



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 02:58 PM EDT

PDB ID : 3CGE / pdb_00003cge
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 : 2.26 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

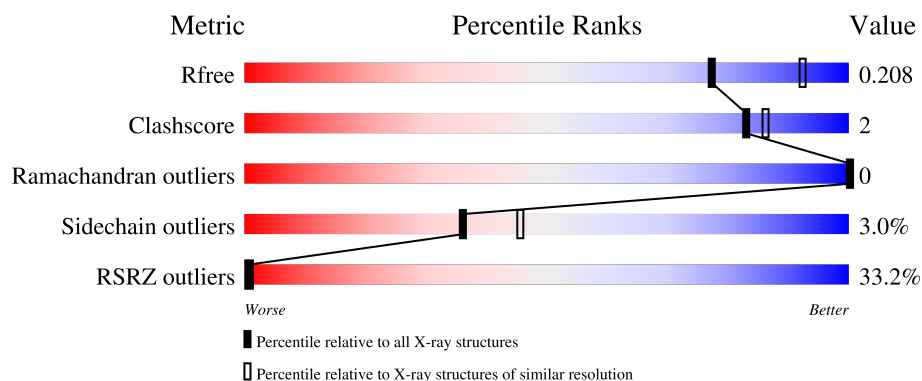
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.26 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	36% 84% 8% 8%
1	B	480	25% 86% 7% 8%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7659 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	2	0
			3491	2205	603	668	15			
1	B	444	Total	C	N	O	S	0	0	0
			3479	2197	602	665	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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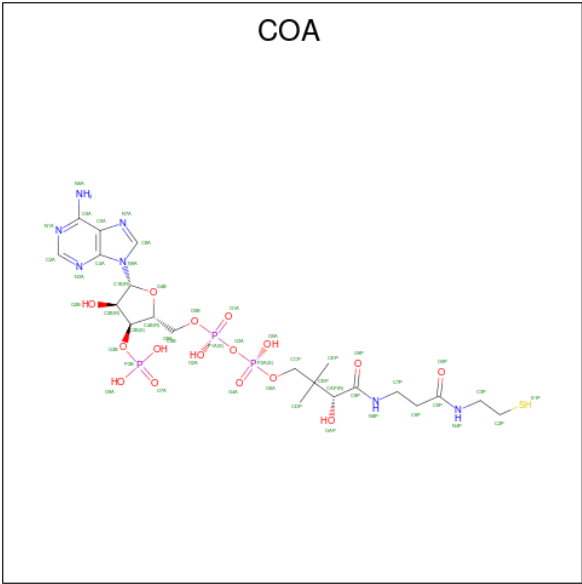
Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	TYR	-	expression tag	UNP Q81TK8
A	-9	ASP	-	expression tag	UNP Q81TK8
A	-8	ASP	-	expression tag	UNP Q81TK8
A	-7	ASP	-	expression tag	UNP Q81TK8
A	-6	ASP	-	expression tag	UNP Q81TK8
A	-5	LYS	-	expression tag	UNP Q81TK8
A	-4	ASP	-	expression tag	UNP 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).



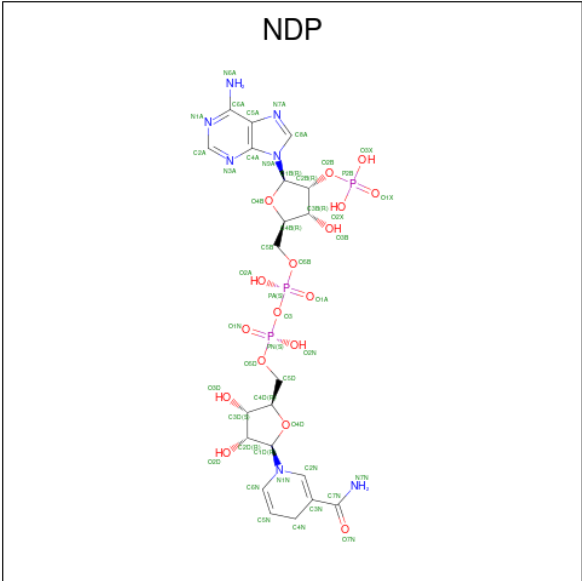
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- 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 NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



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

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

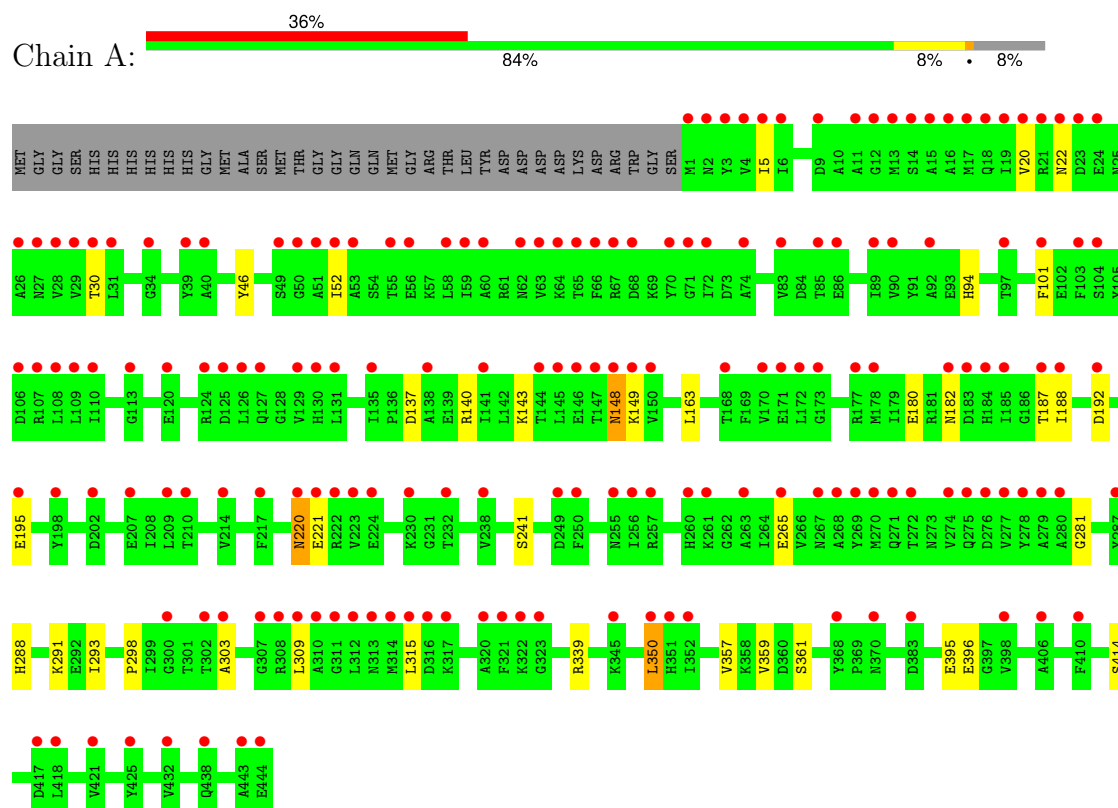
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	189	Total	O	0	0
			189	189		
5	B	202	Total	O	0	0
			202	202		

