wwPDB X-ray Structure Validation Summary Report ⓘ

May 23, 2020 – 02:16 am BST

PDB ID	:	2XLR
Title	:	Joint-functions of protein residues and NADP(H) in oxygen-activation by flavin-containing monooxygenase: Asn78Asp mutant
Authors	:	Orru, R.; Fraaije, M.W.; Mattevi, A.
Deposited on	:	2010-07-21
Resolution	:	2.55 Å(reported)

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

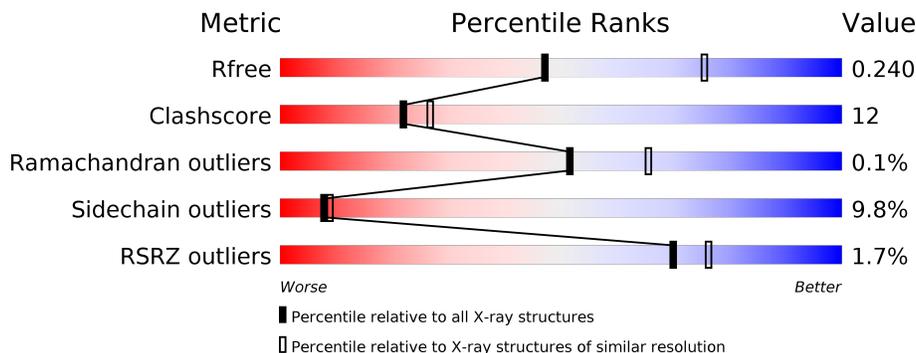|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.55 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	Percentile Ranks	Value
Rfree		0.240
Clashscore		12
Ramachandran outliers		0.1%
Sidechain outliers		9.8%
RSRZ outliers		1.7%

Worse ... *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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 <=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	461	3% / 67% / 23% / 6% ·
1	B	461	77% / 16% · · ·
1	C	461	% / 77% / 16% · · ·
1	D	461	3% / 68% / 23% / 5% ·

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 15348 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 FLAVIN-CONTAINING MONOOXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	446	Total 3652	C 2341	N 605	O 685	S 21	0	0	0
1	B	447	Total 3661	C 2347	N 607	O 686	S 21	0	0	0
1	C	452	Total 3700	C 2373	N 612	O 694	S 21	0	0	0
1	D	447	Total 3658	C 2344	N 606	O 687	S 21	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q83XK4
A	2	ALA	-	expression tag	UNP Q83XK4
A	3	MET	-	expression tag	UNP Q83XK4
A	4	GLY	-	expression tag	UNP Q83XK4
A	5	SER	-	expression tag	UNP Q83XK4
A	78	ASP	ASN	engineered mutation	UNP Q83XK4
A	158	ALA	GLU	conflict	UNP Q83XK4
A	159	ALA	GLU	conflict	UNP Q83XK4
B	1	GLY	-	expression tag	UNP Q83XK4
B	2	ALA	-	expression tag	UNP Q83XK4
B	3	MET	-	expression tag	UNP Q83XK4
B	4	GLY	-	expression tag	UNP Q83XK4
B	5	SER	-	expression tag	UNP Q83XK4
B	78	ASP	ASN	engineered mutation	UNP Q83XK4
B	158	ALA	GLU	conflict	UNP Q83XK4
B	159	ALA	GLU	conflict	UNP Q83XK4
C	1	GLY	-	expression tag	UNP Q83XK4
C	2	ALA	-	expression tag	UNP Q83XK4
C	3	MET	-	expression tag	UNP Q83XK4
C	4	GLY	-	expression tag	UNP Q83XK4
C	5	SER	-	expression tag	UNP Q83XK4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	78	ASP	ASN	engineered mutation	UNP Q83XK4
C	158	ALA	GLU	conflict	UNP Q83XK4
C	159	ALA	GLU	conflict	UNP Q83XK4
D	1	GLY	-	expression tag	UNP Q83XK4
D	2	ALA	-	expression tag	UNP Q83XK4
D	3	MET	-	expression tag	UNP Q83XK4
D	4	GLY	-	expression tag	UNP Q83XK4
D	5	SER	-	expression tag	UNP Q83XK4
D	78	ASP	ASN	engineered mutation	UNP Q83XK4
D	158	ALA	GLU	conflict	UNP Q83XK4
D	159	ALA	GLU	conflict	UNP Q83XK4

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).
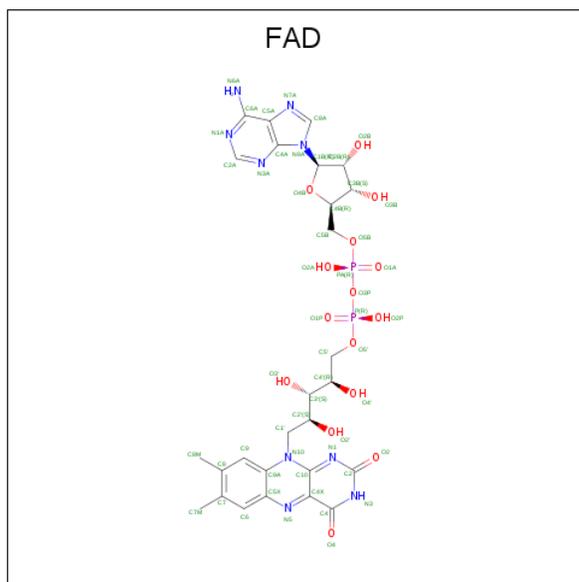
| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).

NAP

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

• Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	53	Total	O	0	0
			53	53		
4	B	85	Total	O	0	0
			85	85		
4	C	91	Total	O	0	0
			91	91		
4	D	44	Total	O	0	0
			44	44		
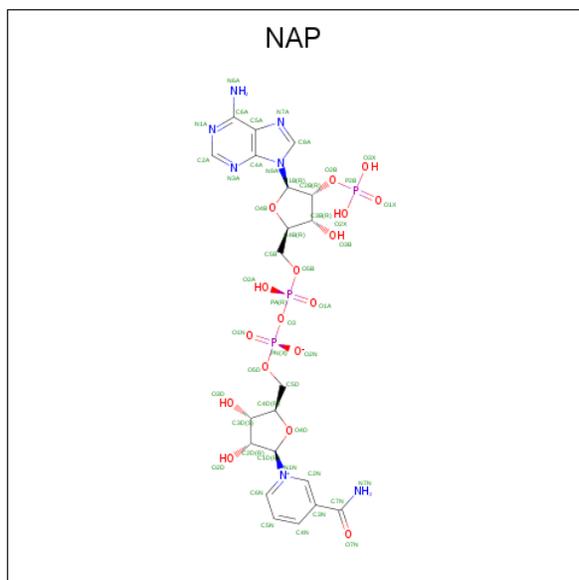
3 Residue-property plots ⓘ

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.

