

# Full wwPDB X-ray Structure Validation Report (i)

May 26, 2020 – 01:32 am BST

PDB ID : 5LBY

Title: Structure of the human quinone reductase 2 (NQO2) in complex with

crenolanib

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Deposited on : 2016-06-17

Resolution : 1.40 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

 $Mol Probity \quad : \quad 4.02b\text{--}467$ 

Mogul: 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.11

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac: 5.8.0158

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

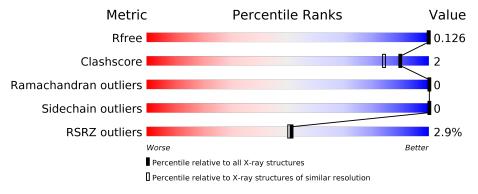
Validation Pipeline (wwPDB-VP) : 2.11

### 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar \; resolution} \\ (\#{\rm Entries, \; resolution \; range(\AA)}) \end{array}$		
$R_{free}$	130704	1714 (1.40-1.40)		
Clashscore	141614	1812 (1.40-1.40)		
Ramachandran outliers	138981	1763 (1.40-1.40)		
Sidechain outliers	138945	1762 (1.40-1.40)		
RSRZ outliers	127900	1674 (1.40-1.40)		

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain						
1	A	237	94%						
1	В	237	88%	8%	<del>-</del>				



# 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4321 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 Ribosyldihydronicotinamide dehydrogenase [quinone].

Mol	Chain	Residues		Atoms				ZeroOcc	AltConf	Trace	
1 A	228	Total	С	N	О	S	0	8	0		
	A	220	1858	1196	310	343	9	U	0		
1	D	220	Total	С	N	О	S	0	7	0	
1	D	B 228	1853	1194	308	342	9	U	1	U	

There are 12 discrepancies between the modelled and reference sequences:

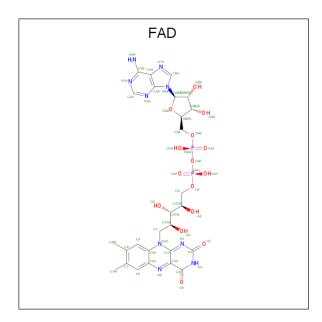
Chain	Residue	Modelled	Actual	Comment	Reference
A	231	HIS	-	expression tag	UNP P16083
A	232	HIS	_	expression tag	UNP P16083
A	233	HIS	-	expression tag	UNP P16083
A	234	HIS	-	expression tag	UNP P16083
A	235	HIS	_	expression tag	UNP P16083
A	236	HIS	_	expression tag	UNP P16083
В	231	HIS	_	expression tag	UNP P16083
В	232	HIS	_	expression tag	UNP P16083
В	233	HIS	-	expression tag	UNP P16083
В	234	HIS	_	expression tag	UNP P16083
В	235	HIS	-	expression tag	UNP P16083
В	236	HIS	_	expression tag	UNP P16083

• Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	В	1	Total Zn 1 1	0	0
2	A	1	Total Zn 1 1	0	0

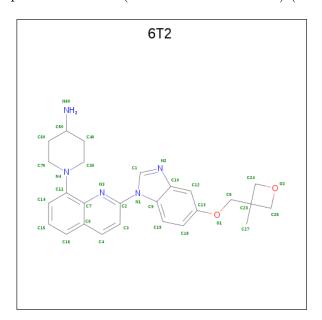
• Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
2	3 A	1	Total	С	N	О	Р	0	0
)		1	53	27	9	15	2	U	
9	D	1	Total	С	N	О	Р	0	0
3	D	1	53	27	9	15	2		

• Molecule 4 is 1-(2-{5-[(3-Methyloxetan-3-yl)methoxy]-1H-benzimidazol-1-yl}quinolin-8-yl)pi peridin-4-amine (three-letter code: 6T2) (formula:  $C_{26}H_{29}N_5O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 33	C 26	N 5	O 2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	В	1	Total 33	C 26	N 5	O 2	0	0

### • Molecule 5 is water.

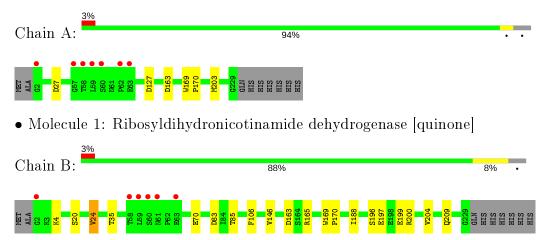
Mol	Chain	Residues	${f Atoms}$	ZeroOcc	AltConf
5	A	234	Total O 234 234	0	0
5	В	202	Total O 202 202	0	0



