



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 03:19 PM UTC

PDB ID : 8ACW / pdb_00008acw
Title : X-ray structure of Na⁺-NQR from *Vibrio cholerae* at 3.4 Å resolution
Authors : Fritz, G.
Deposited on : 2022-07-07
Resolution : 3.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

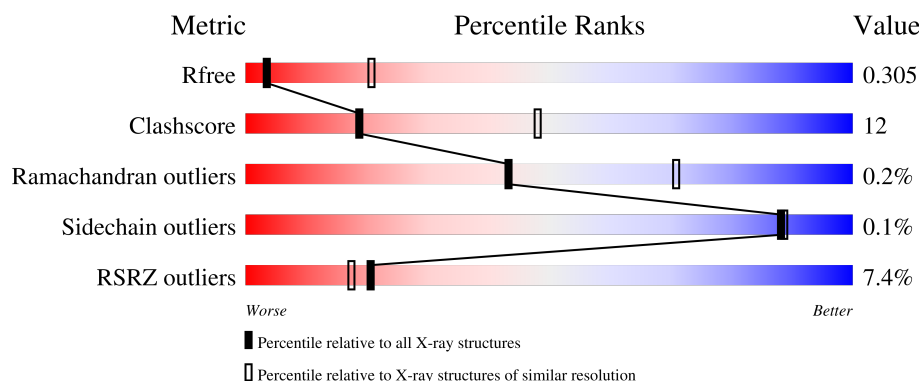
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

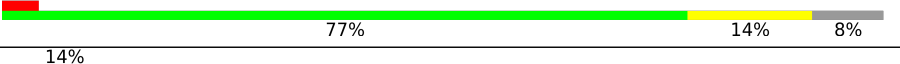
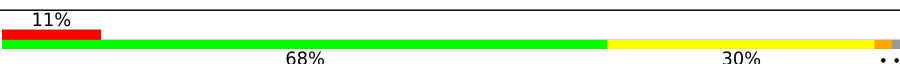
The reported resolution of this entry is 3.40 Å.

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.



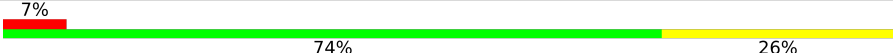
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	468	
2	B	415	
3	C	257	
4	D	210	
5	E	198	

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Mol	Chain	Length	Quality of chain
6	F	408	 A horizontal bar chart showing the quality of chain 6. The bar is divided into three segments: a small red segment at the beginning labeled '7%', a large green segment in the middle labeled '74%', and a yellow segment at the end labeled '26%'.

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	FES	F	1502	-	-	X	-

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 28730 atoms, of which 14422 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 Na(+)-translocating NADH-quinone reductase subunit A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	398	6114	1922	3080	516	582	14	0	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	initiating methionine	UNP A0A655PZA5
A	-20	GLY	-	expression tag	UNP A0A655PZA5
A	-19	SER	-	expression tag	UNP A0A655PZA5
A	-18	SER	-	expression tag	UNP A0A655PZA5
A	-17	HIS	-	expression tag	UNP A0A655PZA5
A	-16	HIS	-	expression tag	UNP A0A655PZA5
A	-15	HIS	-	expression tag	UNP A0A655PZA5
A	-14	HIS	-	expression tag	UNP A0A655PZA5
A	-13	HIS	-	expression tag	UNP A0A655PZA5
A	-12	HIS	-	expression tag	UNP A0A655PZA5
A	-11	SER	-	expression tag	UNP A0A655PZA5
A	-10	SER	-	expression tag	UNP A0A655PZA5
A	-9	GLY	-	expression tag	UNP A0A655PZA5
A	-8	LEU	-	expression tag	UNP A0A655PZA5
A	-7	GLU	-	expression tag	UNP A0A655PZA5
A	-6	VAL	-	expression tag	UNP A0A655PZA5
A	-5	LEU	-	expression tag	UNP A0A655PZA5
A	-4	PHE	-	expression tag	UNP A0A655PZA5
A	-3	GLN	-	expression tag	UNP A0A655PZA5
A	-2	GLY	-	expression tag	UNP A0A655PZA5
A	-1	PRO	-	expression tag	UNP A0A655PZA5
A	0	HIS	-	expression tag	UNP A0A655PZA5

- Molecule 2 is a protein called Na(+)-translocating NADH-quinone reductase subunit B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	380	Total	C	H	N	O	S	0	0	0
			5818	1924	2907	475	490	22			

- Molecule 3 is a protein called Na(+)-translocating NADH-quinone reductase subunit C.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	248	Total	C	H	N	O	S	0	0	0
			3774	1192	1892	324	362	4			

- Molecule 4 is a protein called Na(+)-translocating NADH-quinone reductase subunit D.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	203	Total	C	H	N	O	S	0	0	0
			3188	1031	1635	245	267	10			

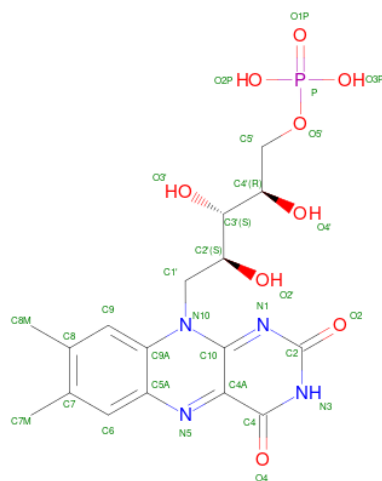
- Molecule 5 is a protein called Na(+)-translocating NADH-quinone reductase subunit E.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
5	E	197	Total	C	H	N	O	S	0	0	0
			3078	1008	1574	229	257	10			

- Molecule 6 is a protein called Na(+)-translocating NADH-quinone reductase subunit F.

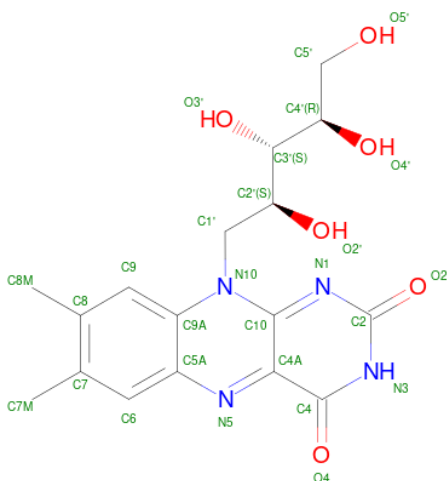
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
6	F	407	Total	C	H	N	O	S	0	0	0
			6259	2025	3098	518	594	24			

- Molecule 7 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P).



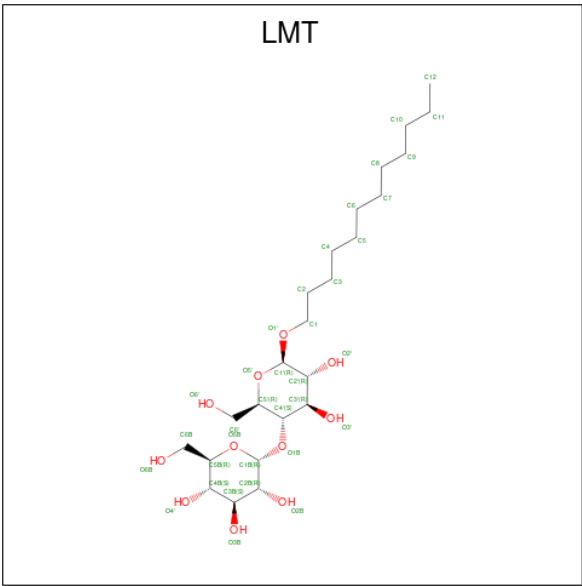
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
7	B	1	Total 49	C 17	H 19	N 4	O 8	P 1	0	0
7	C	1	Total 49	C 17	H 19	N 4	O 8	P 1	0	0

- Molecule 8 is RIBOFLAVIN (CCD ID: RBF) (formula: $C_{17}H_{20}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
8	B	1	Total	C	H	N	O	0	0
			46	17	19	4	6		

- Molecule 9 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).

