



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 01:26 PM EDT

PDB ID : 3HRD / pdb_00003hrd
Title : Crystal structure of nicotinate dehydrogenase
Authors : Wagener, N.; Pierik, A.J.; Hille, R.; Dobbek, H.
Deposited on : 2009-06-09
Resolution : 2.20 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 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

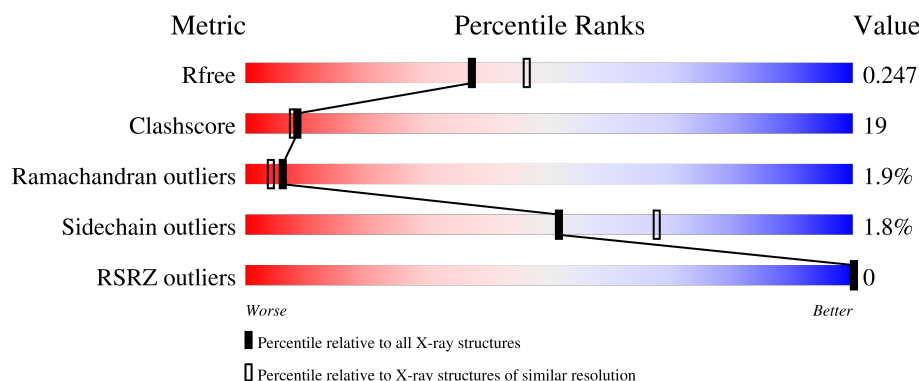
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	425	
1	E	425	
2	B	330	
2	F	330	
3	C	296	

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Mol	Chain	Length	Quality of chain
3	G	296	 55% 40% ..
4	D	160	 75% 24% .
4	H	160	 68% 29% ..

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 19284 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 Nicotinate dehydrogenase large molybdopterin subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	420	Total	C	N	O	S	0	0	0
			3213	2019	558	614	22			
1	E	420	Total	C	N	O	S	0	0	0
			3213	2019	558	614	22			

- Molecule 2 is a protein called Nicotinate dehydrogenase medium molybdopterin subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	330	Total	C	N	O	S	4	0	0
			2410	1506	405	481	18			
2	F	330	Total	C	N	O	S	0	0	0
			2410	1506	405	481	18			

- Molecule 3 is a protein called Nicotinate dehydrogenase FAD-subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	291	Total	C	N	O	S	0	0	0
			2246	1425	385	424	12			
3	G	292	Total	C	N	O	S	0	0	0
			2250	1427	386	425	12			

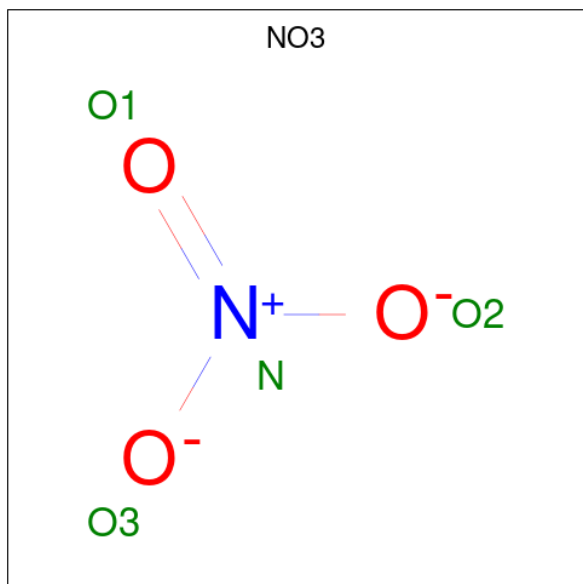
- Molecule 4 is a protein called Nicotinate dehydrogenase small FeS subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	160	Total	C	N	O	S	0	0	0
			1176	724	200	237	15			
4	H	157	Total	C	N	O	S	0	0	0
			1161	715	197	234	15			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	158	ALA	-	expression tag	UNP Q0QLF3
D	159	ALA	-	expression tag	UNP Q0QLF3
D	160	ALA	-	expression tag	UNP Q0QLF3
H	158	ALA	-	expression tag	UNP Q0QLF3
H	159	ALA	-	expression tag	UNP Q0QLF3
H	160	ALA	-	expression tag	UNP Q0QLF3

- Molecule 5 is NITRATE ION (CCD ID: NO3) (formula: NO₃).

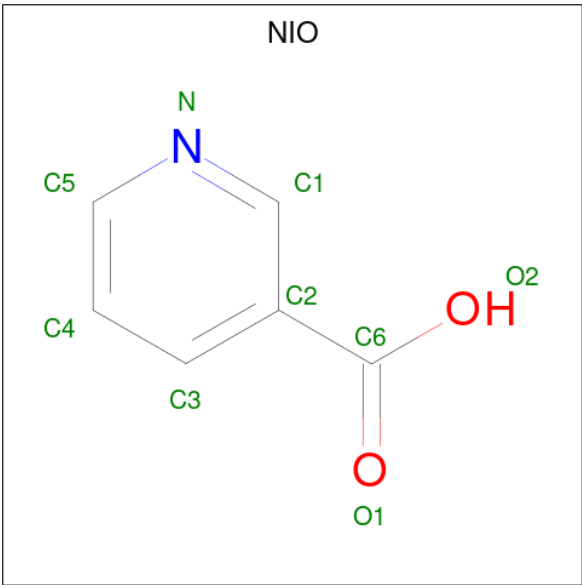


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	N	O	0	0
			4	1	3		
5	C	1	Total	N	O	0	0
			4	1	3		
5	E	1	Total	N	O	0	0
			4	1	3		

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

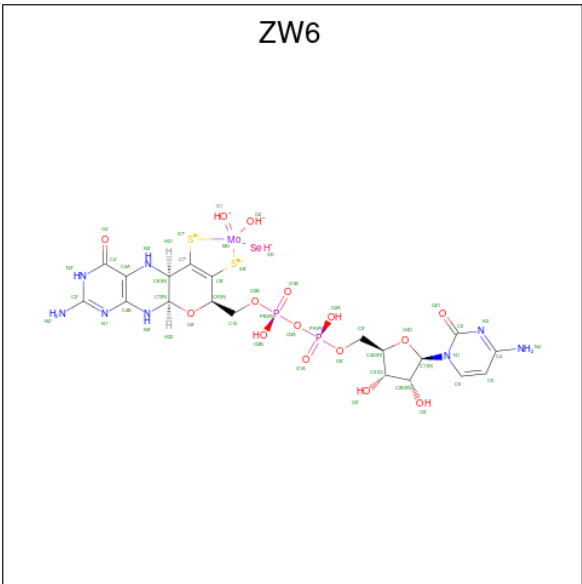
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Mg	0	0
			2	2		

- Molecule 7 is NICOTINIC ACID (CCD ID: NIO) (formula: C₆H₅NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	0
			9	6	1	2		
7	E	1	Total	C	N	O	0	0
			9	6	1	2		

- Molecule 8 is Molybdopterin cytidine dinucleotide hydroxy-oxo-selenol-molybdenum (CCD ID: ZW6) (formula: C₁₉H₂₇MoN₈O₁₅P₂S₂Se).



