



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:01 PM UTC

PDB ID : 4QOG / pdb_00004qog
Title : Crystal structure of fad quinone reductase 2 in complex with melatonin at 1.4Å
Authors : Serriere, J.; Boutin, J.A.; Isabet, T.; Antoine, M.; Ferry, G.
Deposited on : 2014-06-20
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 ⓘ 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

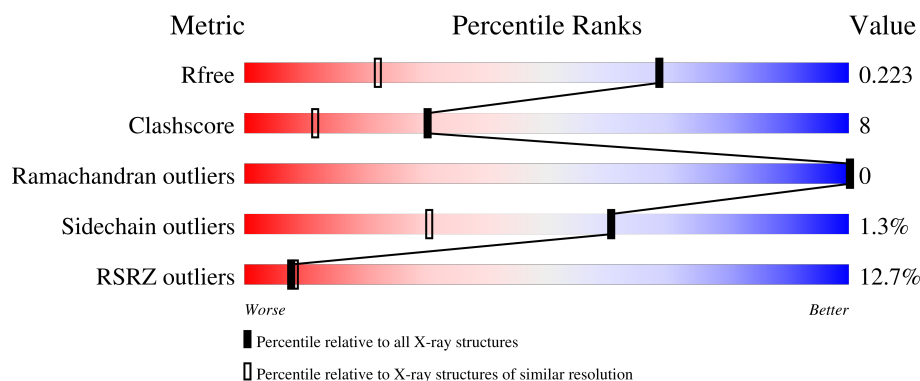
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2563 (1.40-1.40)
Clashscore	190562	2660 (1.40-1.40)
Ramachandran outliers	187476	2611 (1.40-1.40)
Sidechain outliers	187428	2610 (1.40-1.40)
RSRZ outliers	180081	2561 (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 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	231	4% 84% 13% ..
1	B	231	21% 68% 27% ..

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
3	ML1	A	302	-	-	X	-
3	ML1	B	302[A]	-	-	X	-
3	ML1	B	302[B]	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4342 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.

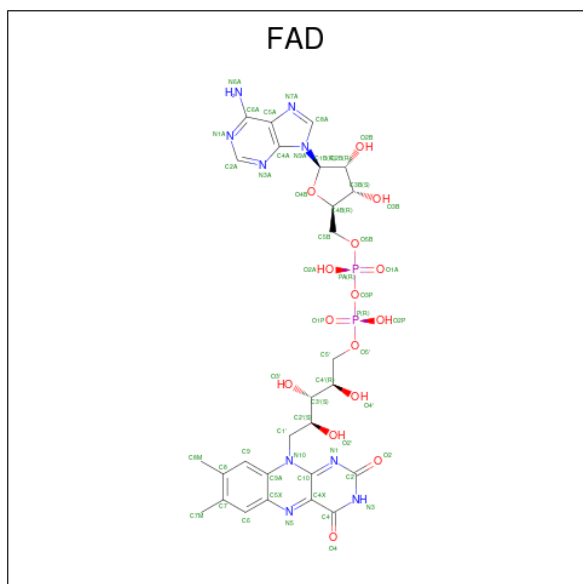
- Molecule 1 is a protein called Ribosyldihyronicotinamide dehydrogenase [quinone].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	228	Total	C	N	O	S	0	7	0
			1864	1198	311	346	9			
1	B	228	Total	C	N	O	S	0	19	0
			1959	1266	321	363	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	46	PHE	LEU	variant	UNP P16083
B	46	PHE	LEU	variant	UNP P16083

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



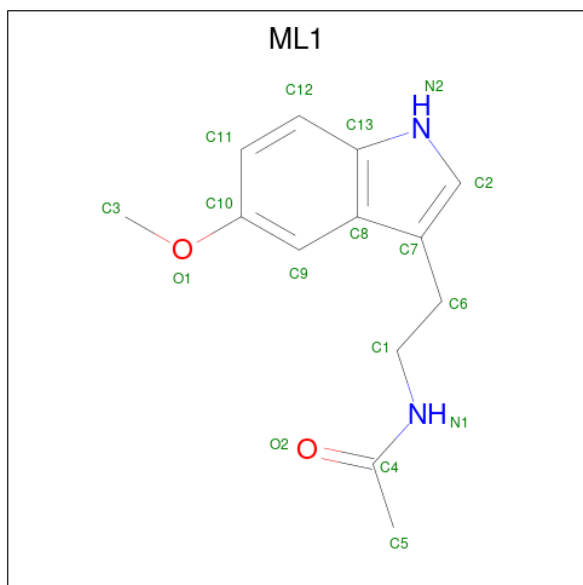
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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