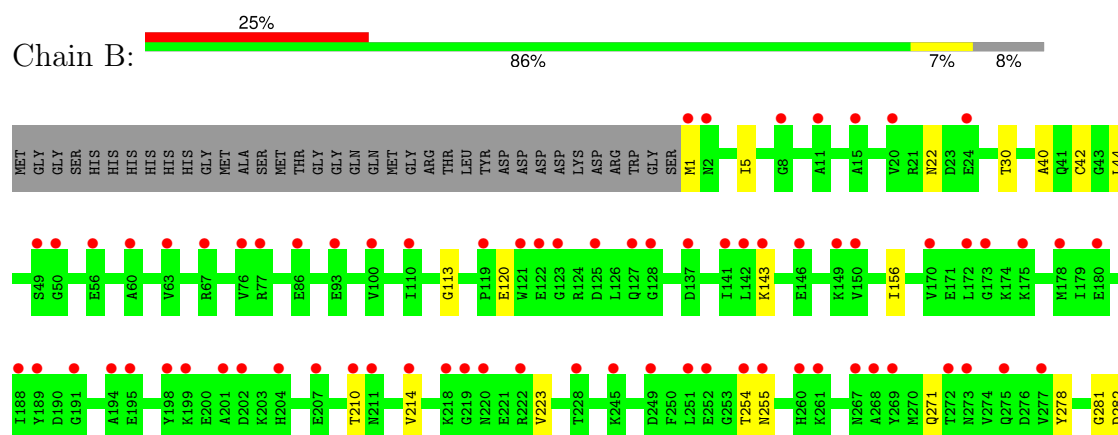
3 Residue-property plots

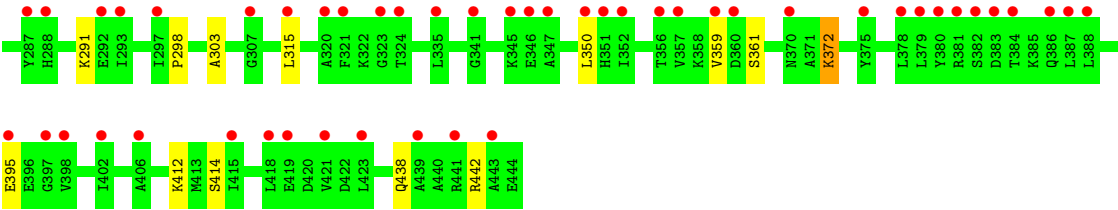
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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	169.33Å 81.60Å 98.38Å 90.00° 104.11° 90.00°	Depositor
Resolution (Å)	42.11 – 2.26 42.11 – 2.26	Depositor EDS
% Data completeness (in resolution range)	99.5 (42.11-2.26) 99.5 (42.11-2.26)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.91 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.177 , 0.214 0.174 , 0.208	Depositor DCC
R_{free} test set	3078 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	38.0	Xtriage
Anisotropy	0.259	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7659	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% 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: NDP, 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	0.49	0/3555	0.75	0/4801
1	B	0.49	0/3537	0.76	0/4777
All	All	0.49	0/7092	0.75	0/9578

There are no bond length outliers.

There are no bond angle outliers.

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	3491	0	3523	19	0
1	B	3479	0	3509	15	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	48	0	26	1	0
4	B	48	0	26	1	0
5	A	189	0	0	1	0
5	B	202	0	0	0	0
All	All	7659	0	7210	34	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 2.

All (34) 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:220:ASN:CG	1:A:221:GLU:H	1.97	0.72
1:A:220:ASN:H	1:A:220:ASN:HD22	1.38	0.71
1:A:220:ASN:CG	1:A:221:GLU:N	2.61	0.58
1:A:137:ASP:OD1	1:A:140:ARG:NH2	2.37	0.57
1:A:291:LYS:HG2	1:A:350:LEU:HD11	1.86	0.57
1:A:359:VAL:HG12	1:A:361:SER:HB2	1.88	0.55
1:B:359:VAL:HG12	1:B:361:SER:HB2	1.92	0.52
1:B:291:LYS:HG2	1:B:350:LEU:HD11	1.90	0.51
1:A:288:HIS:HB3	1:A:291:LYS:HB2	1.93	0.50
1:A:46:TYR:HB2	1:A:52:ILE:HD12	1.93	0.50
1:B:298:PRO:O	4:B:802:NDP:O2D	2.30	0.49
1:A:188:ILE:HD12	1:A:339:ARG:HG2	1.96	0.48
1:B:271:GLN:HG2	1:B:278:TYR:CE2	2.50	0.47
1:B:254:THR:O	1:B:255:ASN:HB2	2.14	0.46
1:A:220:ASN:H	1:A:220:ASN:ND2	2.09	0.46
1:B:156:ILE:HD12	1:B:214:VAL:HG21	1.98	0.46
1:B:438:GLN:O	1:B:442:ARG:HG2	2.15	0.46
1:A:192:ASP:HA	1:A:195:GLU:OE1	2.17	0.45
1:A:94:HIS:HB2	1:A:101:PHE:HE2	1.82	0.44
1:B:113:GLY:HA2	1:B:282:ASP:HB2	1.99	0.44
1:B:5:ILE:HB	1:B:30:THR:HG22	1.98	0.44
1:A:5:ILE:HB	1:A:30:THR:HG22	1.98	0.43
1:B:143:LYS:HB2	1:B:143:LYS:HE2	1.86	0.43
1:A:180:GLU:OE2	1:A:182:ASN:ND2	2.52	0.43
1:A:148:ASN:HD22	1:A:149:LYS:H	1.67	0.42
1:B:22:ASN:HB2	1:B:315:LEU:HD13	2.02	0.42
1:B:372:LYS:HA	1:B:372:LYS:HE3	2.02	0.42
1:A:298:PRO:O	4:A:803:NDP:O2D	2.33	0.41
1:B:40:ALA:HB1	1:B:42:CYS:SG	2.61	0.41
1:B:281:GLY:HA2	1:B:303:ALA:HA	2.02	0.41
1:A:281:GLY:HA2	1:A:303:ALA:HA	2.02	0.41
1:A:22:ASN:HB2	1:A:315:LEU:HD13	2.03	0.41
1:A:395:GLU:HG3	5:A:825:HOH:O	2.21	0.41
1:B:372:LYS:HD3	1:B:395:GLU:OE2	2.21	0.41

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	444/480 (92%)	433 (98%)	11 (2%)	0	100	100
1	B	442/480 (92%)	429 (97%)	13 (3%)	0	100	100
All	All	886/960 (92%)	862 (97%)	24 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	372/398 (94%)	357 (96%)	15 (4%)	28	34
1	B	370/398 (93%)	362 (98%)	8 (2%)	45	56
All	All	742/796 (93%)	719 (97%)	23 (3%)	36	44

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	VAL
1	A	143	LYS
1	A	148	ASN
1	A	163	LEU
1	A	187	THR
1	A	220	ASN
1	A	241	SER
1	A	265[A]	GLU

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Mol	Chain	Res	Type
1	A	265[B]	GLU
1	A	293	ILE
1	A	309	LEU
1	A	350	LEU
1	A	357	VAL
1	A	396	GLU
1	A	414	SER
1	B	1	MET
1	B	44	LEU
1	B	120	GLU
1	B	210	THR
1	B	223	VAL
1	B	372	LYS
1	B	412	LYS
1	B	414	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	127	GLN
1	A	184	HIS
1	A	220	ASN
1	A	275	GLN
1	A	294	HIS
1	A	334	ASN
1	B	2	ASN
1	B	184	HIS
1	B	211	ASN
1	B	220	ASN
1	B	294	HIS
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 ⓘ

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	$\# Z > 2$
2	COA	A	445	-	47,50,50	0.89	3 (6%)	69,75,75	1.69	14 (20%)
3	FAD	B	446	-	58,58,58	0.99	3 (5%)	85,89,89	1.49	15 (17%)
3	FAD	A	446	-	58,58,58	0.96	2 (3%)	85,89,89	1.53	16 (18%)
2	COA	B	445	-	47,50,50	0.91	3 (6%)	69,75,75	1.69	13 (18%)
4	NDP	A	803	-	51,52,52	1.48	4 (7%)	71,80,80	1.50	9 (12%)
4	NDP	B	802	-	51,52,52	1.47	5 (9%)	71,80,80	1.50	9 (12%)

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	COA	A	445	-	-	5/48/64/64	0/3/3/3
3	FAD	B	446	-	-	2/34/50/50	0/6/6/6
3	FAD	A	446	-	-	1/34/50/50	0/6/6/6
2	COA	B	445	-	-	5/48/64/64	0/3/3/3
4	NDP	A	803	-	-	7/34/77/77	0/5/5/5
4	NDP	B	802	-	-	8/34/77/77	0/5/5/5

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	803	NDP	O7N-C7N	7.11	1.41	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	802	NDP	O7N-C7N	7.08	1.41	1.24
3	B	446	FAD	C4X-N5	2.92	1.37	1.30
4	A	803	NDP	C2A-N3A	2.77	1.38	1.33
4	A	803	NDP	C2A-N1A	2.76	1.38	1.33
3	A	446	FAD	C4X-N5	2.67	1.36	1.30
4	B	802	NDP	C2A-N3A	2.63	1.38	1.33
4	B	802	NDP	C2A-N1A	2.63	1.38	1.33
2	B	445	COA	P2A-O3A	2.41	1.62	1.59
2	A	445	COA	P2A-O3A	2.37	1.62	1.59
2	B	445	COA	C8A-N7A	2.26	1.36	1.31
2	A	445	COA	C8A-N7A	2.22	1.36	1.31
3	B	446	FAD	C5A-N7A	-2.20	1.35	1.39
2	B	445	COA	P1A-O3A	2.19	1.61	1.59
4	B	802	NDP	C6N-C5N	2.15	1.39	1.33
4	A	803	NDP	C6N-C5N	2.13	1.39	1.33
3	A	446	FAD	C8A-N7A	2.10	1.35	1.31
4	B	802	NDP	C8A-N7A	2.09	1.35	1.31
3	B	446	FAD	C4A-N9A	-2.08	1.33	1.37
2	A	445	COA	P1A-O3A	2.04	1.61	1.59