- Molecule 1: FLAVIN-CONTAINING MONOOXYGENASE
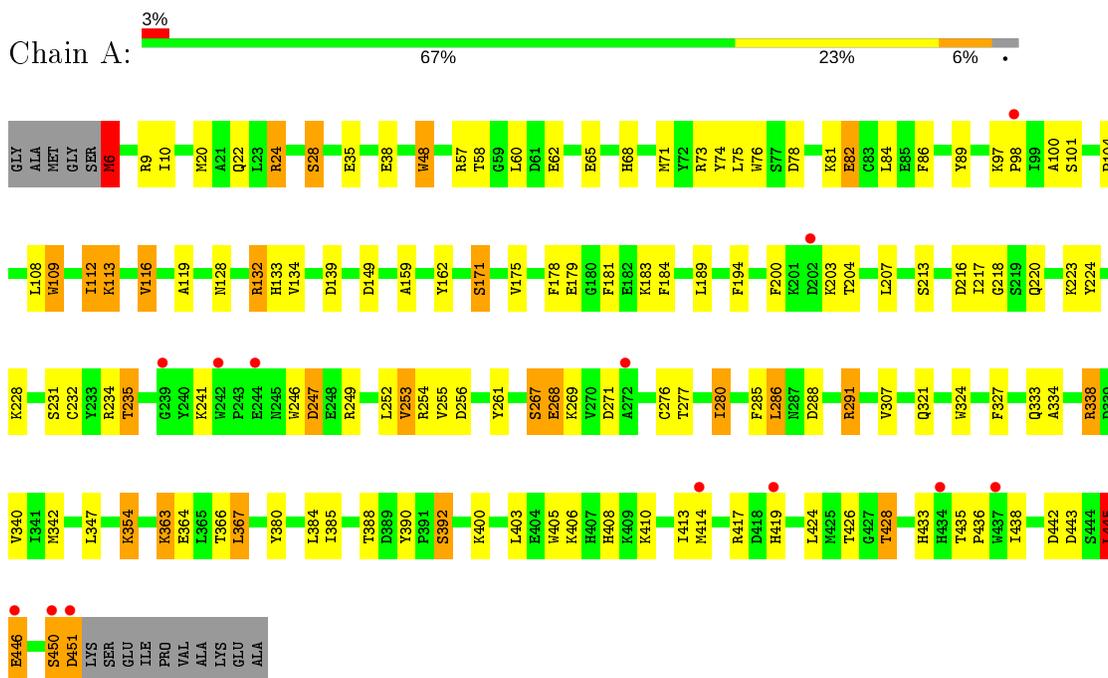
- Molecule 1: FLAVIN-CONTAINING MONOOXYGENASE

- Molecule 1: FLAVIN-CONTAINING MONOOXYGENASE

• Molecule 1: FLAVIN-CONTAINING MONOOXYGENASE

Chain D:
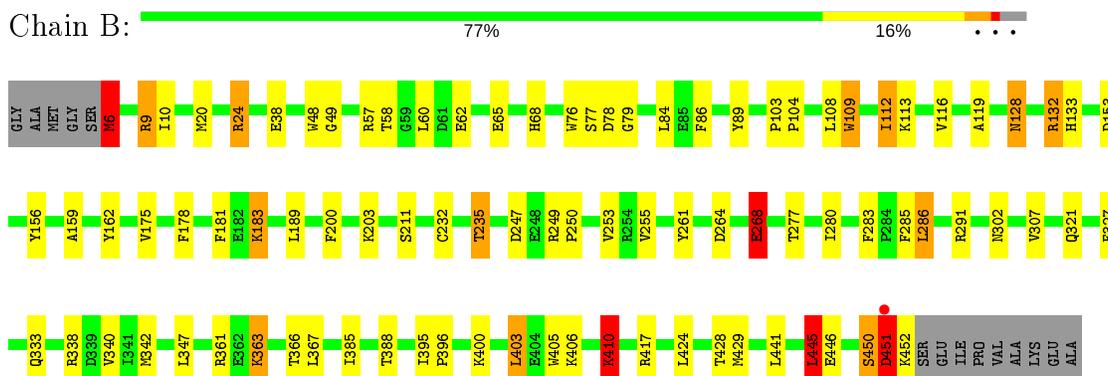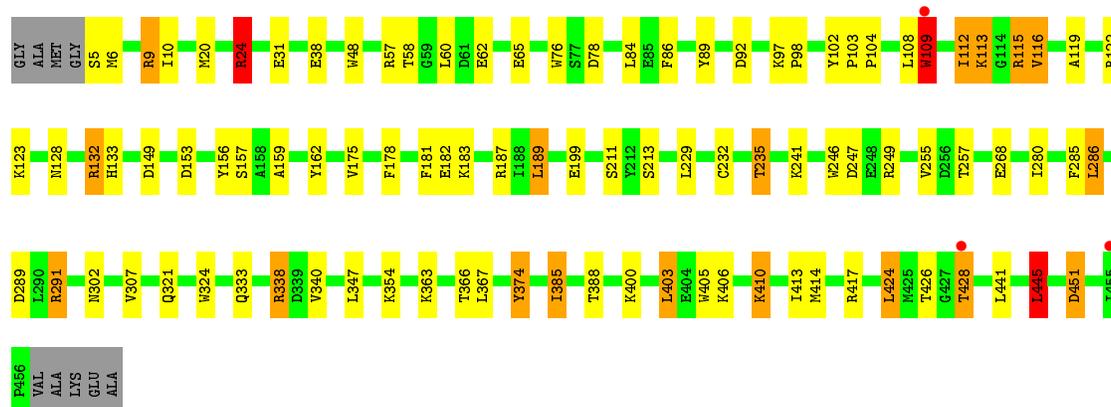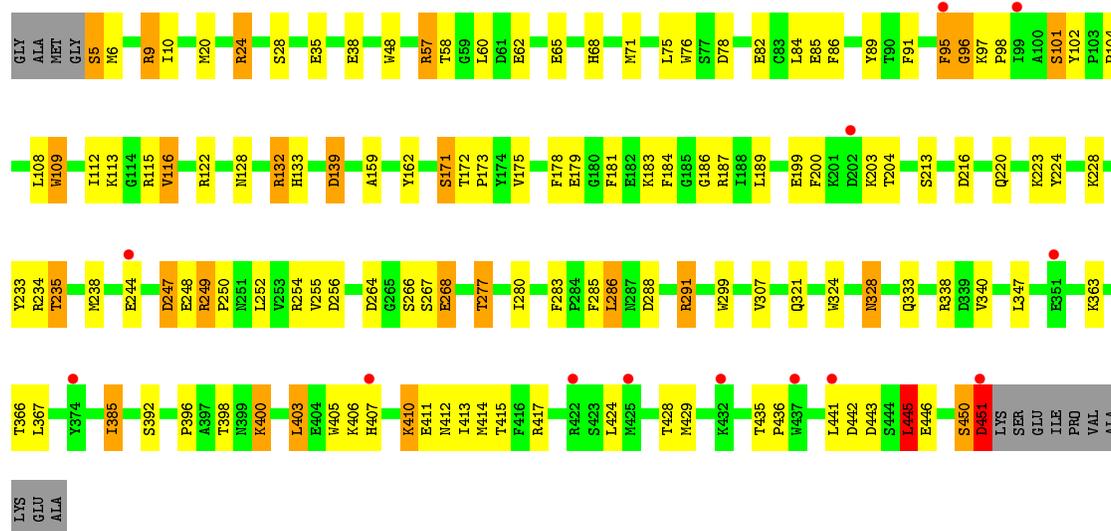
4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	214.06Å 214.06Å 152.81Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	53.51 – 2.55 51.64 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.9 (53.51-2.55) 99.9 (51.64-2.55)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.36 (at 2.55Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.214 , 0.244 0.213 , 0.240	Depositor DCC
R_{free} test set	6422 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	45.1	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 30.9	EDS
L-test for twinning[2]	$<|L|> = 0.50, <L^2> = 0.33$	Xtriage
Estimated twinning fraction	0.028 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	15348	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.83% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAP, 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	1.30	11/3765 (0.3%)	1.13	24/5112 (0.5%)
1	B	1.11	8/3774 (0.2%)	0.93	8/5123 (0.2%)
1	C	1.19	16/3815 (0.4%)	0.99	19/5180 (0.4%)
1	D	1.18	7/3771 (0.2%)	1.00	16/5120 (0.3%)
All	All	1.20	42/15125 (0.3%)	1.01	67/20535 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	451	ASP	CB-CG	-26.44	0.96	1.51
1	C	109	TRP	CE3-CZ3	-19.23	1.05	1.38
1	C	451	ASP	CB-CG	-13.89	1.22	1.51
1	B	451	ASP	CB-CG	-12.51	1.25	1.51
1	A	451	ASP	CA-C	-11.92	1.22	1.52