- Molecule 3 is N-[2-(5-methoxy-1H-indol-3-yl)ethyl]acetamide (CCD ID: ML1) (formula: $C_{13}H_{16}N_2O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	13	2	2		
3	B	1	Total	C	N	O	0	1
			34	26	4	4		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		
4	B	1	Total	Zn	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	211	Total	O	0	0
			211	211		

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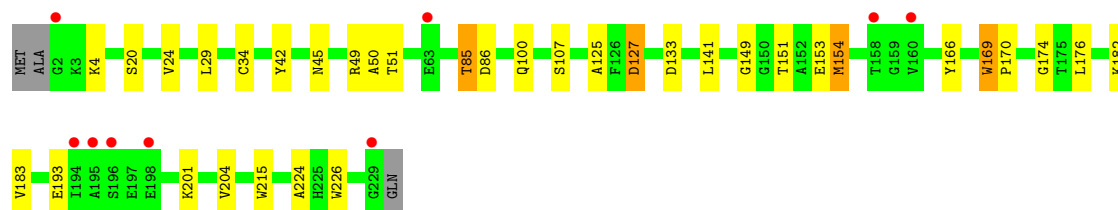
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	149	Total	O	0	0
			149	149		

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.

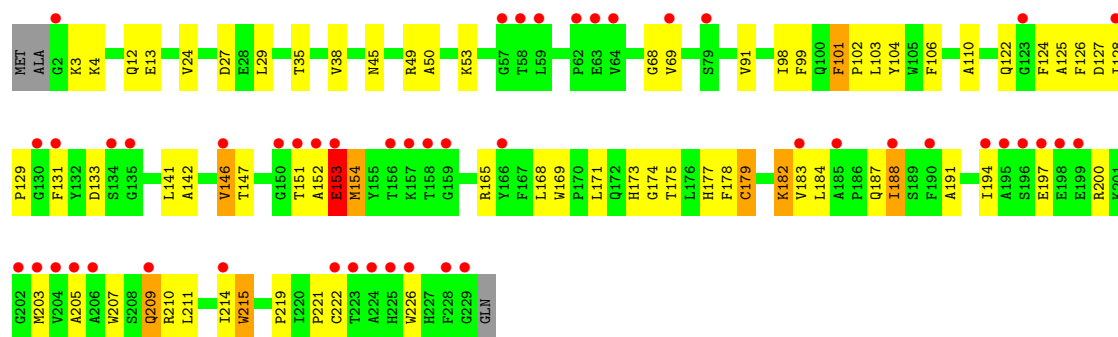
- Molecule 1: Ribosyldihyronicotinamide dehydrogenase [quinone]

Chain A: 



- Molecule 1: Ribosyldihyronicotinamide dehydrogenase [quinone]

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	56.56Å 83.40Å 106.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.81 – 1.40 46.81 – 1.40	Depositor EDS
% Data completeness (in resolution range)	98.0 (46.81-1.40) 98.2 (46.81-1.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 1.40Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.191 , 0.225 0.194 , 0.223	Depositor DCC
R_{free} test set	4918 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	16.1	Xtriage
Anisotropy	0.337	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 35.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4342	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.05% 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: ML1, FAD, ZN

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	1.63	19/1914 (1.0%)	1.36	6/2594 (0.2%)
1	B	1.78	40/2014 (2.0%)	1.51	24/2732 (0.9%)
All	All	1.71	59/3928 (1.5%)	1.44	30/5326 (0.6%)