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	802	NDP	N3A-C2A-N1A	-6.14	119.28	128.58
4	A	803	NDP	N3A-C2A-N1A	-5.65	120.02	128.58
2	A	445	COA	C5A-C4A-N3A	-5.29	119.44	126.72
2	B	445	COA	C5A-C4A-N3A	-5.24	119.50	126.72
3	A	446	FAD	N3A-C2A-N1A	-5.21	120.69	128.58
2	B	445	COA	N3A-C2A-N1A	-4.96	121.08	128.58
2	A	445	COA	N3A-C2A-N1A	-4.94	121.11	128.58
3	B	446	FAD	C5A-C4A-N3A	-4.91	119.95	126.72
3	A	446	FAD	C5A-C4A-N3A	-4.83	120.07	126.72
3	B	446	FAD	N3A-C2A-N1A	-4.54	121.71	128.58
4	A	803	NDP	N9A-C8A-N7A	-4.23	107.93	113.94
4	B	802	NDP	C5A-C4A-N3A	-4.16	120.99	126.72
4	A	803	NDP	C5A-C4A-N3A	-4.14	121.02	126.72
4	B	802	NDP	N9A-C8A-N7A	-3.85	108.47	113.94
4	A	803	NDP	C5A-N7A-C8A	3.66	109.20	103.45
3	A	446	FAD	N9A-C8A-N7A	-3.58	108.86	113.94
2	B	445	COA	N9A-C8A-N7A	-3.54	108.91	113.94
2	B	445	COA	C2A-N3A-C4A	3.54	120.47	111.83
4	B	802	NDP	C2A-N3A-C4A	3.53	120.45	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	445	COA	C2A-N3A-C4A	3.53	120.45	111.83
2	B	445	COA	C2P-C3P-N4P	-3.50	104.37	112.31
2	A	445	COA	N9A-C8A-N7A	-3.48	109.00	113.94
3	A	446	FAD	C2A-N3A-C4A	3.43	120.20	111.83
2	A	445	COA	N3A-C4A-N9A	3.36	132.88	127.17
4	A	803	NDP	C2A-N3A-C4A	3.33	119.96	111.83
2	B	445	COA	N3A-C4A-N9A	3.32	132.81	127.17
2	A	445	COA	C2P-C3P-N4P	-3.30	104.81	112.31
3	B	446	FAD	C2A-N3A-C4A	3.28	119.85	111.83
4	B	802	NDP	C5A-N7A-C8A	3.28	108.61	103.45
3	A	446	FAD	N3A-C4A-N9A	3.22	132.64	127.17
3	B	446	FAD	N9A-C8A-N7A	-3.20	109.39	113.94
2	B	445	COA	C7P-N8P-C9P	3.13	128.18	122.55
2	A	445	COA	C6P-C7P-N8P	-3.09	105.42	112.00
3	B	446	FAD	N3A-C4A-N9A	3.06	132.37	127.17
4	A	803	NDP	N3A-C4A-N9A	2.87	132.05	127.17
2	B	445	COA	C6P-C7P-N8P	-2.87	105.89	112.00
2	A	445	COA	C4A-C5A-N7A	-2.85	107.32	110.58
2	B	445	COA	C4A-C5A-N7A	-2.79	107.39	110.58
3	B	446	FAD	C4-N3-C2	-2.79	120.70	125.64
3	B	446	FAD	C4A-C5A-N7A	-2.77	107.42	110.58
4	A	803	NDP	O4D-C1D-N1N	2.76	113.34	108.08
4	B	802	NDP	N3A-C4A-N9A	2.76	131.85	127.17
3	A	446	FAD	C4A-N9A-C8A	2.76	108.63	105.74
2	A	445	COA	C5A-N7A-C8A	2.69	107.68	103.45
4	B	802	NDP	O4B-C1B-N9A	2.67	113.22	108.09
2	A	445	COA	C3P-N4P-C5P	2.66	127.78	122.82
2	B	445	COA	C5A-N7A-C8A	2.66	107.63	103.45
2	A	445	COA	C7P-N8P-C9P	2.63	127.27	122.55
3	A	446	FAD	C5A-N7A-C8A	2.62	107.56	103.45
3	B	446	FAD	C4X-C4-N3	2.59	119.84	113.25
3	A	446	FAD	C4A-C5A-N7A	-2.56	107.66	110.58
3	B	446	FAD	C4-C4X-N5	2.56	121.74	118.21
3	A	446	FAD	C4-N3-C2	-2.55	121.11	125.64
2	B	445	COA	C4A-N9A-C8A	2.53	108.39	105.74
4	A	803	NDP	C4A-C5A-N7A	-2.50	107.73	110.58
3	B	446	FAD	C5A-N7A-C8A	2.47	107.33	103.45
2	A	445	COA	C4A-N9A-C8A	2.46	108.32	105.74
2	B	445	COA	O6A-CCP-CBP	2.40	114.41	110.55
4	A	803	NDP	C4A-N9A-C8A	2.36	108.22	105.74
3	B	446	FAD	C4A-N9A-C8A	2.33	108.19	105.74
3	A	446	FAD	C4X-C4-N3	2.33	119.18	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	446	FAD	C4X-C10-N10	2.30	119.78	116.48
4	B	802	NDP	C4A-C5A-N7A	-2.27	107.98	110.58
4	B	802	NDP	O4D-C1D-N1N	2.27	112.42	108.08
2	A	445	COA	O6A-CCP-CBP	2.18	114.05	110.55
3	A	446	FAD	O4-C4-C4X	-2.18	120.79	126.53
3	A	446	FAD	C5X-N5-C4X	2.17	121.60	118.09
3	B	446	FAD	C10-C4X-N5	-2.17	120.38	124.81
3	B	446	FAD	C5X-N5-C4X	2.16	121.59	118.09
3	B	446	FAD	O4-C4-C4X	-2.14	120.89	126.53
3	A	446	FAD	C4-C4X-N5	2.11	121.13	118.21
3	A	446	FAD	C10-C4X-N5	-2.09	120.54	124.81
3	A	446	FAD	C4X-C10-N10	2.08	119.47	116.48
2	B	445	COA	C3P-N4P-C5P	2.04	126.62	122.82
2	A	445	COA	C3B-C2B-C1B	2.02	104.33	99.89
3	A	446	FAD	C9A-C5X-N5	-2.01	120.32	122.45

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	445	COA	CEP-CBP-CCP-O6A
4	A	803	NDP	O4D-C1D-N1N-C2N
4	B	802	NDP	O4D-C1D-N1N-C2N
4	A	803	NDP	C2D-C1D-N1N-C6N
4	A	803	NDP	C2D-C1D-N1N-C2N
4	A	803	NDP	C2B-C1B-N9A-C8A
4	B	802	NDP	C2B-C1B-N9A-C8A
2	A	445	COA	CEP-CBP-CCP-O6A
2	B	445	COA	CDP-CBP-CCP-O6A
2	A	445	COA	S1P-C2P-C3P-N4P
2	B	445	COA	S1P-C2P-C3P-N4P
2	A	445	COA	C5B-O5B-P1A-O1A
2	B	445	COA	C5B-O5B-P1A-O1A
4	B	802	NDP	C2D-C1D-N1N-C6N
2	A	445	COA	C3B-O3B-P3B-O9A
3	B	446	FAD	O4B-C4B-C5B-O5B
4	A	803	NDP	O4B-C4B-C5B-O5B
4	B	802	NDP	O4B-C4B-C5B-O5B
4	B	802	NDP	O4B-C1B-N9A-C8A
3	A	446	FAD	O4B-C4B-C5B-O5B
4	A	803	NDP	O4B-C1B-N9A-C8A
4	B	802	NDP	C2D-C1D-N1N-C2N