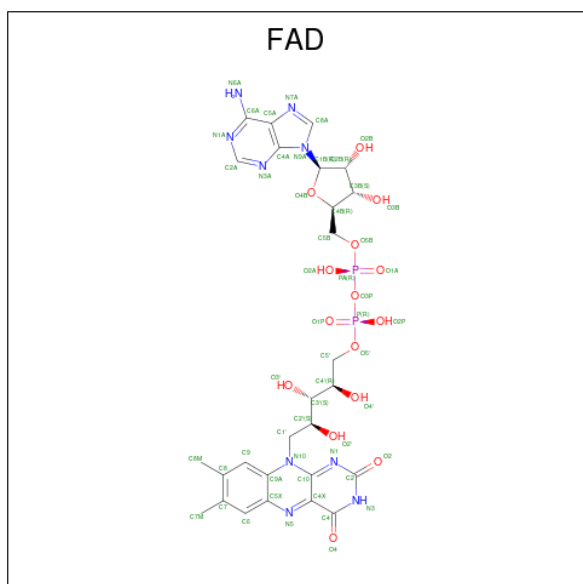
Mol	Chain	Residues	Atoms								ZeroOcc	AltConf
8	B	1	Total	C	Mo	N	O	P	S	Se	0	0
			48	19	1	8	15	2	2	1		

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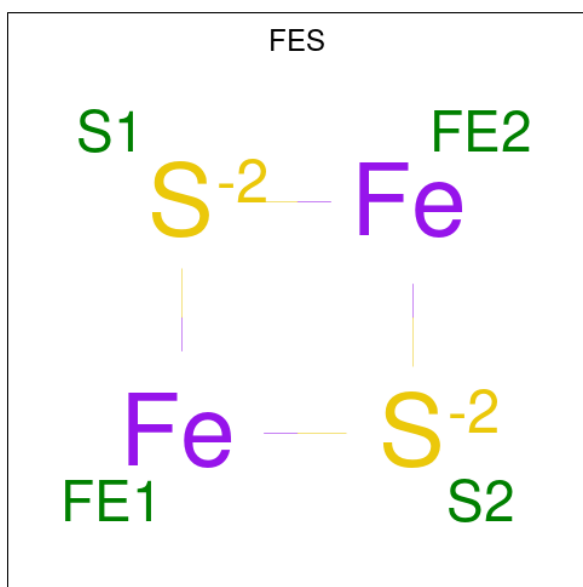
Mol	Chain	Residues	Atoms								ZeroOcc	AltConf
8	F	1	Total	C	Mo	N	O	P	S	Se	0	0
			48	19	1	8	15	2	2	1		

- Molecule 9 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 10 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	D	1	Total	Fe	S	0	0
			4	2	2		
10	D	1	Total	Fe	S	0	0
			4	2	2		
10	H	1	Total	Fe	S	0	0
			4	2	2		
10	H	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 11 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	E	1	Total	Ca	0	0
			1	1		

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	258	Total	O	0	0
			258	258		
12	B	170	Total	O	0	0
			170	170		
12	C	209	Total	O	0	0
			209	209		
12	D	112	Total	O	0	0
			112	112		

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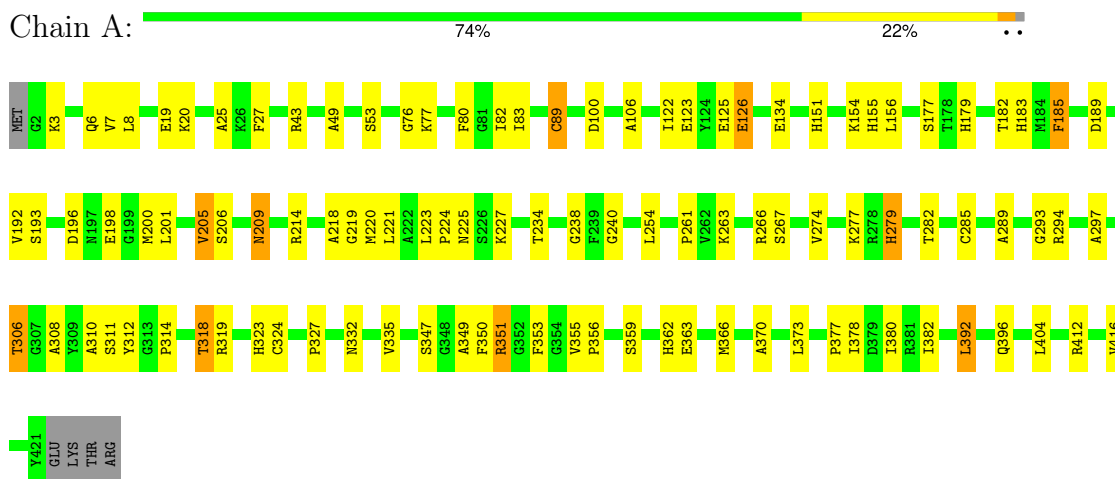
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	E	95	Total 95	O 95	0	0
12	F	59	Total 59	O 59	0	0
12	G	25	Total 25	O 25	0	0
12	H	26	Total 26	O 26	0	0

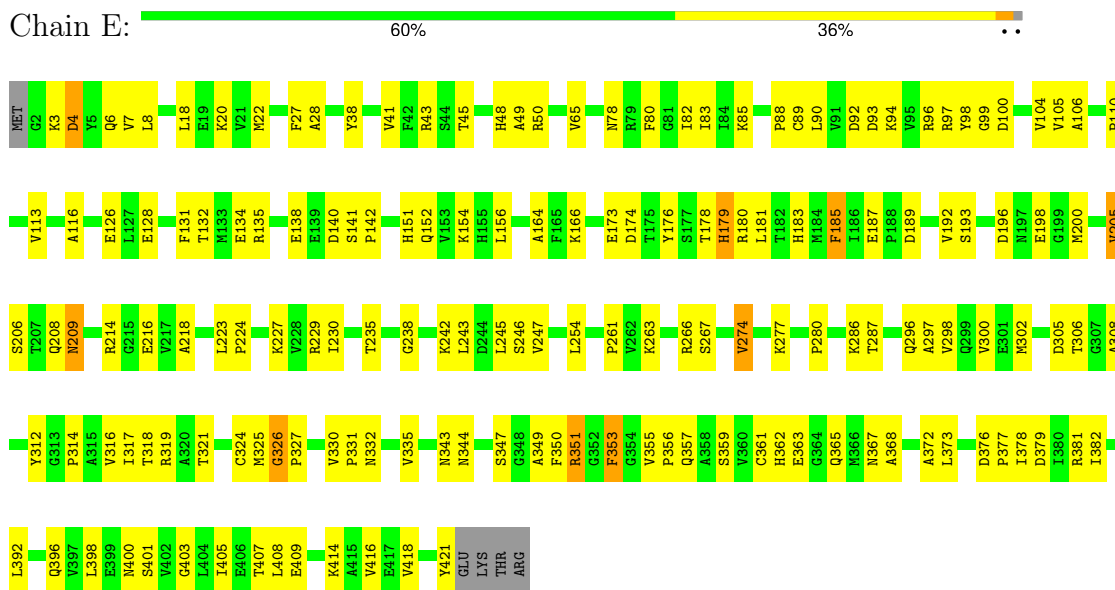
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Nicotinate dehydrogenase large molybdopterin subunit

