



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 07:51 PM UTC

PDB ID : 3CGD / pdb_00003cgd
Title : Pyridine Nucleotide Complexes with Bacillus anthracis Coenzyme A-Disulfide Reductase: A Structural Analysis of Dual NAD(P)H Specificity
Authors : Wallen, J.R.
Deposited on : 2008-03-05
Resolution : 2.25 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

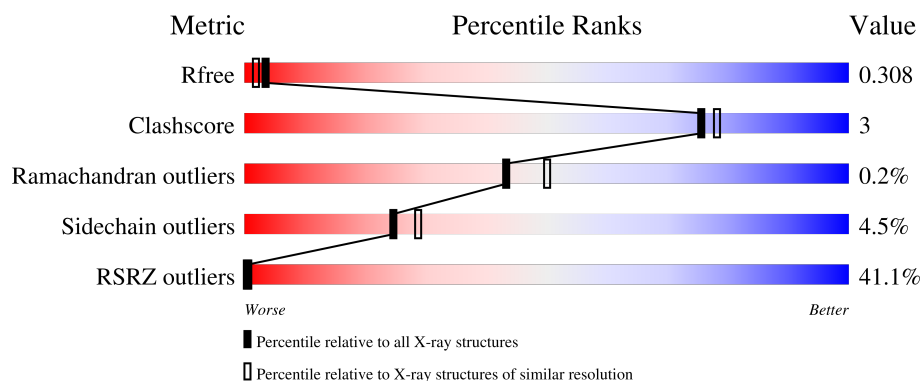
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	480	42% 82%10%8%
1	B	480	34% 82%10%8%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7735 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 Pyridine nucleotide-disulfide oxidoreductase, class I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	444	Total	C	N	O	S	0	3	0
			3496	2208	603	670	15			
1	B	444	Total	C	N	O	S	0	2	0
			3489	2203	603	668	15			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-35	MET	-	expression tag	UNP Q81TK8
A	-34	GLY	-	expression tag	UNP Q81TK8
A	-33	GLY	-	expression tag	UNP Q81TK8
A	-32	SER	-	expression tag	UNP Q81TK8
A	-31	HIS	-	expression tag	UNP Q81TK8
A	-30	HIS	-	expression tag	UNP Q81TK8
A	-29	HIS	-	expression tag	UNP Q81TK8
A	-28	HIS	-	expression tag	UNP Q81TK8
A	-27	HIS	-	expression tag	UNP Q81TK8
A	-26	HIS	-	expression tag	UNP Q81TK8
A	-25	GLY	-	expression tag	UNP Q81TK8
A	-24	MET	-	expression tag	UNP Q81TK8
A	-23	ALA	-	expression tag	UNP Q81TK8
A	-22	SER	-	expression tag	UNP Q81TK8
A	-21	MET	-	expression tag	UNP Q81TK8
A	-20	THR	-	expression tag	UNP Q81TK8
A	-19	GLY	-	expression tag	UNP Q81TK8
A	-18	GLY	-	expression tag	UNP Q81TK8
A	-17	GLN	-	expression tag	UNP Q81TK8
A	-16	GLN	-	expression tag	UNP Q81TK8
A	-15	MET	-	expression tag	UNP Q81TK8
A	-14	GLY	-	expression tag	UNP Q81TK8
A	-13	ARG	-	expression tag	UNP Q81TK8
A	-12	THR	-	expression tag	UNP Q81TK8
A	-11	LEU	-	expression tag	UNP Q81TK8

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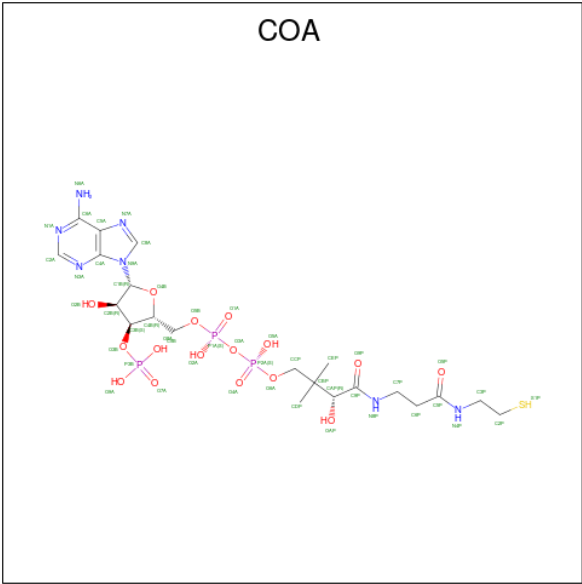
Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	TYR	-	expression tag	UNP Q81TK8
A	-9	ASP	-	expression tag	UNP Q81TK8
A	-8	ASP	-	expression tag	UNP Q81TK8
A	-7	ASP	-	expression tag	UNP Q81TK8
A	-6	ASP	-	expression tag	UNP Q81TK8
A	-5	LYS	-	expression tag	UNP Q81TK8
A	-4	ASP	-	expression tag	UNP Q81TK8
A	-3	ARG	-	expression tag	UNP Q81TK8
A	-2	TRP	-	expression tag	UNP Q81TK8
A	-1	GLY	-	expression tag	UNP Q81TK8
A	0	SER	-	expression tag	UNP Q81TK8
B	-35	MET	-	expression tag	UNP Q81TK8
B	-34	GLY	-	expression tag	UNP Q81TK8
B	-33	GLY	-	expression tag	UNP Q81TK8
B	-32	SER	-	expression tag	UNP Q81TK8
B	-31	HIS	-	expression tag	UNP Q81TK8
B	-30	HIS	-	expression tag	UNP Q81TK8
B	-29	HIS	-	expression tag	UNP Q81TK8
B	-28	HIS	-	expression tag	UNP Q81TK8
B	-27	HIS	-	expression tag	UNP Q81TK8
B	-26	HIS	-	expression tag	UNP Q81TK8
B	-25	GLY	-	expression tag	UNP Q81TK8
B	-24	MET	-	expression tag	UNP Q81TK8
B	-23	ALA	-	expression tag	UNP Q81TK8
B	-22	SER	-	expression tag	UNP Q81TK8
B	-21	MET	-	expression tag	UNP Q81TK8
B	-20	THR	-	expression tag	UNP Q81TK8
B	-19	GLY	-	expression tag	UNP Q81TK8
B	-18	GLY	-	expression tag	UNP Q81TK8
B	-17	GLN	-	expression tag	UNP Q81TK8
B	-16	GLN	-	expression tag	UNP Q81TK8
B	-15	MET	-	expression tag	UNP Q81TK8
B	-14	GLY	-	expression tag	UNP Q81TK8
B	-13	ARG	-	expression tag	UNP Q81TK8
B	-12	THR	-	expression tag	UNP Q81TK8
B	-11	LEU	-	expression tag	UNP Q81TK8
B	-10	TYR	-	expression tag	UNP Q81TK8
B	-9	ASP	-	expression tag	UNP Q81TK8
B	-8	ASP	-	expression tag	UNP Q81TK8
B	-7	ASP	-	expression tag	UNP Q81TK8
B	-6	ASP	-	expression tag	UNP Q81TK8
B	-5	LYS	-	expression tag	UNP Q81TK8

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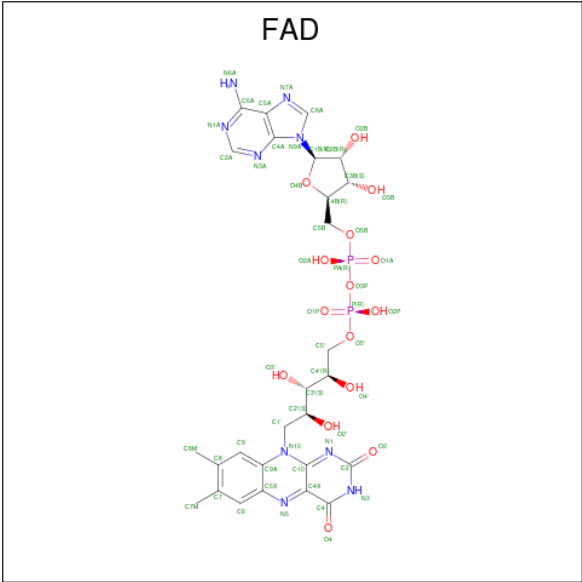
Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	ASP	-	expression tag	UNP Q81TK8
B	-3	ARG	-	expression tag	UNP Q81TK8
B	-2	TRP	-	expression tag	UNP Q81TK8
B	-1	GLY	-	expression tag	UNP Q81TK8
B	0	SER	-	expression tag	UNP Q81TK8

- Molecule 2 is COENZYME A (CCD ID: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).