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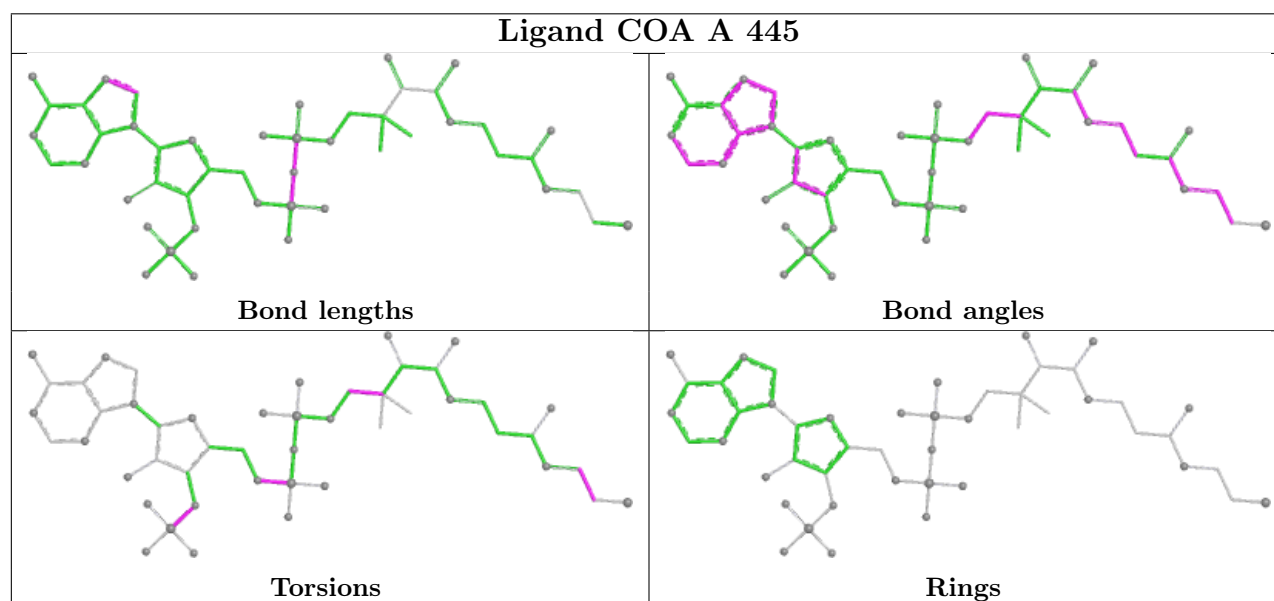
Mol	Chain	Res	Type	Atoms
2	B	445	COA	C3B-O3B-P3B-O9A
4	B	802	NDP	C2B-C1B-N9A-C4A
2	A	445	COA	CDP-CBP-CCP-O6A
4	A	803	NDP	C3B-C4B-C5B-O5B
4	B	802	NDP	C3B-C4B-C5B-O5B
3	B	446	FAD	C3B-C4B-C5B-O5B

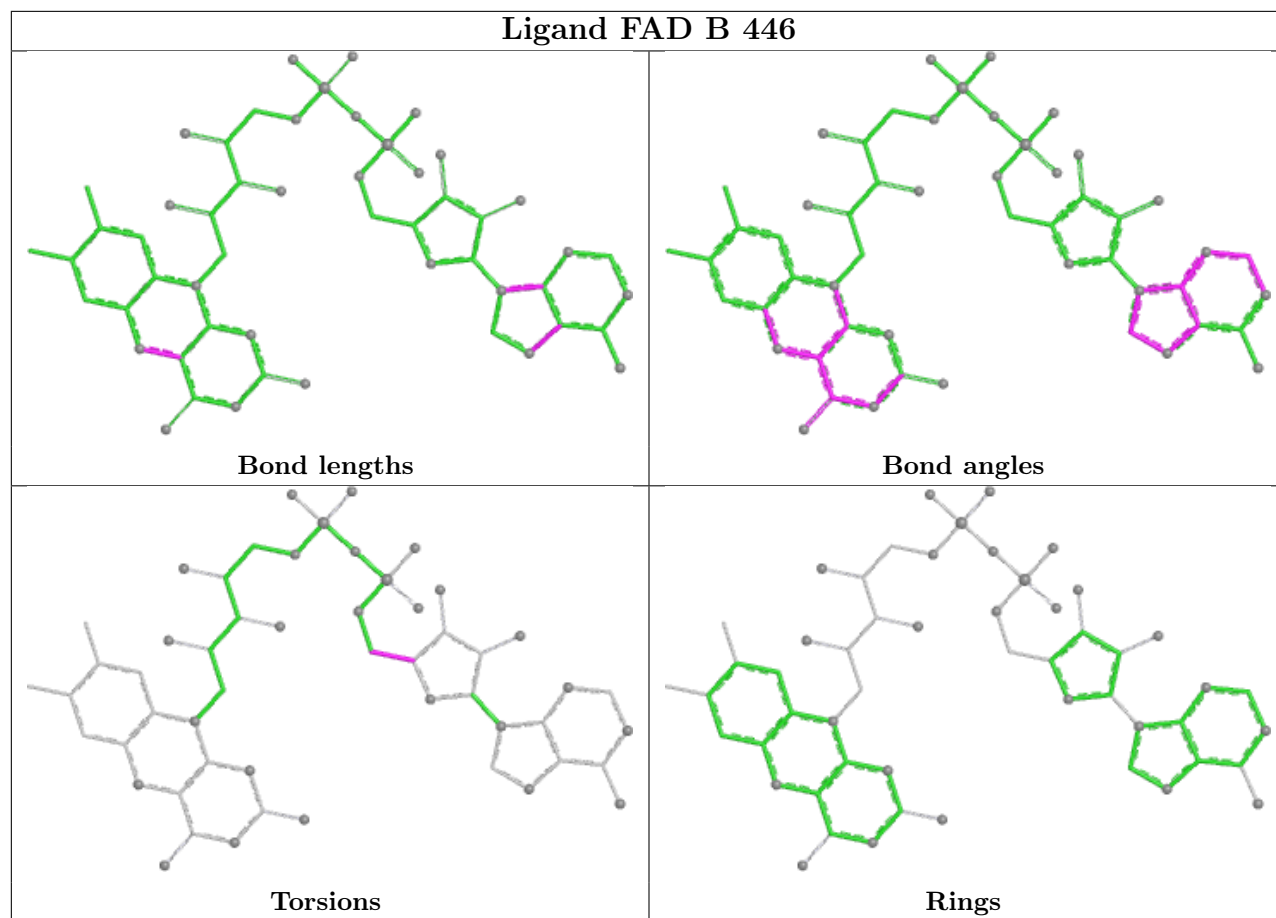
There are no ring outliers.

2 monomers are involved in 2 short contacts:

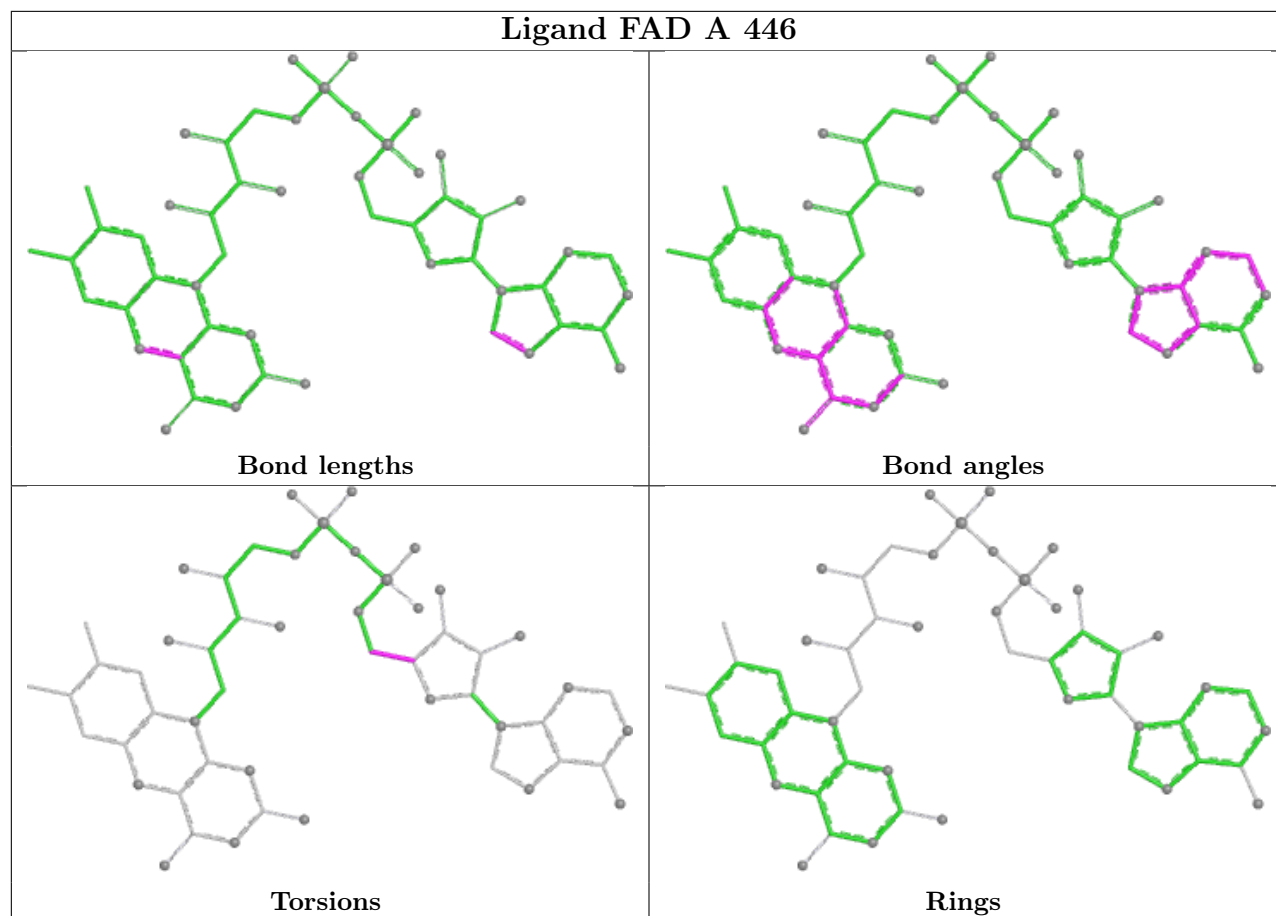
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	803	NDP	1	0
4	B	802	NDP	1	0

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 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.

