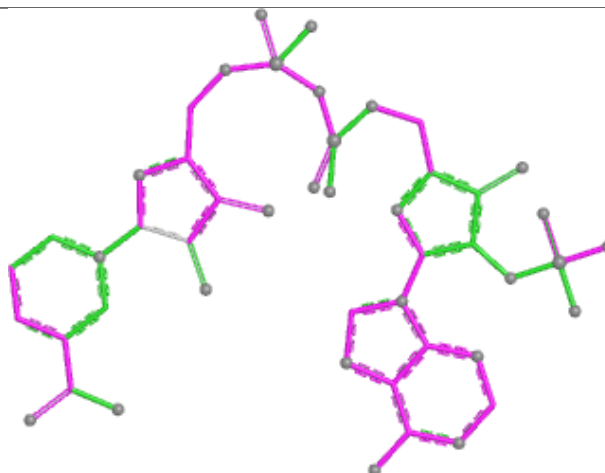
Ligand NAP A 1453



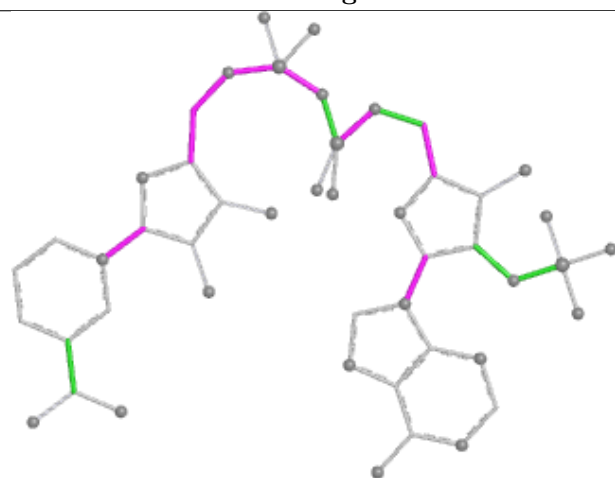
Ligand NAP B 2453



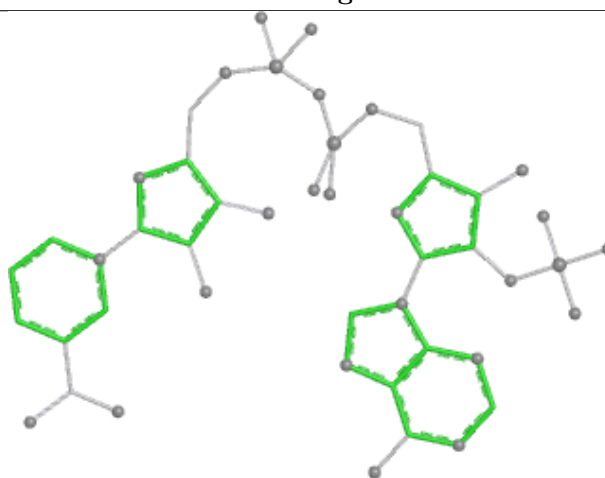
Bond lengths



Bond angles

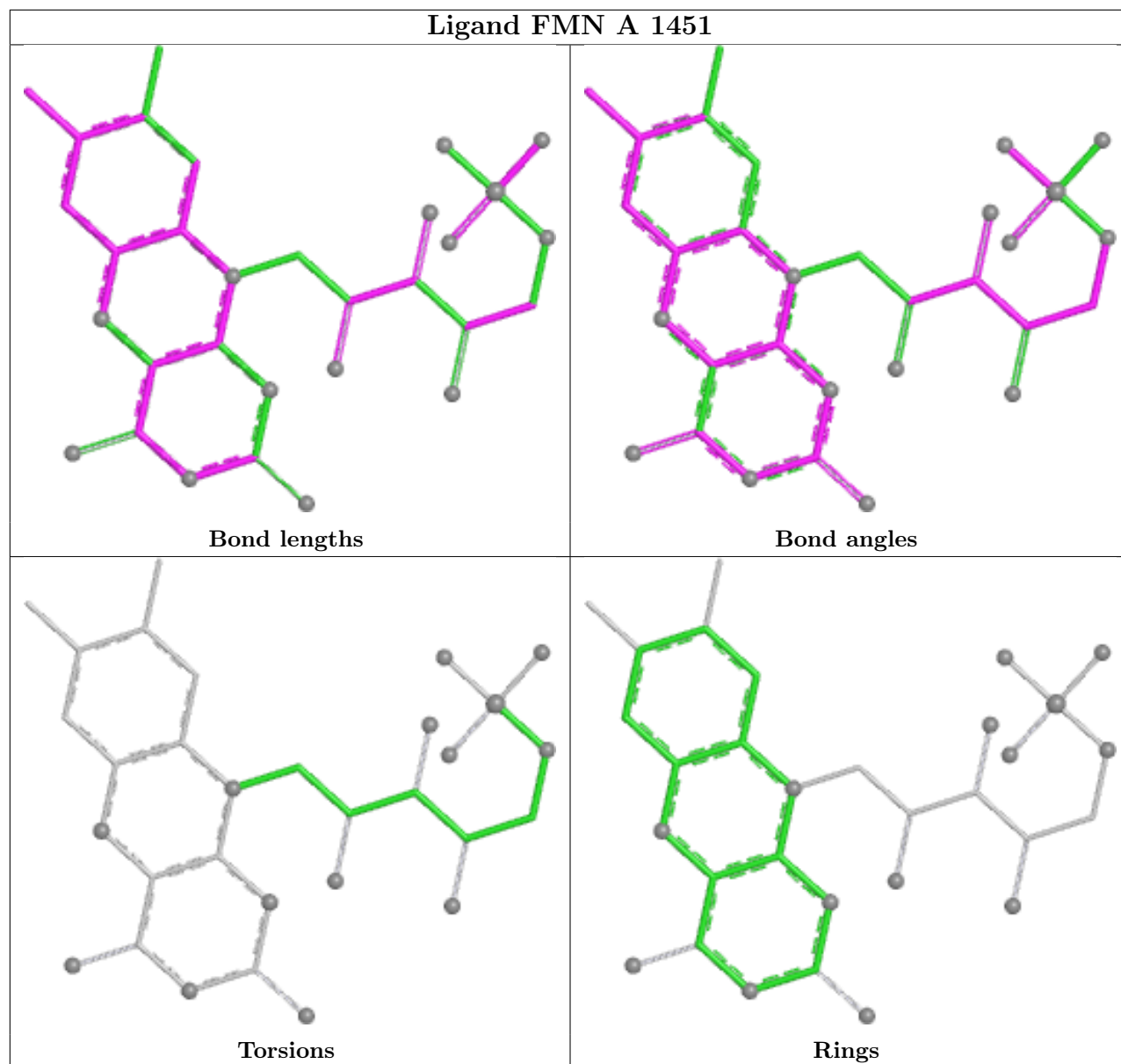