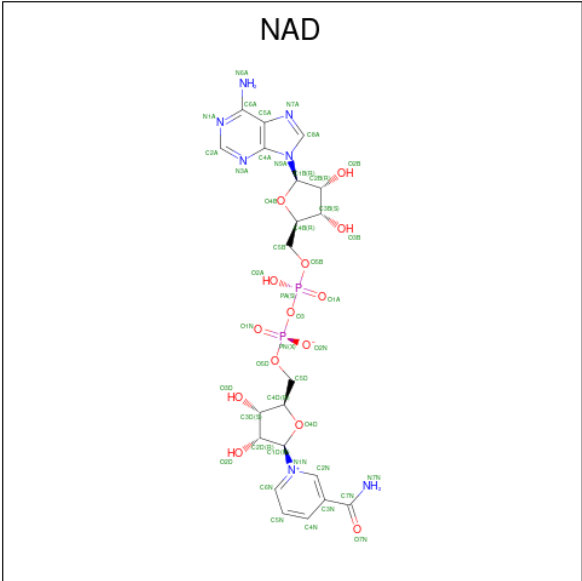
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

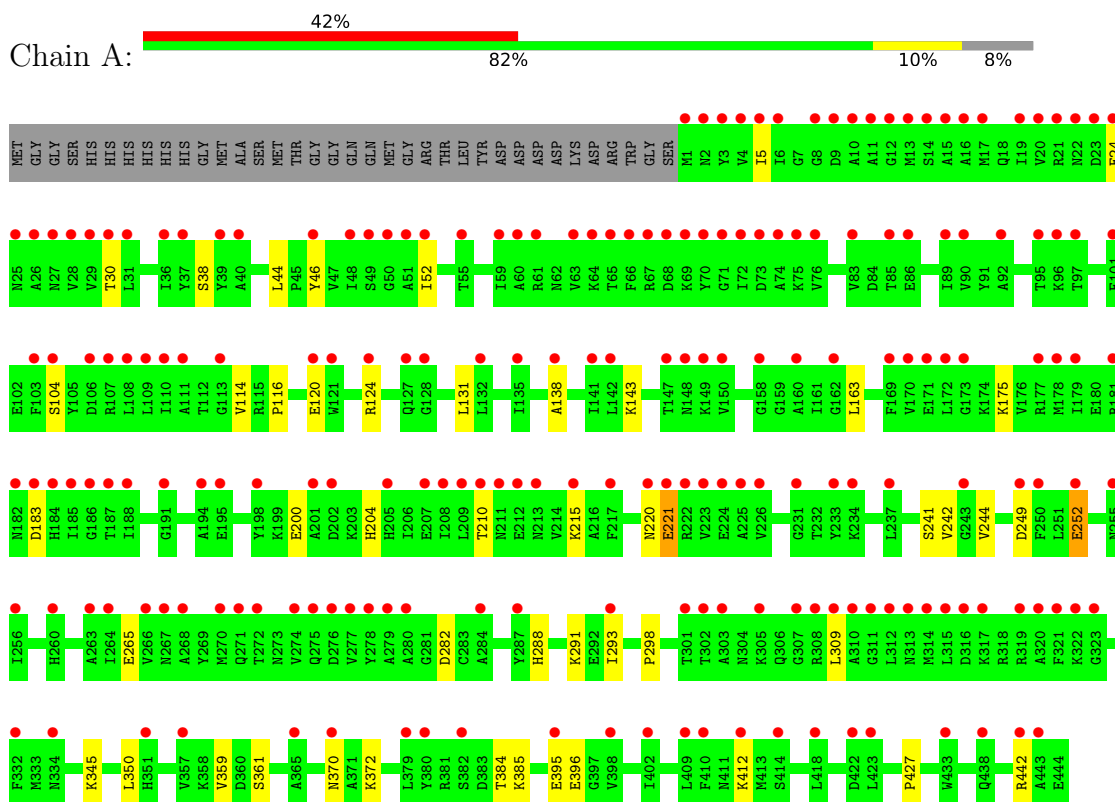
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	229	Total	O	0	0
			229	229		
5	B	231	Total	O	0	0
			231	231		

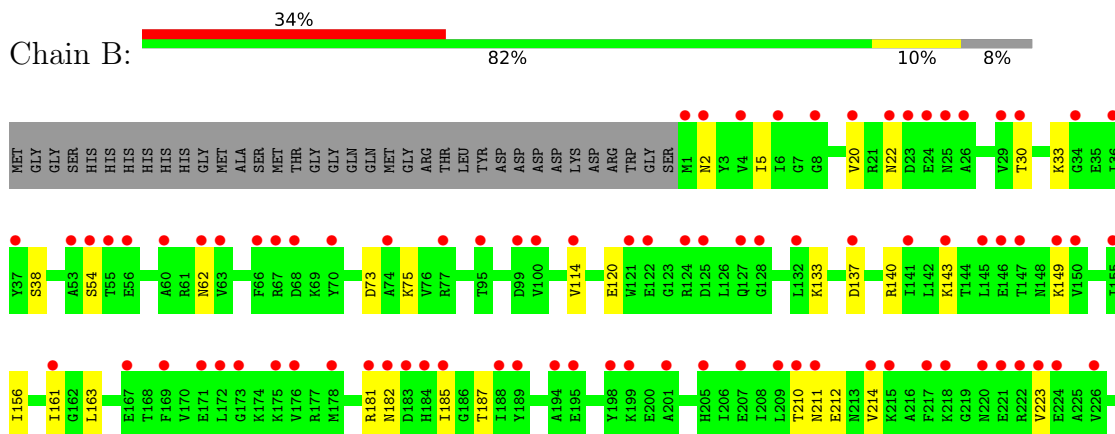
3 Residue-property plots

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: Pyridine nucleotide-disulfide oxidoreductase, class I



- Molecule 1: Pyridine nucleotide-disulfide oxidoreductase, class I





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	169.61Å 81.17Å 98.05Å 90.00° 104.01° 90.00°	Depositor
Resolution (Å)	37.45 – 2.25 37.45 – 2.25	Depositor EDS
% Data completeness (in resolution range)	96.0 (37.45-2.25) 96.0 (37.45-2.25)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.50 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.206 , 0.248 (Not available) , 0.308	Depositor DCC
R_{free} test set	3006 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	32.7	Xtriage
Anisotropy	0.611	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 53.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.38$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7735	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.09% 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: NAD, COA, 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	0.59	0/3563	0.80	3/4812 (0.1%)
1	B	0.56	0/3553	0.80	2/4799 (0.0%)
All	All	0.57	0/7116	0.80	5/9611 (0.1%)

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	B	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	427	PRO	N-CA-C	5.70	117.65	110.70
1	A	242	VAL	N-CA-C	5.52	117.52	111.77
1	A	427	PRO	N-CA-C	5.40	117.29	110.70
1	A	215	LYS	N-CA-C	-5.31	106.86	113.55
1	B	2	ASN	N-CA-C	5.10	116.97	107.99

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	425	TYR	Peptide

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	3496	0	3527	22	0
1	B	3489	0	3519	21	0
2	A	48	0	32	0	0
2	B	48	0	32	0	0
3	A	53	0	31	0	0
3	B	53	0	31	0	0
4	A	44	0	26	2	0
4	B	44	0	26	2	0
5	A	229	0	0	4	0
5	B	231	0	0	3	0
All	All	7735	0	7224	43	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 3.