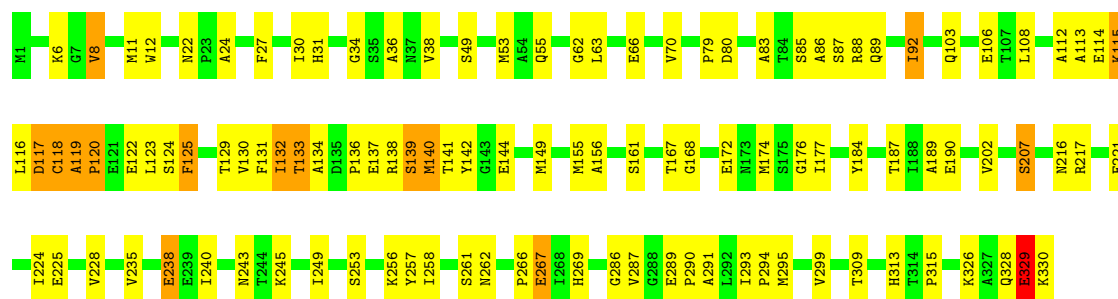


- Molecule 1: Nicotinate dehydrogenase large molybdopterin subunit



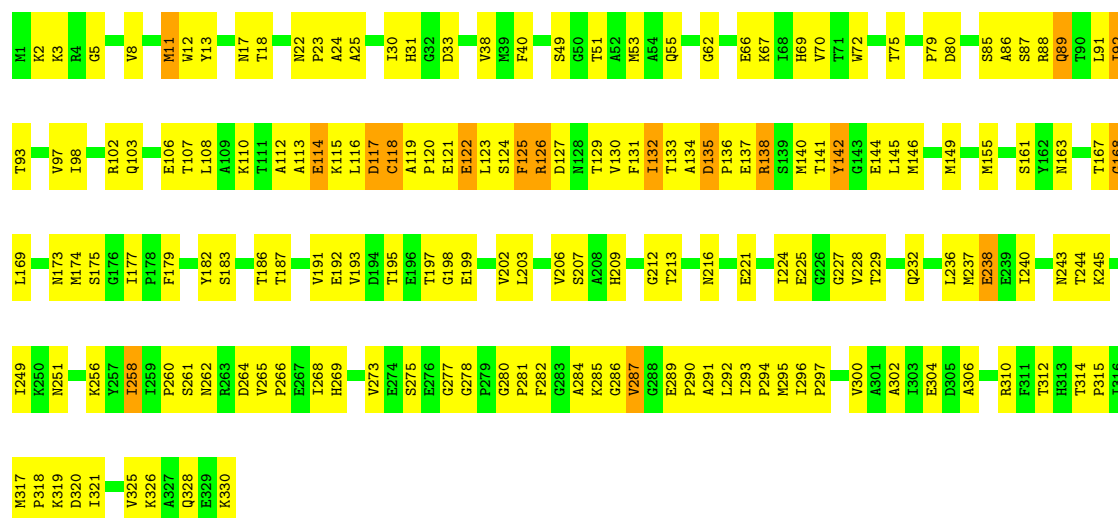
- Molecule 2: Nicotinate dehydrogenase medium molybdopterin subunit

Chain B: 



• Molecule 2: Nicotinate dehydrogenase medium molybdopterin subunit

Chain F: 



• Molecule 3: Nicotinate dehydrogenase FAD-subunit

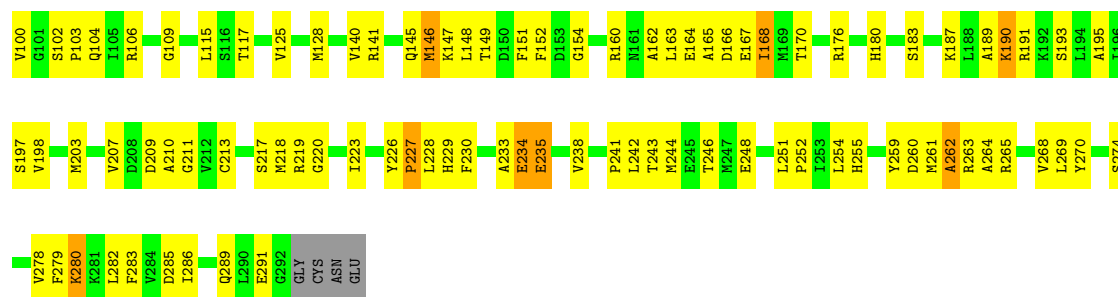
Chain C: 



• Molecule 3: Nicotinate dehydrogenase FAD-subunit

Chain G: 





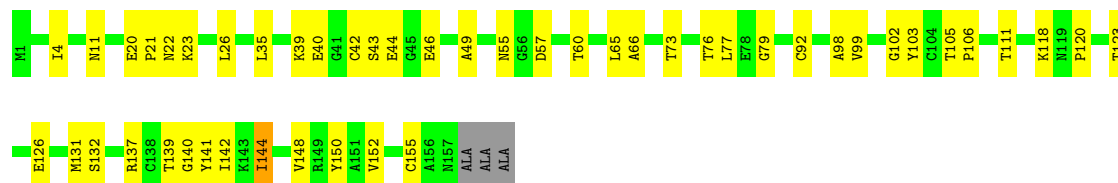
- Molecule 4: Nicotinate dehydrogenase small FeS subunit

Chain D: 75% 24%



- Molecule 4: Nicotinate dehydrogenase small FeS subunit

Chain H: 68% 29%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	97.07Å 71.70Å 214.49Å 90.00° 90.23° 90.00°	Depositor
Resolution (Å)	29.43 – 2.20 29.43 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.6 (29.43-2.20) 98.9 (29.43-2.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 2.20Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.213 , 0.251 0.208 , 0.247	Depositor DCC
R_{free} test set	7408 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	24.5	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 27.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.059 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19284	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% 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: NIO, ZW6, FES, CA, MG, NO3, 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	0.43	0/3273	0.97	12/4432 (0.3%)
1	E	0.33	0/3273	0.87	6/4432 (0.1%)
2	B	0.43	0/2452	1.01	10/3327 (0.3%)
2	F	0.36	0/2452	0.94	8/3327 (0.2%)
3	C	0.43	0/2284	0.94	6/3083 (0.2%)
3	G	0.31	0/2288	0.81	3/3088 (0.1%)
4	D	0.44	0/1188	1.02	7/1609 (0.4%)
4	H	0.36	0/1173	0.94	4/1588 (0.3%)
All	All	0.39	0/18383	0.93	56/24886 (0.2%)

There are no bond length outliers.