The worst 5 of 67 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	451	ASP	CB-CG-OD1	-20.38	99.96	118.30
1	D	249	ARG	NE-CZ-NH2	18.22	129.41	120.30
1	A	451	ASP	CB-CA-C	-17.26	75.88	110.40
1	A	6	MET	CA-C-N	14.04	148.09	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	451	ASP	CB-CG-OD2	11.30	128.47	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	450	SER	Peptide

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	3652	0	3436	118	0
1	B	3661	0	3450	64	0
1	C	3700	0	3487	86	0
1	D	3658	0	3442	93	0
2	A	53	0	31	0	0
2	B	53	0	31	1	0
2	C	53	0	31	0	0
2	D	53	0	31	0	0
3	A	48	0	25	7	0
3	B	48	0	25	5	0
3	C	48	0	25	4	0
3	D	48	0	25	7	0
4	A	53	0	0	7	0
4	B	85	0	0	4	0
4	C	91	0	0	6	0
4	D	44	0	0	0	0
All	All	15348	0	14039	343	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 12.

The worst 5 of 343 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:109:TRP:CH2	1:C:113:LYS:HD3	1.24	1.64
1:C:109:TRP:CZ3	1:C:113:LYS:HD3	1.16	1.63
1:C:109:TRP:CH2	1:C:113:LYS:CD	2.01	1.40
1:C:109:TRP:CZ3	1:C:113:LYS:CD	2.03	1.39
1:A:204:THR:N	1:A:271:ASP:OD2	1.57	1.38

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	444/461 (96%)	426 (96%)	18 (4%)	0	100	100
1	B	445/461 (96%)	434 (98%)	11 (2%)	0	100	100
1	C	450/461 (98%)	438 (97%)	12 (3%)	0	100	100
1	D	445/461 (96%)	430 (97%)	13 (3%)	2 (0%)	34	46
All	All	1784/1844 (97%)	1728 (97%)	54 (3%)	2 (0%)	51	65

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	96	GLY
1	D	450	SER

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	386/397 (97%)	347 (90%)	39 (10%)	7	8
1	B	387/397 (98%)	352 (91%)	35 (9%)	9	11
1	C	392/397 (99%)	355 (91%)	37 (9%)	8	10
1	D	387/397 (98%)	346 (89%)	41 (11%)	6	7
All	All	1552/1588 (98%)	1400 (90%)	152 (10%)	8	9

5 of 152 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	428	THR
1	C	116	VAL
1	D	385	ILE
1	B	441	LEU
1	C	48	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	133	HIS
1	C	45	GLN
1	D	412	ASN
1	B	321	GLN
1	B	407	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
3	NAP	D	501	-	45,52,52	1.75	10 (22%)	56,80,80	1.92	13 (23%)
3	NAP	A	501	-	45,52,52	1.54	8 (17%)	56,80,80	2.04	13 (23%)
2	FAD	A	500	-	51,58,58	1.44	7 (13%)	60,89,89	2.25	13 (21%)
3	NAP	C	501	-	45,52,52	1.43	7 (15%)	56,80,80	1.78	10 (17%)
2	FAD	C	500	-	51,58,58	1.57	8 (15%)	60,89,89	1.97	12 (20%)
3	NAP	B	501	-	45,52,52	1.48	8 (17%)	56,80,80	1.96	12 (21%)
2	FAD	D	500	-	51,58,58	1.56	6 (11%)	60,89,89	2.16	13 (21%)
2	FAD	B	500	-	51,58,58	1.34	6 (11%)	60,89,89	1.94	16 (26%)

