



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 02:49 PM UTC

PDB ID : 6PFZ / pdb_00006pfz
Title : Structure of a NAD-Dependent Persulfide Reductase from *A. fulgidus*
Authors : Sazinsky, M.H.; Shabdar, S.; Garcia-Constineiras, A.; Crane III, E.J.
Deposited on : 2019-06-23
Resolution : 3.10 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

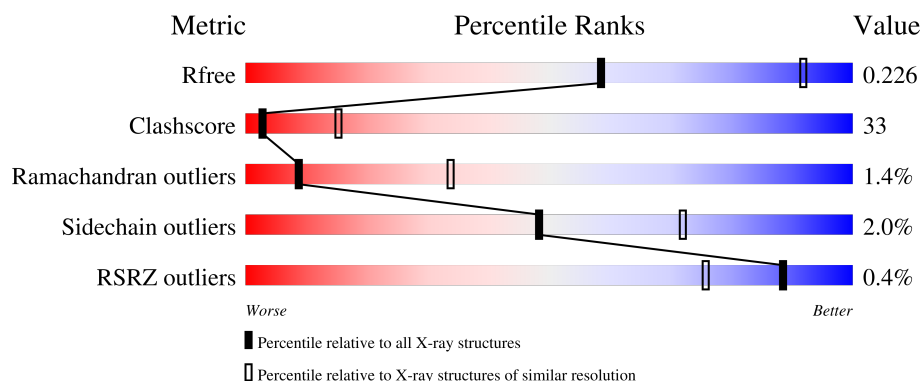
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	551	58% 37% ...
1	B	551	% 56% 40% ..
1	C	551	% 48% 45% ...
1	D	551	54% 41% ...

2 Entry composition [i](#)

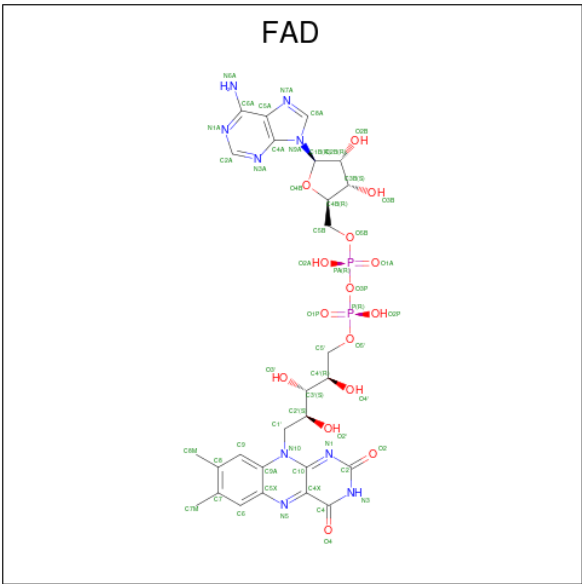
There are 5 unique types of molecules in this entry. The entry contains 16676 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NADH oxidase (NoxA-3).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	536	Total	C	N	O	S	0	0	0
			4044	2560	685	782	17			
1	A	541	Total	C	N	O	S	0	0	0
			4081	2585	691	788	17			
1	B	541	Total	C	N	O	S	0	0	0
			4106	2599	703	787	17			
1	C	535	Total	C	N	O	S	0	0	0
			4023	2551	682	773	17			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



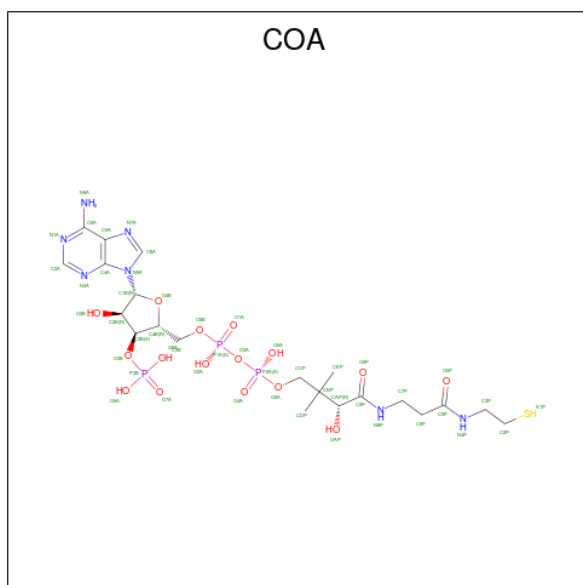
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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		

- Molecule 3 is COENZYME A (CCD ID: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	D	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	B	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	C	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		
4	B	1	Total	Ca	0	0
			1	1		
4	C	2	Total	Ca	0	0
			2	2		

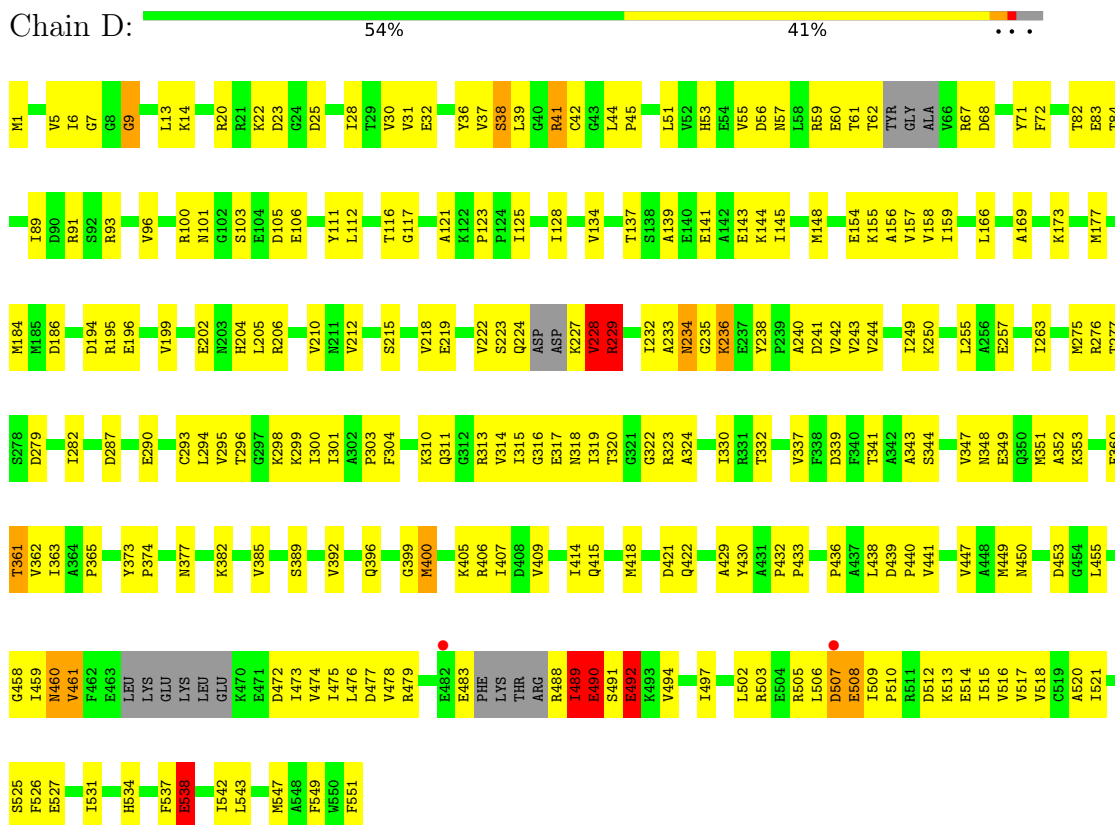
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total 3	O 3	0	0
5	B	11	Total 11	O 11	0	0