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	191	ALA	CA-CB	9.69	1.59	1.52
1	B	146[A]	VAL	C-N	-9.51	1.19	1.33
1	B	146[B]	VAL	C-N	-9.51	1.19	1.33
1	B	187	GLN	CD-NE2	-8.80	1.14	1.33
1	B	221	PRO	CA-C	8.76	1.60	1.52
1	A	107	SER	C-O	-8.31	1.16	1.24
1	B	207	TRP	NE1-CE2	-8.11	1.28	1.37
1	B	38	VAL	C-O	7.91	1.32	1.24
1	B	98	ILE	N-CA	-7.33	1.37	1.46
1	B	142	ALA	CA-C	-7.23	1.43	1.52
1	B	104	TYR	C-O	-7.11	1.16	1.24
1	A	226	TRP	C-O	-6.98	1.16	1.24
1	B	207	TRP	C-O	-6.97	1.16	1.24
1	B	191	ALA	C-O	6.60	1.27	1.23
1	B	183	VAL	N-CA	-6.57	1.38	1.46
1	B	49	ARG	CZ-NH2	-6.40	1.25	1.33
1	B	103	LEU	C-O	-6.21	1.16	1.23
1	A	49	ARG	C-O	-6.21	1.16	1.24
1	B	102	PRO	CA-CB	-6.11	1.46	1.53
1	B	13	GLU	C-O	-6.02	1.18	1.24
1	B	209	GLN	C-N	5.98	1.41	1.33
1	A	169	TRP	N-CA	-5.97	1.41	1.46
1	B	50	ALA	C-O	-5.96	1.16	1.23
1	B	169	TRP	CA-CB	5.91	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	51	THR	C-O	-5.82	1.16	1.23
1	A	154	MET	C-O	-5.81	1.16	1.24
1	A	125	ALA	C-O	-5.76	1.16	1.24
1	B	168	LEU	CA-C	-5.73	1.44	1.52
1	A	100	GLN	C-O	5.70	1.30	1.24
1	A	127	ASP	C-O	-5.67	1.16	1.23
1	A	133	ASP	C-N	-5.65	1.26	1.33
1	B	215	TRP	NE1-CE2	-5.64	1.31	1.37
1	A	50	ALA	C-O	-5.62	1.16	1.23
1	B	222	CYS	N-CA	5.61	1.54	1.46
1	B	188	ILE	CA-C	-5.59	1.45	1.52
1	B	147	THR	C-O	-5.55	1.17	1.23
1	B	191	ALA	CA-C	-5.55	1.49	1.53
1	A	215	TRP	C-O	-5.54	1.16	1.24
1	A	166	TYR	CA-C	5.51	1.59	1.52
1	A	224	ALA	C-O	-5.50	1.17	1.24
1	B	27	ASP	C-O	-5.47	1.17	1.24
1	B	171	LEU	N-CA	5.46	1.53	1.46
1	A	86	ASP	C-O	-5.45	1.17	1.24
1	A	42	TYR	N-CA	5.39	1.53	1.46
1	B	69	VAL	C-O	5.33	1.30	1.24
1	B	210	ARG	CA-CB	5.32	1.61	1.53
1	A	34	CYS	C-O	5.28	1.31	1.23
1	B	45	ASN	C-O	-5.25	1.17	1.23
1	B	152	ALA	C-O	-5.19	1.18	1.24
1	B	211	LEU	CA-C	5.18	1.59	1.52
1	A	183	VAL	CA-CB	5.12	1.60	1.54
1	B	182	LYS	N-CA	-5.12	1.39	1.46
1	B	203	MET	SD-CE	-5.09	1.66	1.79
1	B	173	HIS	CA-C	-5.08	1.47	1.53
1	B	29	LEU	C-O	-5.08	1.17	1.24
1	B	214	ILE	CA-CB	5.08	1.61	1.54
1	A	29	LEU	N-CA	-5.07	1.40	1.46
1	B	99	PHE	C-O	5.07	1.30	1.24
1	B	124	PHE	CA-CB	5.04	1.61	1.53