All (43) 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:A:345:LYS:HE2	5:A:977:HOH:O	1.60	1.01
1:B:137:ASP:OD1	1:B:140:ARG:NH2	2.36	0.58
1:A:244:VAL:HG13	4:A:818:NAD:H51N	1.90	0.53
1:A:395:GLU:HG2	5:A:833:HOH:O	2.09	0.53
1:A:288:HIS:HB3	1:A:291:LYS:HB2	1.92	0.52
1:A:5:ILE:HB	1:A:30:THR:HG22	1.91	0.52
1:A:120:GLU:HA	1:A:124:ARG:HD2	1.92	0.51
1:B:5:ILE:HB	1:B:30:THR:HG22	1.93	0.50
1:A:359:VAL:HG12	1:A:361:SER:HB2	1.94	0.50
1:A:114:VAL:HG13	1:A:282:ASP:HB3	1.94	0.49
1:A:220:ASN:CG	1:A:221:GLU:H	2.19	0.49
1:B:156:ILE:HD12	1:B:214:VAL:HG21	1.94	0.49
1:B:372:LYS:HD3	1:B:395:GLU:OE2	2.12	0.48
1:A:384:THR:O	1:A:385:LYS:HB2	2.14	0.48
1:A:220:ASN:H	1:A:220:ASN:ND2	2.11	0.47
1:B:181:ARG:HE	1:B:182:ASN:ND2	2.12	0.47
1:A:200:GLU:O	1:A:204:HIS:HD2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:THR:O	1:B:255[B]:ASN:HB3	2.15	0.46
1:B:133:LYS:NZ	5:B:894:HOH:O	2.49	0.45
1:B:163:LEU:HD21	1:B:185:ILE:HD12	1.97	0.45
1:A:104:SER:HB2	5:A:979:HOH:O	2.15	0.45
1:B:412:LYS:HA	5:B:911:HOH:O	2.17	0.45
1:B:187:THR:O	1:B:345:LYS:HE3	2.17	0.45
1:B:288:HIS:HB3	1:B:291:LYS:HB2	1.99	0.44
1:A:46:TYR:HB2	1:A:52:ILE:HD12	1.99	0.44
1:B:114:VAL:HG12	1:B:246:PRO:HA	2.00	0.44
1:B:22:ASN:HB2	1:B:315:LEU:HD13	2.00	0.44
1:A:116:PRO:HB2	1:A:131:LEU:HD22	2.00	0.44
1:B:161:ILE:CG1	4:B:819:NAD:H6N	2.48	0.43
1:B:33:LYS:HB3	1:B:33:LYS:HE2	1.79	0.43
1:A:298:PRO:O	4:A:818:NAD:O2D	2.35	0.43
1:A:220:ASN:CG	1:A:221:GLU:N	2.77	0.43
1:A:370:ASN:O	1:A:372:LYS:HG2	2.19	0.42
1:B:73:ASP:OD1	1:B:75:LYS:HE3	2.18	0.42
1:A:345:LYS:HE3	5:A:970:HOH:O	2.19	0.42
1:A:44:LEU:HD22	1:A:138:ALA:HB2	2.02	0.42
1:B:54:SER:HB2	5:B:912:HOH:O	2.20	0.42
1:B:212:GLU:OE2	1:B:233:TYR:OH	2.28	0.41
1:B:161:ILE:HG12	4:B:819:NAD:H6N	2.03	0.41
1:B:345:LYS:H	1:B:345:LYS:HG2	1.67	0.41
1:B:364:MET:O	1:B:365:ALA:C	2.63	0.41

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	445/480 (93%)	429 (96%)	15 (3%)	1 (0%)	43 50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	444/480 (92%)	425 (96%)	18 (4%)	1 (0%)	43	50
All	All	889/960 (93%)	854 (96%)	33 (4%)	2 (0%)	43	50

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	SER
1	B	38	SER

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	373/398 (94%)	354 (95%)	19 (5%)	21	23
1	B	372/398 (94%)	355 (95%)	17 (5%)	24	28
All	All	745/796 (94%)	709 (95%)	36 (5%)	24	25

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	GLU
1	A	143	LYS
1	A	163	LEU
1	A	175	LYS
1	A	183	ASP
1	A	210	THR
1	A	221	GLU
1	A	241	SER
1	A	249[A]	ASP
1	A	249[B]	ASP
1	A	252	GLU
1	A	265[A]	GLU
1	A	265[B]	GLU
1	A	293	ILE

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Mol	Chain	Res	Type
1	A	309	LEU
1	A	350	LEU
1	A	396	GLU
1	A	412	LYS
1	A	442	ARG
1	B	20	VAL
1	B	62	ASN
1	B	120	GLU
1	B	143	LYS
1	B	149	LYS
1	B	210	THR
1	B	211	ASN
1	B	223	VAL
1	B	249[A]	ASP
1	B	249[B]	ASP
1	B	350	LEU
1	B	357	VAL
1	B	372	LYS
1	B	396	GLU
1	B	412	LYS
1	B	414	SER
1	B	442	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	184	HIS
1	A	334	ASN
1	B	2	ASN
1	B	62	ASN
1	B	127	GLN
1	B	182	ASN
1	B	184	HIS
1	B	220	ASN
1	B	334	ASN

5.3.3 RNA ⓘ

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](#)

6 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	FAD	A	446	-	58,58,58	1.02	4 (6%)	85,89,89	1.61	19 (22%)
4	NAD	A	818	-	46,48,48	1.71	5 (10%)	64,73,73	1.56	9 (14%)
2	COA	B	445	-	47,50,50	0.92	3 (6%)	69,75,75	1.66	13 (18%)
3	FAD	B	446	-	58,58,58	1.01	4 (6%)	85,89,89	1.60	18 (21%)
4	NAD	B	819	-	46,48,48	1.68	5 (10%)	64,73,73	1.52	9 (14%)
2	COA	A	445	-	47,50,50	0.86	2 (4%)	69,75,75	1.65	16 (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
3	FAD	A	446	-	-	0/34/50/50	0/6/6/6
4	NAD	A	818	-	-	8/30/62/62	0/5/5/5
2	COA	B	445	-	-	5/48/64/64	0/3/3/3
3	FAD	B	446	-	-	1/34/50/50	0/6/6/6
4	NAD	B	819	-	-	6/30/62/62	0/5/5/5
2	COA	A	445	-	-	6/48/64/64	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	819	NAD	C7N-N7N	8.48	1.48	1.33
4	A	818	NAD	C7N-N7N	8.31	1.48	1.33
4	A	818	NAD	C2A-N3A	3.07	1.39	1.33
4	A	818	NAD	C2N-N1N	2.87	1.38	1.35
4	B	819	NAD	C2N-N1N	2.87	1.38	1.35
3	A	446	FAD	C4X-N5	2.84	1.36	1.30
4	A	818	NAD	C2A-N1A	2.80	1.38	1.33
4	B	819	NAD	C2A-N1A	2.78	1.38	1.33
4	B	819	NAD	C2A-N3A	2.76	1.38	1.33
3	B	446	FAD	C4X-N5	2.73	1.36	1.30
2	B	445	COA	P2A-O3A	2.70	1.62	1.59
3	B	446	FAD	C10-N10	2.43	1.42	1.37
3	A	446	FAD	C10-N10	2.37	1.42	1.37
2	A	445	COA	P2A-O3A	2.26	1.61	1.59
3	A	446	FAD	C8A-N7A	2.23	1.36	1.31
3	B	446	FAD	C5X-N5	-2.21	1.35	1.39
3	A	446	FAD	P-O3P	2.16	1.61	1.59
2	B	445	COA	P1A-O3A	2.13	1.61	1.59
4	A	818	NAD	PA-O3	2.13	1.61	1.59
3	B	446	FAD	C4A-N9A	-2.12	1.33	1.37
4	B	819	NAD	C8A-N7A	2.07	1.35	1.31
2	A	445	COA	C8A-N7A	2.07	1.35	1.31
2	B	445	COA	C8A-N7A	2.02	1.35	1.31