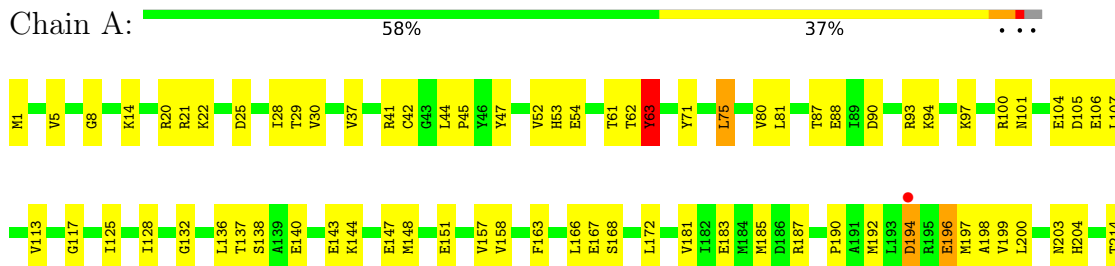
3 Residue-property plots

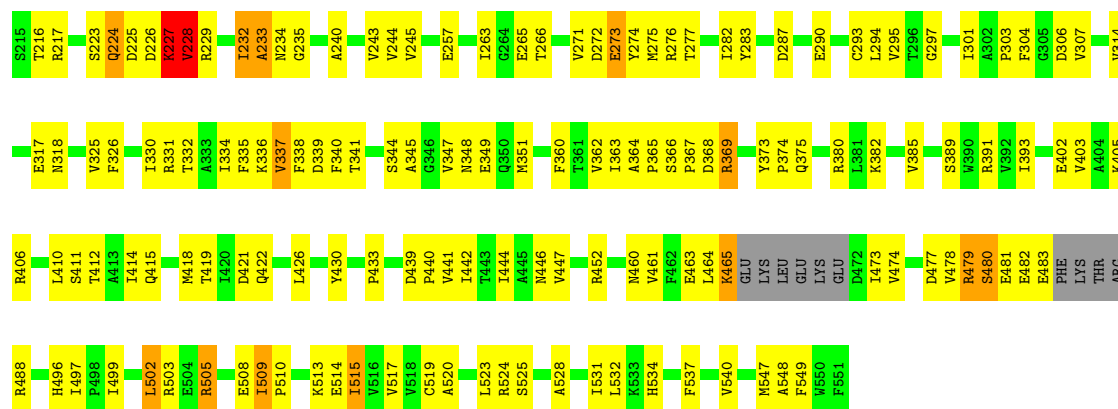
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: NADH oxidase (NoxA-3)

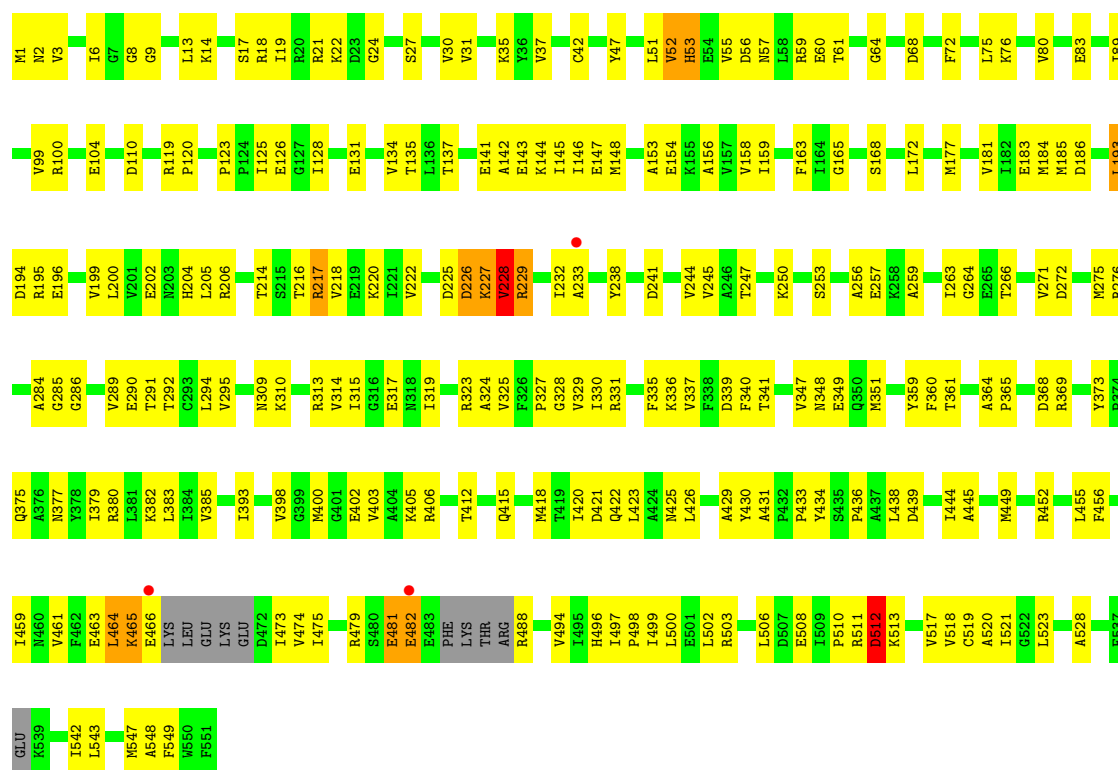


• Molecule 1: NADH oxidase (NoxA-3)

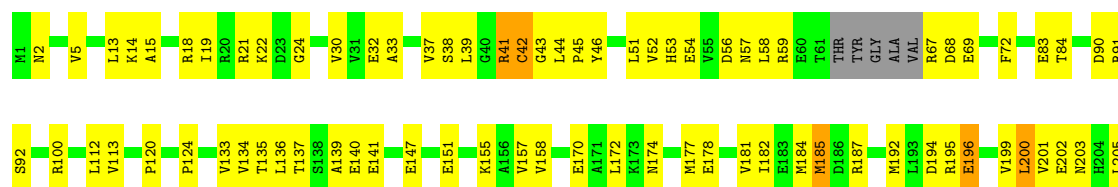




• Molecule 1: NADH oxidase (NoxA-3)



• Molecule 1: NADH oxidase (NoxA-3)



I515	G454	A376	I300	R206
V516	L455	N377	I301	V210
V517	F456	Y378	A302	N211
V518	E457	I379	P303	V212
C519	G458	R380	L381	V213
A520	I459	K382	R313	T214
I521	M460		V314	
G522	V461	K387	I315	R217
L523	F462		G316	V218
R524	E463		E317	E219
S525	L464	V390	N318	K220
F526	K465	R391	I319	I221
F527	F466	V392	T320	V222
A528	LYS			S223
S529	LEU	G399	A324	Q224
R530	GLU	M400	V325	D225
I531	LYS	G401	F326	D226
L532	GLU	F402	P327	K227
K533	ASP	V403	G328	Y228
H534	I473	A404	V329	R229
A535	V474	R405	I330	A230
G536	I475	R406	R331	V231
F537	L476	I407	T332	I232
E538	D477	D408	A333	ALA
K539	V478		I334	N234
V540	R479	T412	F335	
K541	S480	A413	K336	Y238
I542	E481	I414	V337	P239
L543	E482	Q415	F338	A240
E544	E483	A416	D339	D241
G545	F484	G417	F340	
G546		M418	T341	V244
H547	R487	I419	A342	
A548	R488	I420	A343	A256
F549	ILE	D421	S344	
N550	GLU	Q422	A345	L261
F551	SER	L423	G346	
	GLU	A424	V347	T266
	R493	M425	N348	
	V494	L426	E349	I269
	I495		Q350	
	H496	P433	M351	E273
	I497	Y434	A352	Y274
	P498	S435	K353	M275
	I499	P436	E354	R276
	L500	A437		T277
	E501	L438	Y359	S278
	L502	D439	F360	D279
	R503		T361	
	E504	I442	V362	I282
	R505	T443	I363	Y283
	L506	I444	A364	
	D507	A445	P365	D287
	E508	H446		C288
	I509	V447	D368	V289
	P510			E290
	R511	M450		
	D512	R451	Y373	C293
	K513	R452	P374	L294
	E514	D453	Q375	

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.98Å 100.36Å 136.20Å 90.00° 91.89° 90.00°	Depositor
Resolution (Å)	39.48 – 3.10 39.48 – 3.10	Depositor EDS
% Data completeness (in resolution range)	97.9 (39.48-3.10) 97.9 (39.48-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.10_2155	Depositor
R, R_{free}	0.202 , 0.229 0.204 , 0.226	Depositor DCC
R_{free} test set	2879 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	58.6	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 61.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.039 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	16676	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.75% 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: COA, FAD, CA