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	154	MET	CG-SD-CE	10.16	123.25	100.90
1	B	146[A]	VAL	CA-C-N	9.74	137.17	122.65
1	B	146[A]	VAL	C-N-CA	9.74	137.17	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	146[B]	VAL	CA-C-N	9.74	137.17	122.65
1	B	146[B]	VAL	C-N-CA	9.74	137.17	122.65
1	B	101	PHE	O-C-N	9.70	128.73	121.65
1	B	91	VAL	O-C-N	9.32	131.04	121.91
1	B	209	GLN	N-CA-C	7.11	119.03	111.28
1	B	153	GLU	N-CA-CB	-6.27	99.56	109.78
1	A	149	GLY	CA-C-N	6.12	126.15	120.34
1	A	149	GLY	C-N-CA	6.12	126.15	120.34
1	B	210	ARG	N-CA-C	-5.94	104.81	111.28
1	B	91	VAL	CA-C-O	-5.88	114.94	121.17
1	B	12	GLN	O-C-N	5.76	129.35	122.27
1	B	110	ALA	CA-C-O	-5.72	114.45	120.63
1	B	24[A]	VAL	CA-C-O	5.70	126.47	119.58
1	B	24[B]	VAL	CA-C-O	5.70	126.47	119.58
1	B	174	GLY	O-C-N	5.55	128.64	122.54
1	B	174	GLY	N-CA-C	5.46	120.98	113.99
1	A	176	LEU	O-C-N	5.45	127.97	122.09
1	B	177	HIS	O-C-N	-5.43	116.45	122.09
1	B	175	THR	O-C-N	5.40	127.97	121.76
1	A	176	LEU	CA-C-O	-5.40	115.14	120.70
1	B	152	ALA	CA-C-N	5.37	128.87	120.82
1	B	152	ALA	C-N-CA	5.37	128.87	120.82
1	B	101	PHE	CA-C-O	-5.19	115.57	120.34
1	A	193	GLU	N-CA-C	-5.16	105.74	111.36
1	A	85	THR	CA-CB-OG1	-5.12	101.92	109.60
1	B	179	CYS	CA-C-N	-5.10	115.41	122.86
1	B	179	CYS	C-N-CA	-5.10	115.41	122.86

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	1864	0	1813	17	0
1	B	1959	0	1894	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	53	0	31	0	0
2	B	53	0	31	0	0
3	A	17	0	16	7	0
3	B	34	0	32	14	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	211	0	0	6	0
5	B	149	0	0	4	0
All	All	4342	0	3817	66	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 8.