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	NAP	D	501	-	-	13/31/67/67	0/5/5/5
3	NAP	A	501	-	-	13/31/67/67	0/5/5/5
2	FAD	A	500	-	-	3/30/50/50	0/6/6/6
3	NAP	C	501	-	-	6/31/67/67	0/5/5/5
2	FAD	C	500	-	-	4/30/50/50	0/6/6/6
3	NAP	B	501	-	-	11/31/67/67	0/5/5/5
2	FAD	D	500	-	-	3/30/50/50	0/6/6/6
2	FAD	B	500	-	-	4/30/50/50	0/6/6/6

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	500	FAD	C10-N1	5.95	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	501	NAP	O4B-C1B	5.52	1.48	1.41
2	C	500	FAD	C4X-N5	4.87	1.40	1.33
2	D	500	FAD	C4X-N5	4.67	1.40	1.33
2	C	500	FAD	C2A-N3A	4.35	1.39	1.32

The worst 5 of 102 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	FAD	C1'-N10-C9A	9.39	125.69	118.29
2	D	500	FAD	C1'-N10-C9A	8.45	124.94	118.29
2	B	500	FAD	C1'-N10-C9A	7.30	124.04	118.29
2	D	500	FAD	N3A-C2A-N1A	-7.05	117.66	128.68
2	A	500	FAD	C4-N3-C2	7.00	121.05	115.14

There are no chirality outliers.

5 of 57 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	501	NAP	C5B-O5B-PA-O1A
3	D	501	NAP	C5B-O5B-PA-O2A
3	D	501	NAP	C3B-C4B-C5B-O5B
3	D	501	NAP	C5D-O5D-PN-O3
3	D	501	NAP	C5D-O5D-PN-O1N

There are no ring outliers.