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	0.84	2/4139 (0.0%)	1.08	23/5609 (0.4%)
1	B	0.85	1/4163 (0.0%)	1.04	13/5634 (0.2%)
1	C	0.95	7/4079 (0.2%)	1.01	15/5527 (0.3%)
1	D	0.84	0/4099	1.08	21/5552 (0.4%)
All	All	0.87	10/16480 (0.1%)	1.05	72/22322 (0.3%)

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	496	HIS	CE1-NE2	-7.43	1.25	1.32
1	A	509	ILE	N-CA	-6.73	1.40	1.46
1	C	185	MET	SD-CE	-6.63	1.62	1.79
1	C	540	VAL	C-O	-6.18	1.17	1.24
1	C	496	HIS	CG-ND1	-5.97	1.31	1.38

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	228	VAL	N-CA-C	12.06	134.42	109.34
1	A	63	TYR	N-CA-C	-10.16	96.83	110.55
1	A	232	ILE	N-CA-C	9.63	123.68	108.85
1	A	229	ARG	N-CA-C	9.28	122.70	108.42
1	C	502	LEU	N-CA-C	9.25	121.36	111.28

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	4081	0	4098	217	0
1	B	4106	0	4152	266	0
1	C	4023	0	4026	364	0
1	D	4044	0	4057	276	0
2	A	53	0	31	2	0
2	B	53	0	31	3	0
2	C	53	0	31	6	0
2	D	53	0	31	5	0
3	A	48	0	32	8	0
3	B	48	0	32	8	0
3	C	48	0	32	12	0
3	D	48	0	32	8	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0
5	A	3	0	0	0	0
5	B	11	0	0	0	0
All	All	16676	0	16585	1092	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 33.

The worst 5 of 1092 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:495:ILE:CD1	1:C:508:GLU:HG2	1.37	1.54
1:C:495:ILE:HD11	1:C:508:GLU:CG	1.37	1.53
1:C:509:ILE:HG21	1:C:537:PHE:CE2	1.53	1.42
1:C:509:ILE:HG21	1:C:537:PHE:CZ	1.54	1.41
1:C:529:SER:CB	1:C:542:ILE:HD11	1.54	1.36

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	535/551 (97%)	506 (95%)	24 (4%)	5 (1%)	14	44
1	B	533/551 (97%)	494 (93%)	36 (7%)	3 (1%)	21	52
1	C	525/551 (95%)	476 (91%)	36 (7%)	13 (2%)	4	21
1	D	526/551 (96%)	492 (94%)	26 (5%)	8 (2%)	8	32
All	All	2119/2204 (96%)	1968 (93%)	122 (6%)	29 (1%)	9	34

5 of 29 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	228	VAL
1	D	489	ILE
1	D	492	GLU
1	A	227	LYS
1	A	233	ALA

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	423/446 (95%)	417 (99%)	6 (1%)	59	76
1	B	428/446 (96%)	418 (98%)	10 (2%)	44	70
1	C	415/446 (93%)	405 (98%)	10 (2%)	43	69
1	D	420/446 (94%)	413 (98%)	7 (2%)	53	74
All	All	1686/1784 (94%)	1653 (98%)	33 (2%)	48	72

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	277	THR
1	C	426	LEU
1	C	508	GLU
1	A	465	LYS
1	A	369	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	425	ASN
1	C	350	GLN
1	A	422	GLN
1	C	101	ASN
1	A	375	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FAD	A	901	-	58,58,58	2.08	17 (29%)	85,89,89	1.98	24 (28%)
3	COA	D	902	-	47,50,50	2.41	11 (23%)	69,75,75	2.30	25 (36%)
3	COA	C	902	-	47,50,50	2.61	13 (27%)	69,75,75	2.63	30 (43%)
3	COA	B	902	-	47,50,50	2.48	12 (25%)	69,75,75	2.19	19 (27%)
3	COA	A	902	-	47,50,50	2.59	13 (27%)	69,75,75	2.46	24 (34%)
2	FAD	C	901	-	58,58,58	2.02	18 (31%)	85,89,89	1.85	24 (28%)
2	FAD	B	901	-	58,58,58	1.95	18 (31%)	85,89,89	1.73	18 (21%)
2	FAD	D	901	-	58,58,58	1.86	17 (29%)	85,89,89	1.86	20 (23%)

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
2	FAD	A	901	-	-	11/34/50/50	0/6/6/6
3	COA	D	902	-	-	5/48/64/64	0/3/3/3
3	COA	C	902	-	-	13/48/64/64	0/3/3/3
3	COA	B	902	-	-	13/48/64/64	0/3/3/3
3	COA	A	902	-	-	22/48/64/64	0/3/3/3
2	FAD	C	901	-	-	10/34/50/50	0/6/6/6
2	FAD	B	901	-	-	3/34/50/50	0/6/6/6
2	FAD	D	901	-	-	5/34/50/50	0/6/6/6

The worst 5 of 119 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	902	COA	P2A-O3A	8.33	1.68	1.59
3	A	902	COA	P1A-O3A	7.26	1.67	1.59
3	C	902	COA	P1A-O3A	6.87	1.66	1.59
3	A	902	COA	P2A-O3A	6.72	1.66	1.59
3	D	902	COA	P2A-O3A	6.43	1.66	1.59

The worst 5 of 184 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	902	COA	C4A-N9A-C8A	8.40	114.56	105.74
3	D	902	COA	C4A-N9A-C8A	8.12	114.26	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	902	COA	C4A-N9A-C8A	7.84	113.97	105.74
3	A	902	COA	C2P-C3P-N4P	-7.53	95.22	112.31
3	B	902	COA	C4A-N9A-C8A	7.33	113.44	105.74

There are no chirality outliers.

5 of 82 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	901	FAD	C5B-O5B-PA-O1A
2	A	901	FAD	C3'-C4'-C5'-O5'
2	A	901	FAD	O4'-C4'-C5'-O5'
2	A	901	FAD	C5'-O5'-P-O3P
2	A	901	FAD	PA-O3P-P-O5'

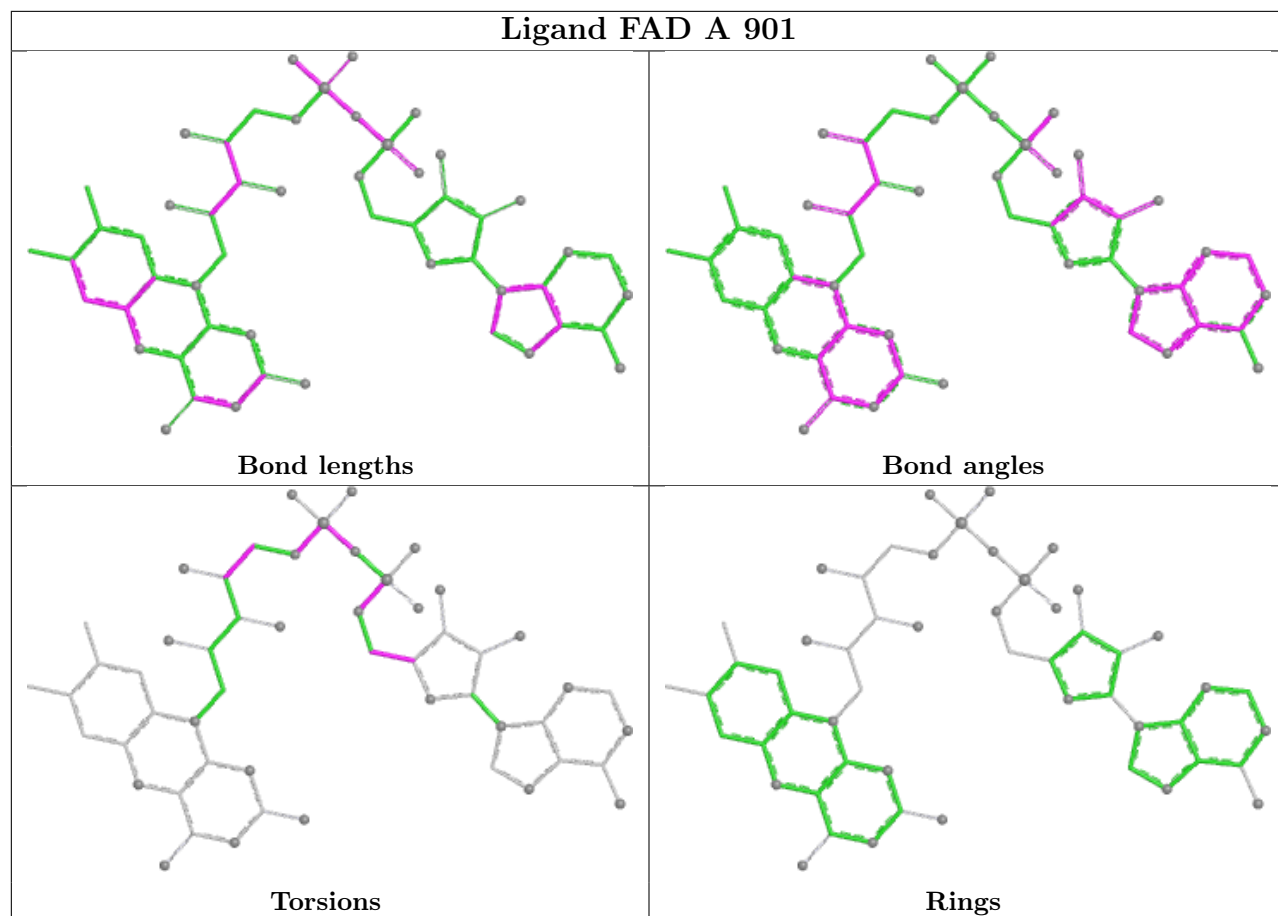
There are no ring outliers.