All (66) 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)
3:B:302[A]:ML1:H2	3:B:302[A]:ML1:C4	1.52	1.36
3:B:302[A]:ML1:H2	3:B:302[A]:ML1:O2	1.30	1.26
1:A:85:THR:HG22	5:A:559:HOH:O	1.51	1.08
3:B:302[A]:ML1:H2	3:B:302[A]:ML1:N1	1.70	1.06
1:A:151:THR:H	1:A:154:MET:HE3	1.22	1.02
3:B:302[B]:ML1:H12A	5:B:521:HOH:O	1.60	1.01
3:B:302[A]:ML1:C4	3:B:302[A]:ML1:C2	2.40	0.99
3:B:302[A]:ML1:O2	3:B:302[A]:ML1:C2	2.15	0.95
3:A:302:ML1:H31	1:B:106[B]:PHE:CE1	2.03	0.92
1:B:151:THR:OG1	1:B:154:MET:HG3	1.80	0.81
3:B:302[A]:ML1:N1	3:B:302[A]:ML1:C2	2.34	0.80
3:A:302:ML1:C3	1:B:106[B]:PHE:CE1	2.64	0.79
1:B:205:ALA:O	1:B:209:GLN:HG3	1.85	0.76
1:B:122:GLN:HG3	1:B:127[A]:ASP:HA	1.69	0.74
1:B:122:GLN:NE2	1:B:128[A]:ILE:H	1.87	0.72
1:A:174:GLY:HA3	1:B:106[B]:PHE:CD1	2.24	0.72
3:B:302[B]:ML1:H2	3:B:302[B]:ML1:C4	2.20	0.72
3:A:302:ML1:H31	1:B:106[B]:PHE:HE1	1.53	0.71
1:B:182:LYS:HB3	1:B:219:PRO:HB3	1.73	0.70
1:B:126[B]:PHE:HZ	3:B:302[B]:ML1:H11	1.58	0.68
1:B:122:GLN:CG	1:B:127[A]:ASP:HA	2.26	0.64
1:B:68:GLY:HA3	3:B:302[B]:ML1:C4	2.27	0.64
1:B:101:PHE:CZ	1:B:146[B]:VAL:HG12	2.33	0.64
1:B:197:GLU:OE2	1:B:200:ARG:NH1	2.26	0.64
3:A:302:ML1:H31	1:B:106[B]:PHE:CZ	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:302:ML1:C3	1:B:106[B]:PHE:HE1	2.06	0.62
1:A:24:VAL:HG13	5:A:513:HOH:O	1.98	0.62
1:A:85:THR:CG2	5:A:559:HOH:O	2.27	0.60
1:A:174:GLY:CA	1:B:106[B]:PHE:CE1	2.87	0.58
1:B:133[A]:ASP:HB2	5:B:463:HOH:O	2.03	0.57
1:A:151:THR:N	1:A:154:MET:HE3	2.07	0.56
1:B:141:LEU:HD22	1:B:184:LEU:HD21	1.88	0.56
1:B:122:GLN:NE2	1:B:128[A]:ILE:N	2.56	0.54
1:B:126[B]:PHE:HZ	3:B:302[B]:ML1:C1	2.20	0.52
1:B:131[A]:PHE:CB	1:B:178:PHE:CZ	2.93	0.52
1:B:151:THR:OG1	1:B:153:GLU:HB2	2.10	0.51
3:A:302:ML1:H32	1:B:106[B]:PHE:CE1	2.44	0.50
1:A:45[B]:ASN:OD1	5:A:565:HOH:O	2.19	0.49
1:A:174:GLY:HA2	1:B:106[B]:PHE:CE1	2.47	0.49
1:A:174:GLY:CA	1:B:106[B]:PHE:CD1	2.95	0.49
1:A:24:VAL:CG1	5:A:513:HOH:O	2.58	0.48
1:B:122:GLN:HA	1:B:126[A]:PHE:O	2.13	0.48
1:B:153:GLU:CD	5:B:471:HOH:O	2.55	0.48
1:A:141:LEU:HD23	1:A:182[B]:LYS:HB2	1.97	0.47
1:B:68:GLY:HA3	3:B:302[B]:ML1:O2	2.15	0.46
1:B:125:ALA:HB1	1:B:179:CYS:SG	2.56	0.46
1:B:182:LYS:HB3	1:B:219:PRO:CB	2.43	0.46
1:B:178:PHE:CD1	3:B:302[A]:ML1:H33	2.53	0.44
1:A:4[A]:LYS:HD2	5:A:604:HOH:O	2.18	0.44
1:B:131[A]:PHE:CD2	1:B:178:PHE:CE1	3.05	0.44
1:A:20:SER:O	1:A:24:VAL:HG13	2.18	0.44
1:B:3:LYS:HB3	1:B:215:TRP:CH2	2.54	0.43
1:B:141:LEU:HD22	1:B:184:LEU:CD2	2.48	0.43
1:B:165:ARG:HD3	1:B:226:TRP:CE3	2.54	0.43
1:B:131[A]:PHE:CG	1:B:178:PHE:CZ	3.07	0.42
3:A:302:ML1:H51	1:B:154:MET:HE1	2.01	0.42
1:B:4[B]:LYS:HG2	1:B:35:THR:HB	2.00	0.42
1:A:24:VAL:HG11	1:A:204:VAL:CG1	2.49	0.42
1:A:182[B]:LYS:HB2	1:A:182[B]:LYS:HE3	1.91	0.42
1:B:53:LYS:HE2	5:B:478:HOH:O	2.20	0.42
1:B:146[B]:VAL:CG2	1:B:188:ILE:HG12	2.50	0.42
1:B:128[A]:ILE:HA	1:B:129[A]:PRO:HA	1.79	0.42
1:B:146[B]:VAL:O	1:B:146[B]:VAL:HG23	2.20	0.41
1:A:169:TRP:HB3	1:A:170:PRO:HD3	2.01	0.41
1:B:68:GLY:CA	3:B:302[B]:ML1:C4	2.98	0.40
1:B:101:PHE:CZ	1:B:146[A]:VAL:HG22	2.57	0.40

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	233/231 (101%)	224 (96%)	9 (4%)	0	100	100
1	B	245/231 (106%)	238 (97%)	7 (3%)	0	100	100
All	All	478/462 (104%)	462 (97%)	16 (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	Percentiles	
1	A	200/195 (103%)	197 (98%)	3 (2%)	57	26
1	B	210/195 (108%)	208 (99%)	2 (1%)	68	40
All	All	410/390 (105%)	405 (99%)	5 (1%)	61	34