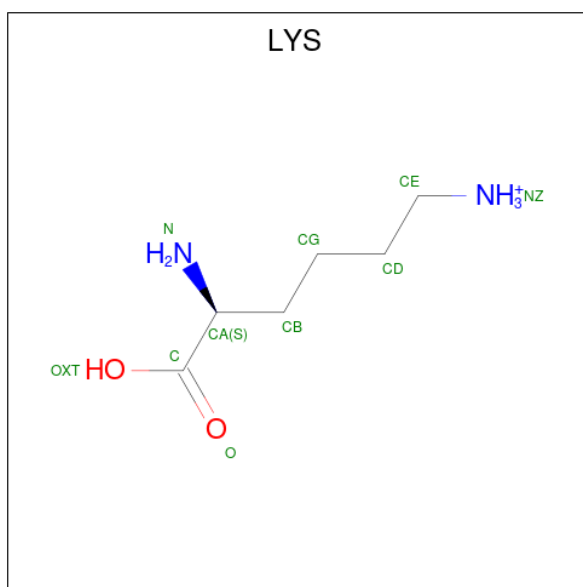


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total	C	H	O	0	0
			80	24	45	11		
9	D	1	Total	C	H	O	0	0
			81	24	46	11		
9	E	1	Total	C	H	O	0	0
			80	24	45	11		

- Molecule 10 is POTASSIUM ION (CCD ID: K) (formula: K).

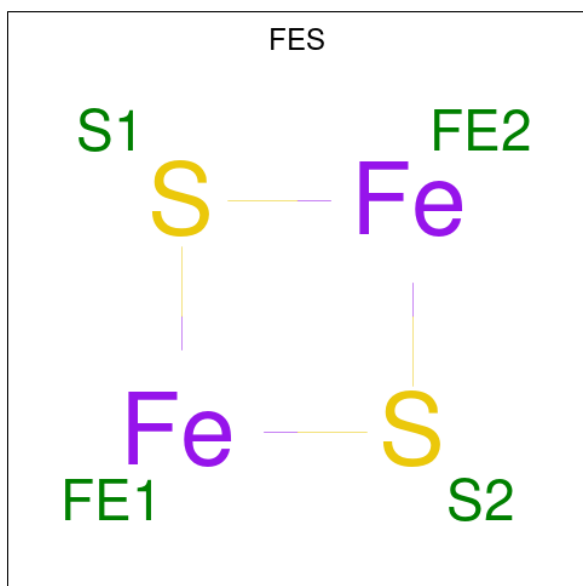
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	1	Total	K	0	0
			1	1		

- Molecule 11 is LYSINE (CCD ID: LYS) (formula: C₆H₁₅N₂O₂).



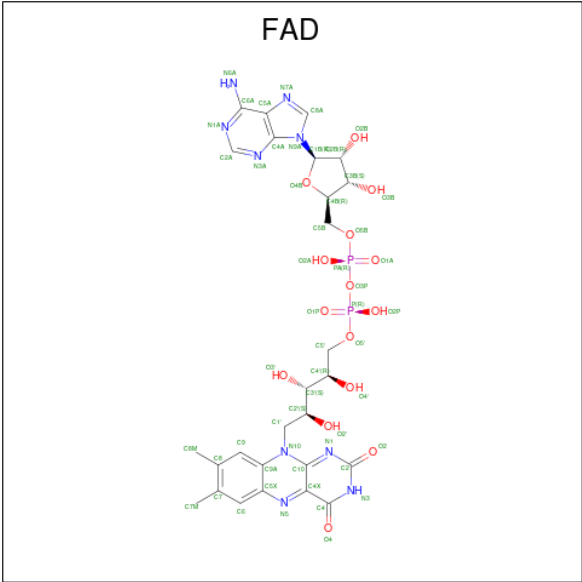
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	D	1	Total	C	H	N	O	0	0
			21	6	12	2	1		

- Molecule 12 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	E	1	Total	Fe S	0	0
			4	2 2		
12	F	1	Total	Fe S	0	0
			4	2 2		

- Molecule 13 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$).

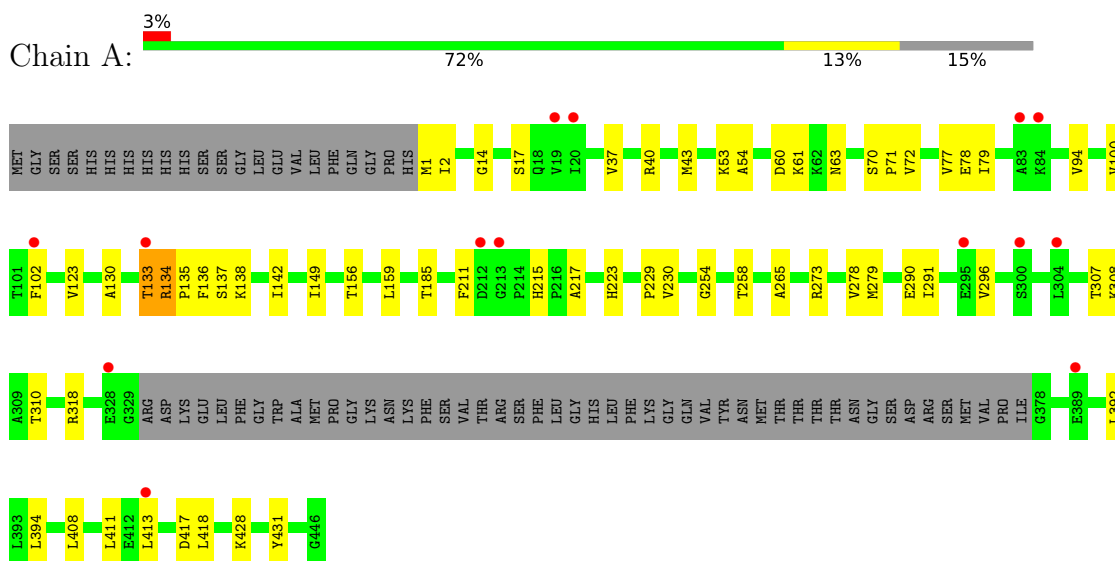


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	F	1	Total	C	H	N	O	P	
			84	27	31	9	15	2	

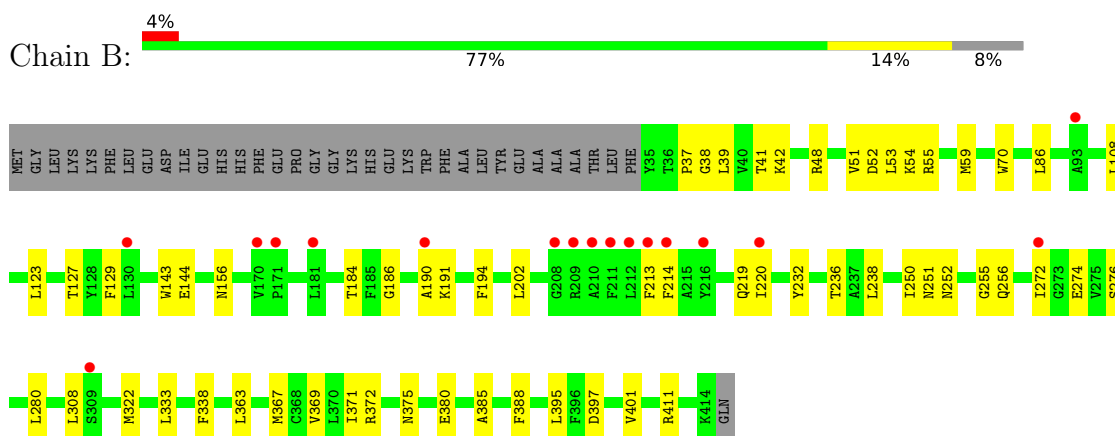
3 Residue-property plots [i](#)