8 monomers are involved in 52 short contacts:

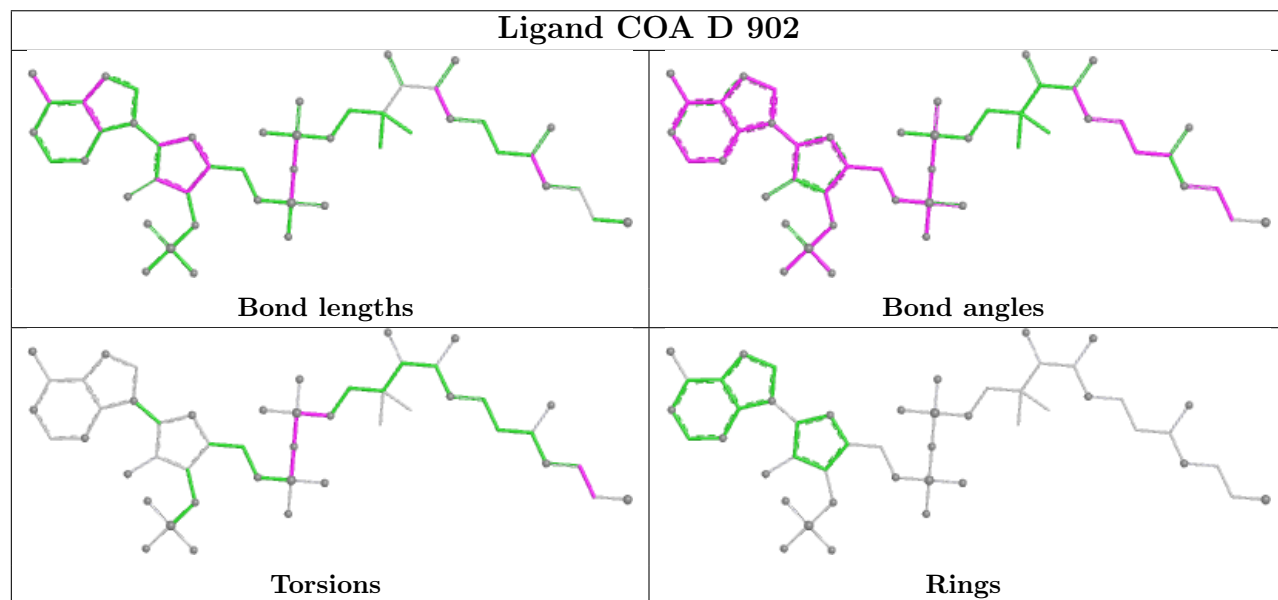
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	FAD	2	0
3	D	902	COA	8	0
3	C	902	COA	12	0
3	B	902	COA	8	0
3	A	902	COA	8	0
2	C	901	FAD	6	0
2	B	901	FAD	3	0
2	D	901	FAD	5	0

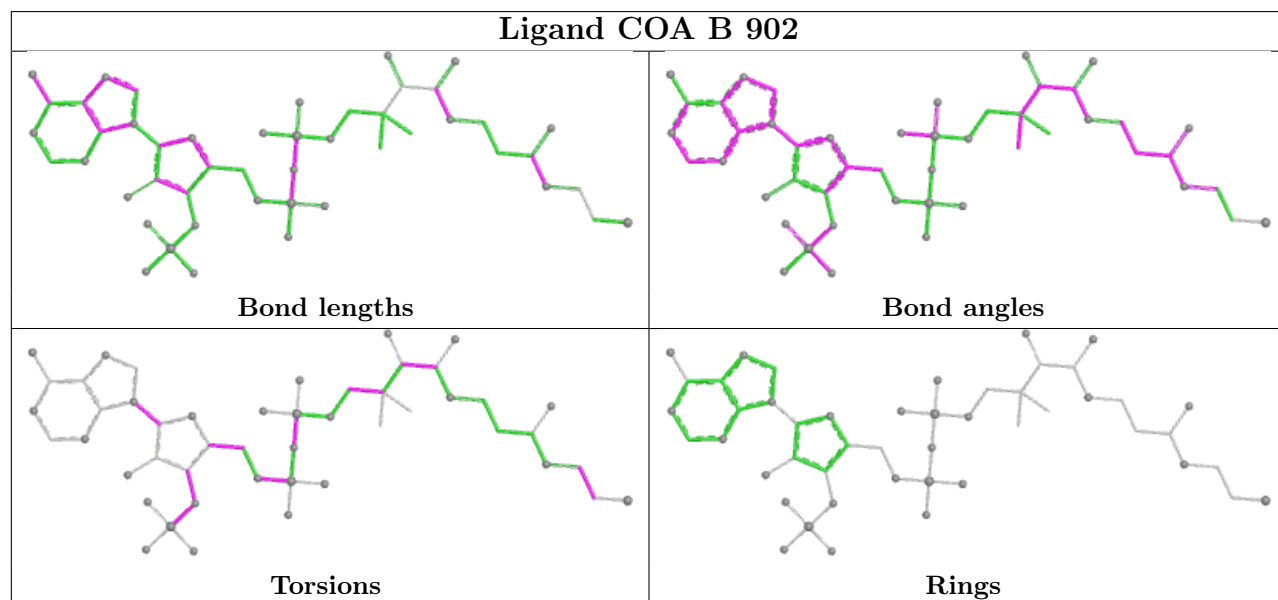
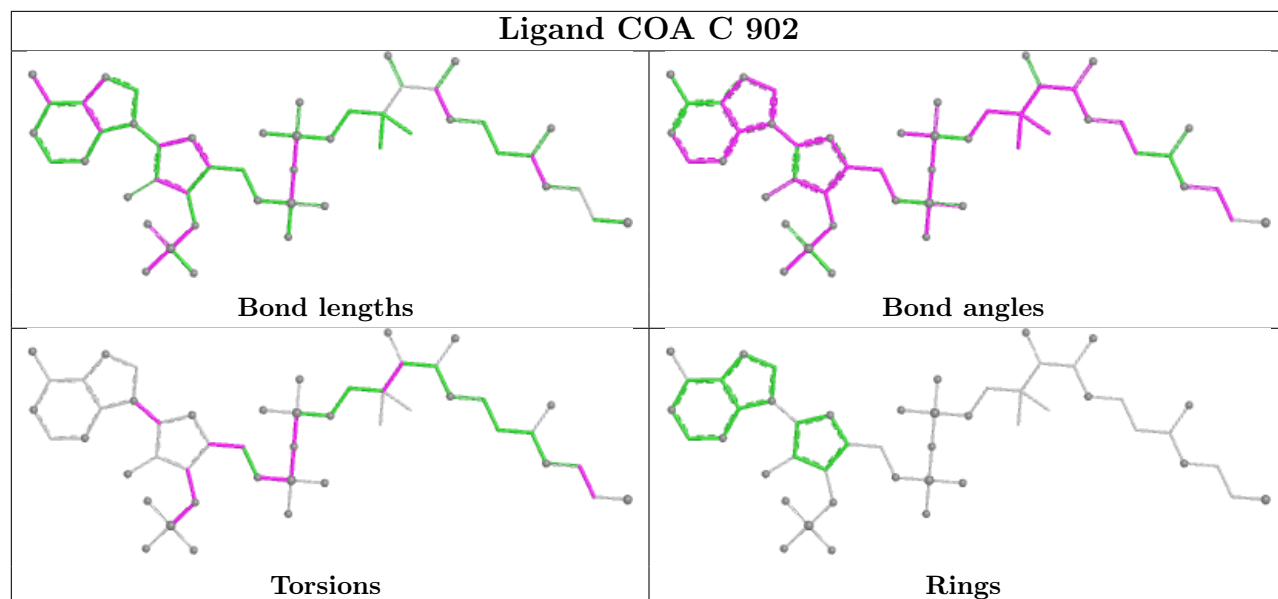
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