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127	ASP
1	A	153	GLU
1	A	201	LYS
1	B	153	GLU
1	B	194	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	GLN
1	B	100	GLN
1	B	212	GLN
1	B	225	HIS

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 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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	$\# Z > 2$
2	FAD	A	301	-	58,58,58	1.45	7 (12%)	85,89,89	0.95	3 (3%)
2	FAD	B	301	-	58,58,58	1.85	9 (15%)	85,89,89	1.16	8 (9%)
3	ML1	B	302[B]	-	18,18,18	0.43	0	24,24,24	0.57	0
3	ML1	B	302[A]	-	18,18,18	0.50	0	24,24,24	0.36	0
3	ML1	A	302	-	18,18,18	0.37	0	24,24,24	0.33	0

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	FAD	A	301	-	-	5/34/50/50	0/6/6/6
2	FAD	B	301	-	-	7/34/50/50	0/6/6/6
3	ML1	B	302[B]	-	-	2/8/8/8	0/2/2/2
3	ML1	B	302[A]	-	-	3/8/8/8	0/2/2/2
3	ML1	A	302	-	-	2/8/8/8	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	FAD	P-O3P	7.88	1.68	1.59
2	B	301	FAD	PA-O3P	-6.82	1.52	1.59
2	A	301	FAD	P-O3P	6.09	1.66	1.59
2	A	301	FAD	PA-O3P	4.73	1.64	1.59
2	B	301	FAD	C10-N1	4.05	1.41	1.33
2	A	301	FAD	P-O5'	-3.89	1.44	1.59
2	A	301	FAD	PA-O1A	-3.79	1.37	1.50
2	B	301	FAD	O2-C2	3.21	1.30	1.24
2	B	301	FAD	C2-N3	-2.98	1.32	1.39
2	A	301	FAD	C2-N1	-2.44	1.31	1.36
2	B	301	FAD	C1'-C2'	2.26	1.55	1.52
2	B	301	FAD	C2-N1	-2.15	1.31	1.36
2	B	301	FAD	P-O5'	-2.14	1.51	1.59
2	A	301	FAD	P-O2P	-2.11	1.45	1.55
2	B	301	FAD	O4'-C4'	-2.11	1.38	1.43
2	A	301	FAD	C10-N1	2.06	1.37	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	FAD	O2A-PA-O3P	4.15	118.49	107.27
2	A	301	FAD	O2-C2-N1	-3.53	115.94	121.80
2	B	301	FAD	O5'-P-O1P	3.25	121.81	108.94
2	B	301	FAD	O3P-PA-O1A	-2.97	101.76	110.70
2	B	301	FAD	C1'-N10-C9A	-2.65	115.48	120.63
2	B	301	FAD	O3P-P-O1P	-2.49	103.21	110.70
2	B	301	FAD	O2A-PA-O5B	2.31	118.05	107.57
2	A	301	FAD	O5B-C5B-C4B	-2.17	101.61	108.99
2	B	301	FAD	O4'-C4'-C3'	-2.16	104.20	109.25
2	A	301	FAD	C4X-C10-N10	2.15	119.56	116.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	FAD	O3'-C3'-C2'	-2.09	104.19	108.93

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	302[A]	ML1	N1-C1-C6-C7
3	B	302[A]	ML1	C5-C4-N1-C1
3	B	302[A]	ML1	O2-C4-N1-C1
3	B	302[B]	ML1	C5-C4-N1-C1
3	B	302[B]	ML1	O2-C4-N1-C1
3	A	302	ML1	C5-C4-N1-C1
3	A	302	ML1	O2-C4-N1-C1
2	B	301	FAD	C2B-C1B-N9A-C8A
2	A	301	FAD	C2B-C1B-N9A-C8A
2	B	301	FAD	P-O3P-PA-O2A
2	A	301	FAD	C5B-O5B-PA-O2A
2	B	301	FAD	C5B-O5B-PA-O2A
2	A	301	FAD	C2B-C1B-N9A-C4A
2	B	301	FAD	C2B-C1B-N9A-C4A
2	A	301	FAD	C4'-C5'-O5'-P
2	B	301	FAD	C4'-C5'-O5'-P
2	A	301	FAD	O4B-C1B-N9A-C8A
2	B	301	FAD	P-O3P-PA-O1A
2	B	301	FAD	O4B-C1B-N9A-C8A