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: Na(+)-translocating NADH-quinone reductase subunit A

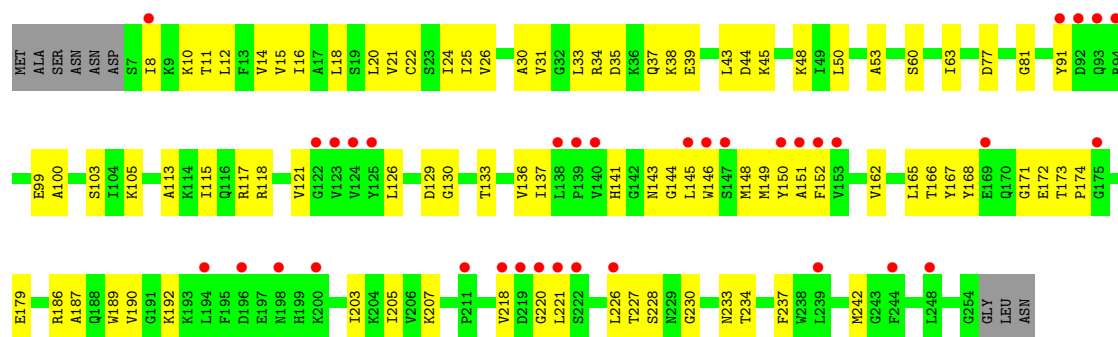


- Molecule 2: Na(+)-translocating NADH-quinone reductase subunit B

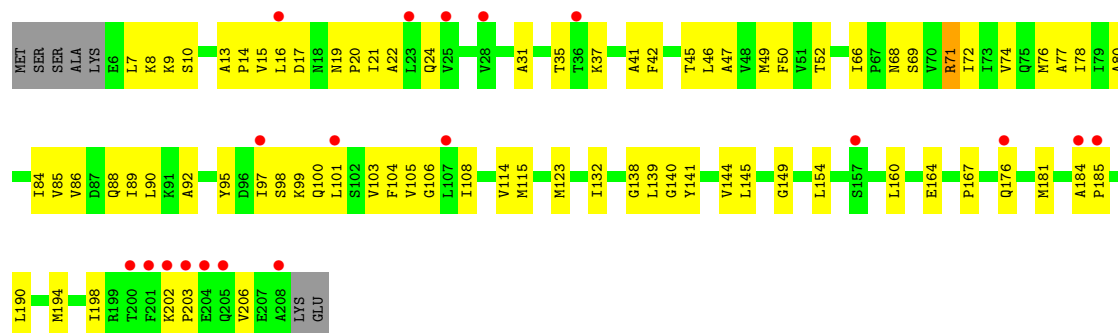


- Molecule 3: Na(+)-translocating NADH-quinone reductase subunit C

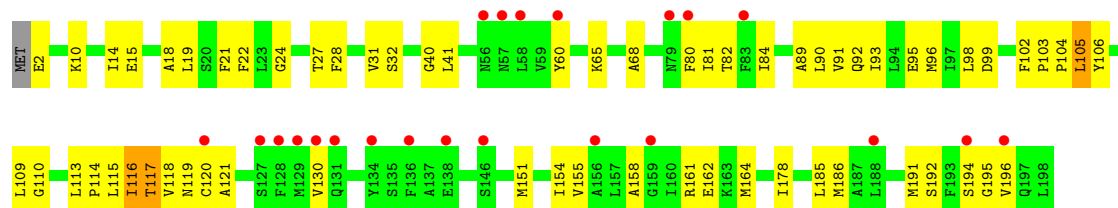




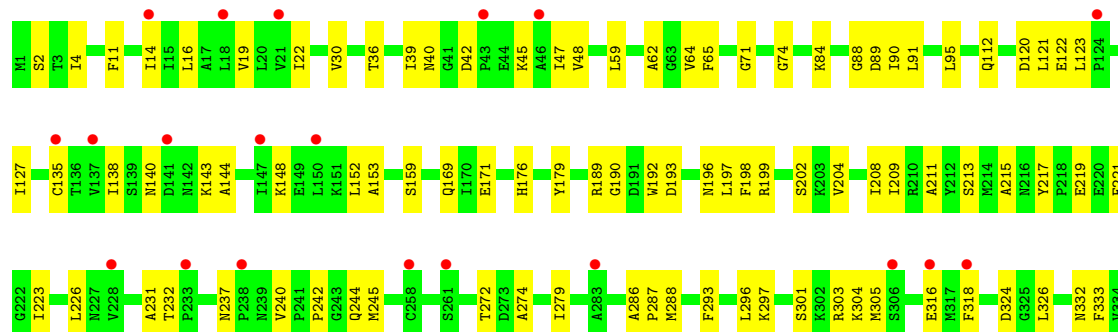
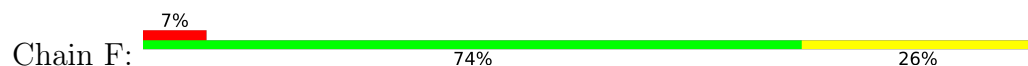
• Molecule 4: Na(+)-translocating NADH-quinone reductase subunit D



• Molecule 5: Na(+)-translocating NADH-quinone reductase subunit E



• Molecule 6: Na(+)-translocating NADH-quinone reductase subunit F





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.72Å 142.94Å 103.39Å 90.00° 109.93° 90.00°	Depositor
Resolution (Å)	48.60 – 3.40 48.60 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.60-3.40) 99.4 (48.60-3.40)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.04 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.20.1-4487	Depositor
R, R_{free}	0.270 , 0.306 0.271 , 0.305	Depositor DCC
R_{free} test set	1788 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	157.3	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 130.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	28730	wwPDB-VP
Average B, all atoms (Å ²)	217.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, K, RBF, LMT, FMN, FES

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	0.21	0/3087	0.57	2/4185 (0.0%)
2	B	0.19	0/2998	0.51	0/4083
3	C	0.27	0/1914	0.71	0/2583
4	D	0.30	0/1585	0.83	0/2153
5	E	0.30	0/1537	0.87	2/2084 (0.1%)
6	F	0.27	0/3239	0.66	1/4384 (0.0%)
All	All	0.25	0/14360	0.67	5/19472 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	134	ARG	N-CA-C	7.01	125.30	109.81
6	F	190	GLY	N-CA-C	5.54	118.93	112.50
1	A	133	THR	N-CA-C	-5.44	100.83	109.96
5	E	105	LEU	N-CA-C	5.36	120.69	114.04
5	E	116	ILE	N-CA-C	-5.36	105.50	110.53

There are no chirality outliers.

There are no planarity outliers.

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	3034	3080	3082	47	0
2	B	2911	2907	2907	47	0
3	C	1882	1892	1892	76	0
4	D	1553	1635	1635	67	0
5	E	1504	1574	1574	74	0
6	F	3161	3098	3098	85	0
7	B	30	19	19	2	0
7	C	30	19	19	4	0
8	B	27	19	20	0	0
9	B	35	45	44	2	0
9	D	35	46	46	0	0
9	E	35	45	44	1	0
10	B	1	0	0	0	0
11	D	9	12	12	0	0
12	E	4	0	0	0	0
12	F	4	0	0	2	0
13	F	53	31	31	3	0
All	All	14308	14422	14423	342	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 342 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:310:THR:OG1	2:B:42:LYS:NZ	1.97	0.97
3:C:172:GLU:OE1	3:C:227:THR:OG1	1.85	0.95
2:B:236:THR:HG21	7:B:501:FMN:H5'2	1.65	0.78
3:C:118:ARG:NH1	3:C:242:MET:O	2.17	0.77
4:D:72:ILE:HG21	5:E:117:THR:HG21	1.66	0.77