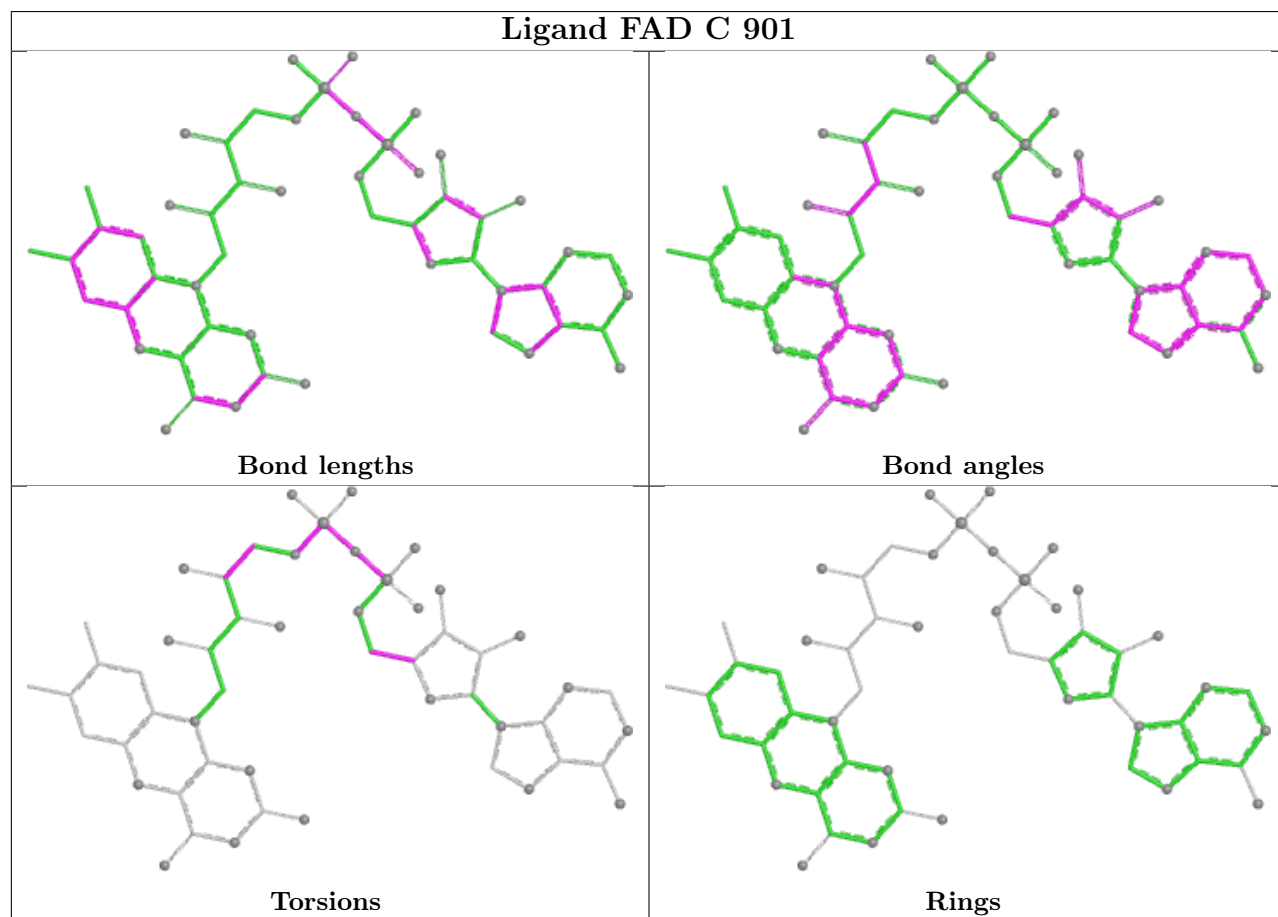
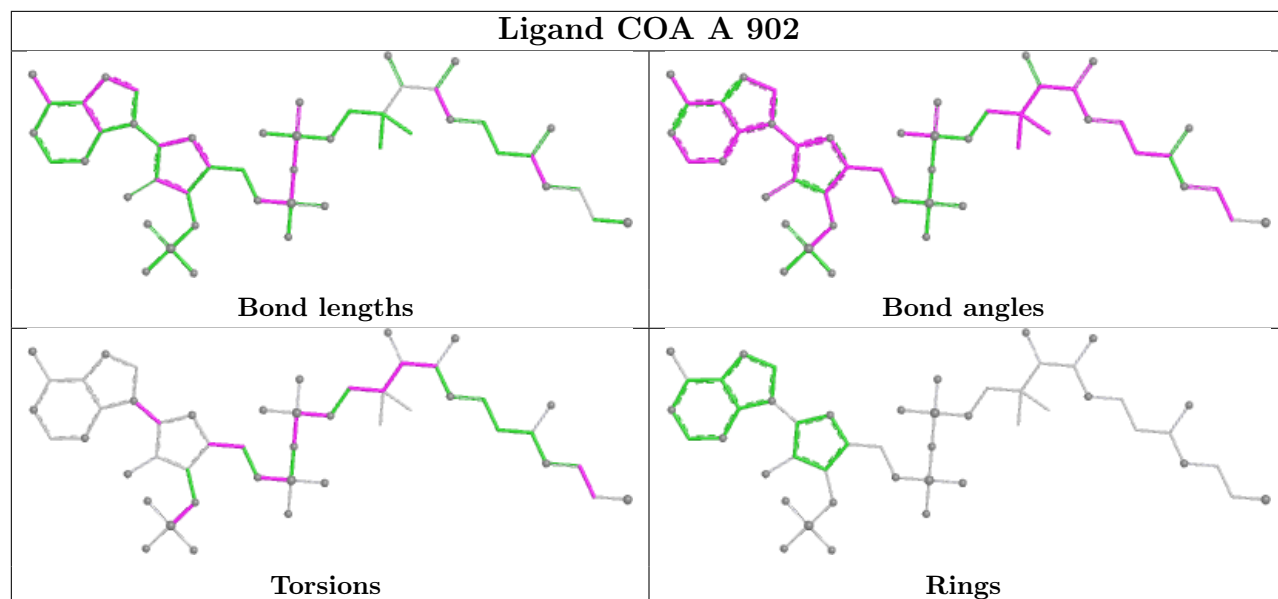
Ligand FAD A 901