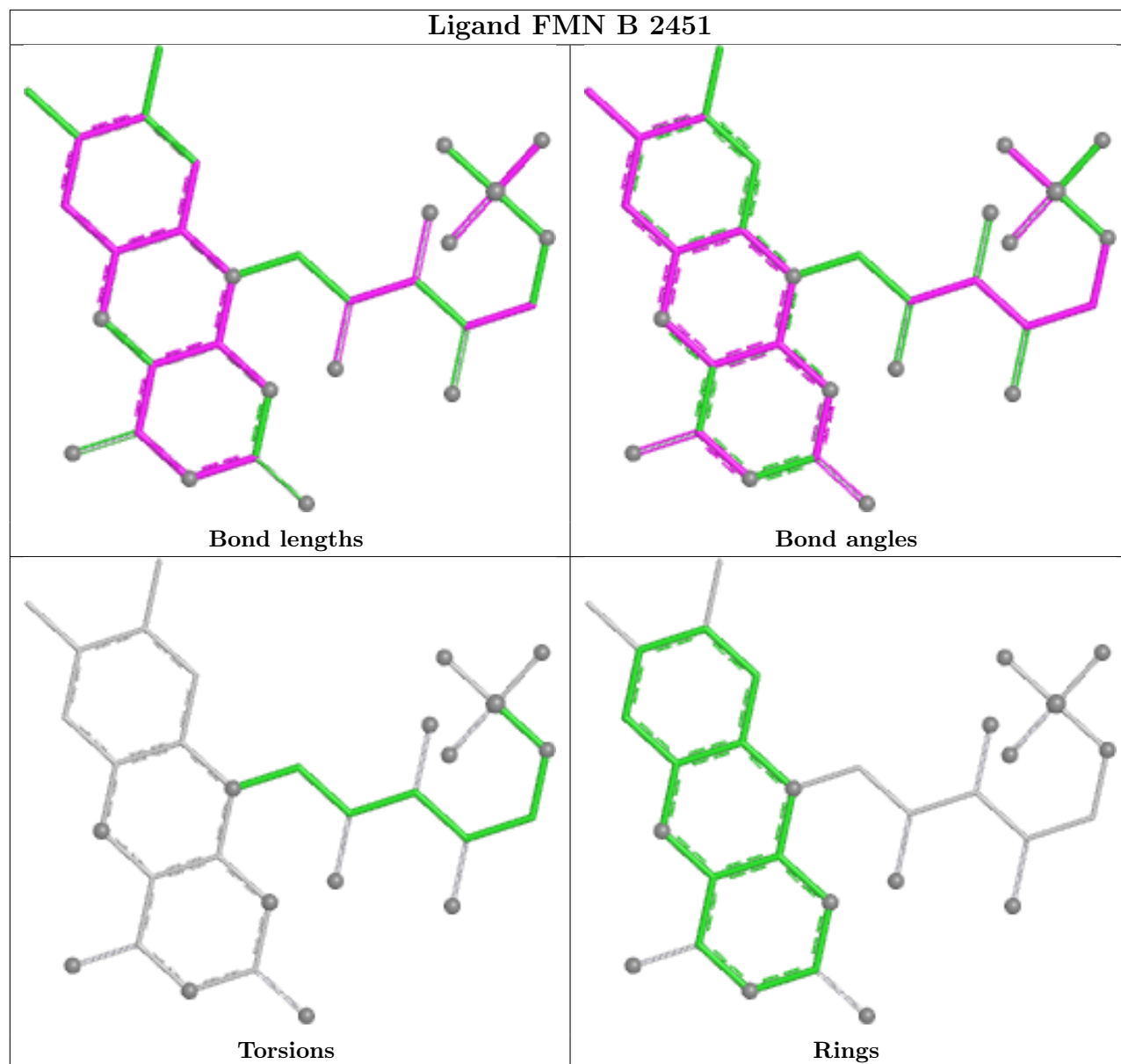
Torsions



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%)	0.32	20 (3%) 50 52	28, 52, 88, 99	0
1	B	616/688 (89%)	0.45	28 (4%) 38 40	24, 61, 93, 100	0
All	All	1246/1376 (90%)	0.38	48 (3%) 43 45	24, 56, 92, 100	0

The worst 5 of 48 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1413	ILE	3.9
1	B	2902	LEU	3.9
1	A	948	VAL	3.6
1	B	3410	SER	3.4
1	A	946	ASP	3.3

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](#)