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	394/468 (84%)	388 (98%)	6 (2%)	0	100	100
2	B	378/415 (91%)	371 (98%)	7 (2%)	0	100	100
3	C	246/257 (96%)	244 (99%)	2 (1%)	0	100	100
4	D	201/210 (96%)	196 (98%)	5 (2%)	0	100	100
5	E	195/198 (98%)	186 (95%)	6 (3%)	3 (2%)	8	30
6	F	405/408 (99%)	400 (99%)	5 (1%)	0	100	100
All	All	1819/1956 (93%)	1785 (98%)	31 (2%)	3 (0%)	43	71

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	117	THR
5	E	115	LEU
5	E	110	GLY

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	334/395 (85%)	334 (100%)	0	100	100
2	B	292/320 (91%)	292 (100%)	0	100	100
3	C	198/205 (97%)	198 (100%)	0	100	100
4	D	170/176 (97%)	169 (99%)	1 (1%)	78	80
5	E	164/165 (99%)	164 (100%)	0	100	100
6	F	337/337 (100%)	337 (100%)	0	100	100
All	All	1495/1598 (94%)	1494 (100%)	1 (0%)	88	89

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	71	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
6	F	227	ASN
6	F	330	ASN
3	C	216	HIS
4	D	205	GLN
5	E	57	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	FMN	C	1000	3	29,32,33	1.11	2 (6%)	41,47,50	1.35	7 (17%)
12	FES	E	202	4,5	0,4,4	-	-	-		
13	FAD	F	1501	-	58,58,58	0.33	0	85,89,89	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	LMT	E	201	-	36,36,36	1.15	4 (11%)	47,47,47	1.01	3 (6%)
9	LMT	D	301	-	36,36,36	1.07	3 (8%)	47,47,47	1.08	3 (6%)
8	RBF	B	502	-	29,29,29	0.59	0	42,43,43	0.69	1 (2%)
7	FMN	B	501	2	29,32,33	1.11	2 (6%)	41,47,50	1.39	8 (19%)
11	LYS	D	302	-	7,8,9	0.49	0	3,8,10	0.32	0
12	FES	F	1502	6	0,4,4	-	-	-	-	-
9	LMT	B	503	-	36,36,36	1.18	5 (13%)	47,47,47	1.15	3 (6%)

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
7	FMN	C	1000	3	-	0/15/17/18	0/3/3/3
12	FES	E	202	4,5	-	-	0/1/1/1
13	FAD	F	1501	-	-	8/34/50/50	0/6/6/6
9	LMT	E	201	-	-	10/21/61/61	0/2/2/2
9	LMT	D	301	-	-	12/21/61/61	0/2/2/2
8	RBF	B	502	-	-	0/14/14/14	0/3/3/3
7	FMN	B	501	2	-	6/15/17/18	0/3/3/3
11	LYS	D	302	-	-	1/6/7/9	-
12	FES	F	1502	6	-	-	0/1/1/1
9	LMT	B	503	-	-	10/21/61/61	0/2/2/2

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	1000	FMN	C4A-N5	3.50	1.38	1.30
7	B	501	FMN	C4A-N5	3.40	1.38	1.30
9	E	201	LMT	O3'-C3'	-2.89	1.35	1.43
7	B	501	FMN	C10-N1	2.69	1.38	1.33
9	B	503	LMT	O3'-C3'	-2.65	1.36	1.43

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	1000	FMN	C5A-C9A-N10	3.54	121.17	117.97
7	B	501	FMN	C4-N3-C2	-3.42	119.56	125.64
7	B	501	FMN	C9A-C5A-N5	-3.22	119.04	122.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	503	LMT	C3'-C4'-C5'	-2.96	104.38	110.93
9	E	201	LMT	C3'-C4'-C5'	-2.92	104.47	110.93

There are no chirality outliers.

5 of 47 torsion outliers are listed below:

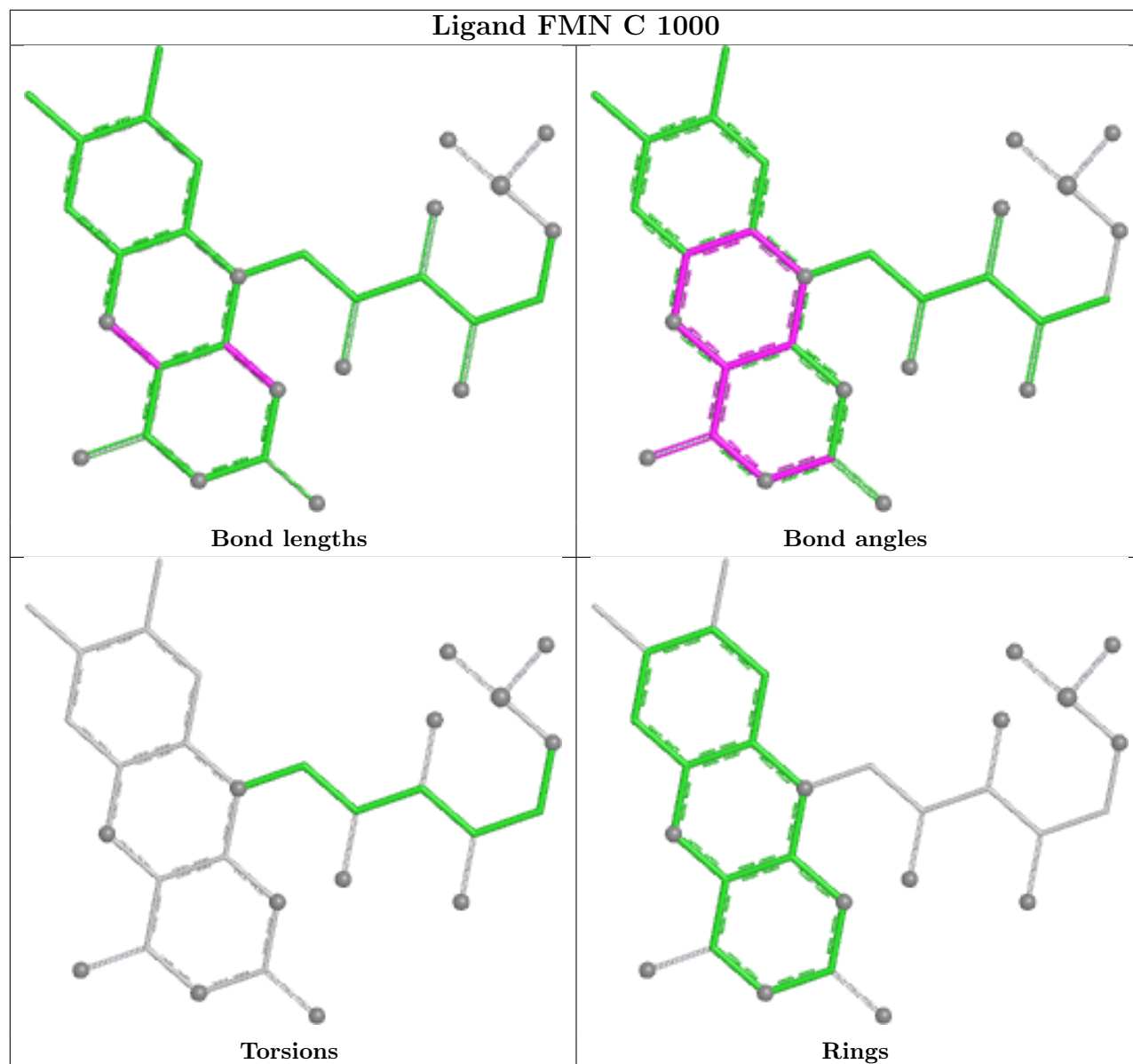
Mol	Chain	Res	Type	Atoms
7	B	501	FMN	C2'-C3'-C4'-O4'
7	B	501	FMN	O3'-C3'-C4'-O4'
7	B	501	FMN	C3'-C4'-C5'-O5'
7	B	501	FMN	O4'-C4'-C5'-O5'
9	B	503	LMT	O5'-C1'-O1'-C1