# 3 Residue-property plots (i)

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

• Molecule 1: Ribosyldihydronicotinamide dehydrogenase [quinone]





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	61.59Å 79.40Å 106.57Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.30 - 1.40	Depositor
resolution (A)	44.27 - 1.40	EDS
% Data completeness	93.0 (44.30-1.40)	Depositor
(in resolution range)	93.0 (44.27-1.40)	EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	3.79 (at 1.40Å)	Xtriage
Refinement program	REFMAC 5.8.0151	Depositor
P. P.	0.105 , $0.125$	Depositor
$R, R_{free}$	0.105 , $0.126$	DCC
$R_{free}$ test set	4820 reflections $(4.99%)$	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	11.3	Xtriage
Anisotropy	0.400	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.39 , 47.0	EDS
L-test for twinning <sup>2</sup>	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	4321	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.83% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of <|L|>,  $< L^2>$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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: ZN, 6T2, 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	0.85	0/1913	0.89	5/2595~(0.2%)	
	1	В	0.83	0/1908	0.89	$7/2589 \; (0.3\%)$	
	All	All	0.84	0/3821	0.89	12/5184~(0.2%)	

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$Ideal(^{o})$
1	A	127	ASP	CB-CG-OD1	8.74	126.16	118.30
1	В	163	ASP	CB-CG-OD1	8.30	125.77	118.30
1	A	127	ASP	CB-CG-OD2	-7.59	111.47	118.30
1	A	27	ASP	CB-CG-OD2	-7.16	111.86	118.30
1	В	24[A]	VAL	CG1-CB-CG2	6.72	121.65	110.90
1	В	24[B]	VAL	CG1-CB-CG2	6.72	121.65	110.90
1	В	165	ARG	NE-CZ-NH2	-6.59	117.00	120.30
1	В	83	ASP	CB-CG-OD1	6.26	123.93	118.30
1	В	70	GLU	OE1-CD-OE2	-5.60	116.58	123.30
1	В	106	PHE	CB-CG-CD1	5.59	124.71	120.80
1	A	163	ASP	CB-CG-OD1	5.59	123.33	118.30
1	A	203	MET	CG-SD-CE	-5.07	92.09	100.20

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	$\mathbf{H}(\mathbf{model})$	$\mathbf{H}(\mathbf{added})$	Clashes	Symm-Clashes
1	A	1858	0	1820	1	0
1	В	1853	0	1820	13	0
2	A	1	0	0	0	0
2	В	1	0	0	0	0
3	A	53	0	31	0	0
3	В	53	0	31	0	0
4	A	33	0	0	0	0
4	В	33	0	0	0	0
5	A	234	0	0	0	0
5	В	202	0	0	5	0
All	All	4321	0	3702	14	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 (14) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{aligned} &  ext{Interatomic} \ &  ext{distance} \ &  ext{(Å)} \end{aligned}$	Clash overlap (Å)	
1:B:20:SER:O	1:B:24[B]:VAL:HG23	1.81	0.80	
1:B:85[A]:THR:HG21	5:B:530:HOH:O	1.82	0.79	
1:B:209[A]:GLN:HG3	5:B:529:HOH:O	1.89	0.72	
1:B:24[B]:VAL:HG21	1:B:204:VAL:CG1	2.28	0.63	
1:B:146[B]:VAL:CG1	1:B:188:ILE:HG12	2.37	0.54	
1:B:24[B]:VAL:HG12	5:B:497:HOH:O	2.10	0.52	
1:B:24[A]:VAL:HG13	5:B:522:HOH:O	2.11	0.50	
1:B:169:TRP:HB3	1:B:170:PRO:HD3	1.94	0.49	
1:B:197:GLU:OE1	1:B:200:ARG:NH2	2.48	0.46	
1:B:85[A]:THR:CG2	5:B:530:HOH:O	2.53	0.45	
1:B:196:SER:OG	1:B:199:GLU:HG3	2.18	0.43	
1:B:4:LYS:HG2	1:B:35:THR:HB	2.00	0.43	
1:B:24[B]:VAL:HG21	1:B:204:VAL:HG13	2.00	0.42	
1:A:169:TRP:HB3	1:A:170:PRO:HD3	2.03	0.41	

There are no symmetry-related clashes.