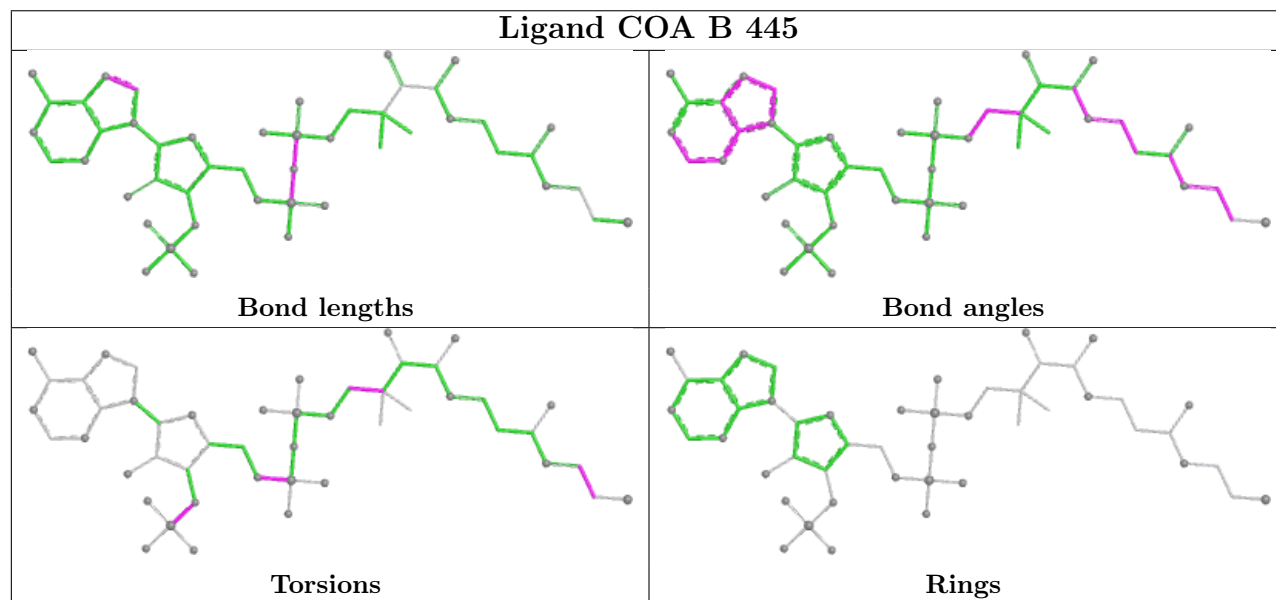


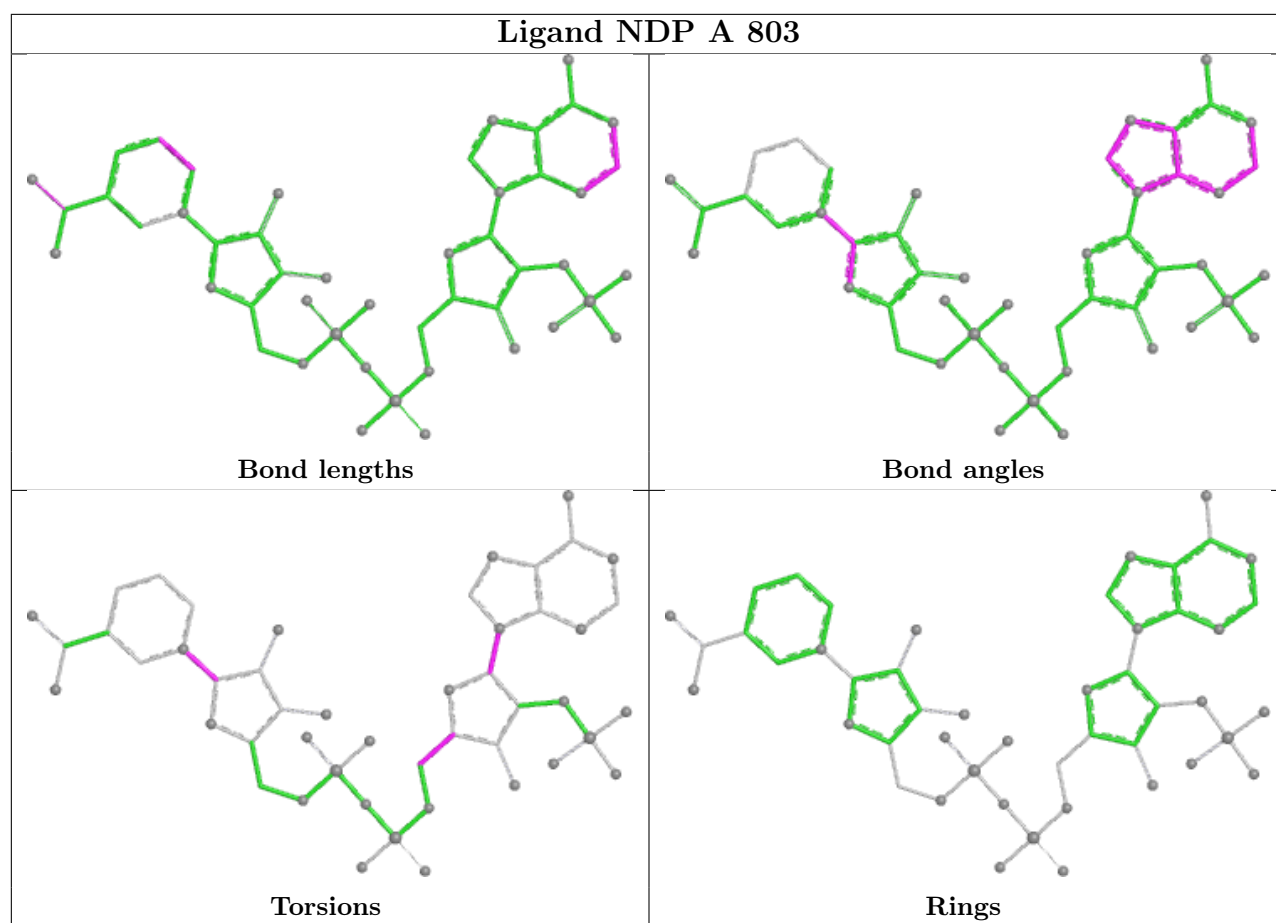


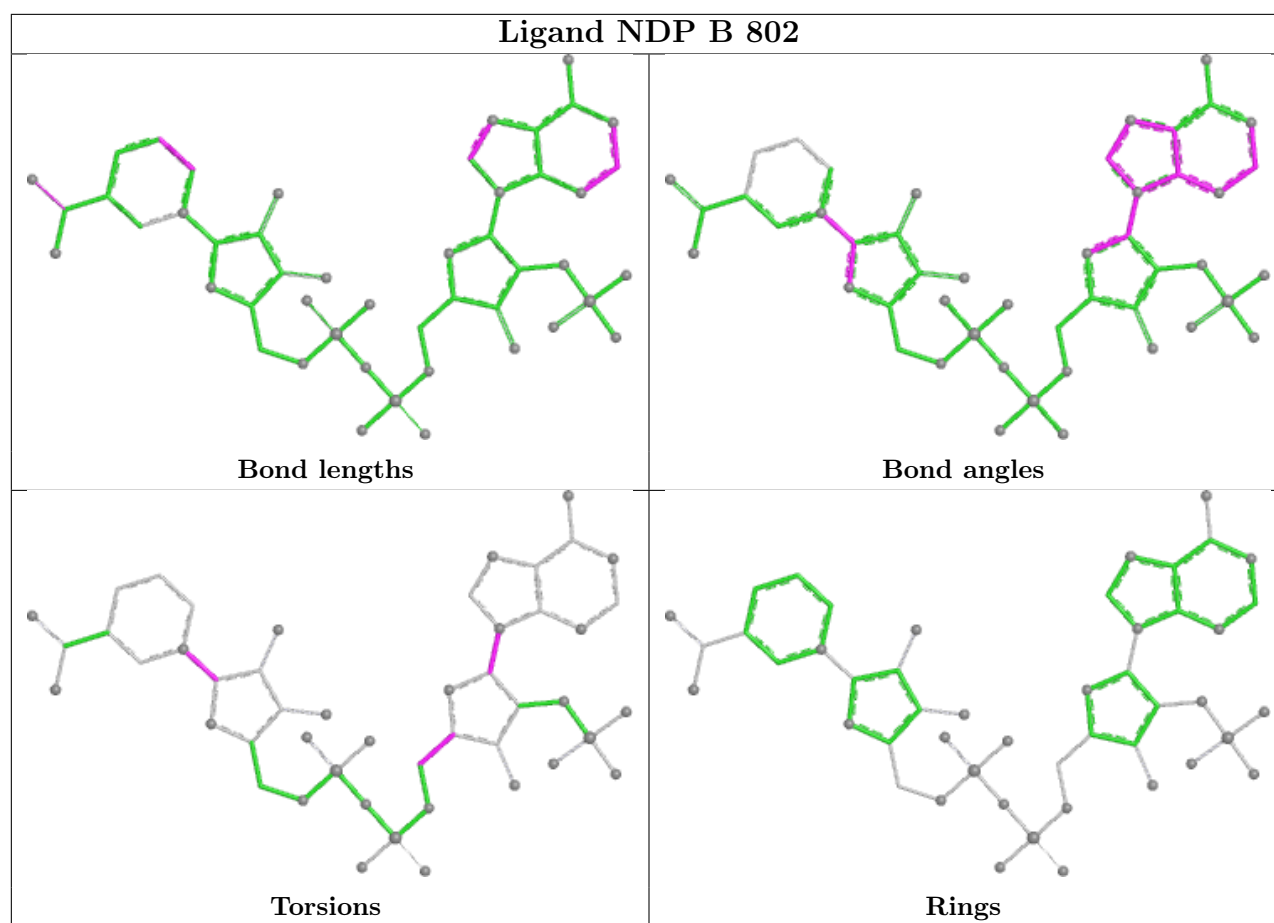
Ligand FAD A 446



Ligand COA B 445







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(Å ²)	Q<0.9
1	A	444/480 (92%)	1.88	174 (39%) 1 0	32, 58, 67, 71	2 (0%)
1	B	444/480 (92%)	1.68	121 (27%) 1 1	50, 58, 66, 72	0
All	All	888/960 (92%)	1.78	295 (33%) 1 0	32, 58, 66, 72	2 (0%)

All (295) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	5.7
1	A	29	VAL	5.0
1	B	1	MET	4.9
1	A	4	VAL	4.6
1	B	260	HIS	4.6
1	A	15	ALA	4.2
1	A	188	ILE	4.1
1	A	310	ALA	3.9
1	A	19	ILE	3.9
1	B	188	ILE	3.9
1	A	89	ILE	3.9
1	B	255	ASN	3.9
1	A	277	VAL	3.8
1	A	5	ILE	3.8
1	A	20	VAL	3.8
1	A	147	THR	3.8
1	B	351	HIS	3.8
1	A	249	ASP	3.7
1	B	24	GLU	3.7
1	A	311	GLY	3.7
1	A	28	VAL	3.7
1	A	40	ALA	3.7
1	B	443	ALA	3.7
1	A	64	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	350	LEU	3.6
1	A	315	LEU	3.5
1	A	275	GLN	3.5
1	A	279	ALA	3.5
1	A	72	ILE	3.5
1	A	2	ASN	3.5
1	A	70	TYR	3.5
1	B	359	VAL	3.4
1	A	312	LEU	3.4
1	A	120	GLU	3.4
1	A	168	THR	3.4
1	A	12	GLY	3.4
1	A	224	GLU	3.3
1	A	26	ALA	3.3
1	A	260	HIS	3.3
1	A	149	LYS	3.3
1	B	261	LYS	3.3
1	A	278	TYR	3.3
1	A	11	ALA	3.2
1	A	16	ALA	3.2
1	A	220	ASN	3.2
1	A	14	SER	3.2
1	A	198	TYR	3.2
1	A	261	LYS	3.2
1	A	74	ALA	3.2
1	A	223	VAL	3.2
1	B	347	ALA	3.2
1	A	217	PHE	3.2
1	B	382	SER	3.2
1	A	309	LEU	3.2
1	A	313	ASN	3.1
1	A	108	LEU	3.1
1	A	106	ASP	3.1
1	A	51	ALA	3.1
1	A	110	ILE	3.1
1	A	23	ASP	3.1
1	B	370	ASN	3.1
1	A	268	ALA	3.1
1	A	63	VAL	3.1
1	A	438[A]	GLN	3.0
1	B	50	GLY	3.0
1	B	195	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	267	ASN	3.0
1	A	316	ASP	3.0
1	B	315	LEU	3.0
1	A	127	GLN	3.0
1	B	149	LYS	3.0
1	A	49	SER	3.0
1	B	173	GLY	3.0
1	A	178	MET	3.0
1	B	60	ALA	2.9
1	B	268	ALA	2.9
1	A	85	THR	2.9
1	B	189	TYR	2.9
1	B	418	LEU	2.9
1	A	272	THR	2.9
1	A	27	ASN	2.9
1	A	323	GLY	2.9
1	B	220	ASN	2.9
1	B	287	TYR	2.9
1	B	345	LYS	2.9
1	B	214	VAL	2.8
1	A	18	GLN	2.8
1	A	124	ARG	2.8
1	B	210	THR	2.8
1	B	123	GLY	2.8
1	A	31	LEU	2.8
1	B	170	VAL	2.8
1	B	207	GLU	2.8
1	A	131	LEU	2.8
1	B	150	VAL	2.8
1	A	125	ASP	2.7
1	A	148	ASN	2.7
1	A	370	ASN	2.7
1	B	378	LEU	2.7
1	A	138	ALA	2.7
1	A	66	PHE	2.7
1	A	238	VAL	2.7
1	B	20	VAL	2.7
1	A	255	ASN	2.7
1	B	228	THR	2.7
1	B	402	ILE	2.7
1	B	245	LYS	2.7
1	B	201	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	103	PHE	2.7
1	B	125	ASP	2.7
1	A	171	GLU	2.7
1	B	49	SER	2.7
1	B	218	LYS	2.7
1	A	144	THR	2.7
1	A	232	THR	2.7
1	B	384	THR	2.7
1	A	50	GLY	2.7
1	A	314	MET	2.7
1	B	178	MET	2.7
1	B	269	TYR	2.6
1	A	274	VAL	2.6
1	B	76	VAL	2.6
1	B	137	ASP	2.6
1	A	173	GLY	2.6
1	A	307	GLY	2.6
1	A	322	LYS	2.6
1	B	352	ILE	2.6
1	B	292	GLU	2.6
1	A	443	ALA	2.6
1	A	182	ASN	2.6
1	A	417	ASP	2.6
1	A	30	THR	2.6
1	B	272	THR	2.6
1	A	104	SER	2.6
1	A	207	GLU	2.6
1	A	113	GLY	2.6