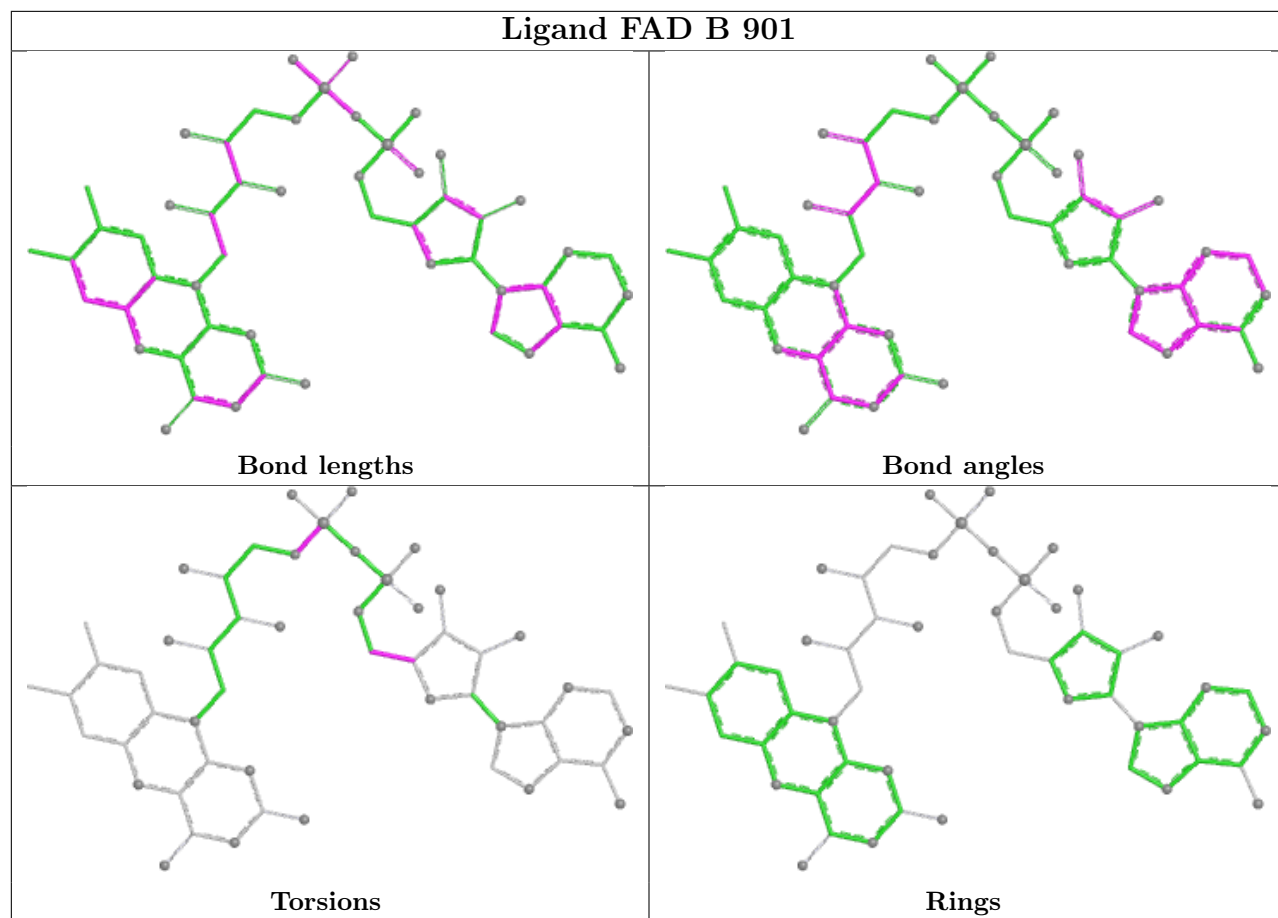


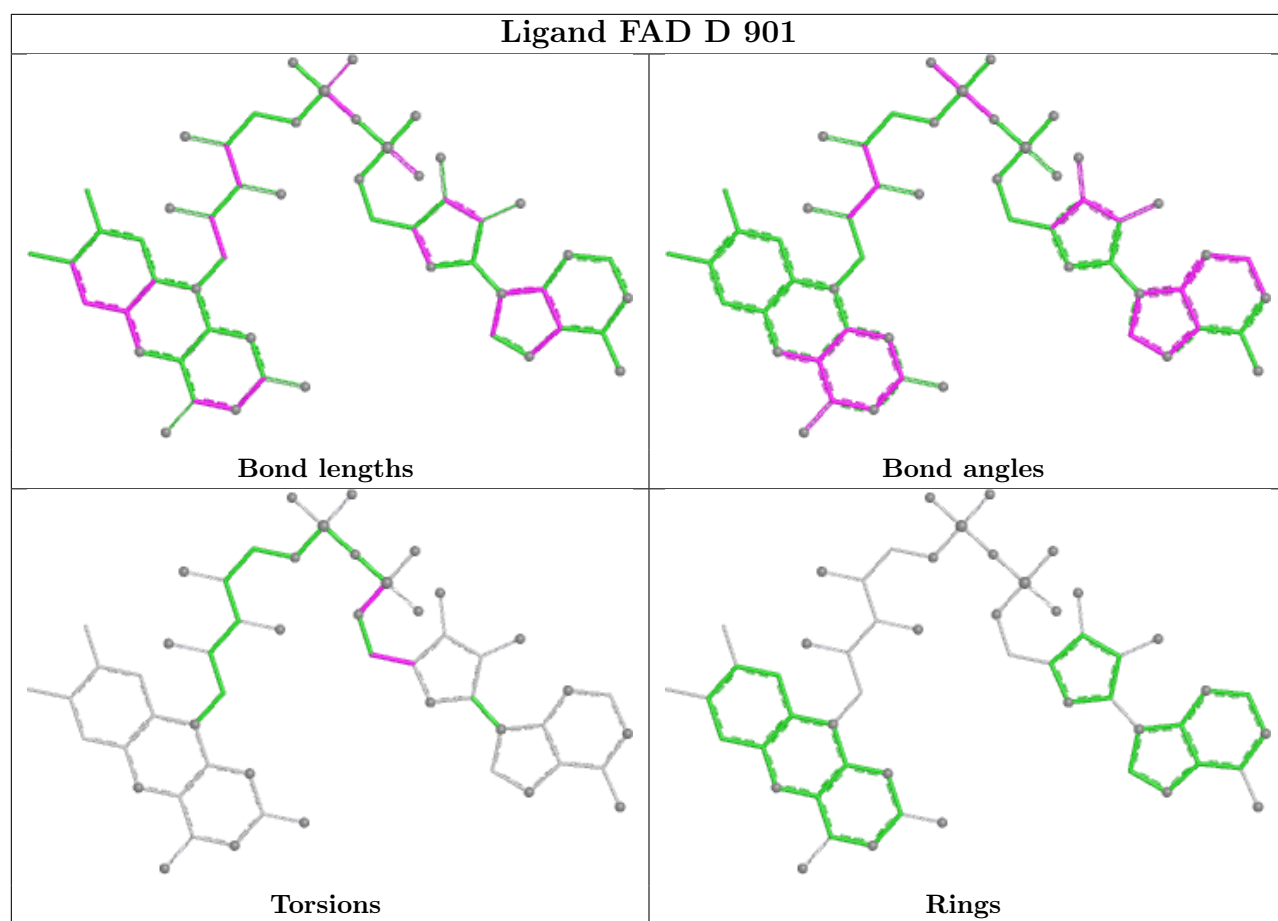
Ligand COA D 902











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	541/551 (98%)	-0.27	1 (0%) 91 83	26, 47, 71, 87	0
1	B	541/551 (98%)	-0.24	3 (0%) 85 70	23, 48, 72, 97	0
1	C	535/551 (97%)	-0.04	3 (0%) 85 70	39, 60, 84, 174	0
1	D	536/551 (97%)	-0.17	2 (0%) 88 76	33, 58, 83, 112	0
All	All	2153/2204 (97%)	-0.18	9 (0%) 88 76	23, 53, 79, 174	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	194	ASP	3.7
1	D	507	ASP	2.5
1	C	513	LYS	2.4
1	B	233	ALA	2.3
1	D	482	GLU	2.2

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](#)