### 5.3 Torsion angles (i)

#### 5.3.1 Protein backbone (i)

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

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

Mol	Chain	${f Analysed}$	Favoured Allowed		Outliers	Percentiles	
1	A	233/237~(98%)	227 (97%)	6 (3%)	0	100	100
1	В	233/237~(98%)	226 (97%)	7 (3%)	0	100	100
All	All	466/474~(98%)	453 (97%)	13 (3%)	0	100	100

There are no Ramachandran outliers to report.

#### 5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Perce	ercentiles	
1	A	200/201 (100%)	200 (100%)	0	100	100	
1	В	$200/201 \; (100\%)$	200 (100%)	0	100	100	
All	All	400/402 (100%)	400 (100%)	0	100	100	

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	GLN
1	В	100	GLN
1	В	172	GLN



#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	Во	Bond lengths			Bond angles		
MIGI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z >2
3	FAD	В	301	-	51,58,58	1.45	4 (7%)	60,89,89	2.11	13 (21%)
4	6T2	A	303	-	38,38,38	2.57	5 (13%)	46,56,56	3.88	9 (19%)
4	6T2	В	303	-	38,38,38	2.62	8 (21%)	46,56,56	4.59	11 (23%)
3	FAD	A	302	-	51,58,58	1.63	6 (11%)	60,89,89	1.98	10 (16%)

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	$\operatorname{Res}$	Link	Chirals	${f Torsions}$	Rings
3	FAD	В	301	-	-	5/30/50/50	0/6/6/6
4	6T2	A	303	_	-	0/11/32/32	0/6/6/6
4	6T2	В	303	_	-	0/11/32/32	0/6/6/6
3	FAD	A	302	-	-	6/30/50/50	0/6/6/6



All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$Ideal(\AA)$
4	В	303	6T2	O2-C24	13.29	1.64	1.45
4	A	303	6T2	O2-C24	12.07	1.62	1.45
3	A	302	FAD	C4X-C10	7.61	1.46	1.38
3	В	301	FAD	C4X-C10	6.50	1.45	1.38
4	A	303	6T2	O2-C26	-6.31	1.36	1.45
4	A	303	6T2	C26-C23	-5.47	1.46	1.54
4	В	303	6T2	O2-C26	-4.13	1.39	1.45
3	A	302	FAD	C4-N3	3.84	1.39	1.33
3	В	301	FAD	C1'-N10	-3.32	1.44	1.48
4	В	303	6T2	C19-C18	2.95	1.42	1.36
4	A	303	6T2	C70-N4	2.71	1.51	1.46
4	В	303	6T2	C1-N2	-2.63	1.30	1.34
4	В	303	6T2	C40-C50	2.62	1.58	1.51
4	В	303	6T2	C26-C23	-2.60	1.50	1.54
3	A	302	FAD	C2A-N3A	2.53	1.36	1.32
3	A	302	FAD	C5'-C4'	2.51	1.55	1.51
3	A	302	FAD	C2B-C1B	-2.23	1.50	1.53
3	A	302	FAD	C8A-N7A	-2.22	1.30	1.34
3	В	301	FAD	C2A-N1A	2.21	1.38	1.33
3	В	301	FAD	C2A-N3A	2.18	1.35	1.32
4	В	303	6T2	C12-C13	2.16	1.40	1.37
4	В	303	6T2	C2-N1	-2.06	1.38	1.44
4	A	303	6T2	C12-C13	2.02	1.40	1.37

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
4	В	303	6T2	O2-C24-C23	-25.45	78.93	91.85
4	A	303	6T2	O2-C24-C23	-22.21	80.58	91.85
4	В	303	6T2	C26-C23-C24	13.24	95.11	84.31
3	В	301	FAD	C4-N3-C2	10.69	124.17	115.14
4	A	303	6T2	C26-C23-C24	10.64	92.99	84.31
3	A	302	FAD	C4-N3-C2	9.89	123.49	115.14
4	В	303	6T2	C26-O2-C24	5.99	96.47	91.11
3	В	301	FAD	C4-C4X-C10	-5.17	116.53	119.95
3	A	302	FAD	C4X-C4-N3	-4.91	116.71	123.43
4	В	303	6T2	O2-C26-C23	-4.75	89.44	91.85
3	В	301	FAD	C4X-C4-N3	-4.55	117.21	123.43
3	В	301	FAD	N3A-C2A-N1A	-4.28	121.98	128.68
4	В	303	6T2	C11-C7-N3	4.25	122.49	118.70
3	A	302	FAD	C1'-N10-C9A	4.12	121.53	118.29
3	A	302	FAD	C4-C4X-C10	-4.07	117.26	119.95