1	B	323	GLY	2.6
1	A	83	VAL	2.6
1	B	277	VAL	2.6
1	A	6	ILE	2.6
1	A	52	ILE	2.6
1	A	221	GLU	2.5
1	A	350	LEU	2.5
1	B	346	GLU	2.5
1	A	280	ALA	2.5
1	B	191	GLY	2.5
1	B	219	GLY	2.5
1	A	410	PHE	2.5
1	B	421	VAL	2.5
1	A	67	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	308	ARG	2.5
1	B	397	GLY	2.5
1	A	184	HIS	2.5
1	A	351	HIS	2.5
1	A	321	PHE	2.5
1	B	293	ILE	2.5
1	A	368	TYR	2.5
1	B	335	LEU	2.5
1	B	379	LEU	2.5
1	A	71	GLY	2.5
1	A	271	GLN	2.5
1	B	386	GLN	2.5
1	A	24	GLU	2.5
1	A	177	ARG	2.5
1	A	195	GLU	2.5
1	B	441	ARG	2.5
1	A	39	TYR	2.5
1	A	22	ASN	2.5
1	A	21	ARG	2.4
1	A	222	ARG	2.4
1	A	3	TYR	2.4
1	B	172	LEU	2.4
1	B	387	LEU	2.4
1	A	68	ASP	2.4
1	A	202	ASP	2.4
1	B	398	VAL	2.4
1	A	109	LEU	2.4
1	A	276	ASP	2.4
1	B	360	ASP	2.4
1	B	56	GLU	2.4
1	A	59	ILE	2.4
1	A	345	LYS	2.4
1	A	421	VAL	2.4
1	A	269	TYR	2.4
1	A	183	ASP	2.4
1	A	265[A]	GLU	2.4
1	A	92	ALA	2.4
1	A	65	THR	2.4
1	A	150	VAL	2.4
1	A	270	MET	2.4
1	B	63	VAL	2.4
1	B	77	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	86	GLU	2.4
1	A	62	ASN	2.3
1	A	303	ALA	2.3
1	A	9	ASP	2.3
1	B	383	ASP	2.3
1	A	300	GLY	2.3
1	A	320	ALA	2.3
1	A	13	MET	2.3
1	A	55	THR	2.3
1	A	97	THR	2.3
1	B	395	GLU	2.3
1	B	251	LEU	2.3
1	B	175	LYS	2.3
1	B	11	ALA	2.3
1	A	210	THR	2.3
1	A	302	THR	2.3
1	B	275	GLN	2.3
1	B	110	ILE	2.3
1	B	141	ILE	2.3
1	B	202	ASP	2.3
1	B	324	THR	2.3
1	B	204	HIS	2.3
1	B	127	GLN	2.3
1	B	252	GLU	2.3
1	A	230	LYS	2.3
1	A	90	VAL	2.3
1	A	209	LEU	2.2
1	B	406	ALA	2.2
1	A	141	ILE	2.2
1	A	256	ILE	2.2
1	B	297	ILE	2.2
1	A	130	HIS	2.2
1	A	146	GLU	2.2
1	B	375	TYR	2.2
1	A	185	ILE	2.2
1	A	172	LEU	2.2
1	B	2	ASN	2.2
1	B	222	ARG	2.2
1	B	249	ASP	2.2
1	B	267	ASN	2.2
1	A	34	GLY	2.2
1	B	128	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	86	GLU	2.2
1	B	419	GLU	2.2
1	A	187	THR	2.2
1	A	126	LEU	2.2
1	A	135	ILE	2.2
1	A	192	ASP	2.2
1	B	180	GLU	2.2
1	B	380	TYR	2.1
1	A	129	VAL	2.1
1	A	432	VAL	2.1
1	B	100	VAL	2.1
1	A	101	PHE	2.1
1	A	444	GLU	2.1
1	B	8	GLY	2.1
1	A	53	ALA	2.1
1	B	320	ALA	2.1
1	A	287	TYR	2.1
1	A	145	LEU	2.1
1	B	423	LEU	2.1
1	A	56	GLU	2.1
1	B	146	GLU	2.1
1	A	107	ARG	2.1
1	A	17	MET	2.1
1	A	58	LEU	2.1
1	A	425	TYR	2.1
1	B	198	TYR	2.1
1	B	415	ILE	2.1
1	A	250	PHE	2.1
1	B	307	GLY	2.1
1	A	263	ALA	2.1
1	A	317	LYS	2.1
1	B	15	ALA	2.1
1	B	122	GLU	2.1
1	B	142	LEU	2.1
1	A	383	ASP	2.1
1	B	288	HIS	2.1
1	A	214	VAL	2.1
1	B	357	VAL	2.1
1	B	321	PHE	2.1
1	B	341	GLY	2.1
1	A	257	ARG	2.1
1	B	121	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	199	LYS	2.0
1	B	254	THR	2.0
1	B	356	THR	2.0
1	A	352	ILE	2.0
1	A	170	VAL	2.0
1	A	398	VAL	2.0
1	B	381	ARG	2.0
1	B	93	GLU	2.0
1	A	60	ALA	2.0
1	A	406	ALA	2.0
1	B	194	ALA	2.0
1	B	439	ALA	2.0
1	A	418	LEU	2.0
1	B	211	ASN	2.0
1	B	273	ASN	2.0
1	B	388	LEU	2.0
1	B	67	ARG	2.0
1	B	119	PRO	2.0
1	B	143	LYS	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.