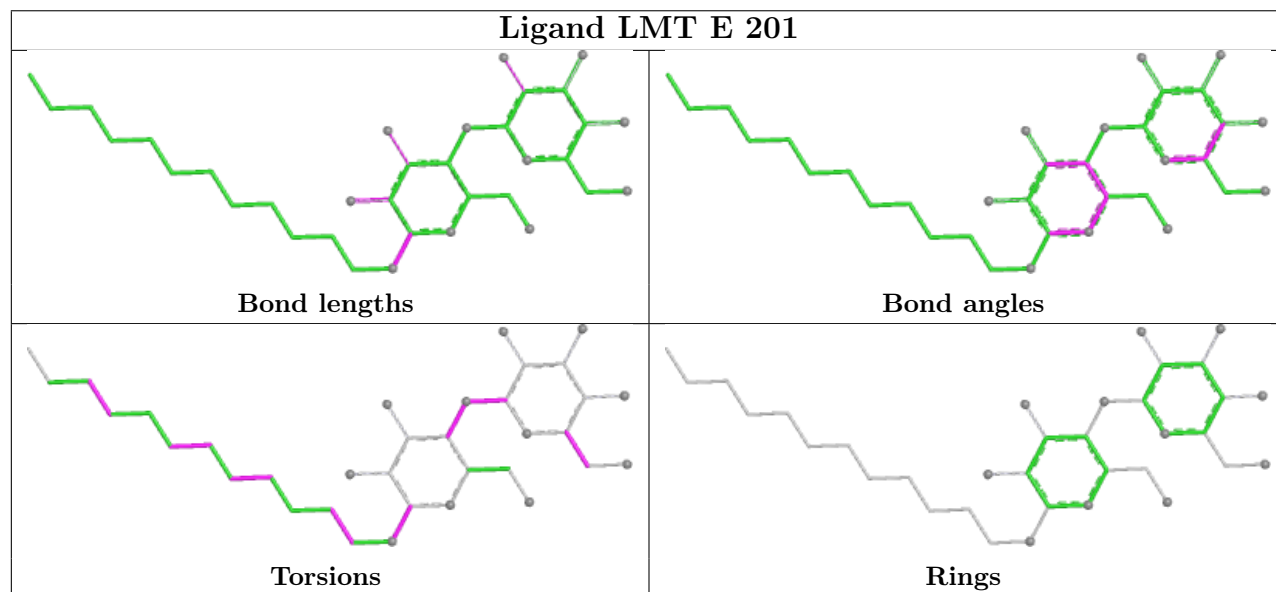
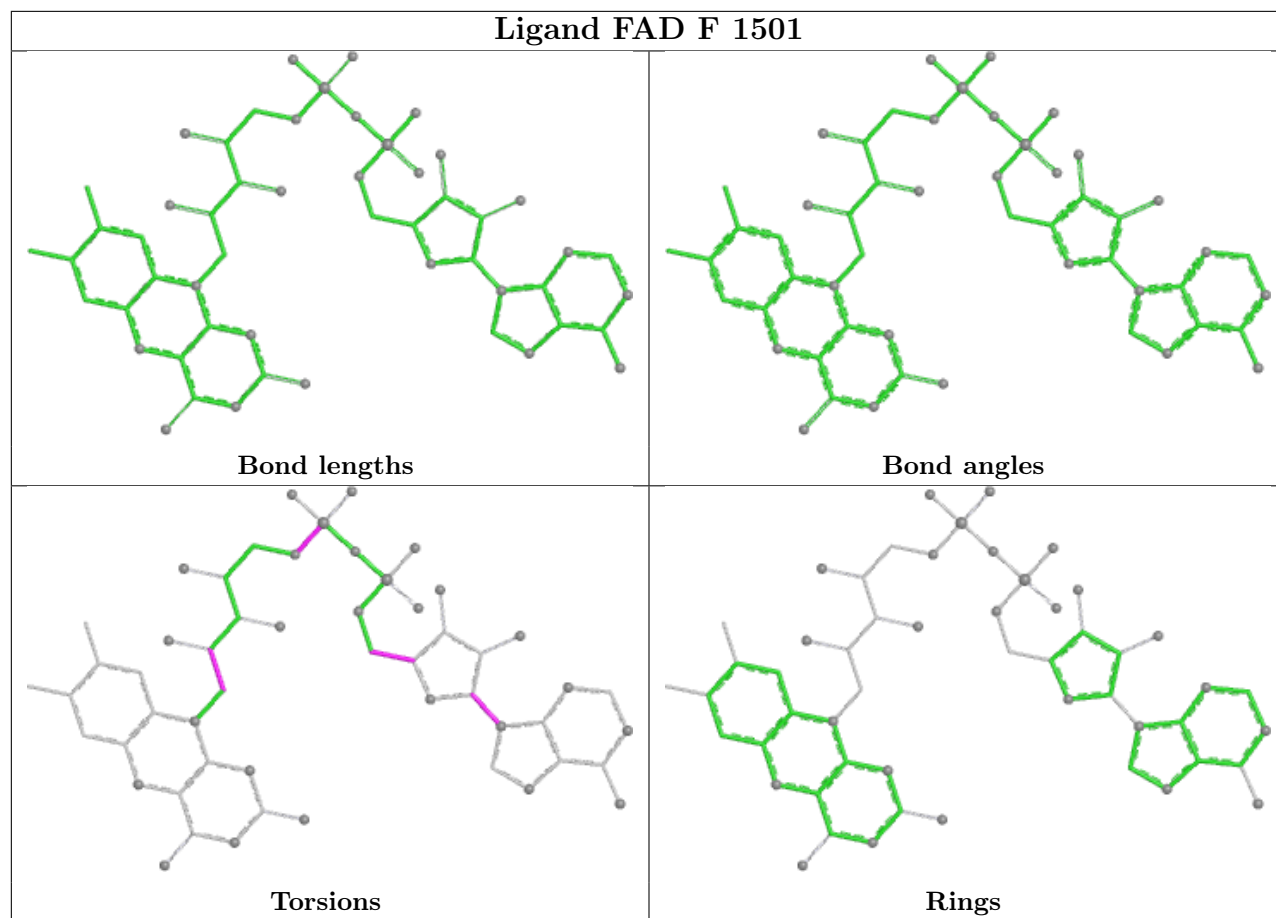
There are no ring outliers.

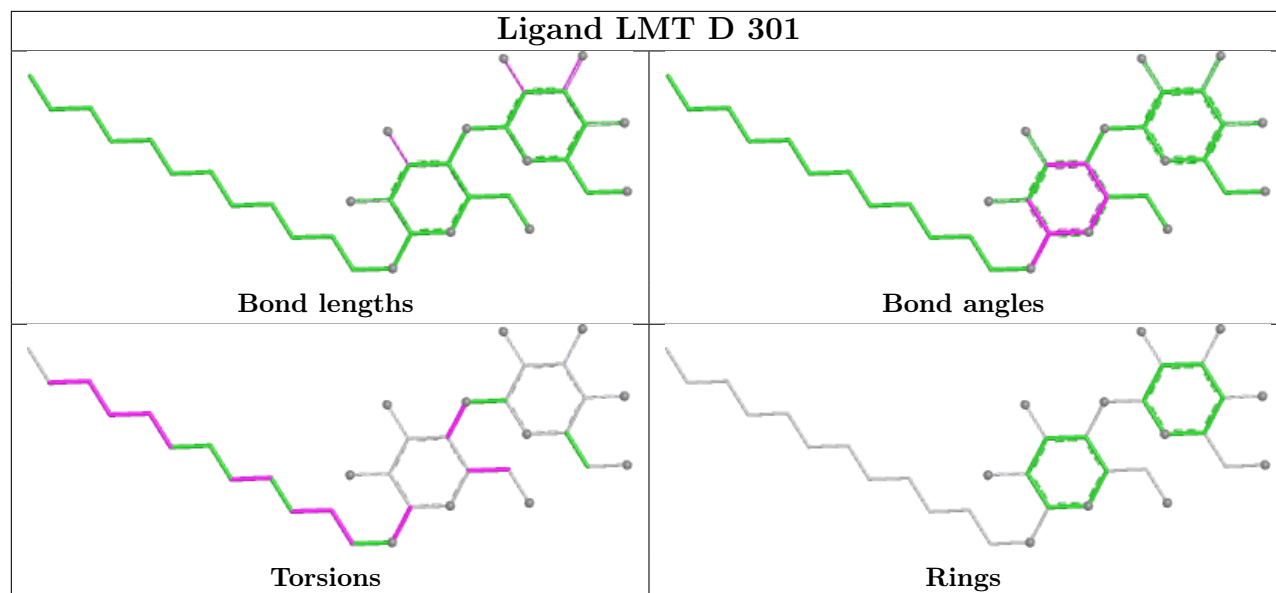
6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	1000	FMN	4	0
13	F	1501	FAD	3	0
9	E	201	LMT	1	0
7	B	501	FMN	2	0
12	F	1502	FES	2	0
9	B	503	LMT	2	0