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Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(^o)$	$\mathbf{Ideal}(^o)$
4	Α	303	6T2	C11-C7-N3	3.58	121.90	118.70
3	В	301	FAD	C1'-N10-C9A	3.26	120.86	118.29
3	В	301	FAD	C1B-N9A-C4A	-3.15	121.11	126.64
4	Α	303	6T2	O1-C13-C12	-3.06	113.62	123.96
3	Α	302	FAD	C3B-C2B-C1B	3.04	105.56	100.98
3	В	301	FAD	C5X-C9A-N10	2.85	119.78	117.72
4	A	303	6T2	C26-O2-C24	2.83	93.64	91.11
3	A	302	FAD	N3A-C2A-N1A	-2.75	124.38	128.68
3	В	301	FAD	C2A-N1A-C6A	2.73	123.43	118.75
3	A	302	FAD	C4A-C5A-N7A	-2.72	106.56	109.40
3	A	302	FAD	C4X-C10-N10	-2.62	117.61	120.30
4	В	303	6T2	C14-C11-N4	2.57	125.69	122.18
4	A	303	6T2	C13-C12-C10	-2.54	116.61	119.27
4	В	303	6T2	C30-C40-C50	-2.53	106.02	110.82
4	В	303	6T2	C6-C7-N3	-2.47	119.35	122.64
3	В	301	FAD	C4A-C5A-N7A	-2.45	106.85	109.40
4	В	303	6T2	C16-C6-C7	2.42	122.22	118.26
4	В	303	6T2	O1-C13-C12	-2.36	115.97	123.96
4	A	303	6T2	C6-C7-N3	-2.36	119.50	122.64
3	В	301	FAD	C4X-N5-C5X	2.34	119.11	116.77
4	A	303	6T2	N3-C2-N1	2.30	117.54	114.66
4	A	303	6T2	C14-C11-N4	2.26	125.27	122.18
4	В	303	6T2	C16-C6-C4	-2.24	117.95	123.19
3	A	302	FAD	O4B-C4B-C3B	2.24	109.54	105.11
3	В	301	FAD	C4X-C10-N10	-2.12	118.13	120.30
3	A	302	FAD	O4B-C1B-C2B	-2.10	103.86	106.93
3	В	301	FAD	C4-C4X-N5	2.04	120.92	118.60
3	В	301	FAD	C9A-N10-C10	-2.03	119.26	121.91

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	В	301	FAD	C5B-O5B-PA-O1A
3	A	302	FAD	C5B-O5B-PA-O1A
3	A	302	FAD	C5B-O5B-PA-O2A
3	В	301	FAD	C5B-O5B-PA-O3P
3	A	302	FAD	C4B-C5B-O5B-PA
3	В	301	FAD	C5B-O5B-PA-O2A
3	A	302	FAD	C5B-O5B-PA-O3P
3	В	301	FAD	P-O3P-PA-O1A
3	A	302	FAD	P-O3P-PA-O1A

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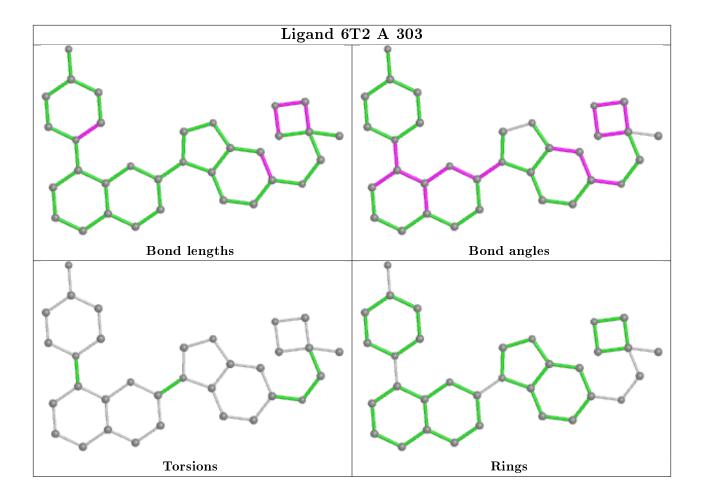
Mol	Chain	Res	Type	Atoms
3	В	301	FAD	C4'-C5'-O5'-P
3	A	302	FAD	C4'-C5'-O5'-P

There are no ring outliers.