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	818	NAD	N3A-C2A-N1A	-5.55	120.19	128.58
4	B	819	NAD	N3A-C2A-N1A	-5.54	120.19	128.58
3	A	446	FAD	N3A-C2A-N1A	-5.41	120.39	128.58
2	B	445	COA	C5A-C4A-N3A	-5.20	119.56	126.72
3	B	446	FAD	C5A-C4A-N3A	-5.04	119.78	126.72
2	A	445	COA	C5A-C4A-N3A	-5.02	119.80	126.72
3	A	446	FAD	C5A-C4A-N3A	-5.01	119.82	126.72
3	B	446	FAD	N3A-C2A-N1A	-4.92	121.13	128.58
2	B	445	COA	N3A-C2A-N1A	-4.81	121.31	128.58
2	A	445	COA	N3A-C2A-N1A	-4.60	121.62	128.58
4	A	818	NAD	N9A-C8A-N7A	-4.33	107.79	113.94
4	A	818	NAD	C5A-C4A-N3A	-4.30	120.80	126.72
4	B	819	NAD	C5A-C4A-N3A	-4.09	121.09	126.72
4	B	819	NAD	N9A-C8A-N7A	-4.03	108.21	113.94
3	A	446	FAD	C2A-N3A-C4A	3.78	121.06	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	818	NAD	C5A-N7A-C8A	3.57	109.06	103.45
3	B	446	FAD	C2A-N3A-C4A	3.55	120.50	111.83
3	B	446	FAD	N9A-C8A-N7A	-3.45	109.04	113.94
2	B	445	COA	C2A-N3A-C4A	3.45	120.25	111.83
3	A	446	FAD	N9A-C8A-N7A	-3.45	109.05	113.94
2	B	445	COA	N3A-C4A-N9A	3.43	133.01	127.17
2	A	445	COA	C6P-C7P-N8P	-3.38	104.81	112.00
4	B	819	NAD	C5A-N7A-C8A	3.35	108.72	103.45
4	A	818	NAD	C2A-N3A-C4A	3.34	119.99	111.83
2	A	445	COA	N3A-C4A-N9A	3.31	132.80	127.17
2	B	445	COA	N9A-C8A-N7A	-3.31	109.24	113.94
2	A	445	COA	C2A-N3A-C4A	3.29	119.88	111.83
4	B	819	NAD	C2A-N3A-C4A	3.25	119.76	111.83
2	A	445	COA	N9A-C8A-N7A	-3.24	109.34	113.94
4	B	819	NAD	C6N-N1N-C2N	-3.23	119.13	121.88
3	A	446	FAD	N3A-C4A-N9A	3.22	132.64	127.17
3	B	446	FAD	C4A-C5A-N7A	-3.14	106.99	110.58
4	A	818	NAD	N3A-C4A-N9A	3.09	132.42	127.17
3	B	446	FAD	N3A-C4A-N9A	3.04	132.34	127.17
2	A	445	COA	C7P-N8P-C9P	2.82	127.62	122.55
4	B	819	NAD	N3A-C4A-N9A	2.81	131.95	127.17
3	A	446	FAD	C4A-N9A-C8A	2.77	108.65	105.74
2	B	445	COA	C3P-N4P-C5P	2.73	127.91	122.82
3	A	446	FAD	C4A-C5A-N7A	-2.70	107.49	110.58
4	A	818	NAD	C6N-N1N-C2N	-2.70	119.58	121.88
2	B	445	COA	C6P-C7P-N8P	-2.69	106.28	112.00
3	A	446	FAD	C5X-N5-C4X	2.67	122.41	118.09
2	A	445	COA	C2P-C3P-N4P	-2.66	106.26	112.31
3	B	446	FAD	C4A-N9A-C8A	2.66	108.53	105.74
3	A	446	FAD	C4-N3-C2	-2.66	120.92	125.64
4	A	818	NAD	C4A-N9A-C8A	2.62	108.49	105.74
3	B	446	FAD	C5A-N7A-C8A	2.61	107.55	103.45
2	B	445	COA	C7P-C6P-C5P	-2.61	108.05	112.39
3	B	446	FAD	C4-N3-C2	-2.57	121.08	125.64
2	B	445	COA	C2P-C3P-N4P	-2.53	106.56	112.31
3	B	446	FAD	C5X-N5-C4X	2.53	122.18	118.09
2	B	445	COA	C4A-N9A-C8A	2.51	108.38	105.74
2	A	445	COA	C4A-C5A-N7A	-2.51	107.71	110.58
3	A	446	FAD	C4X-C4-N3	2.51	119.64	113.25
2	B	445	COA	C4A-C5A-N7A	-2.50	107.73	110.58
2	B	445	COA	C7P-N8P-C9P	2.44	126.93	122.55
3	A	446	FAD	C5A-N7A-C8A	2.44	107.28	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	445	COA	C4A-N9A-C8A	2.43	108.29	105.74
2	A	445	COA	C5A-N7A-C8A	2.43	107.26	103.45
3	B	446	FAD	C4X-C4-N3	2.41	119.40	113.25
2	B	445	COA	C5A-N7A-C8A	2.40	107.22	103.45
4	B	819	NAD	C4A-N9A-C8A	2.38	108.23	105.74
4	B	819	NAD	C4A-C5A-N7A	-2.38	107.86	110.58
4	A	818	NAD	C4A-C5A-N7A	-2.37	107.87	110.58
2	A	445	COA	O6A-CCP-CBP	2.37	114.35	110.55
3	A	446	FAD	O3P-PA-O1A	-2.32	103.72	110.70
2	A	445	COA	C7P-C6P-C5P	-2.29	108.57	112.39
3	B	446	FAD	O3P-PA-O1A	-2.26	103.91	110.70
3	A	446	FAD	O4-C4-C4X	-2.22	120.66	126.53
3	A	446	FAD	C10-C4X-N5	-2.20	120.31	124.81
3	A	446	FAD	O4B-C1B-N9A	2.17	112.26	108.09
3	B	446	FAD	C4X-C10-N10	2.17	119.59	116.48
2	A	445	COA	C3P-N4P-C5P	2.15	126.83	122.82
3	B	446	FAD	C10-C4X-N5	-2.15	120.42	124.81
3	B	446	FAD	O2P-P-O3P	-2.13	101.52	107.27
3	B	446	FAD	C4X-C10-N1	-2.13	119.38	124.59
3	A	446	FAD	C9A-C5X-N5	-2.11	120.21	122.45
3	A	446	FAD	C10-N1-C2	2.11	121.42	116.85
3	B	446	FAD	O4-C4-C4X	-2.08	121.05	126.53
3	A	446	FAD	C4-C4X-N5	2.07	121.06	118.21
3	A	446	FAD	C4X-C10-N1	-2.06	119.54	124.59
2	A	445	COA	O3A-P2A-O4A	-2.04	104.56	110.70
2	A	445	COA	C3B-C2B-C1B	2.04	104.37	99.89
3	B	446	FAD	C10-N1-C2	2.01	121.21	116.85

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	445	COA	C5B-O5B-P1A-O1A
2	A	445	COA	CDP-CBP-CCP-O6A
2	A	445	COA	CEP-CBP-CCP-O6A
2	A	445	COA	CAP-CBP-CCP-O6A
2	B	445	COA	CDP-CBP-CCP-O6A
2	B	445	COA	CEP-CBP-CCP-O6A
2	B	445	COA	CAP-CBP-CCP-O6A
4	A	818	NAD	C2D-C1D-N1N-C2N
4	A	818	NAD	C2D-C1D-N1N-C6N
4	B	819	NAD	C2D-C1D-N1N-C2N

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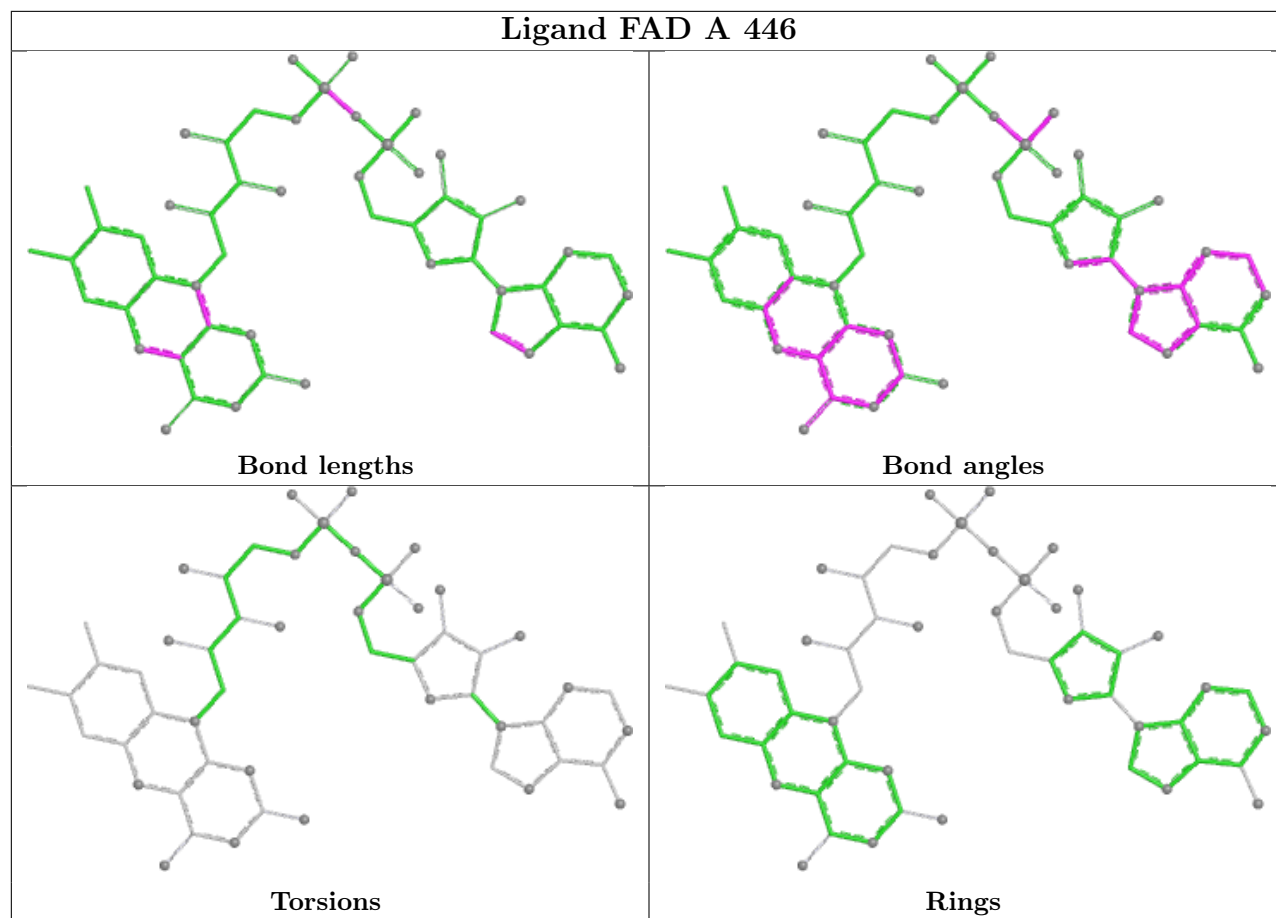
Mol	Chain	Res	Type	Atoms
4	B	819	NAD	C2D-C1D-N1N-C6N
4	B	819	NAD	C3B-C4B-C5B-O5B
4	B	819	NAD	O4B-C4B-C5B-O5B
4	A	818	NAD	O4B-C4B-C5B-O5B
4	A	818	NAD	C3B-C4B-C5B-O5B
4	A	818	NAD	O4D-C4D-C5D-O5D
2	B	445	COA	S1P-C2P-C3P-N4P
2	A	445	COA	C5B-O5B-P1A-O2A
2	A	445	COA	C5B-O5B-P1A-O3A
2	B	445	COA	C5B-O5B-P1A-O1A
4	A	818	NAD	C5D-O5D-PN-O1N
4	A	818	NAD	PA-O3-PN-O2N
4	B	819	NAD	PA-O3-PN-O1N
4	B	819	NAD	PA-O3-PN-O2N
3	B	446	FAD	O4B-C4B-C5B-O5B
4	A	818	NAD	C3D-C4D-C5D-O5D