5 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	501	NAP	7	0
3	A	501	NAP	7	0
3	C	501	NAP	4	0
3	B	501	NAP	5	0
2	B	500	FAD	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.
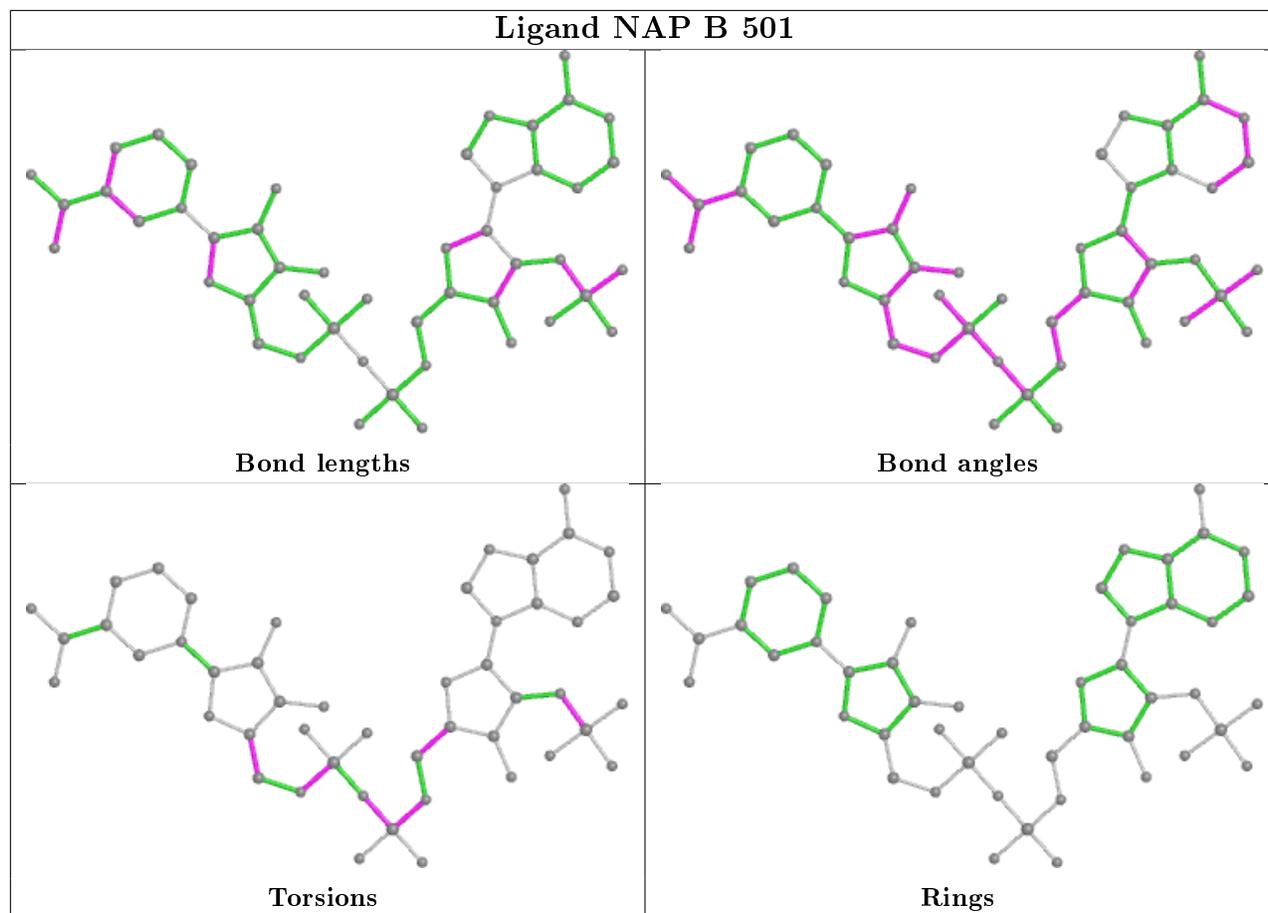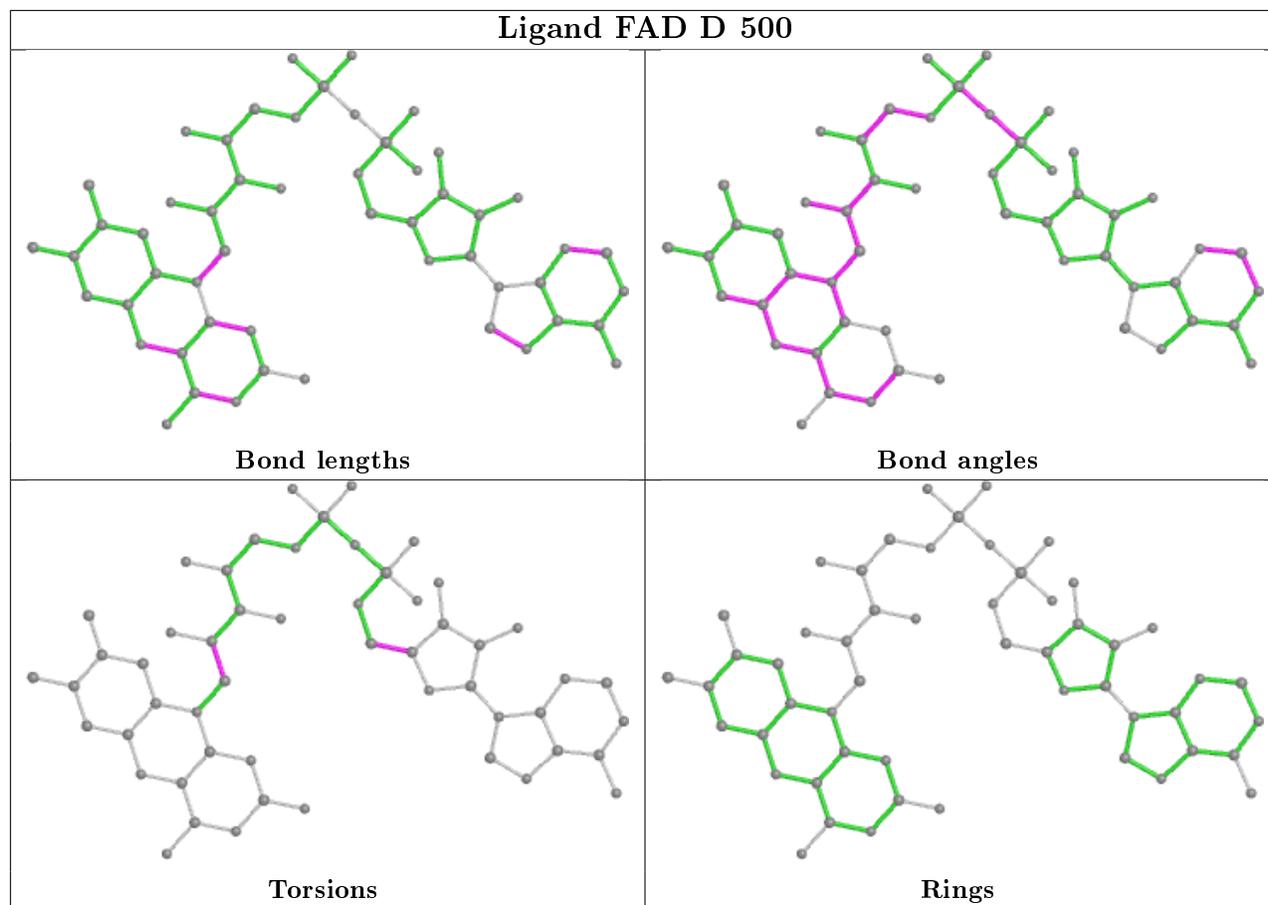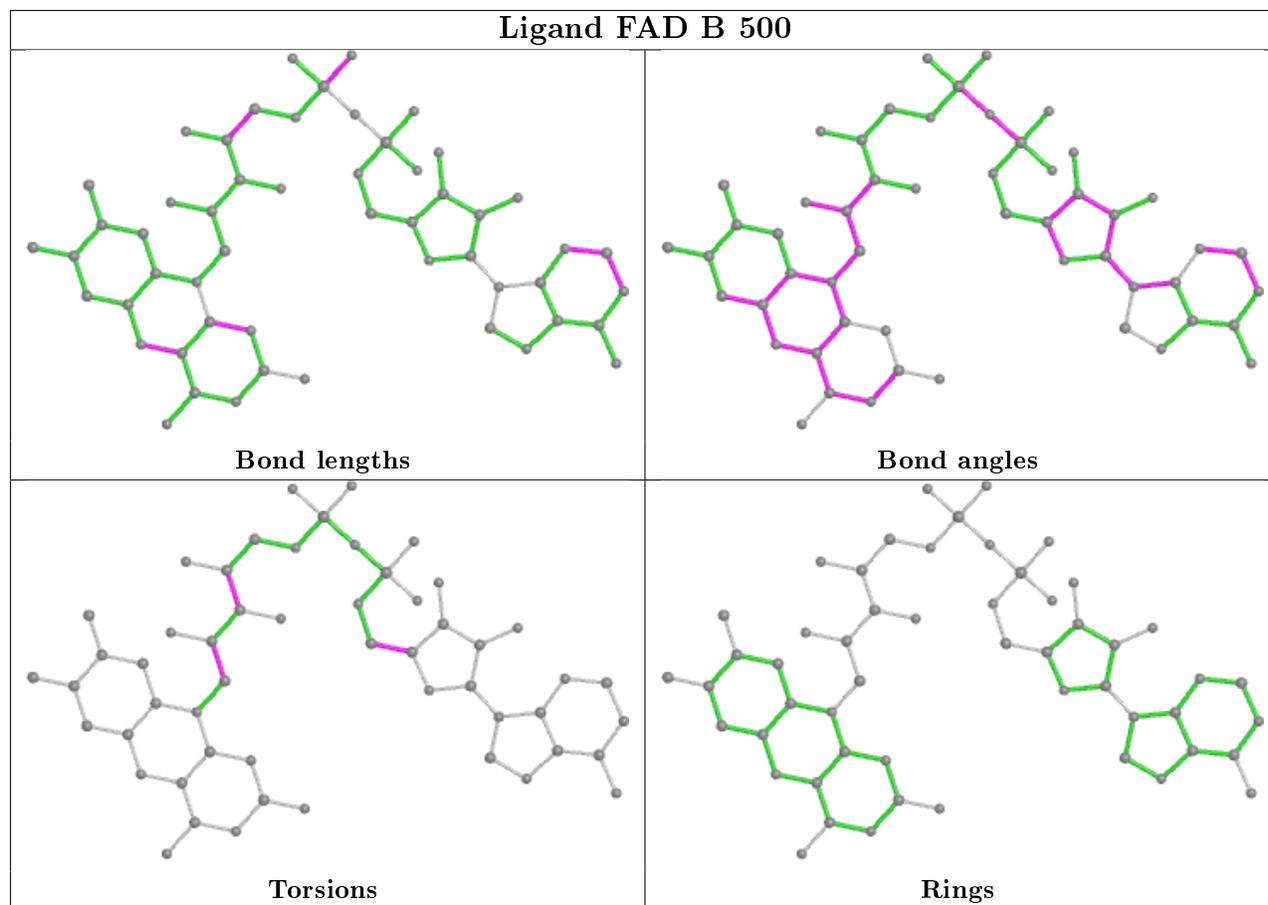
Ligand NAP D 501	
Bond lengths	Bond angles
Torsions	Rings