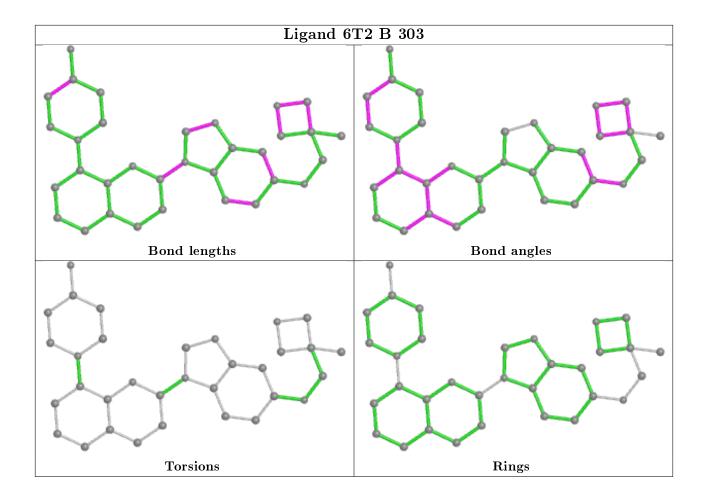
No monomer is involved in short contacts.

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

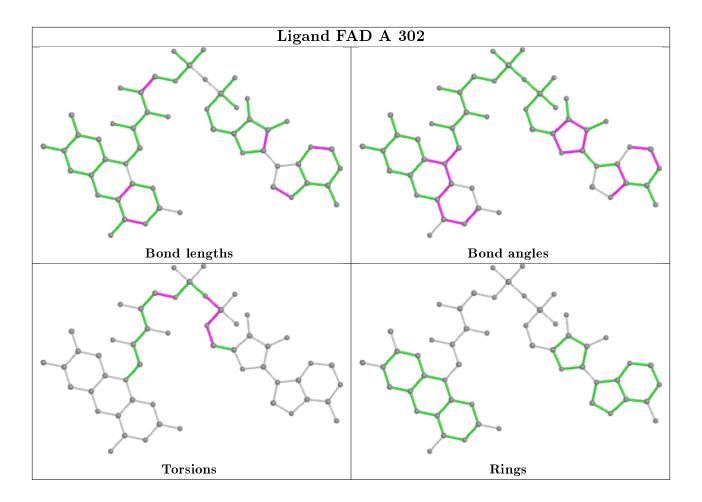












## 5.7 Other polymers (i)

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,  $95^{th}$  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 $>$	$\#\mathrm{RSRZ}{>}2$	$OWAB( m \AA^2)$	Q<0.9
1	A	228/237~(96%)	-0.43	7 (3%) 49 48	7, 11, 28, 59	0
1	В	$228/237 \ (96\%)$	-0.48	6 (2%) 56 55	7, 13, 31, 62	0
All	All	456/474 (96%)	-0.46	13 (2%) 51 50	7, 12, 31, 62	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	59	LEU	4.9
1	В	63	GLU	3.8
1	В	61	ASN	3.7
1	В	60	SER	3.5
1	A	62	PRO	3.2
1	В	2	GLY	2.9
1	A	63	GLU	2.8
1	A	58	THR	2.7
1	A	60	SER	2.6
1	A	57	GLY	2.3
1	A	59	LEU	2.2
1	В	58	THR	2.2
1	A	2	GLY	2.1