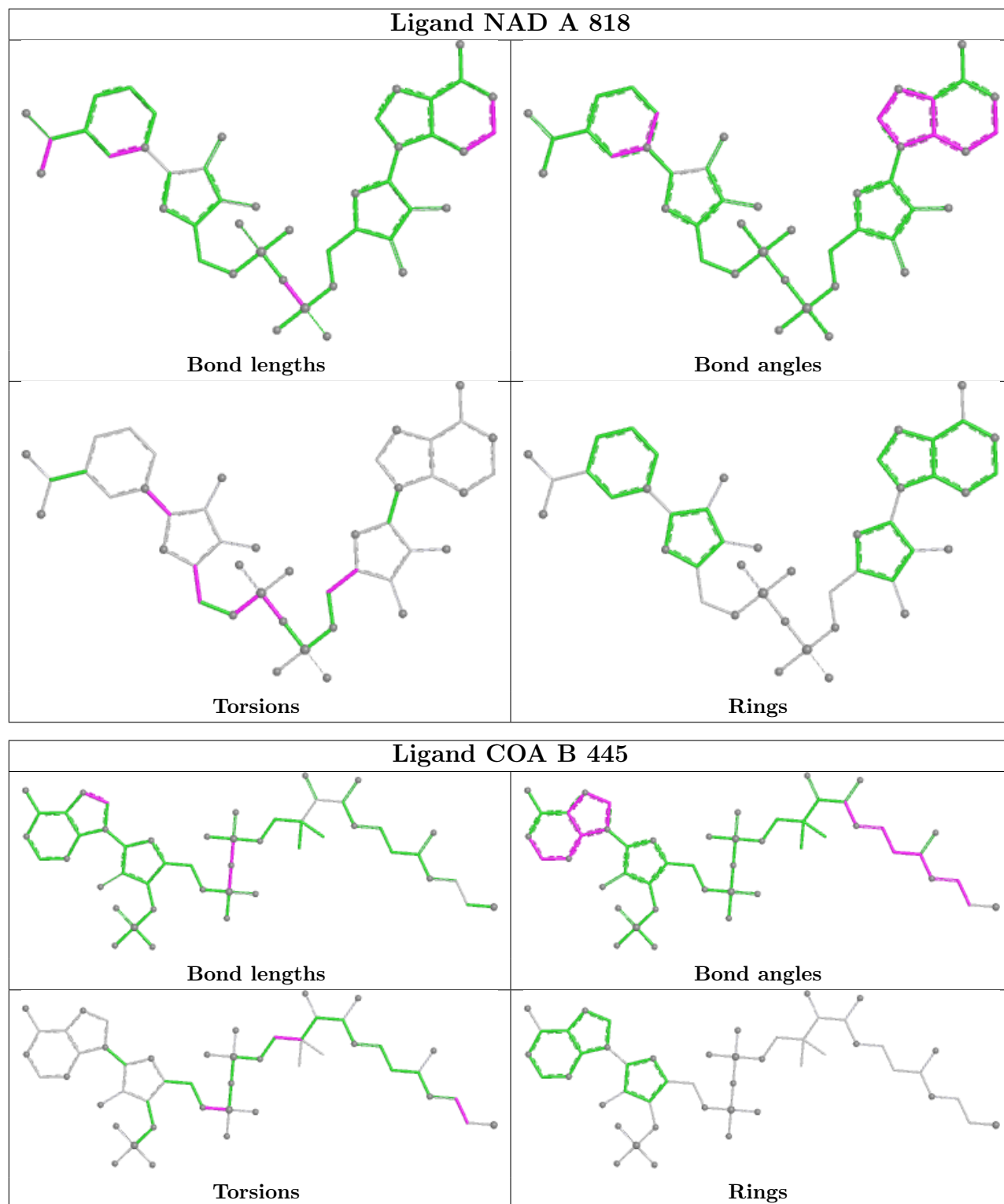
There are no ring outliers.

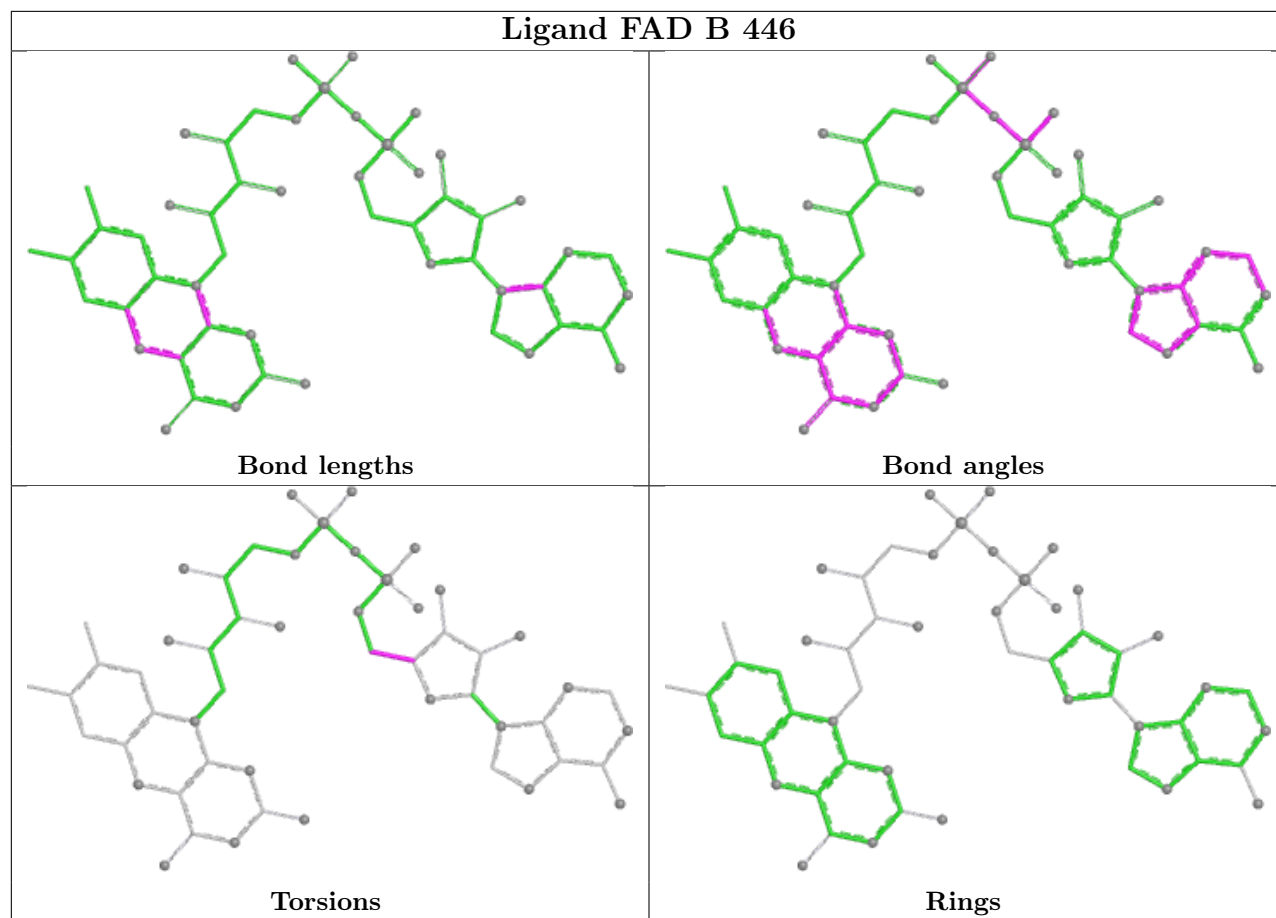
2 monomers are involved in 4 short contacts:

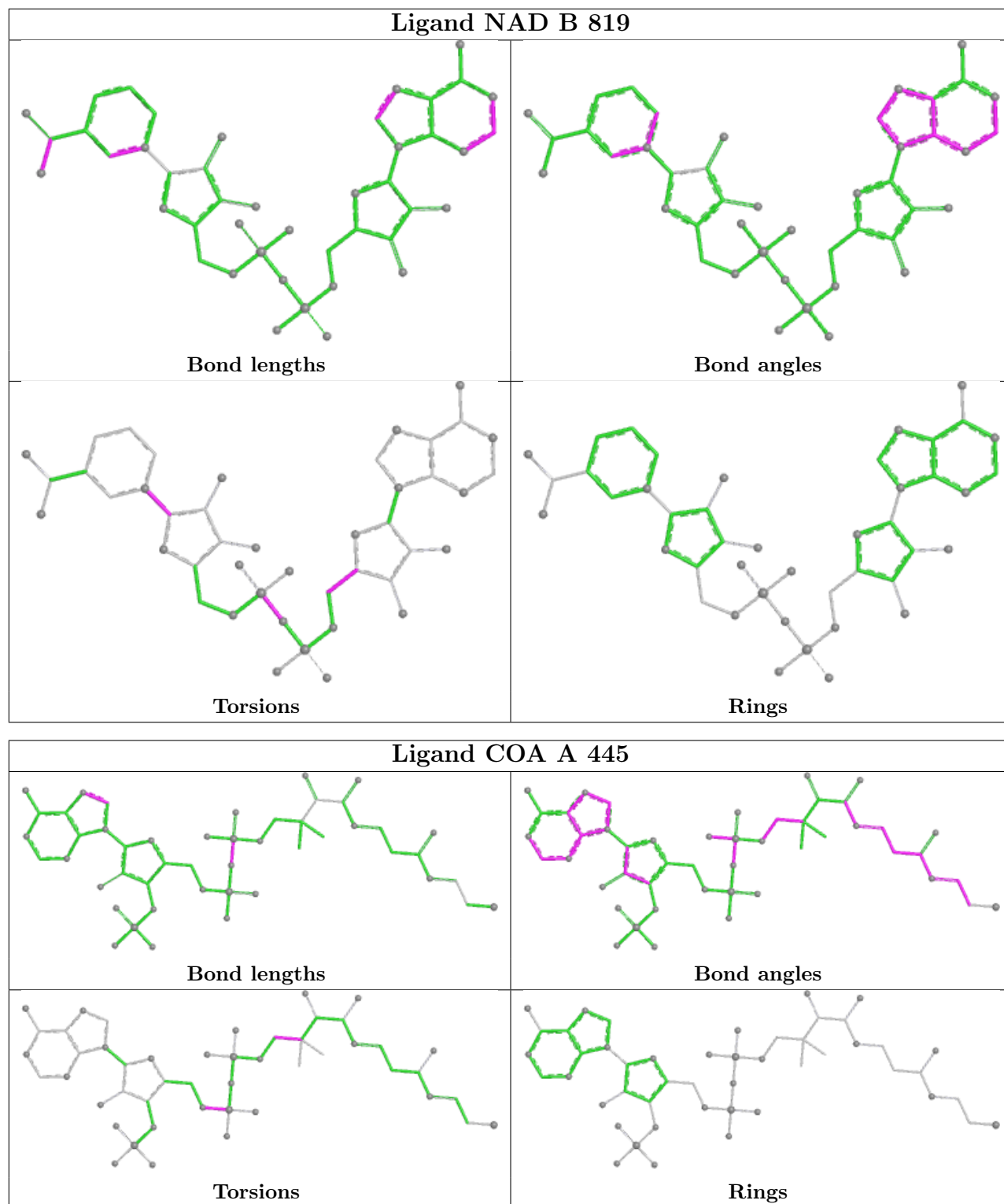
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	818	NAD	2	0
4	B	819	NAD	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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(Å ²)	Q<0.9
1	A	444/480 (92%)	1.99	204 (45%) 0 0	25, 46, 55, 62	3 (0%)
1	B	444/480 (92%)	1.83	161 (36%) 1 0	28, 46, 54, 61	2 (0%)
All	All	888/960 (92%)	1.91	365 (41%) 0 0	25, 46, 55, 62	5 (0%)