Ligand NAP A 501

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD A 500

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP C 501

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD C 500

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP B 501

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD D 500

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD B 500

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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(Å²)	Q<0.9
1	A	446/461 (96%)	-0.05	13 (2%)	51	59	25, 41, 60, 72	0
1	B	447/461 (96%)	-0.17	1 (0%)	95	97	25, 40, 60, 74	0
1	C	452/461 (98%)	-0.14	3 (0%)	87	90	24, 41, 60, 86	0
1	D	447/461 (96%)	-0.04	13 (2%)	51	59	25, 41, 60, 72	1 (0%)
All	All	1792/1844 (97%)	-0.10	30 (1%)	70	76	24, 41, 60, 86	1 (0%)

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	244	GLU	3.9
1	A	451	ASP	3.4
1	C	455	ILE	3.2
1	D	202	ASP	3.1
1	B	451	ASP	2.9

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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($Å^2$)	Q<0.9
3	NAP	A	501	48/48	0.94	0.14	45,55,74,76	0
3	NAP	D	501	48/48	0.96	0.12	46,55,74,75	0
3	NAP	B	501	48/48	0.96	0.13	45,54,74,75	0
3	NAP	C	501	48/48	0.97	0.14	44,54,74,75	0
2	FAD	D	500	53/53	0.97	0.12	21,30,49,50	0
2	FAD	A	500	53/53	0.98	0.13	22,30,49,50	0
2	FAD	C	500	53/53	0.99	0.15	22,29,48,49	0
2	FAD	B	500	53/53	0.99	0.14	22,29,48,50	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 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
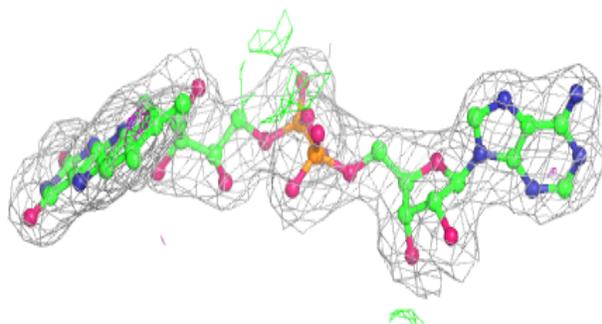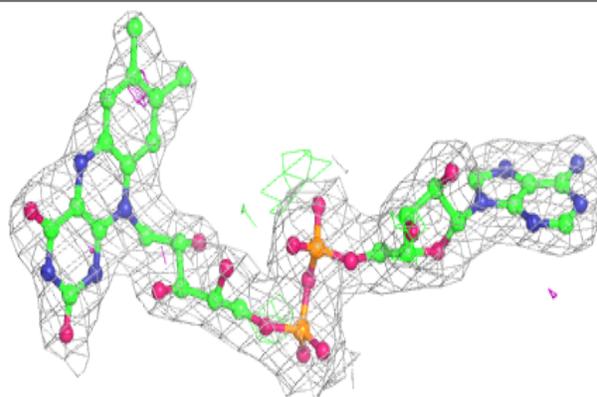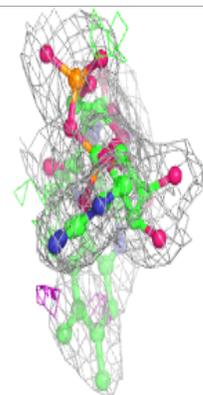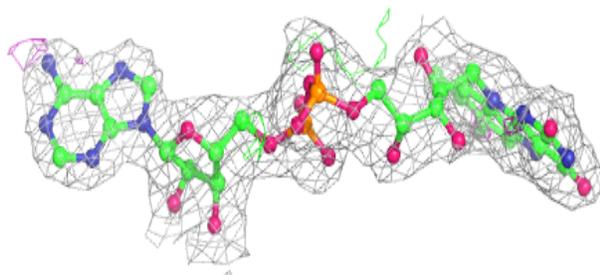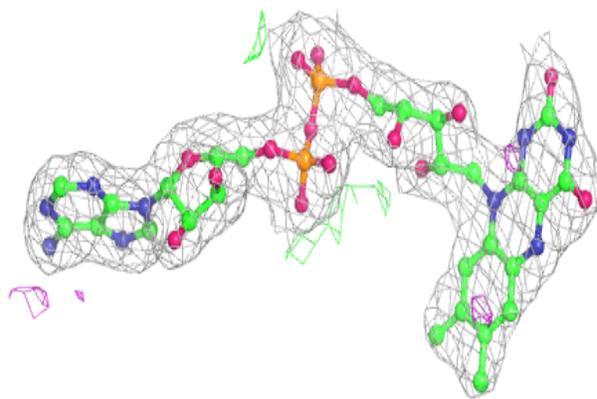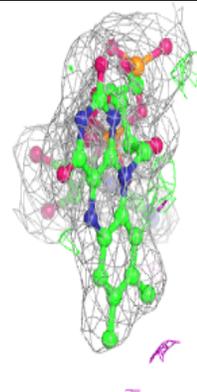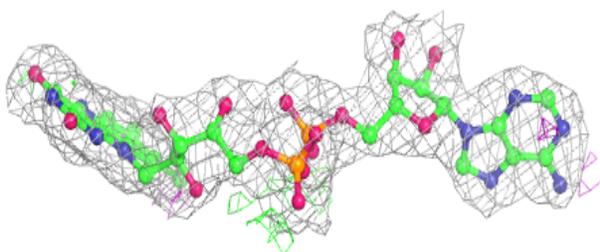mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)
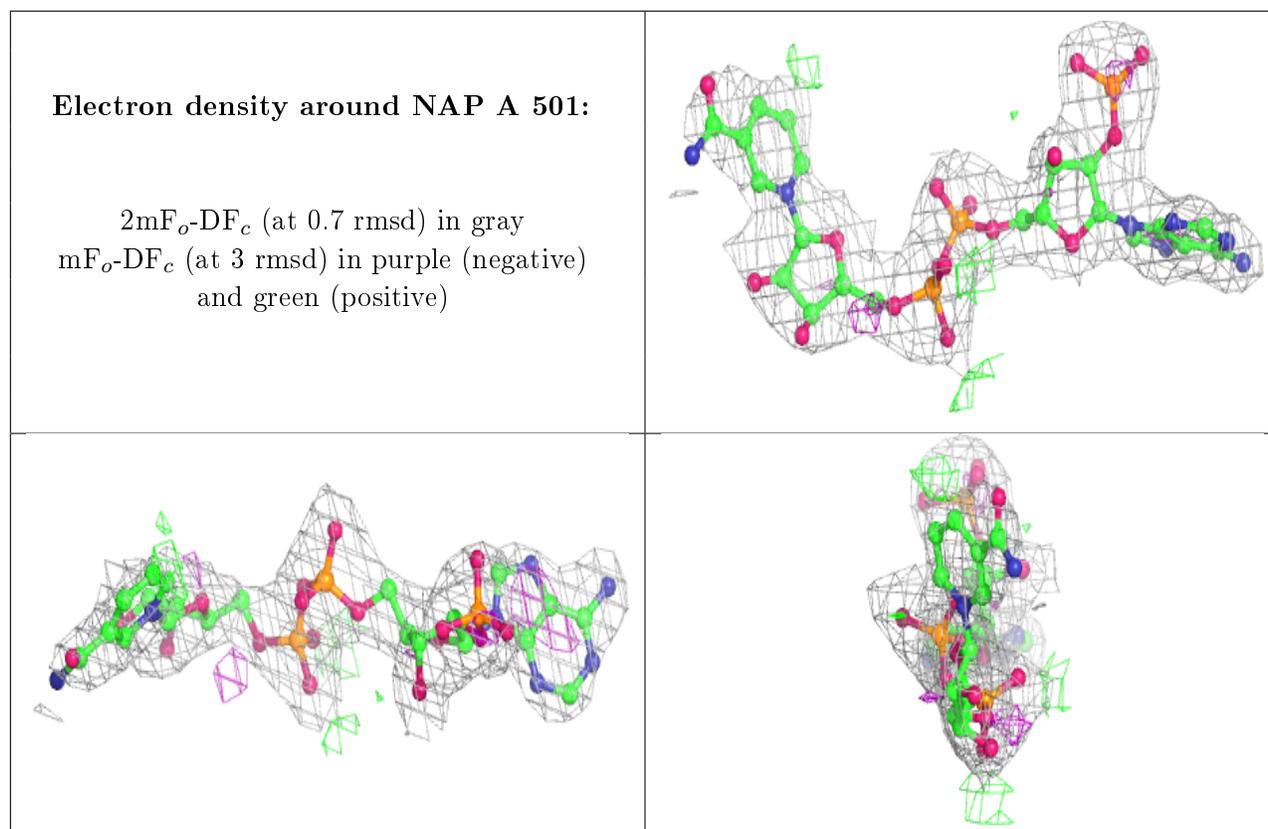
Electron density around NAP D 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
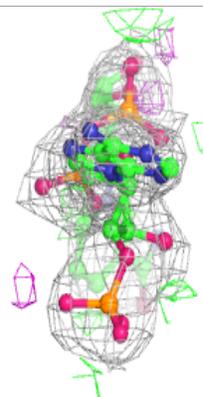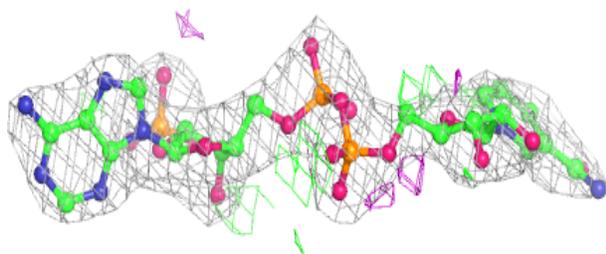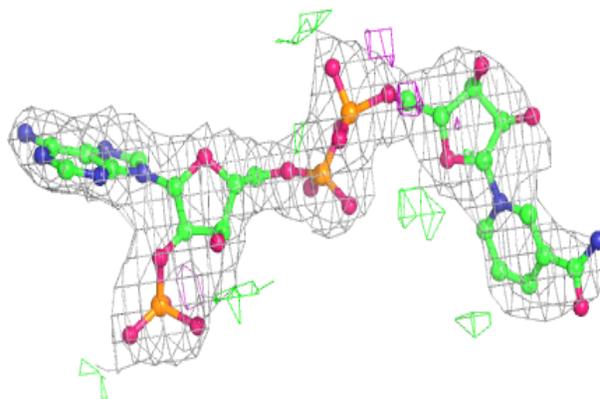