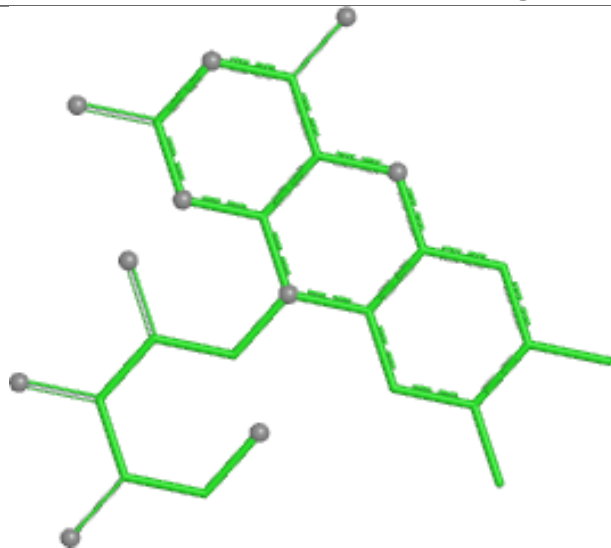
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



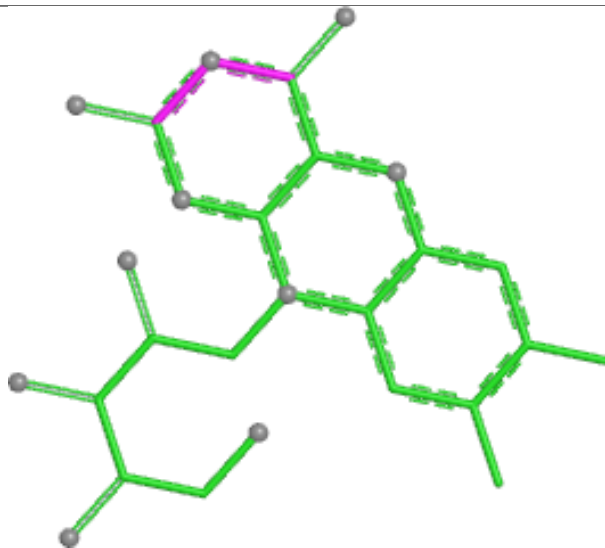




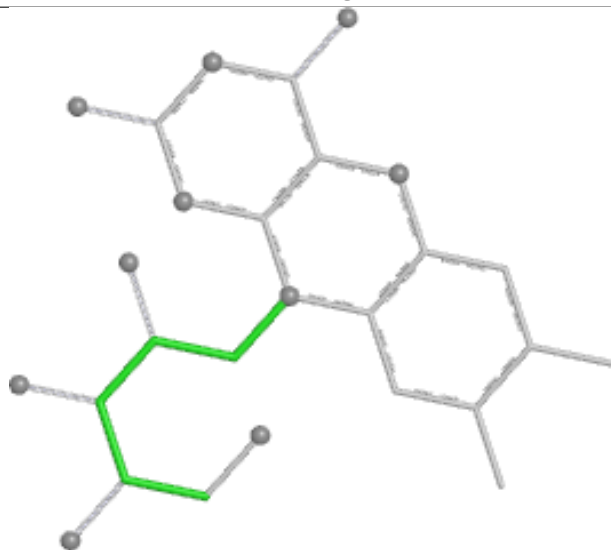
Ligand RBF B 502



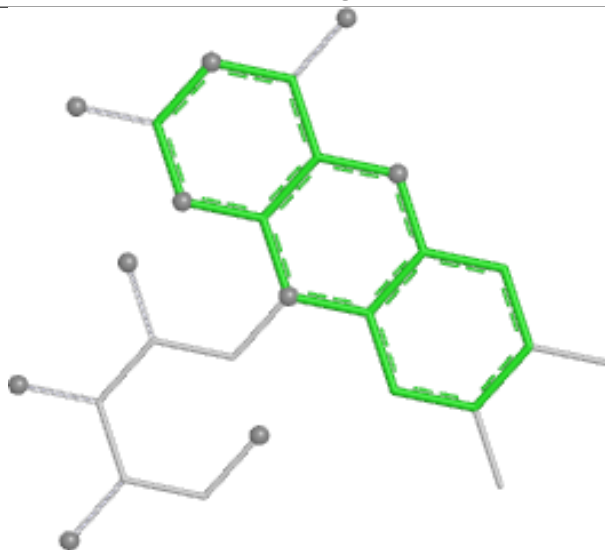
Bond lengths



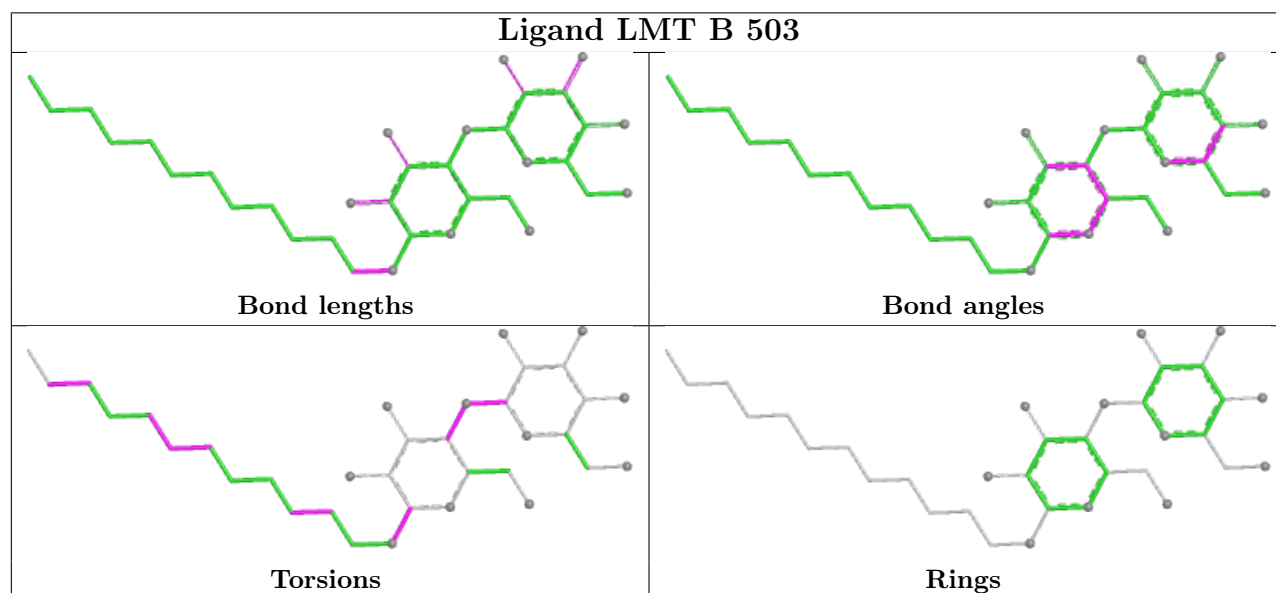
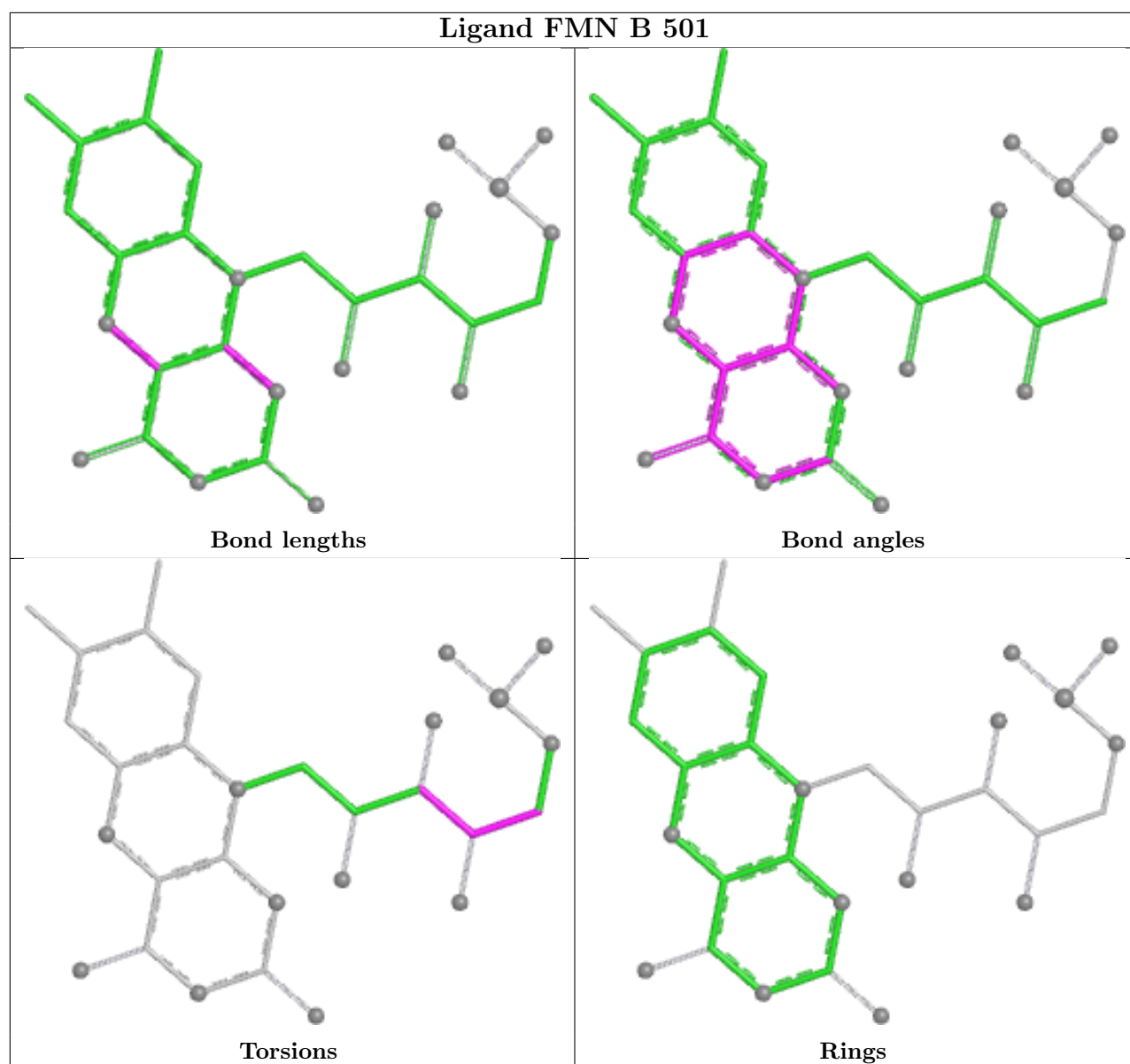
Bond angles



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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	398/468 (85%)	-0.06	14 (3%)	47	34	135, 183, 237, 308	0
2	B	380/415 (91%)	0.06	17 (4%)	38	28	115, 187, 275, 423	0
3	C	248/257 (96%)	0.50	35 (14%)	6	8	188, 266, 337, 416	0
4	D	203/210 (96%)	0.20	19 (9%)	14	14	127, 203, 271, 388	0
5	E	197/198 (99%)	0.45	22 (11%)	10	11	135, 204, 270, 353	0
6	F	407/408 (99%)	0.23	29 (7%)	22	18	140, 250, 319, 387	0
All	All	1833/1956 (93%)	0.19	136 (7%)	20	17	115, 210, 309, 423	0

The worst 5 of 136 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	201	PHE	7.1
1	A	83	ALA	7.0