### 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 carbohydrates in this entry.

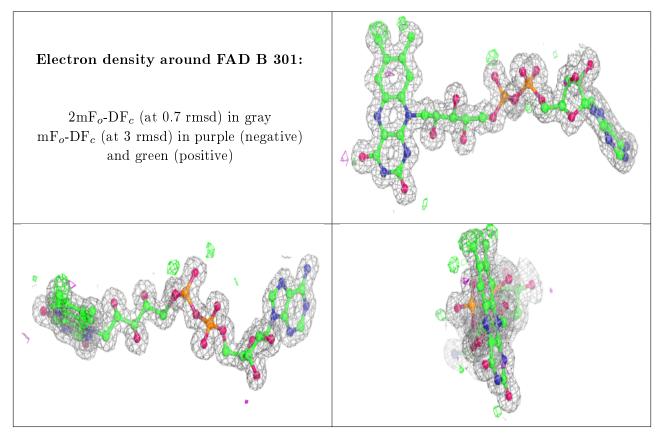


### 6.4 Ligands (i)

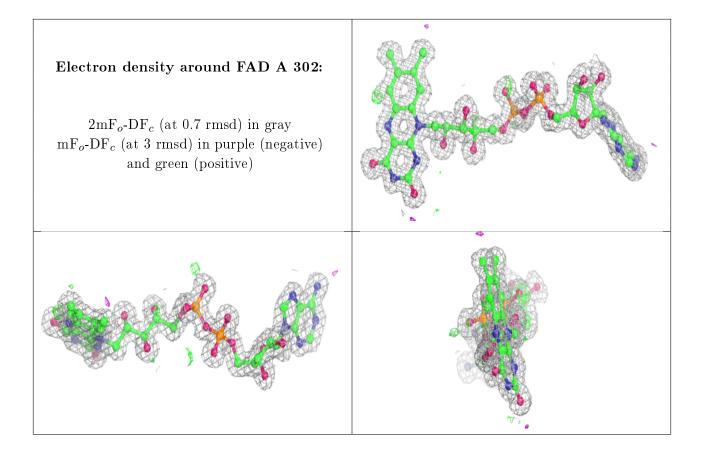
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median,  $95^{th}$  percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
3	FAD	В	301	53/53	0.98	0.06	6,10,21,32	0
3	FAD	A	302	53/53	0.98	0.06	6,8,15,27	0
4	6T2	A	303	33/33	0.98	0.06	8,9,20,26	0
4	6T2	В	303	33/33	0.98	0.05	9,11,24,34	0
2	ZN	A	301	1/1	1.00	0.07	7,7,7,7	1
2	ZN	В	302	1/1	1.00	0.07	9,9,9,9	1

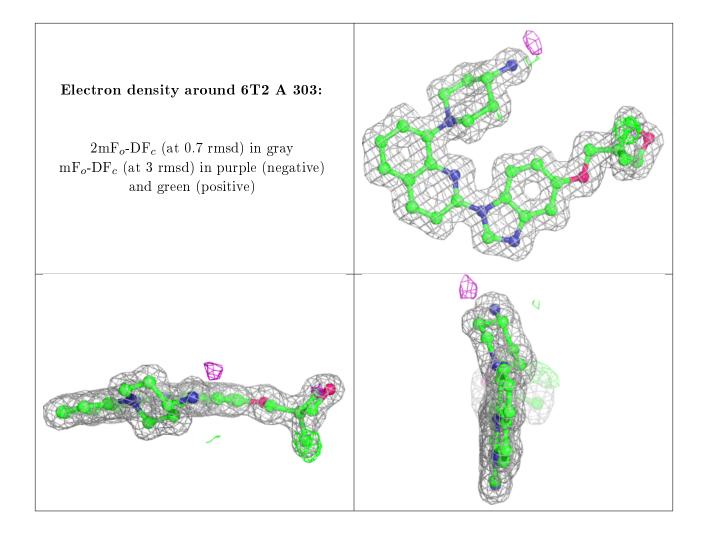
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



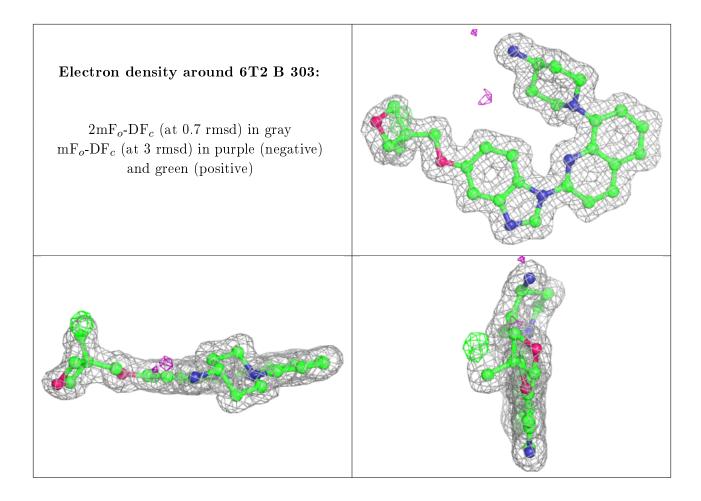












# 6.5 Other polymers (i)

There are no such residues in this entry.