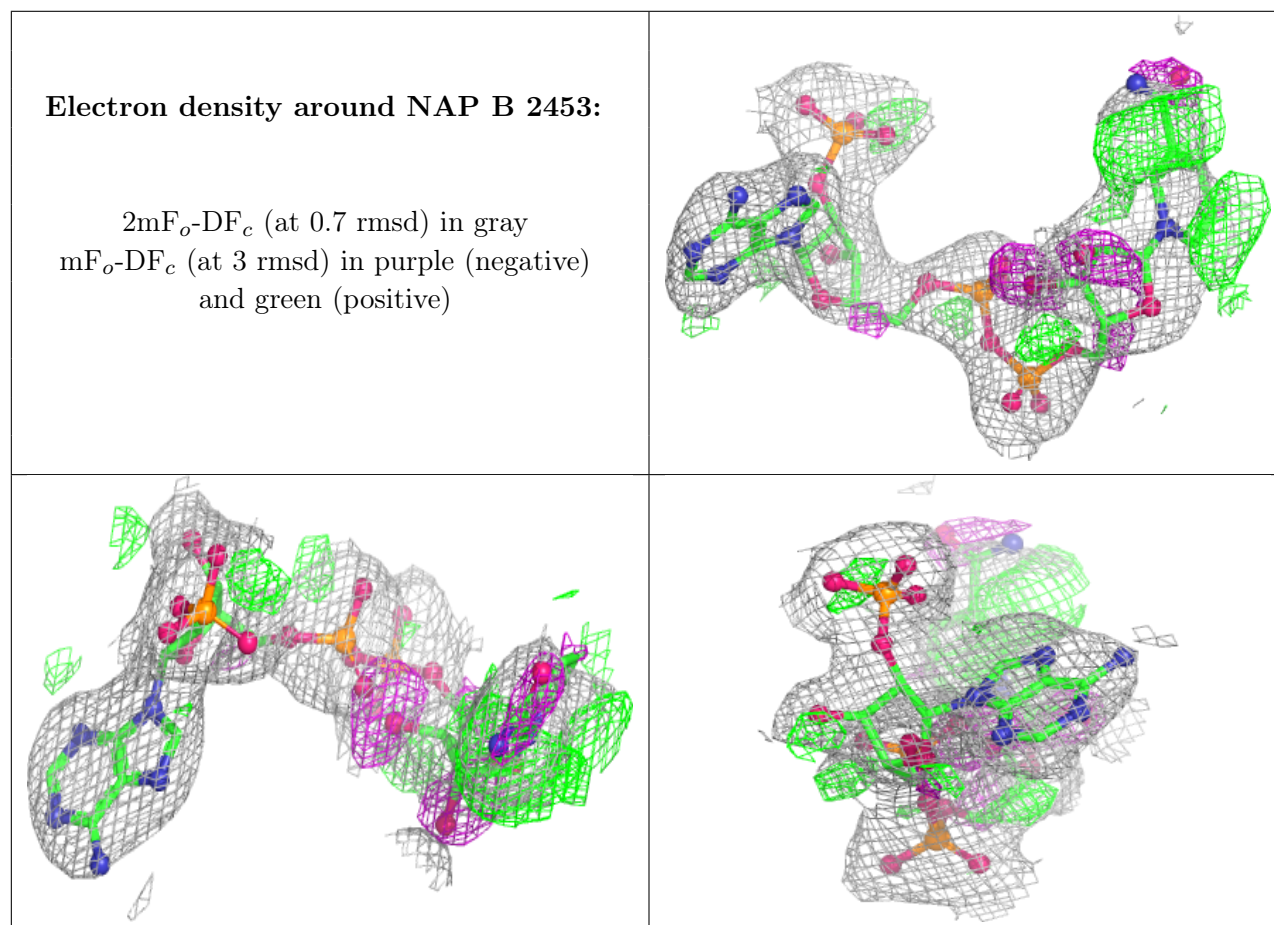
There are no oligosaccharides in this entry.

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.