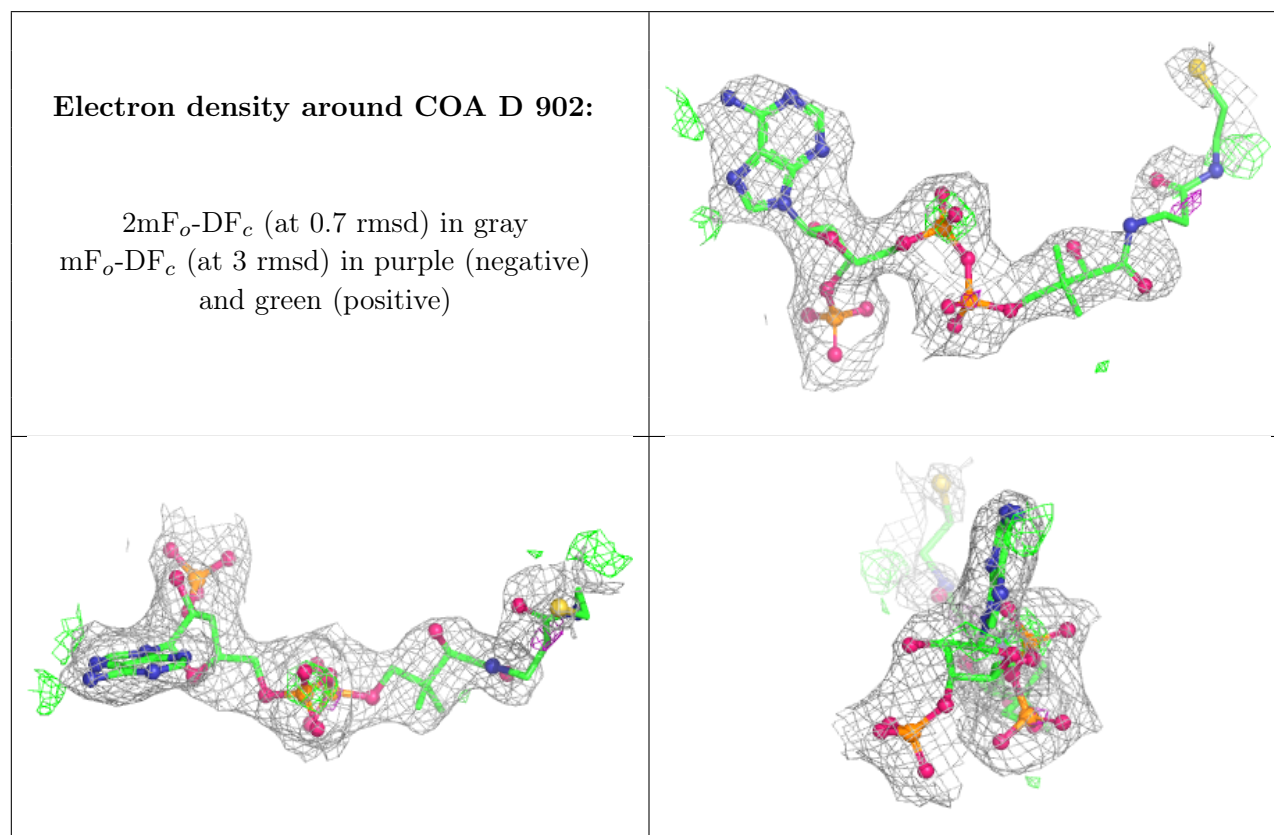
There are no oligosaccharides in this entry.

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.

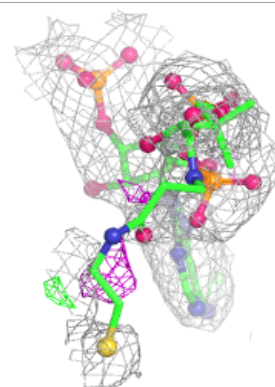
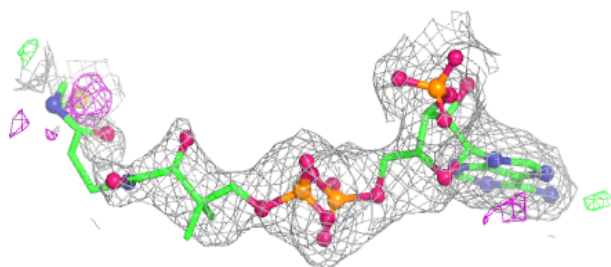
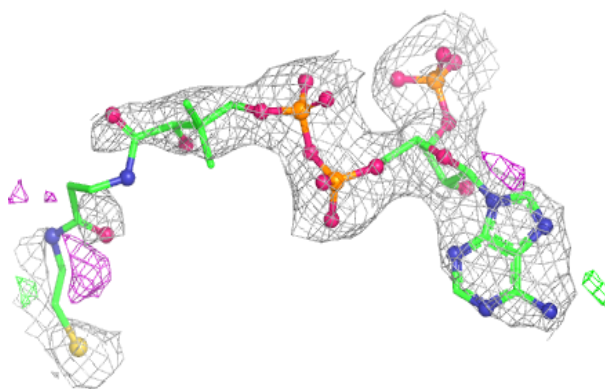
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CA	A	903	1/1	0.76	0.37	122,122,122,122	0
4	CA	C	904	1/1	0.78	0.24	102,102,102,102	0
4	CA	B	903	1/1	0.85	0.20	69,69,69,69	0
3	COA	D	902	48/48	0.88	0.12	34,60,89,221	0
4	CA	C	903	1/1	0.90	0.09	62,62,62,62	0
3	COA	B	902	48/48	0.91	0.11	37,62,88,91	0
3	COA	A	902	48/48	0.92	0.10	31,53,84,91	0
3	COA	C	902	48/48	0.92	0.12	41,79,121,123	0
2	FAD	B	901	53/53	0.94	0.11	39,64,80,101	0
2	FAD	C	901	53/53	0.94	0.08	27,45,61,74	0
2	FAD	D	901	53/53	0.96	0.07	28,47,63,67	0
2	FAD	A	901	53/53	0.96	0.07	29,45,56,68	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.

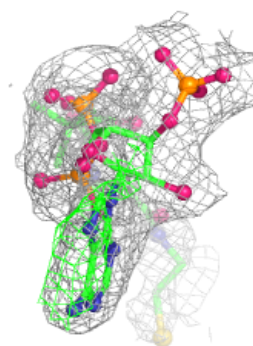
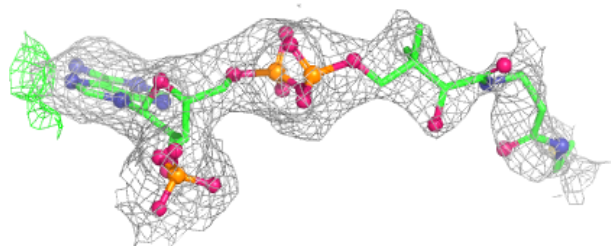
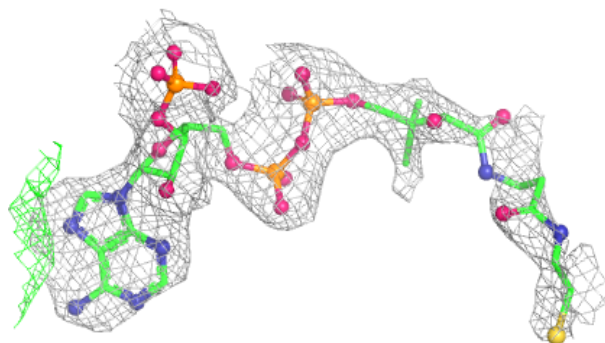


Electron density around COA B 902:

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

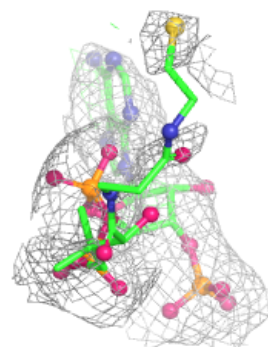
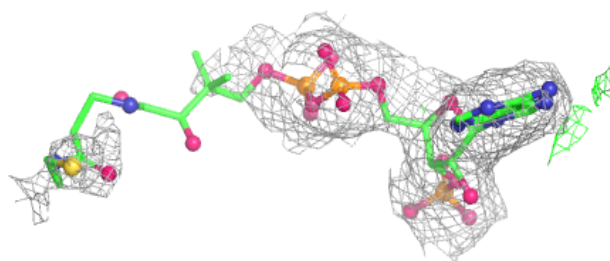
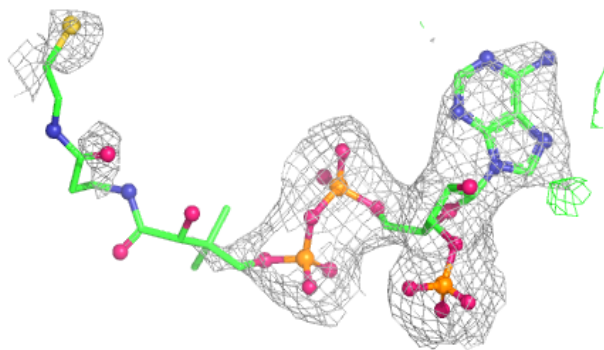
**Electron density around COA A 902:**