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	198	VAL	N-CA-C	-9.25	103.86	111.81
2	F	136	PRO	N-CA-C	-9.13	103.24	114.20
1	A	185	PHE	N-CA-C	-8.28	98.83	110.50
2	B	258	ILE	N-CA-C	8.23	120.72	108.54
2	B	286	GLY	N-CA-C	7.89	122.32	112.14

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	3213	0	3193	86	0
1	E	3213	0	3194	142	0
2	B	2410	0	2391	120	0
2	F	2410	0	2391	183	0
3	C	2246	0	2281	53	0
3	G	2250	0	2284	117	0
4	D	1176	0	1168	23	0
4	H	1161	0	1153	34	0
5	A	4	0	0	0	0
5	C	4	0	0	1	0
5	E	4	0	0	0	0
6	A	2	0	0	0	0
7	B	9	0	4	0	0
7	E	9	0	4	2	0
8	B	48	0	0	4	0
8	F	48	0	0	0	0
9	C	53	0	31	1	0
9	G	53	0	31	1	0
10	D	8	0	0	0	0
10	H	8	0	0	0	0
11	E	1	0	0	0	0
12	A	258	0	0	8	0
12	B	170	0	0	5	0
12	C	209	0	0	8	1
12	D	112	0	0	2	0
12	E	95	0	0	3	0
12	F	59	0	0	10	0
12	G	25	0	0	1	0
12	H	26	0	0	0	0
All	All	19284	0	18125	691	1

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 19.

The worst 5 of 691 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)
2:B:295:MET:HE2	2:B:299:VAL:HG23	1.28	1.12
1:A:19:GLU:HG2	1:E:198:GLU:HA	1.39	1.03
1:A:327:PRO:HB3	2:B:12:TRP:HB2	1.44	1.00
2:B:119:ALA:HB3	2:B:120:PRO:HD3	1.43	0.99
2:B:132:ILE:HD13	2:B:136:PRO:HG3	1.46	0.97

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:C:299:HOH:O	12:C:300:HOH:O[2_455]	2.07	0.13

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	418/425 (98%)	399 (96%)	16 (4%)	3 (1%)	18	19
1	E	418/425 (98%)	383 (92%)	30 (7%)	5 (1%)	10	8
2	B	328/330 (99%)	300 (92%)	15 (5%)	13 (4%)	2	1
2	F	328/330 (99%)	289 (88%)	27 (8%)	12 (4%)	2	1
3	C	289/296 (98%)	275 (95%)	13 (4%)	1 (0%)	36	42
3	G	290/296 (98%)	255 (88%)	27 (9%)	8 (3%)	4	2
4	D	158/160 (99%)	152 (96%)	4 (2%)	2 (1%)	9	8
4	H	155/160 (97%)	145 (94%)	9 (6%)	1 (1%)	21	23
All	All	2384/2422 (98%)	2198 (92%)	141 (6%)	45 (2%)	6	4

5 of 45 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	114	GLU
2	B	115	LYS
2	B	117	ASP
2	B	125	PHE
2	B	133	THR

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	344/349 (99%)	337 (98%)	7 (2%)	48	64
1	E	344/349 (99%)	339 (98%)	5 (2%)	57	73
2	B	252/252 (100%)	247 (98%)	5 (2%)	48	64
2	F	252/252 (100%)	248 (98%)	4 (2%)	55	71
3	C	241/246 (98%)	232 (96%)	9 (4%)	30	41
3	G	241/246 (98%)	237 (98%)	4 (2%)	53	69
4	D	129/129 (100%)	129 (100%)	0	100	100
4	H	129/129 (100%)	129 (100%)	0	100	100
All	All	1932/1952 (99%)	1898 (98%)	34 (2%)	51	68

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	135	ASP
2	F	142	TYR
3	G	168	ILE
3	C	12	LEU
2	B	330	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	344	ASN
2	F	55	GLN
1	E	362	HIS
2	F	17	ASN
2	F	232	GLN

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](#)

Of 16 ligands modelled in this entry, 3 are monoatomic - leaving 13 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
8	ZW6	B	5662	-	44,53,53	1.37	7 (15%)	54,86,86	1.69	13 (24%)
10	FES	H	908	4	0,4,4	-	-	-		
10	FES	D	907	4	0,4,4	-	-	-		
10	FES	D	908	4	0,4,4	-	-	-		
7	NIO	E	5660	-	9,9,9	2.48	4 (44%)	11,11,11	1.56	3 (27%)
12	ZW6	F	331	-	44,53,53	1.49	8 (18%)	54,86,86	1.66	12 (22%)
5	NO3	C	5659	-	1,3,3	0.20	0	0,3,3	-	-
9	FAD	G	900	-	58,58,58	2.60	22 (37%)	85,89,89	1.12	7 (8%)
9	FAD	C	900	-	58,58,58	2.64	22 (37%)	85,89,89	1.10	6 (7%)
5	NO3	E	5662	-	1,3,3	0.38	0	0,3,3	-	-
5	NO3	A	5658	-	1,3,3	0.27	0	0,3,3	-	-
7	NIO	B	5661	-	9,9,9	2.50	3 (33%)	11,11,11	1.65	4 (36%)
10	FES	H	907	4	0,4,4	-	-	-		

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
8	ZW6	B	5662	-	-	3/22/78/78	0/6/6/6
10	FES	H	908	4	-	-	0/1/1/1
10	FES	D	907	4	-	-	0/1/1/1
10	FES	D	908	4	-	-	0/1/1/1
7	NIO	E	5660	-	-	0/4/4/4	0/1/1/1
12	ZW6	F	331	-	-	3/22/78/78	0/6/6/6
9	FAD	G	900	-	-	12/34/50/50	0/6/6/6
9	FAD	C	900	-	-	8/34/50/50	0/6/6/6
7	NIO	B	5661	-	-	0/4/4/4	0/1/1/1
10	FES	H	907	4	-	-	0/1/1/1

The worst 5 of 66 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	900	FAD	P-O3P	-13.19	1.45	1.59
9	G	900	FAD	P-O3P	-12.30	1.46	1.59
9	G	900	FAD	PA-O2A	-4.56	1.34	1.55
9	C	900	FAD	PA-O2A	-4.53	1.34	1.55
9	G	900	FAD	PA-O3P	4.52	1.64	1.59