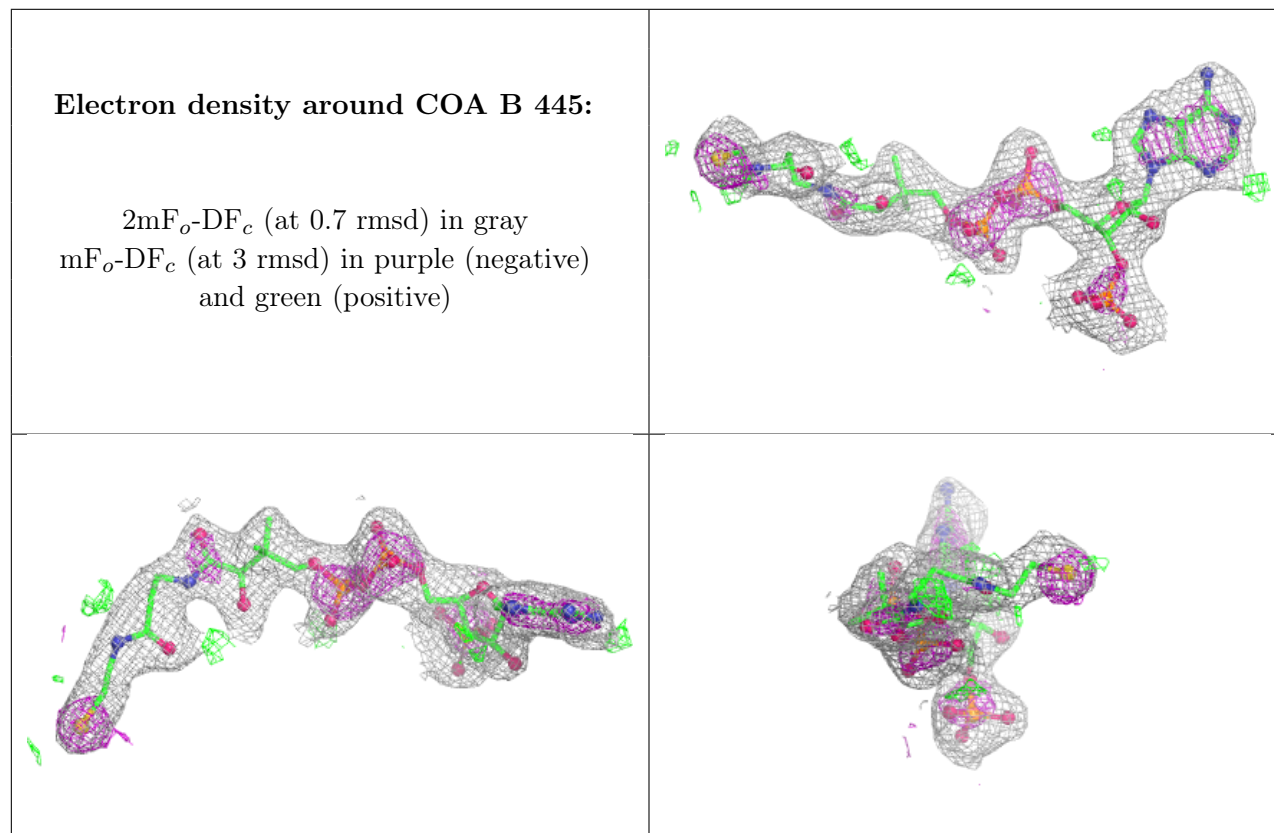
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	COA	B	445	48/48	0.89	0.17	50,57,65,65	0
2	COA	A	445	48/48	0.90	0.15	52,59,66,67	0
4	NDP	A	803	48/48	0.91	0.14	42,46,52,54	0
4	NDP	B	802	48/48	0.92	0.12	42,46,49,50	0

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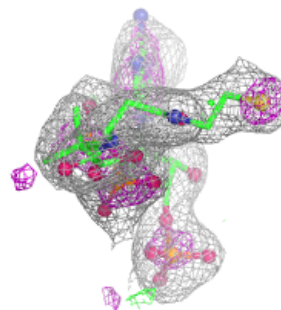
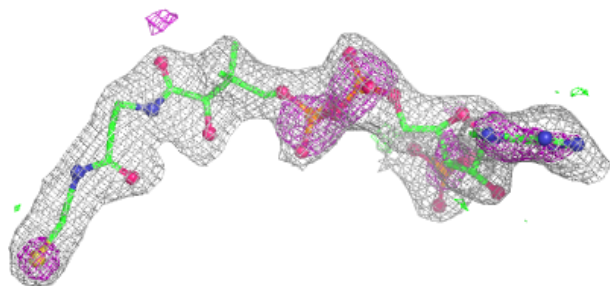
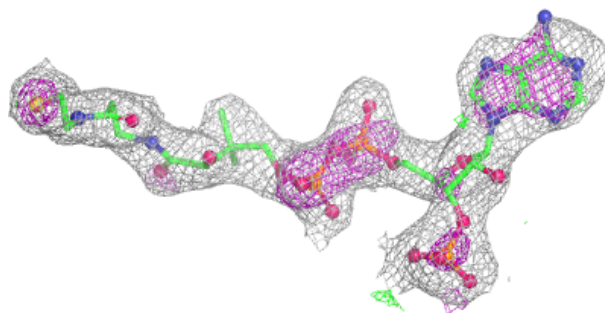
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	FAD	A	446	53/53	0.94	0.12	31,36,39,39	0
3	FAD	B	446	53/53	0.94	0.12	30,34,37,37	0

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.