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

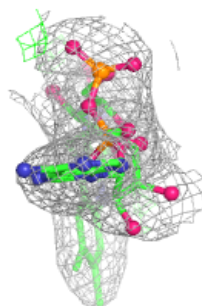
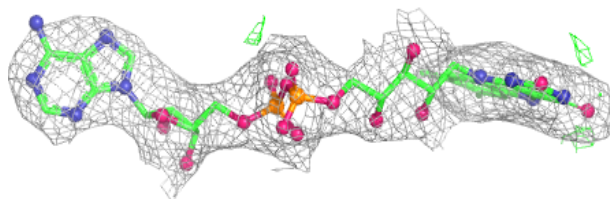
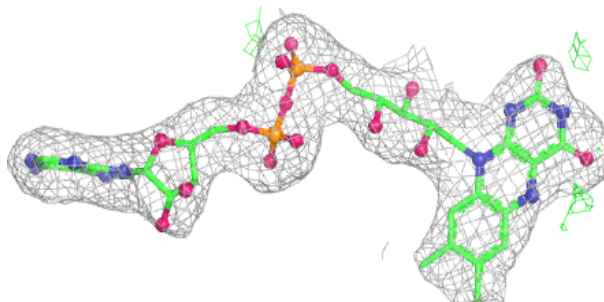


Electron density around COA C 902:

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

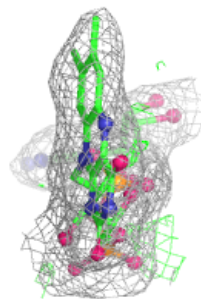
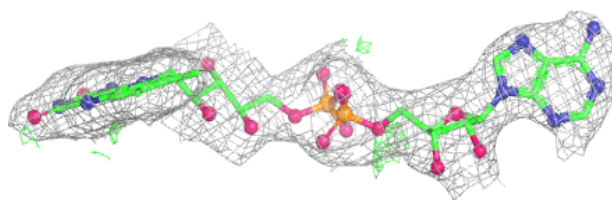
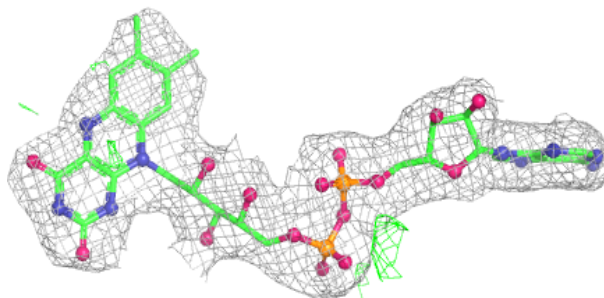
**Electron density around FAD B 901:**

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

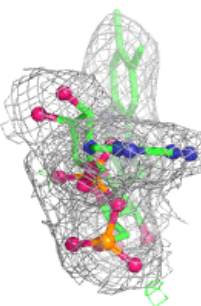
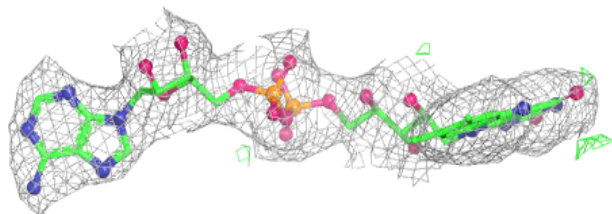
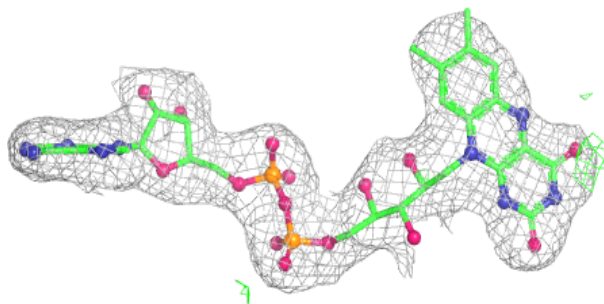


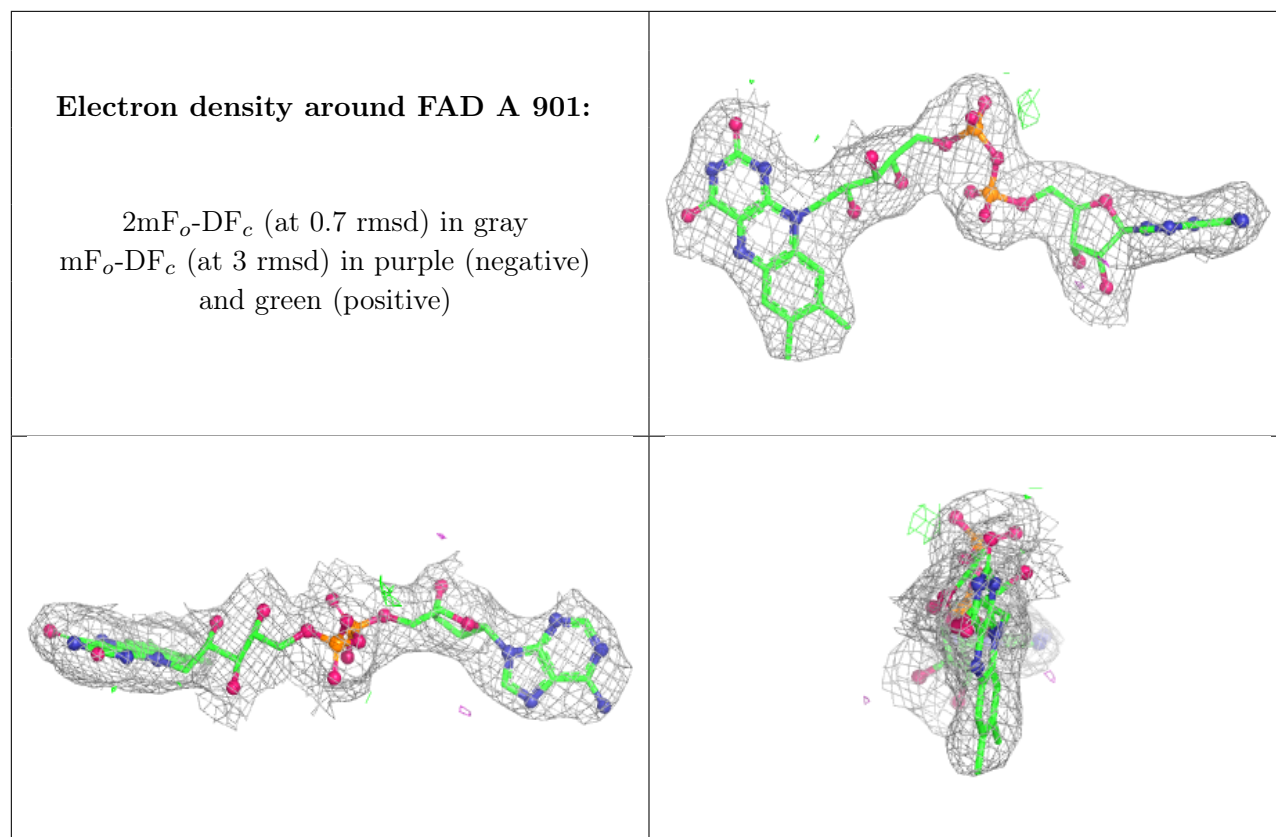
Electron density around FAD C 901:

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

**Electron density around FAD D 901:**

$2mF_o-DF_c$ (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.