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	5662	ZW6	C7-C6'-N5'	5.64	113.41	107.87
12	F	331	ZW6	C7-C6'-N5'	5.42	113.19	107.87
12	F	331	ZW6	O9'-C9'-C8'	3.95	114.66	109.09
8	B	5662	ZW6	O9'-C7-N8'	3.88	112.12	108.61
12	F	331	ZW6	C7'-C8'-S8'	-3.86	117.96	120.15

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

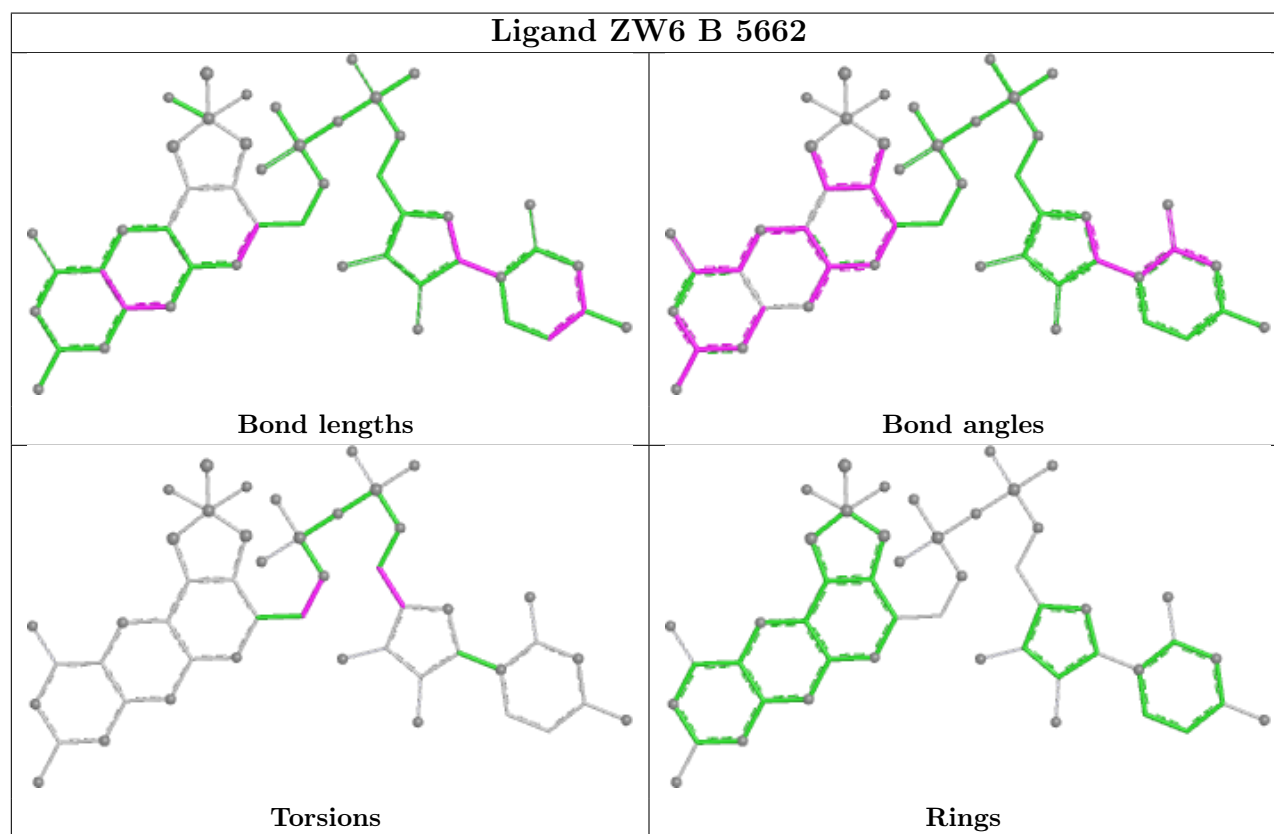
Mol	Chain	Res	Type	Atoms
9	C	900	FAD	N10-C1'-C2'-O2'
9	C	900	FAD	N10-C1'-C2'-C3'
9	G	900	FAD	N10-C1'-C2'-O2'
9	G	900	FAD	N10-C1'-C2'-C3'
9	G	900	FAD	C2'-C3'-C4'-O4'