Electron density around NAP B 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
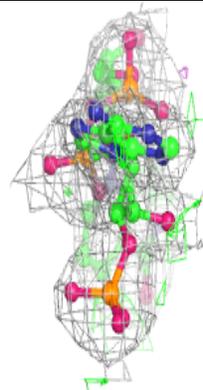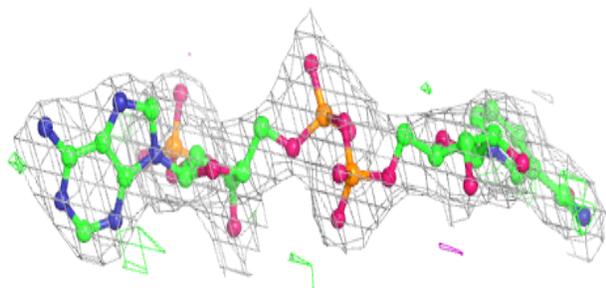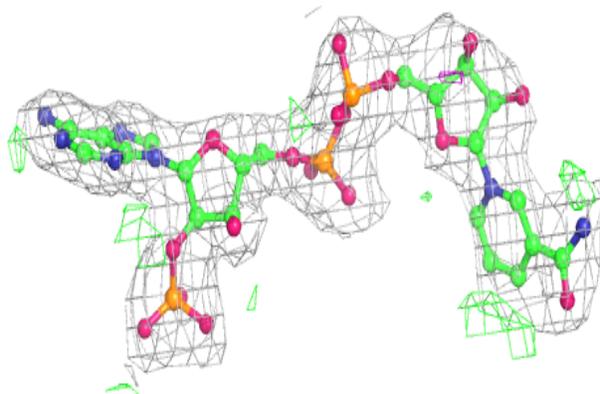
Electron density around NAP C 501:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
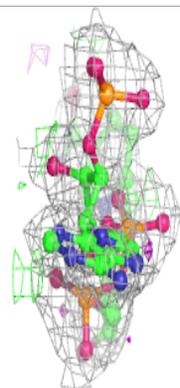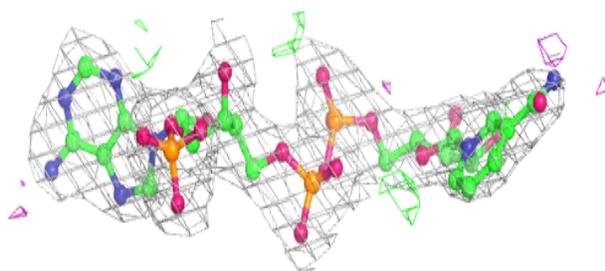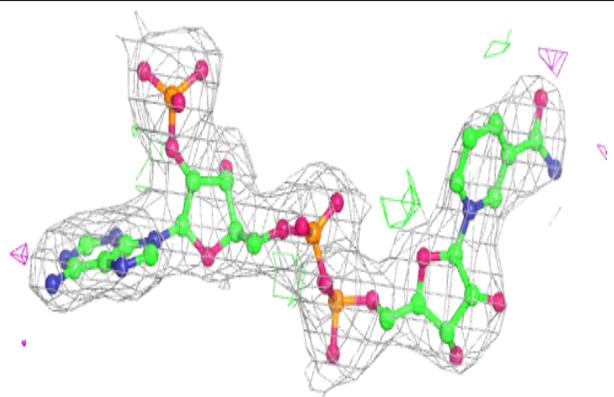
Electron density around FAD D 500:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
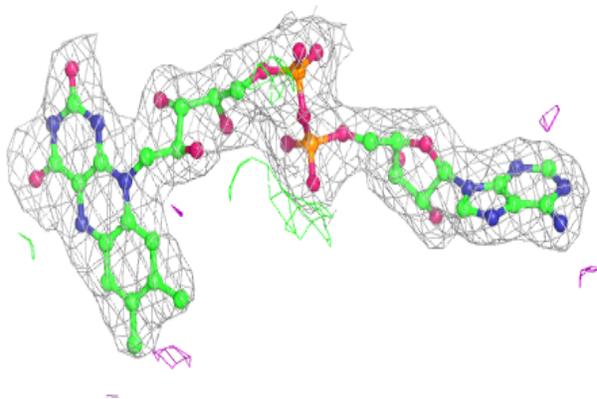$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
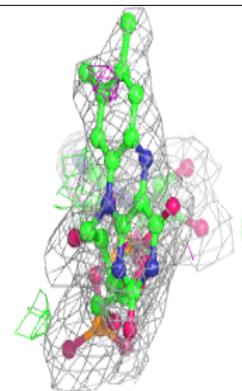
Electron density around FAD A 500:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
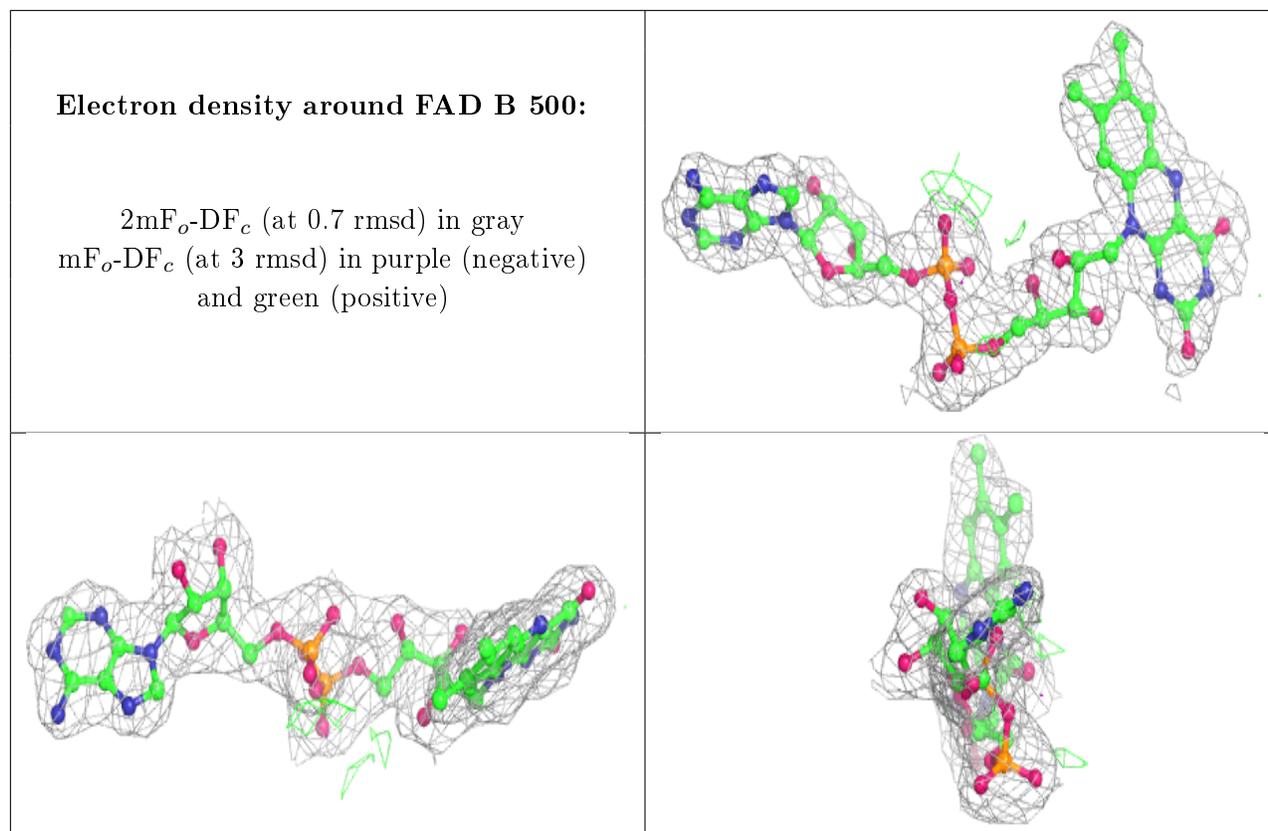mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around FAD C 500:

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 500:

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

6.5 Other polymers (i)

There are no such residues in this entry.