All (365) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	198	TYR	7.4
1	A	185	ILE	5.1
1	A	4	VAL	4.8
1	A	182	ASN	4.6
1	A	70	TYR	4.6
1	A	28	VAL	4.6
1	A	29	VAL	4.6
1	A	1	MET	4.3
1	B	188	ILE	4.3
1	B	24	GLU	4.2
1	A	312	LEU	4.0
1	A	310	ALA	4.0
1	A	173	GLY	4.0
1	A	217	PHE	4.0
1	A	2	ASN	3.9
1	B	351	HIS	3.9
1	A	14	SER	3.9
1	A	74	ALA	3.8
1	B	370	ASN	3.8
1	A	66	PHE	3.8
1	A	313	ASN	3.7
1	A	92	ALA	3.7
1	A	19	ILE	3.7
1	A	323	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	198	TYR	3.7
1	A	72	ILE	3.6
1	A	12	GLY	3.6
1	A	311	GLY	3.6
1	A	277	VAL	3.6
1	A	15	ALA	3.6
1	A	187	THR	3.6
1	A	10	ALA	3.6
1	B	25	ASN	3.6
1	B	418	LEU	3.5
1	A	316	ASP	3.5
1	A	150	VAL	3.5
1	A	31	LEU	3.5
1	B	189	TYR	3.5
1	B	62	ASN	3.5
1	A	178	MET	3.5
1	A	171	GLU	3.5
1	B	1	MET	3.4
1	B	214	VAL	3.4
1	B	181	ARG	3.4
1	A	147	THR	3.4
1	A	280	ALA	3.4
1	B	143	LYS	3.4
1	B	277	VAL	3.4
1	A	67	ARG	3.4
1	A	279	ALA	3.4
1	B	220	ASN	3.4
1	B	185	ILE	3.3
1	B	261	LYS	3.3
1	A	71	GLY	3.3
1	A	307	GLY	3.3
1	A	110	ILE	3.3
1	A	184	HIS	3.3
1	A	11	ALA	3.3
1	A	6	ILE	3.3
1	A	120	GLU	3.3
1	A	207	GLU	3.3
1	B	345	LYS	3.3
1	A	20	VAL	3.3
1	B	60	ALA	3.2
1	A	181	ARG	3.2
1	B	2	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	59	ILE	3.2
1	B	268	ALA	3.2
1	B	173	GLY	3.2
1	A	309	LEU	3.2
1	A	90	VAL	3.2
1	A	278	TYR	3.2
1	B	63	VAL	3.2
1	B	211	ASN	3.2
1	A	5	ILE	3.2
1	B	352	ILE	3.2
1	B	55	THR	3.2
1	B	254	THR	3.2
1	B	384	THR	3.2
1	A	252	GLU	3.1
1	A	370	ASN	3.1
1	B	287	TYR	3.1
1	A	209	LEU	3.1
1	B	378	LEU	3.1
1	B	255[A]	ASN	3.1
1	A	266	VAL	3.1
1	B	100	VAL	3.1
1	A	3	TYR	3.1
1	A	314	MET	3.1
1	B	36	ILE	3.1
1	A	97	THR	3.1
1	A	260	HIS	3.1
1	A	202	ASP	3.1
1	B	402	ILE	3.0
1	A	64	LYS	3.0
1	B	201	ALA	3.0
1	B	443	ALA	3.0
1	B	357	VAL	3.0
1	A	208	ILE	3.0
1	B	293	ILE	3.0
1	B	275	GLN	3.0
1	B	218	LYS	3.0
1	B	441	ARG	3.0
1	A	183	ASP	3.0
1	B	252	GLU	3.0
1	A	315	LEU	3.0
1	A	89	ILE	3.0
1	A	128	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	255	ASN	3.0
1	A	212	GLU	3.0
1	B	150	VAL	2.9
1	A	21	ARG	2.9
1	A	188	ILE	2.9
1	A	51	ALA	2.9
1	A	65	THR	2.9
1	A	186	GLY	2.9
1	B	182	ASN	2.9
1	A	63	VAL	2.9
1	B	20	VAL	2.9
1	A	48	ILE	2.9
1	A	224	GLU	2.9
1	A	8	GLY	2.9
1	B	350	LEU	2.9
1	A	27	ASN	2.9
1	A	250	PHE	2.8
1	B	369	PRO	2.8
1	B	37	TYR	2.8
1	B	342	LEU	2.8
1	B	359	VAL	2.8
1	B	161	ILE	2.8
1	B	323	GLY	2.8
1	A	221	GLU	2.8
1	B	221	GLU	2.8
1	B	269	TYR	2.8
1	B	315	LEU	2.8
1	A	322	LYS	2.8
1	B	347	ALA	2.8
1	A	101	PHE	2.8
1	A	308	ARG	2.8
1	A	68	ASP	2.7
1	A	243	GLY	2.7
1	A	132	LEU	2.7
1	A	442	ARG	2.7
1	A	76	VAL	2.7
1	B	260	HIS	2.7
1	B	289	VAL	2.7
1	A	271	GLN	2.7
1	B	141	ILE	2.7
1	A	191	GLY	2.7
1	A	172	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	77	ARG	2.7
1	A	410	PHE	2.7
1	A	276	ASP	2.7
1	B	210	THR	2.7
1	A	382	SER	2.7
1	B	379	LEU	2.7
1	A	148	ASN	2.7
1	B	171	GLU	2.7
1	A	158	GLY	2.7
1	A	104	SER	2.7
1	B	172	LEU	2.7
1	B	251	LEU	2.7
1	A	205	HIS	2.6
1	A	160	ALA	2.6
1	B	175	LYS	2.6
1	A	16	ALA	2.6
1	A	106	ASP	2.6
1	A	61	ARG	2.6
1	A	177	ARG	2.6
1	B	222	ARG	2.6
1	B	4	VAL	2.6
1	B	147	THR	2.6
1	A	75	LYS	2.6
1	A	365	ALA	2.6
1	B	67	ARG	2.6
1	A	22	ASN	2.6
1	B	183	ASP	2.6
1	A	39	TYR	2.6
1	A	274	VAL	2.6
1	B	380	TYR	2.6
1	B	54	SER	2.6
1	A	142	LEU	2.6
1	B	419	GLU	2.6
1	B	417	ASP	2.6
1	A	332	PHE	2.6
1	B	432	VAL	2.6
1	A	141	ILE	2.6
1	A	284	ALA	2.5
1	B	74	ALA	2.5
1	B	440	ALA	2.5
1	A	17	MET	2.5
1	B	217	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	149	LYS	2.5
1	A	135	ILE	2.5
1	A	275	GLN	2.5
1	A	13	MET	2.5
1	A	320	ALA	2.5
1	A	69	LYS	2.5
1	B	253	GLY	2.5
1	A	301	THR	2.5
1	B	205	HIS	2.5
1	B	29	VAL	2.5
1	B	386	GLN	2.5
1	B	195	GLU	2.5
1	B	207	GLU	2.5
1	B	145	LEU	2.5
1	B	388	LEU	2.5
1	A	40	ALA	2.5
1	A	55	THR	2.5
1	A	127	GLN	2.5
1	B	176	VAL	2.5
1	B	433	TRP	2.5
1	B	425	TYR	2.5
1	A	108	LEU	2.5
1	A	270	MET	2.5
1	A	96	LYS	2.5
1	A	249[A]	ASP	2.5
1	B	23	ASP	2.5
1	A	303	ALA	2.5
1	B	26	ALA	2.5
1	B	194	ALA	2.5
1	A	210	THR	2.4
1	B	56	GLU	2.4
1	B	124	ARG	2.4
1	A	36	ILE	2.4
1	B	290	ILE	2.4
1	B	178	MET	2.4
1	A	26	ALA	2.4
1	A	201	ALA	2.4
1	A	302	THR	2.4
1	A	256	ILE	2.4
1	A	351	HIS	2.4
1	A	267	ASN	2.4
1	B	146	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	231	GLY	2.4
1	A	272	THR	2.4
1	A	83	VAL	2.4
1	B	132	LEU	2.4
1	A	24	GLU	2.4
1	A	195	GLU	2.4
1	B	316	ASP	2.4
1	B	414	SER	2.4
1	A	321	PHE	2.4
1	B	122	GLU	2.4
1	A	433	TRP	2.4
1	A	233	TYR	2.3
1	B	375	TYR	2.3
1	B	8	GLY	2.3
1	B	149	LYS	2.3
1	A	85	THR	2.3
1	B	382	SER	2.3
1	B	169	PHE	2.3
1	A	319	ARG	2.3
1	A	25	ASN	2.3
1	A	211	ASN	2.3
1	A	50	GLY	2.3
1	A	95	THR	2.3
1	A	226	VAL	2.3
1	B	398	VAL	2.3
1	A	237	LEU	2.3
1	A	220	ASN	2.3
1	A	334	ASN	2.3
1	B	199	LYS	2.3
1	B	383	ASP	2.3
1	A	113	GLY	2.3
1	B	167	GLU	2.3
1	B	256	ILE	2.3
1	A	223	VAL	2.3
1	A	109	LEU	2.3
1	B	53	ALA	2.3
1	B	381	ARG	2.3
1	B	356	THR	2.3
1	B	224	GLU	2.3
1	A	169	PHE	2.2
1	A	409	LEU	2.2
1	A	73	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	125	ASP	2.2
1	B	307	GLY	2.2
1	A	30	THR	2.2
1	A	46	TYR	2.2
1	A	225	ALA	2.2
1	A	263	ALA	2.2
1	A	287	TYR	2.2
1	B	30	THR	2.2
1	B	121	TRP	2.2
1	B	6	ILE	2.2
1	A	418	LEU	2.2
1	B	209	LEU	2.2
1	B	34	GLY	2.2
1	A	194	ALA	2.2
1	B	385	LYS	2.2
1	B	426	ALA	2.2
1	B	264	ILE	2.2
1	B	393	ILE	2.2
1	A	170	VAL	2.2
1	A	103	PHE	2.2
1	B	321	PHE	2.2
1	A	23	ASP	2.2
1	A	422	ASP	2.2
1	B	349	GLY	2.2
1	A	86	GLU	2.2
1	A	215	LYS	2.2
1	B	70	TYR	2.2
1	B	297	ILE	2.2
1	B	226	VAL	2.2
1	A	49	SER	2.2
1	A	111	ALA	2.2
1	B	413	MET	2.1
1	A	357	VAL	2.1
1	B	404	VAL	2.1
1	A	305	LYS	2.1
1	B	395	GLU	2.1
1	B	127	GLN	2.1
1	A	60	ALA	2.1
1	A	443	ALA	2.1
1	B	95	THR	2.1
1	B	258	THR	2.1
1	B	338	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	423	LEU	2.1
1	B	358	LYS	2.1
1	B	412	LYS	2.1
1	B	423	LEU	2.1
1	A	9	ASP	2.1
1	B	184	HIS	2.1
1	A	107	ARG	2.1
1	B	215	LYS	2.1
1	B	346	GLU	2.1
1	A	37	TYR	2.1
1	A	293	ILE	2.1
1	A	380	TYR	2.1
1	B	68	ASP	2.1
1	B	223	VAL	2.1
1	B	66	PHE	2.1
1	A	138	ALA	2.1
1	A	234	LYS	2.1
1	A	412	LYS	2.1
1	A	379	LEU	2.1
1	A	438[A]	GLN	2.1
1	B	99	ASP	2.1
1	B	137	ASP	2.1
1	B	155	ILE	2.1
1	B	114	VAL	2.1
1	B	341	GLY	2.1
1	A	124	ARG	2.1
1	A	222	ARG	2.1
1	A	317	LYS	2.0
1	A	268	ALA	2.0
1	B	406	ALA	2.0
1	A	213	ASN	2.0
1	B	325	LEU	2.0
1	B	335	LEU	2.0
1	A	52	ILE	2.0
1	A	264	ILE	2.0
1	A	398	VAL	2.0
1	A	162	GLY	2.0
1	B	128	GLY	2.0
1	A	121	TRP	2.0
1	A	395	GLU	2.0
1	A	414	SER	2.0
1	B	320	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	22	ASN	2.0
1	B	267	ASN	2.0
1	B	376	LEU	2.0
1	A	179	ILE	2.0
1	A	402	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