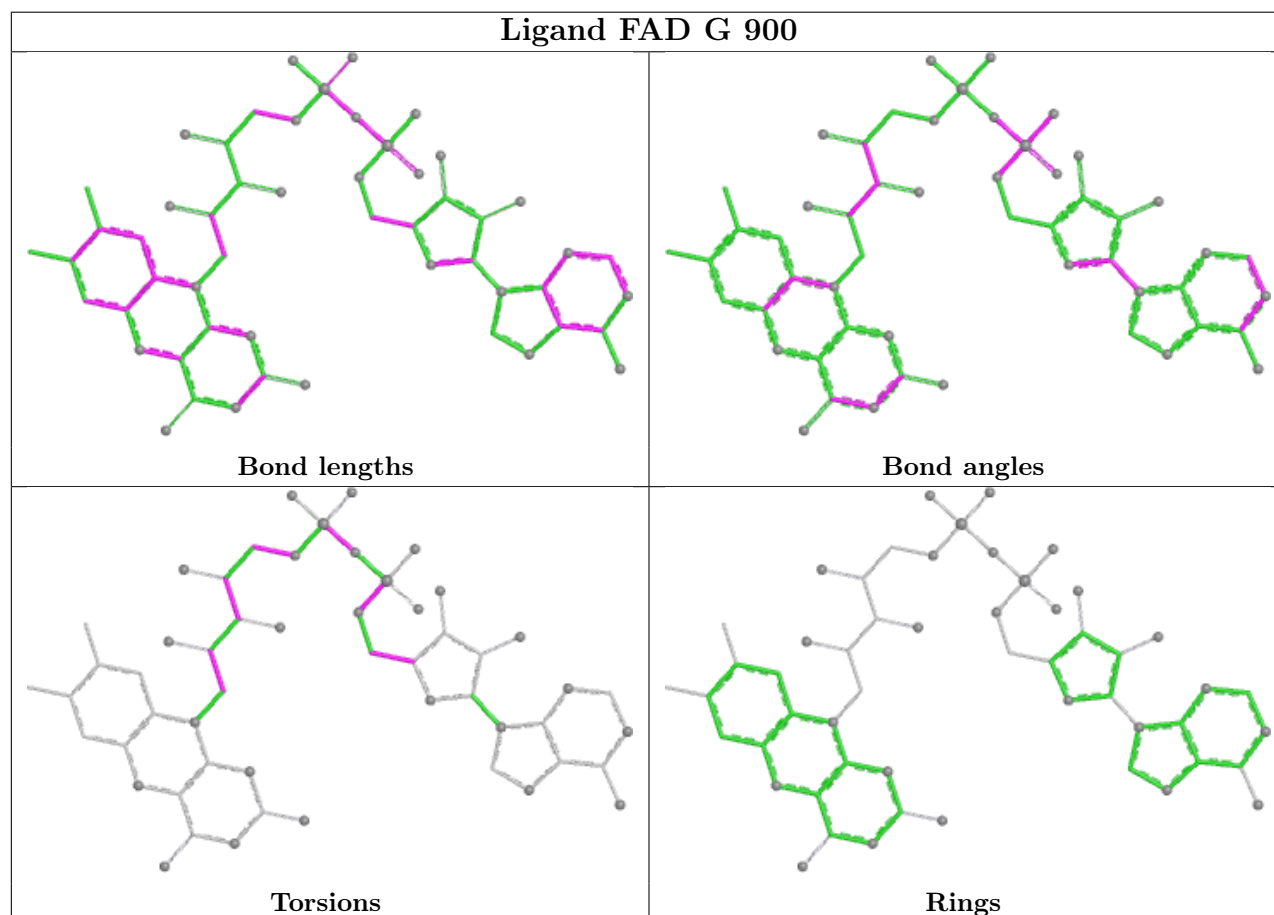
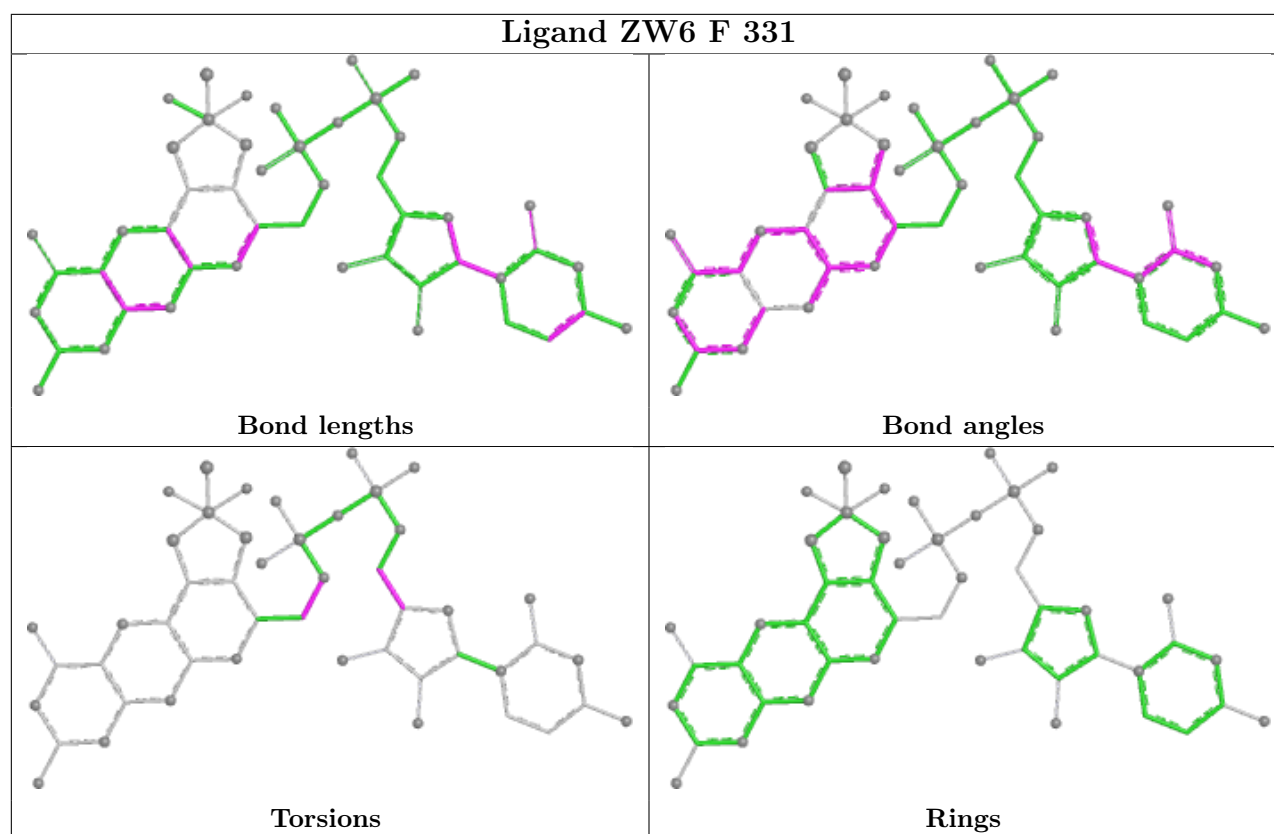
There are no ring outliers.