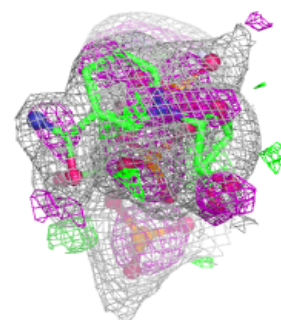
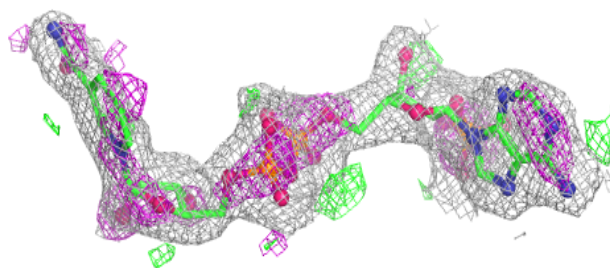
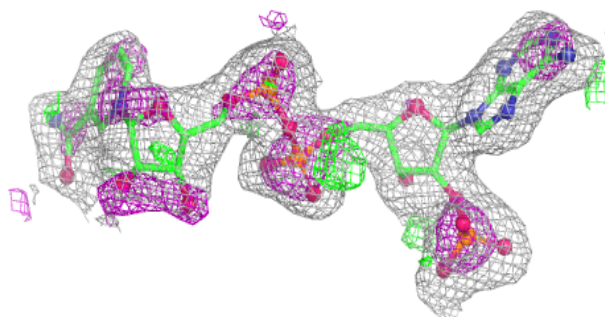


Electron density around COA A 445:

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

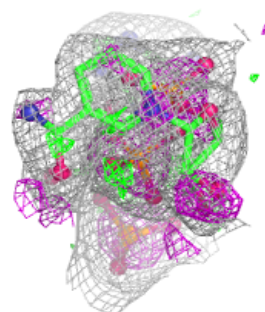
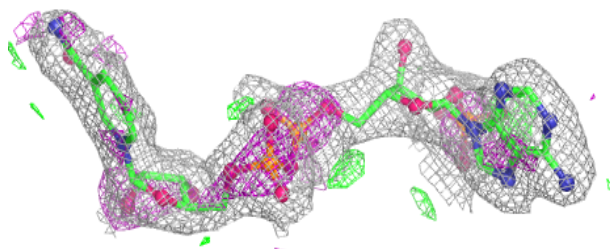
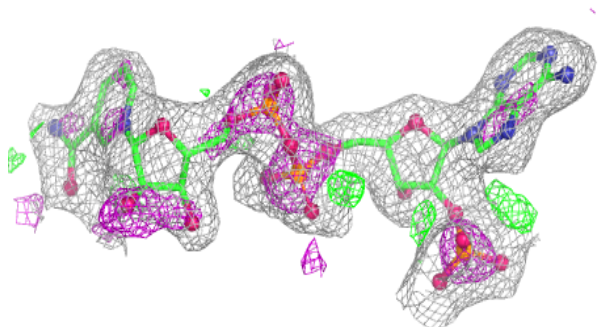
**Electron density around NDP A 803:**

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

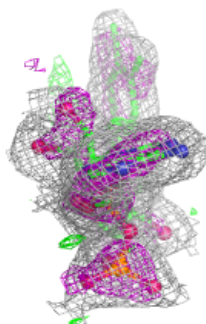
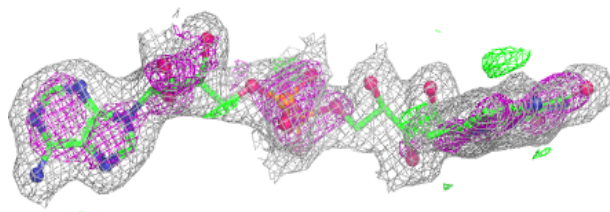
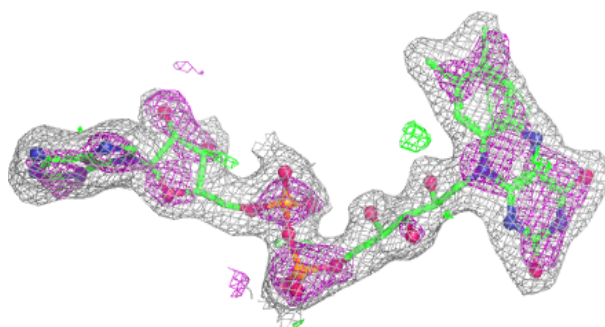


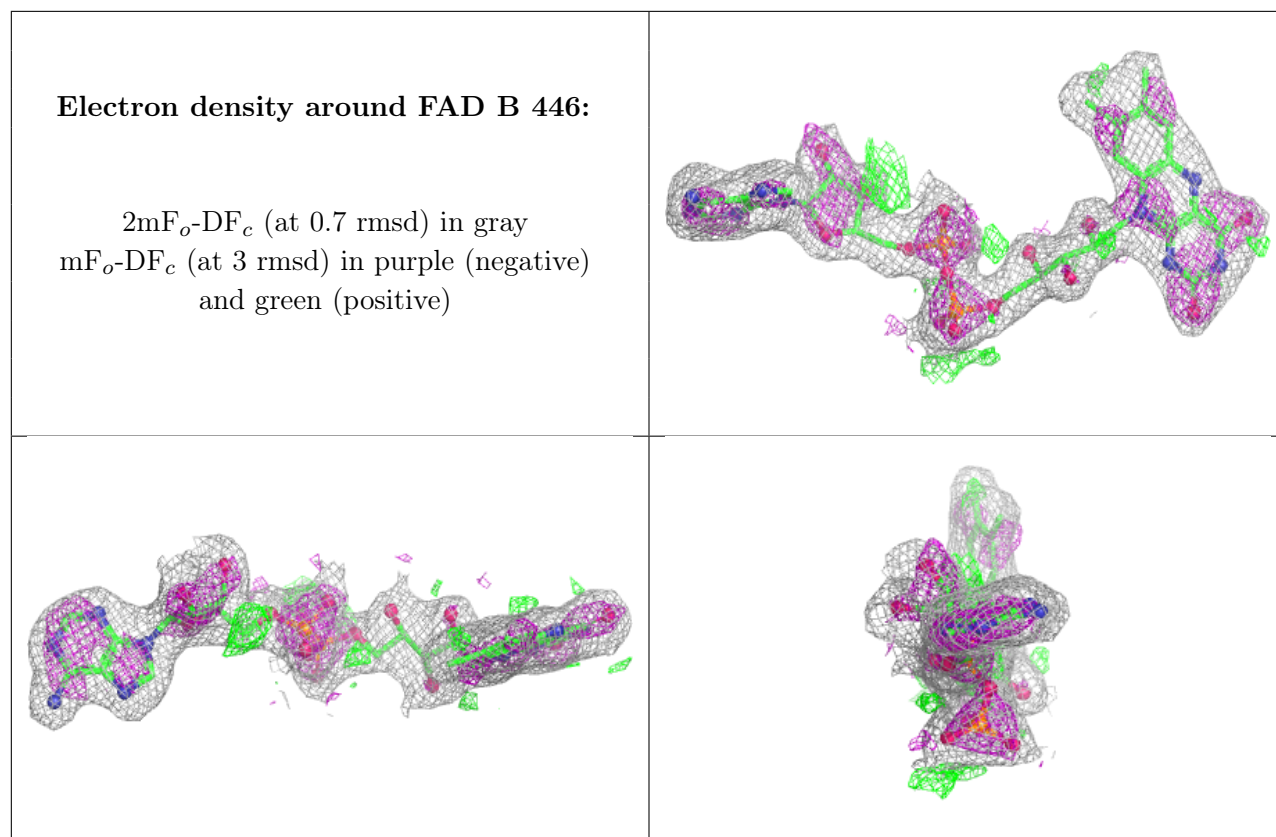
Electron density around NDP B 802:

$2mF_o-DF_c$ (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)





6.5 Other polymers [i](#)

There are no such residues in this entry.