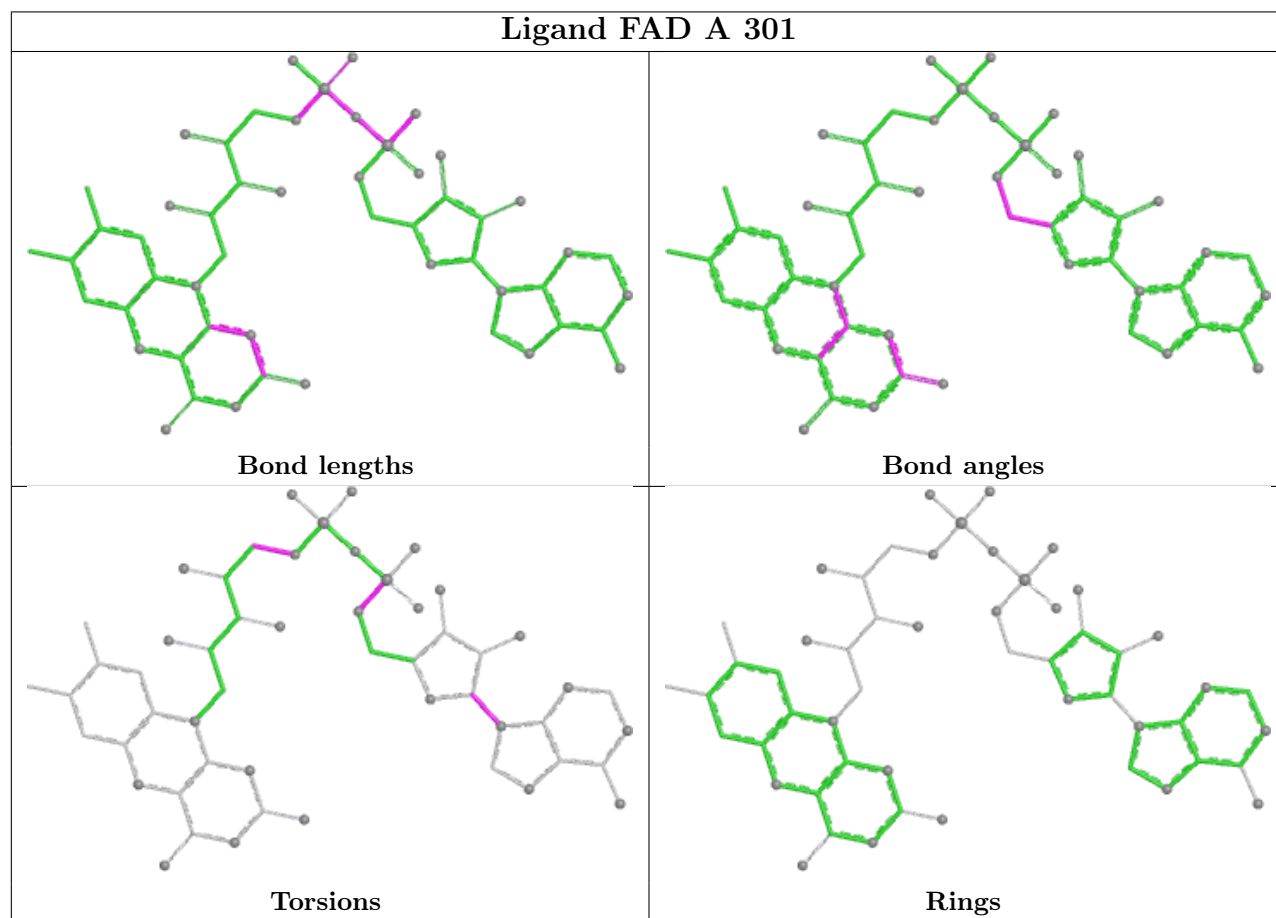
There are no ring outliers.