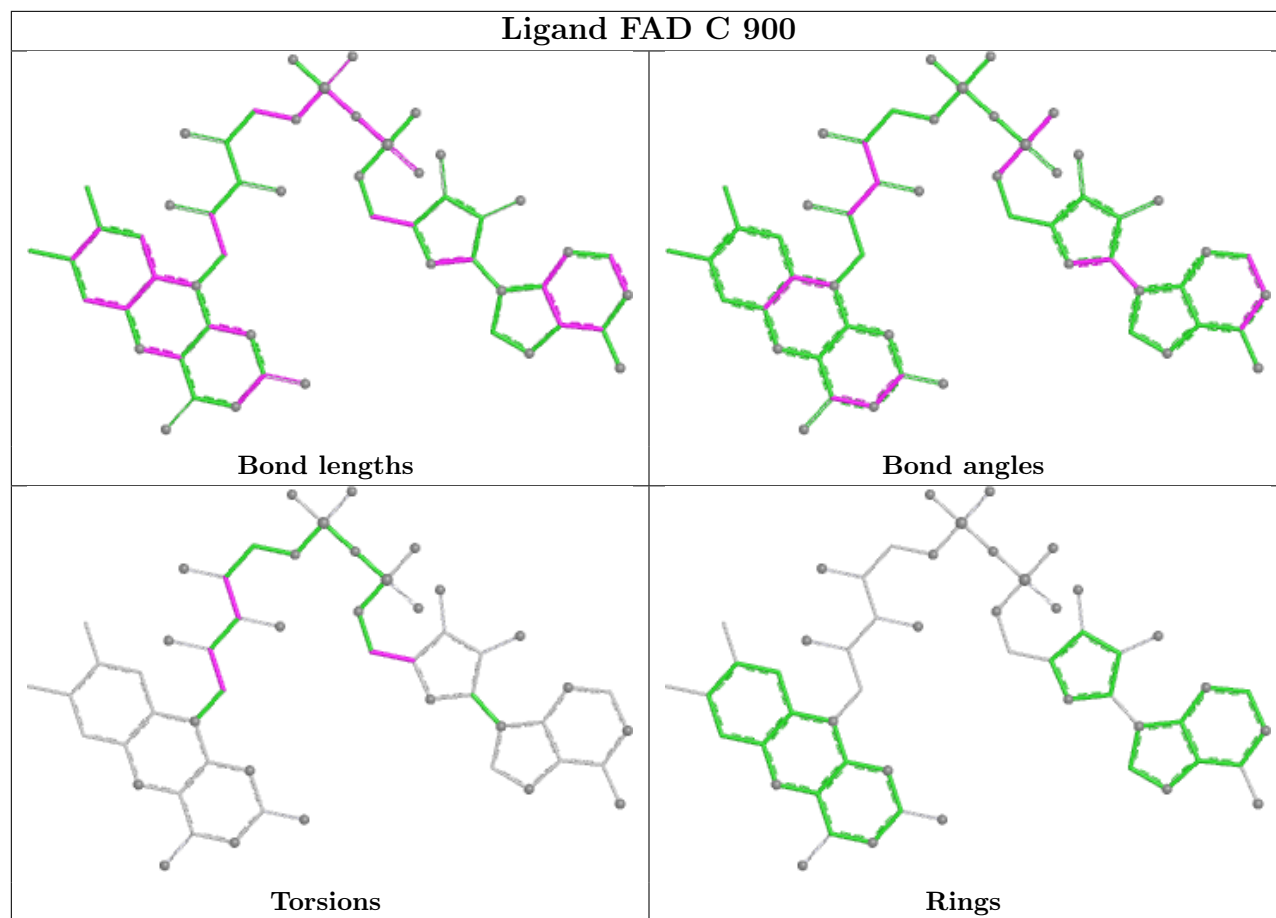
6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	5662	ZW6	4	0
7	E	5660	NIO	2	0
12	F	331	ZW6	3	0
5	C	5659	NO3	1	0
9	G	900	FAD	1	0
9	C	900	FAD	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 [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	420/425 (98%)	-1.69	0 100 100	4, 20, 32, 69	1 (0%)
1	E	420/425 (98%)	-1.41	0 100 100	20, 42, 72, 85	0
2	B	330/330 (100%)	-1.58	0 100 100	9, 20, 77, 115	1 (0%)
2	F	330/330 (100%)	-1.37	0 100 100	20, 42, 81, 101	0
3	C	291/296 (98%)	-1.66	0 100 100	9, 20, 43, 62	1 (0%)
3	G	292/296 (98%)	-1.12	0 100 100	35, 63, 89, 123	1 (0%)
4	D	160/160 (100%)	-1.70	0 100 100	10, 17, 38, 52	0
4	H	157/160 (98%)	-1.48	0 100 100	26, 37, 56, 70	0
All	All	2400/2422 (99%)	-1.50	0 100 100	4, 30, 75, 123	4 (0%)

There are no RSRZ outliers to report.

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](#)

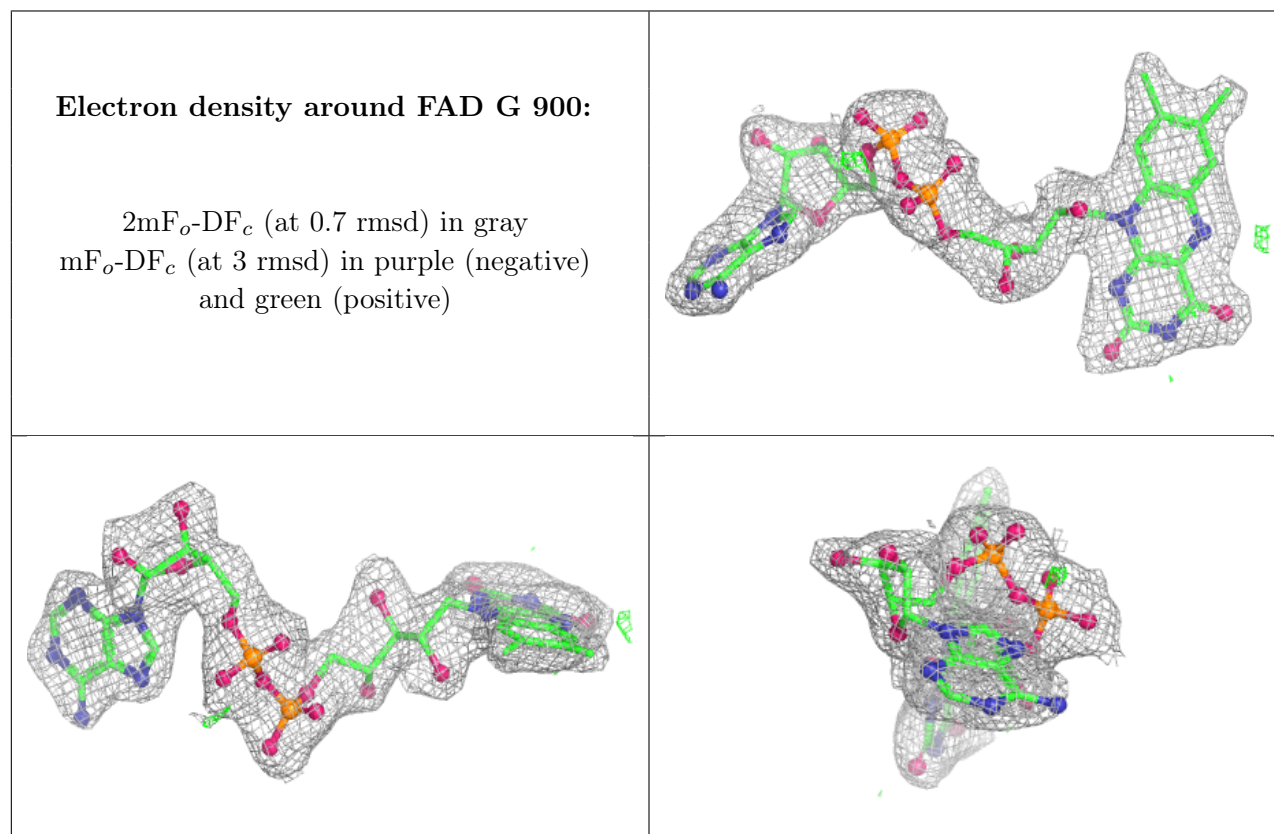
There are no oligosaccharides in this entry.

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.