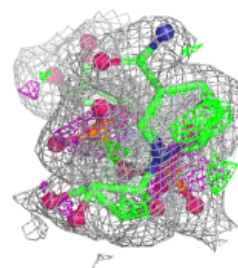
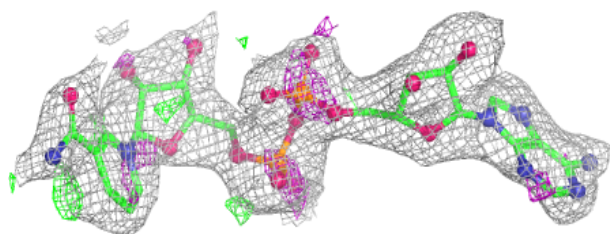
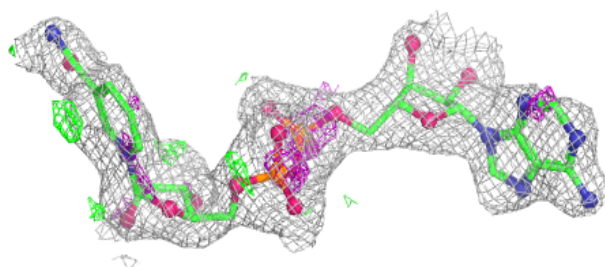
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAD	A	818	44/44	0.89	0.16	53,57,62,62	0
4	NAD	B	819	44/44	0.89	0.15	53,56,60,60	0
3	FAD	A	446	53/53	0.90	0.15	37,45,54,54	0
2	COA	A	445	48/48	0.90	0.16	50,59,70,70	0
2	COA	B	445	48/48	0.90	0.16	48,58,69,70	0
3	FAD	B	446	53/53	0.92	0.15	36,43,52,52	0

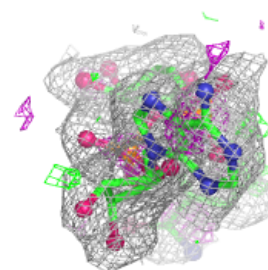
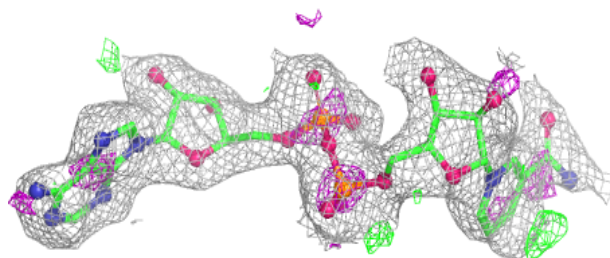
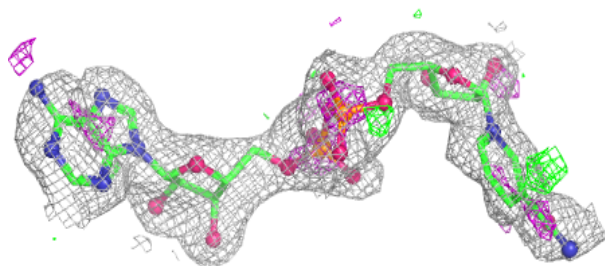
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD A 818:

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

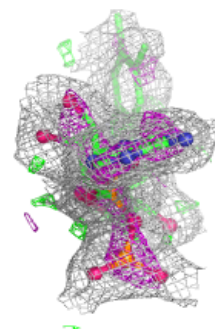
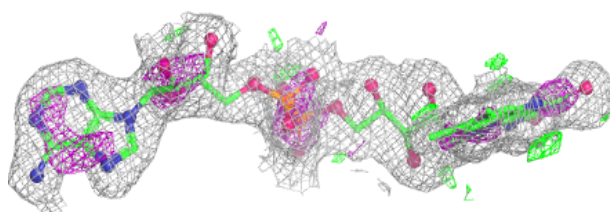
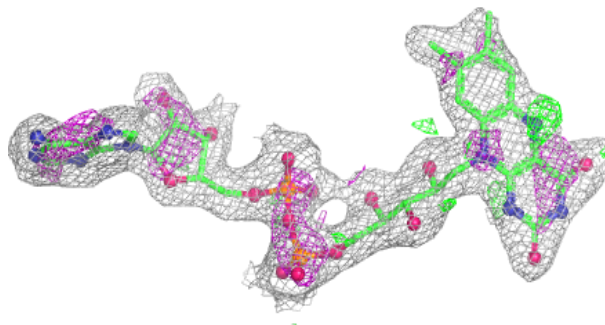
**Electron density around NAD B 819:**

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

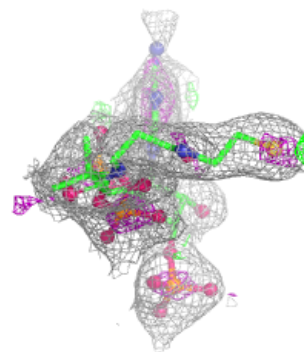
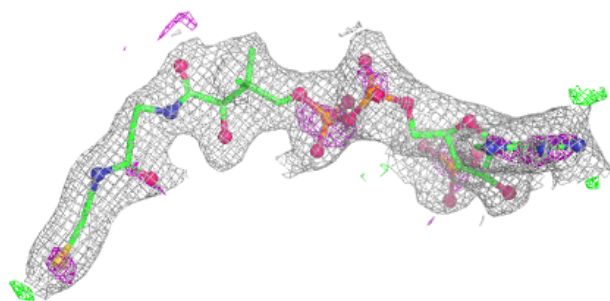
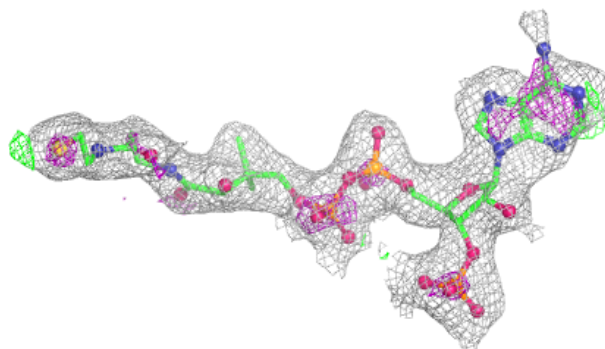


Electron density around FAD A 446:

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

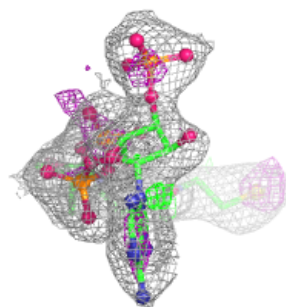
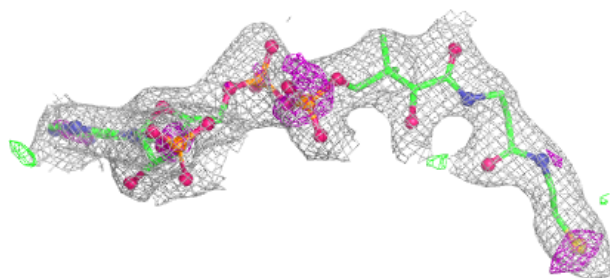
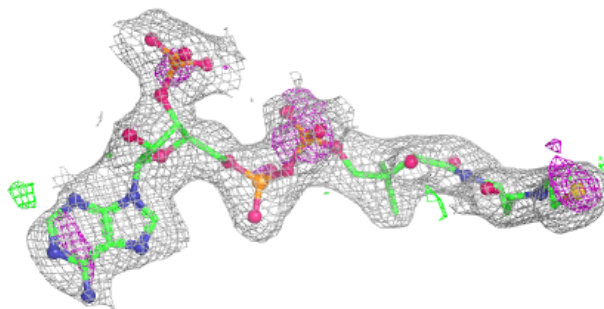
**Electron density around COA A 445:**

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

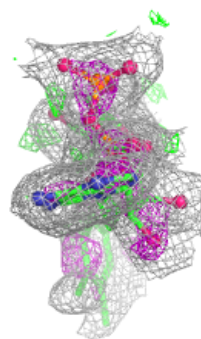
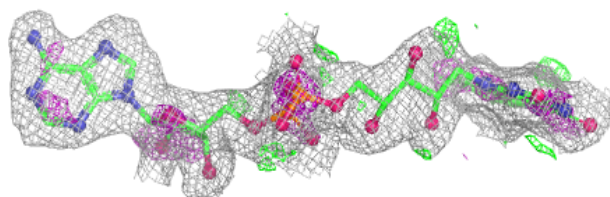
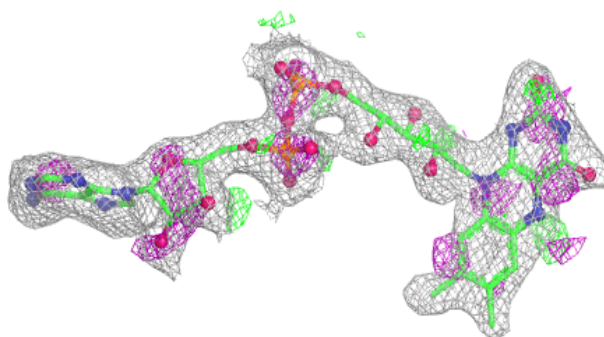


Electron density around COA B 445:

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

**Electron density around FAD B 446:**

$2mF_o-DF_c$ (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.