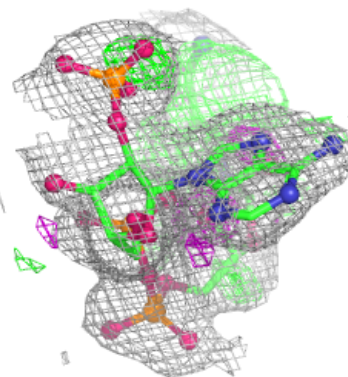
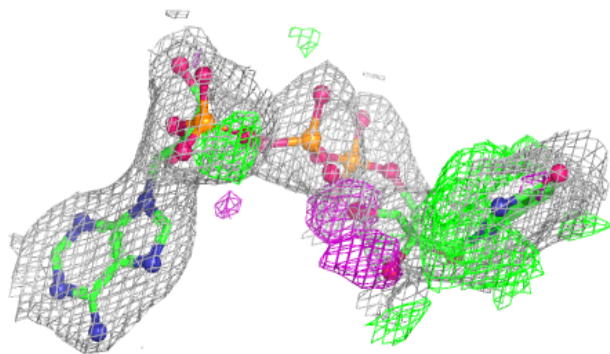
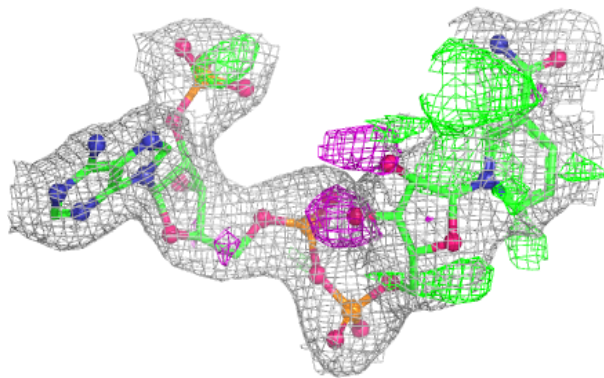
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO3	A	1500	4/4	0.81	0.12	67,68,68,68	4
2	SO3	B	2500	4/4	0.81	0.09	79,80,81,82	0
5	NAP	B	2453	48/48	0.84	0.12	40,47,59,61	0
5	NAP	A	1453	48/48	0.87	0.11	27,44,54,56	0
3	FMN	B	2451	31/31	0.94	0.09	45,49,53,54	0
3	FMN	A	1451	31/31	0.95	0.07	32,35,38,41	0
4	FAD	A	1452	53/53	0.96	0.07	17,30,51,53	0
4	FAD	B	2452	53/53	0.96	0.07	17,29,59,59	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.



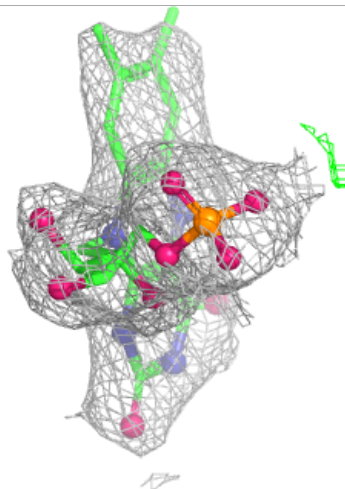
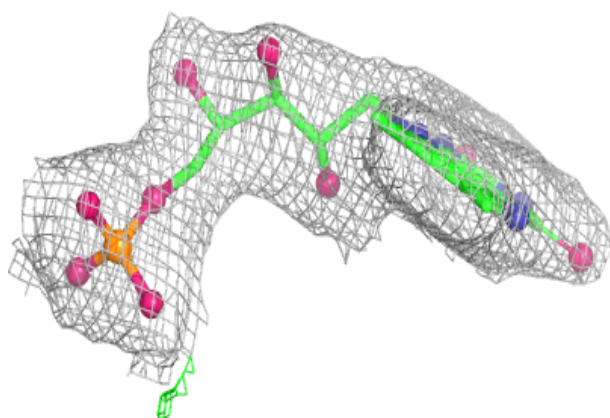
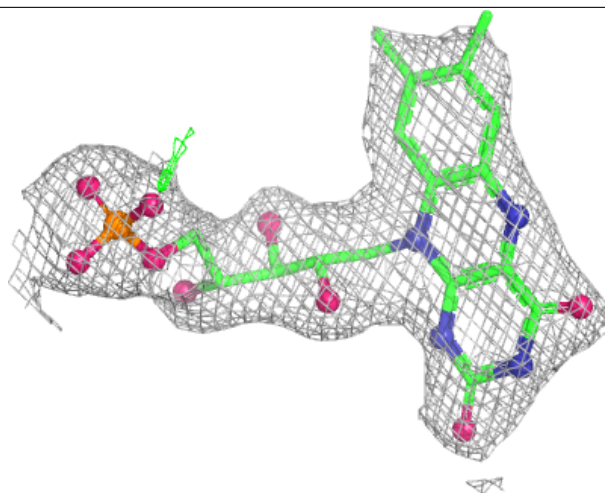
Electron density around NAP A 1453:

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



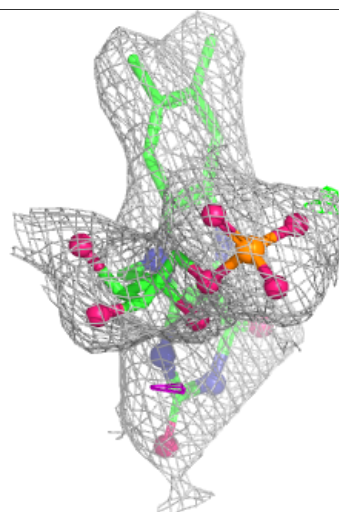
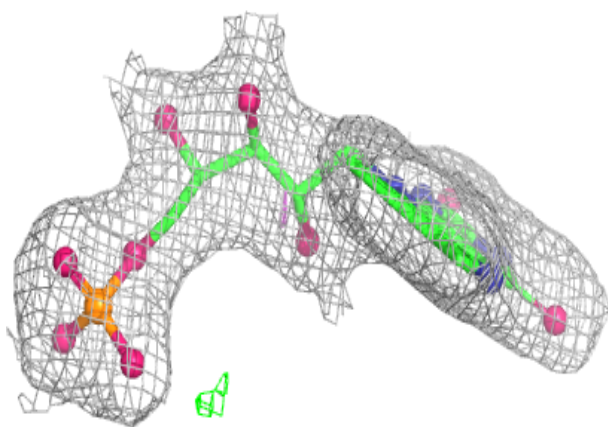
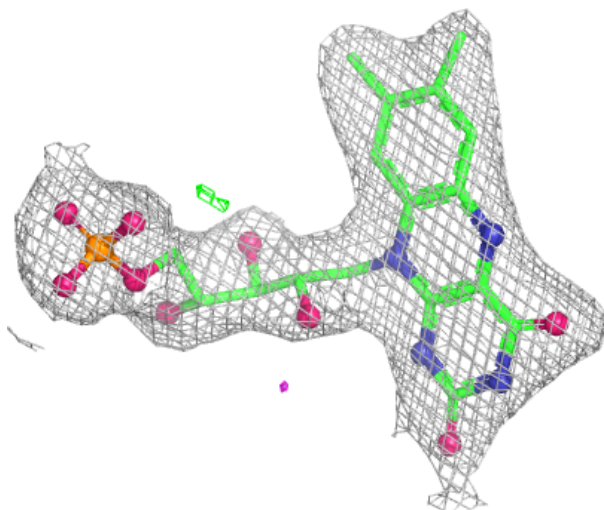
Electron density around FMN B 2451:

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



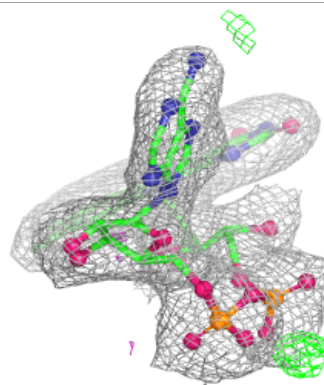
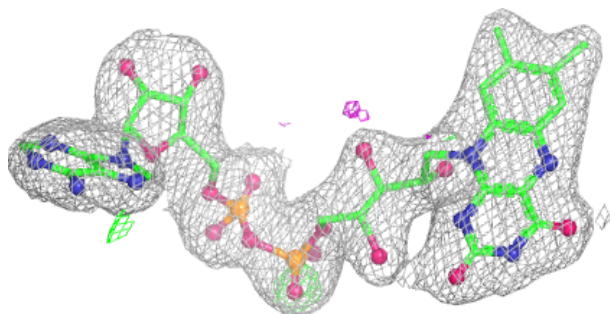
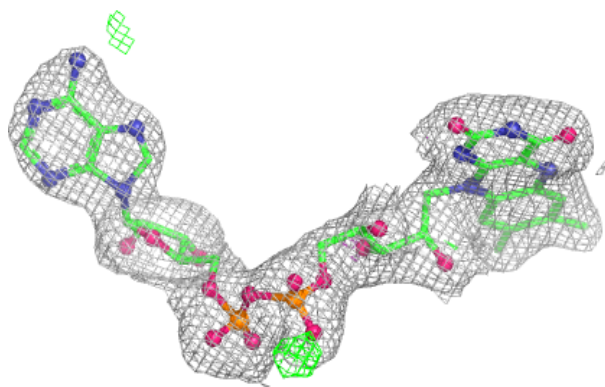
Electron density around FMN A 1451:

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

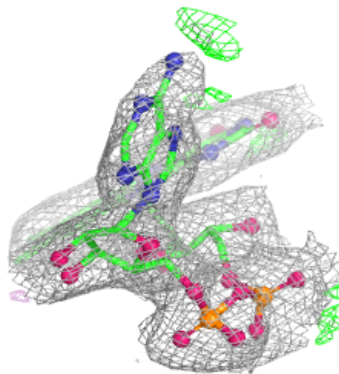
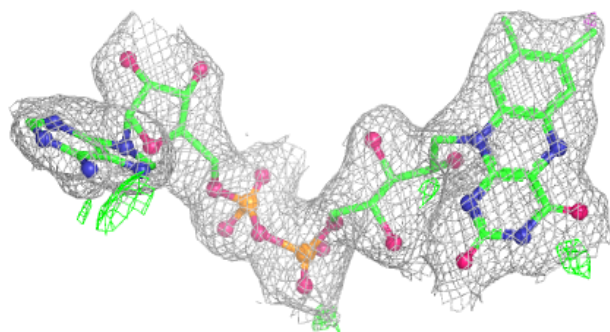
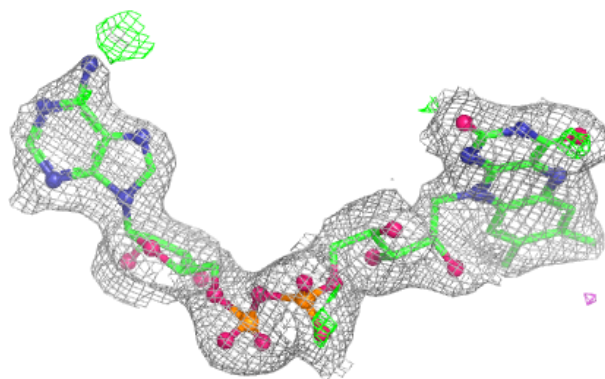


Electron density around FAD A 1452:

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

**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)



6.5 Other polymers [i](#)

There are no such residues in this entry.