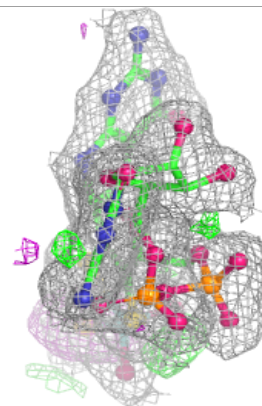
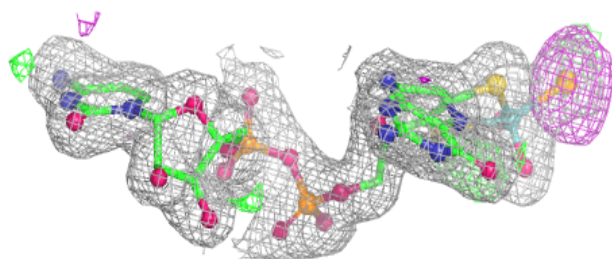
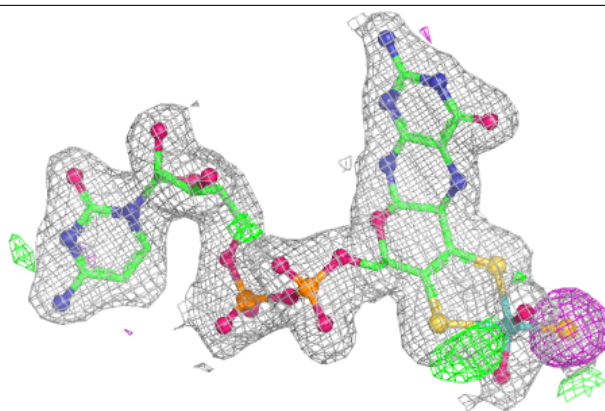
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NO3	C	5659	4/4	0.99	0.03	29,31,32,32	0
5	NO3	E	5662	4/4	0.99	0.03	44,44,44,45	0
7	NIO	B	5661	9/9	0.99	0.07	24,25,26,26	9
7	NIO	E	5660	9/9	0.99	0.04	42,42,44,44	0
9	FAD	G	900	53/53	0.99	0.03	36,41,44,49	0
11	CA	E	5663	1/1	0.99	0.04	48,48,48,48	0
6	MG	A	426	1/1	1.00	0.01	21,21,21,21	0
8	ZW6	B	5662	48/48	1.00	0.02	9,15,21,23	1
12	ZW6	F	331	48/48	1.00	0.02	24,32,36,38	1
9	FAD	C	900	53/53	1.00	0.02	1,12,18,20	0
6	MG	A	427	1/1	1.00	0.03	23,23,23,23	0
10	FES	D	907	4/4	1.00	0.01	10,11,13,13	0
10	FES	D	908	4/4	1.00	0.01	11,12,15,15	0
10	FES	H	907	4/4	1.00	0.01	27,29,30,31	0
10	FES	H	908	4/4	1.00	0.01	36,36,37,37	0
5	NO3	A	5658	4/4	1.00	0.01	20,20,21,23	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.

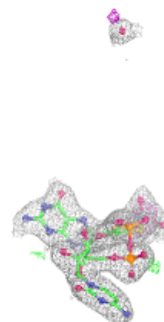
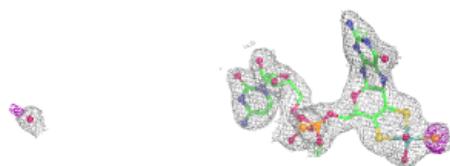
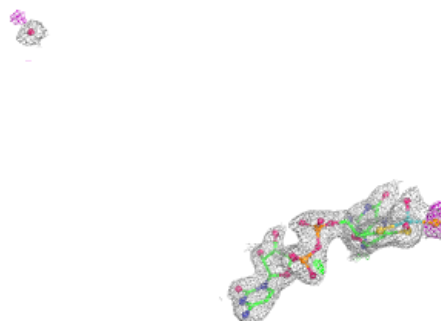


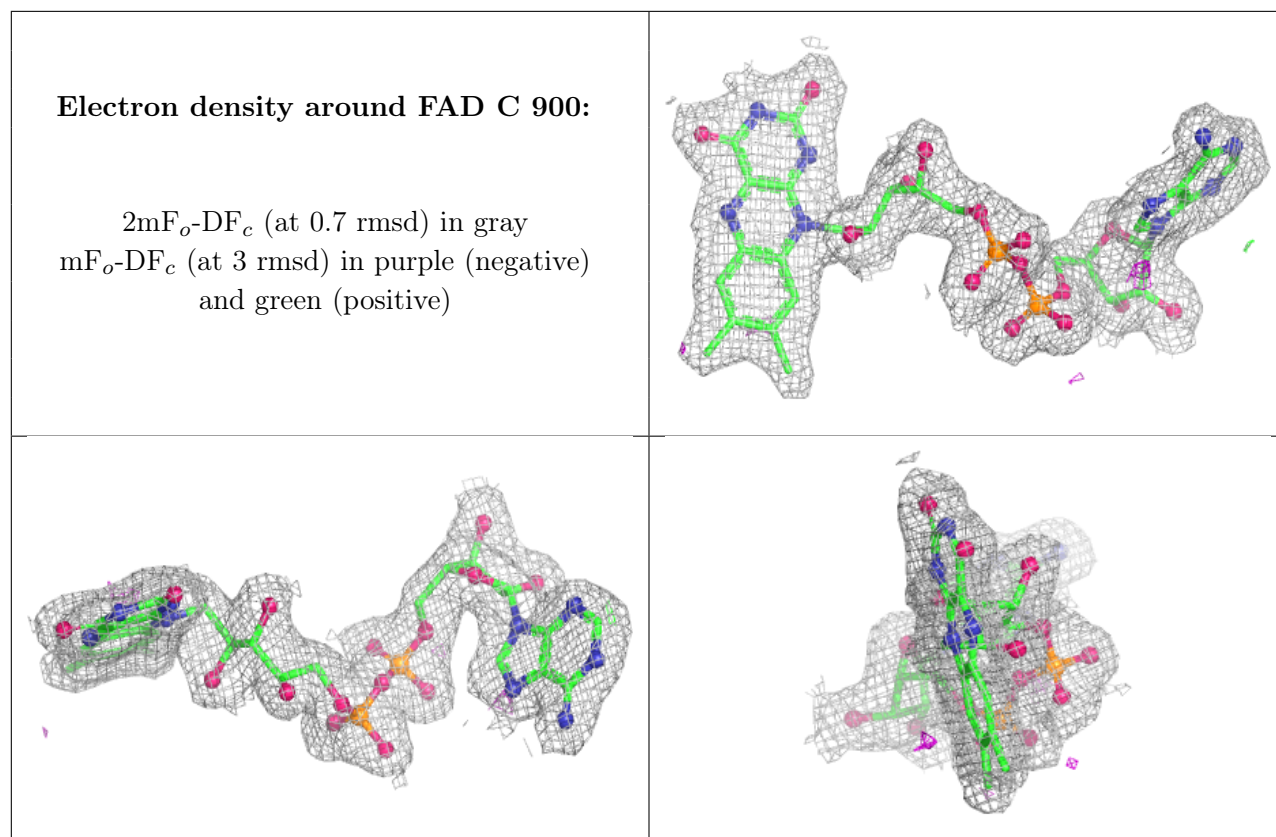
Electron density around ZW6 B 5662:

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

**Electron density around ZW6 F 331:**

$2mF_o-DF_c$ (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.