6	F	258	CYS	6.5
3	C	244	PHE	6.1
4	D	204	GLU	6.0

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

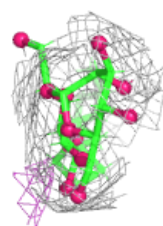
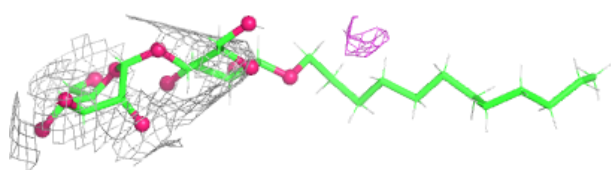
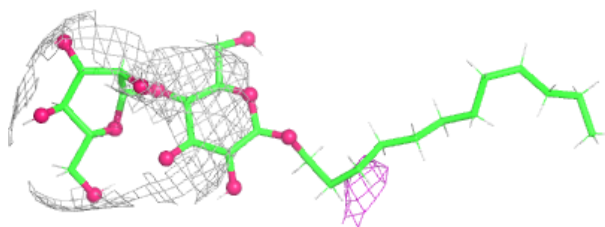
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
9	LMT	B	503	35/35	0.62	0.13	119,194,235,263	0
11	LYS	D	302	9/10	0.67	0.14	176,253,302,314	0
13	FAD	F	1501	53/53	0.70	0.13	163,244,303,314	0
9	LMT	D	301	35/35	0.82	0.11	148,223,265,279	0
7	FMN	B	501	30/31	0.87	0.10	138,177,225,243	0
8	RBF	B	502	27/27	0.88	0.10	142,180,238,246	0
9	LMT	E	201	35/35	0.88	0.11	126,187,257,269	0
7	FMN	C	1000	30/31	0.91	0.11	150,188,244,266	0
12	FES	F	1502	4/4	0.93	0.06	308,329,350,371	0
12	FES	E	202	4/4	0.96	0.07	123,163,173,376	0
10	K	B	504	1/1	0.97	0.04	155,155,155,155	0

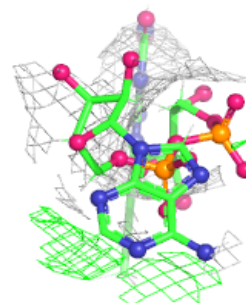
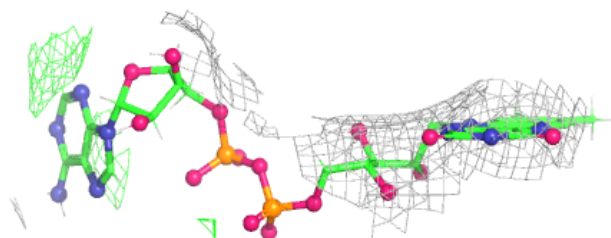
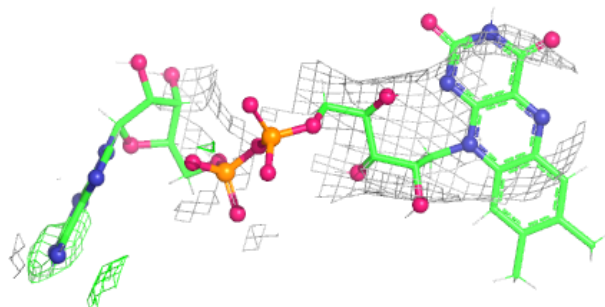
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LMT B 503:

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

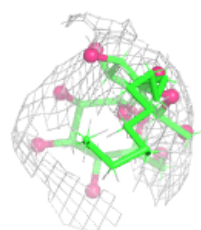
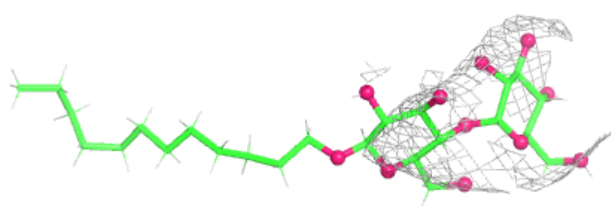
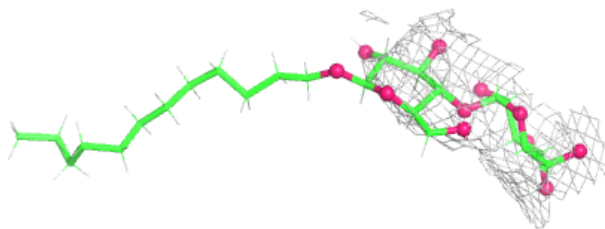
**Electron density around FAD F 1501:**

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

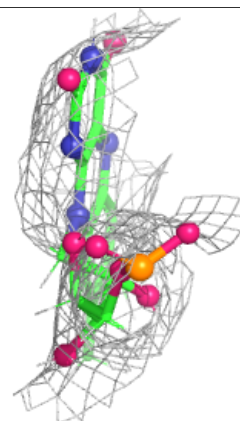
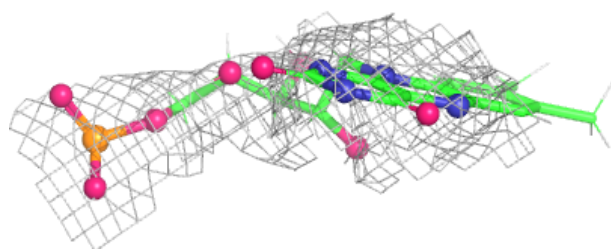
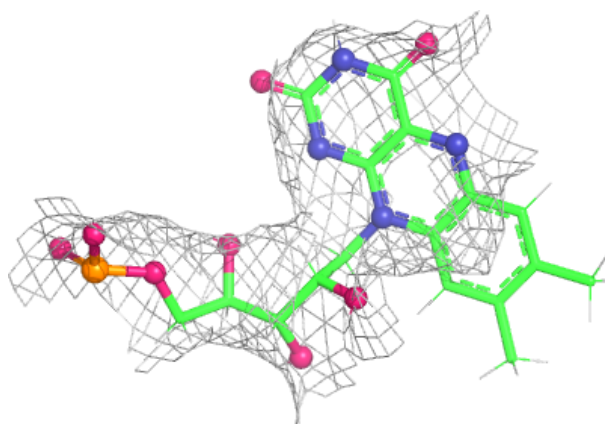


Electron density around LMT D 301:

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

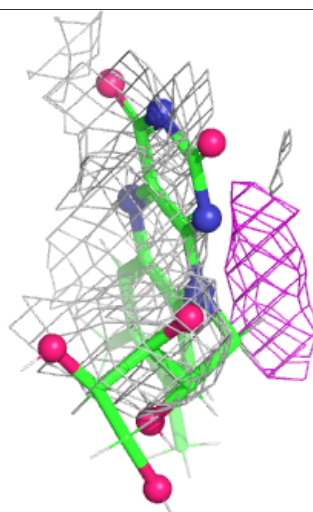
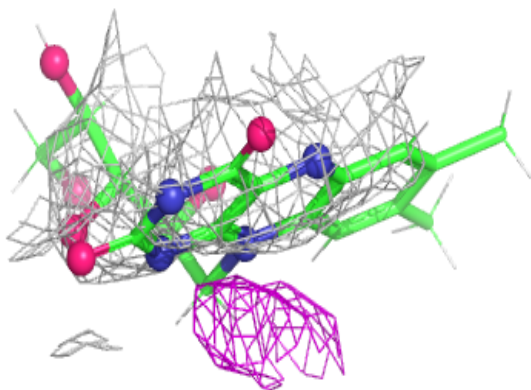
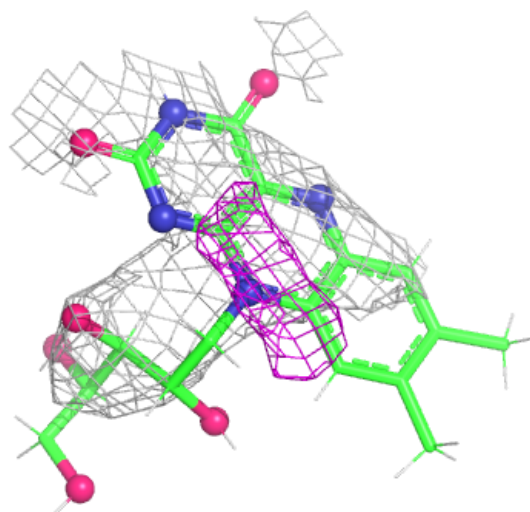
**Electron density around FMN B 501:**

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



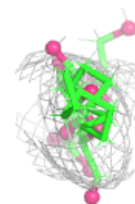
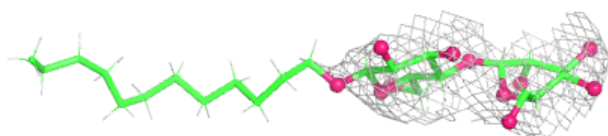
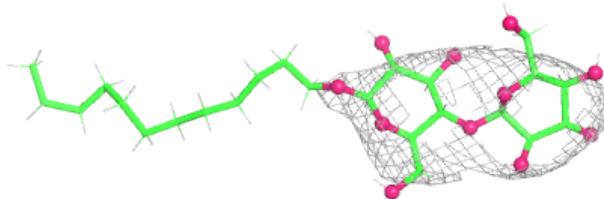
Electron density around RBF B 502:

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

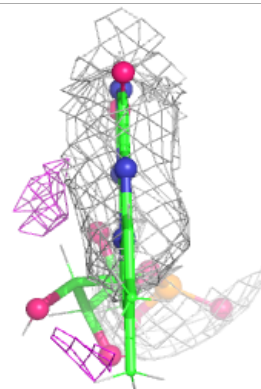
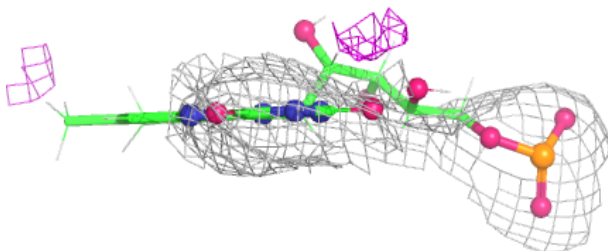
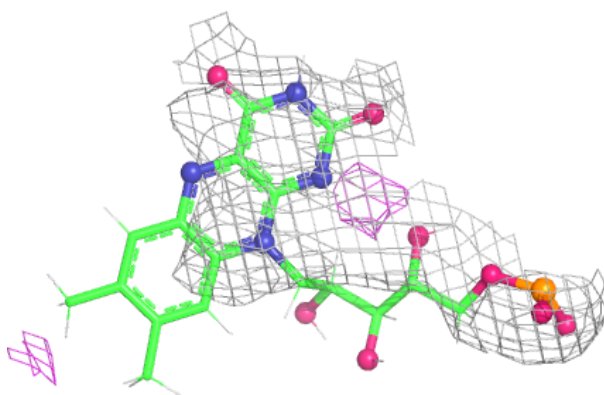


Electron density around LMT E 201:

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

**Electron density around FMN C 1000:**

$2mF_o-DF_c$ (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.