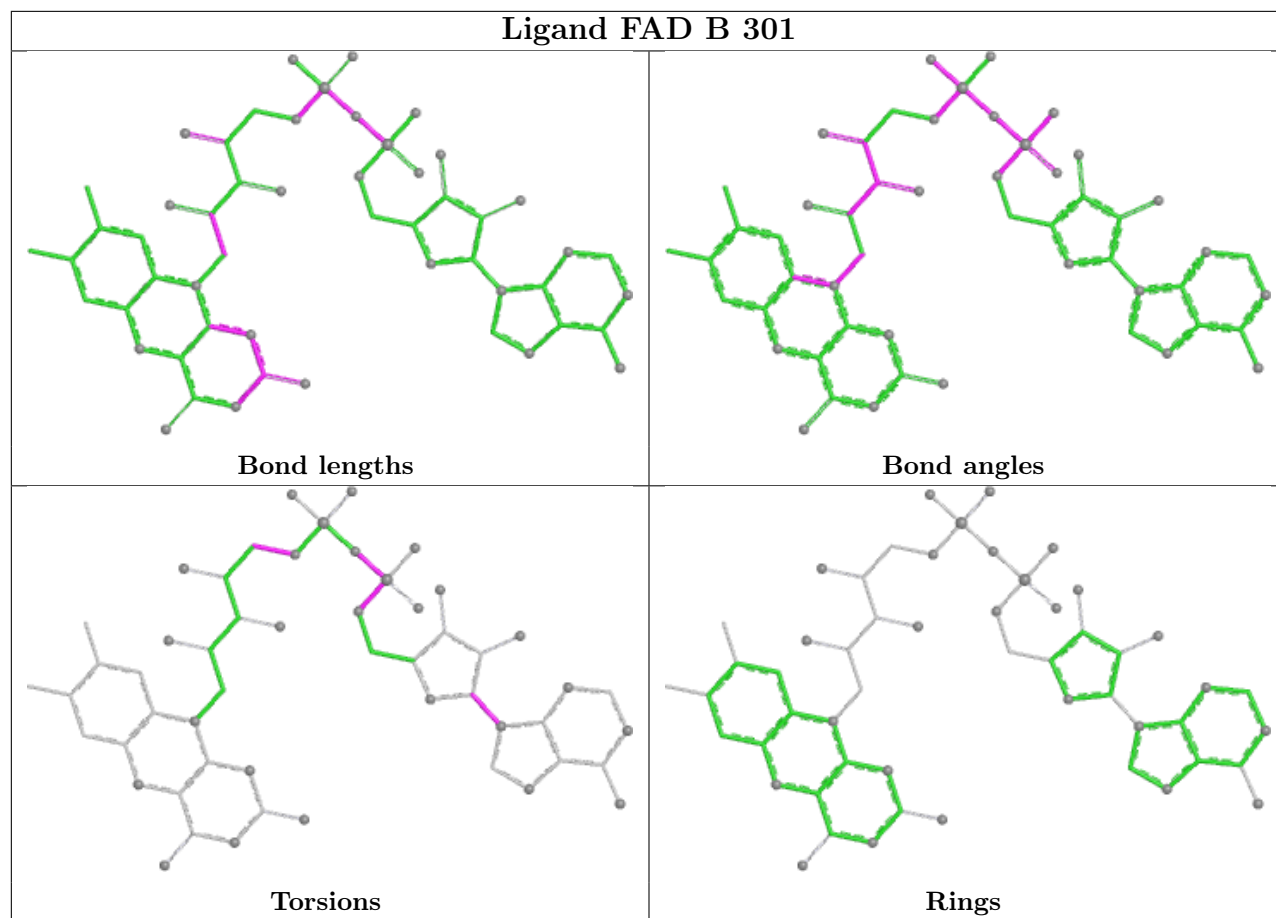
3 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	302[B]	ML1	7	0
3	B	302[A]	ML1	7	0
3	A	302	ML1	7	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	146[A]:VAL	C	147:THR	N	1.19
1	B	146[B]:VAL	C	147:THR	N	1.18

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	228/231 (98%)	0.06	9 (3%) 43 45	5, 16, 34, 59	7 (3%)
1	B	228/231 (98%)	1.03	49 (21%) 2 2	7, 20, 40, 60	19 (8%)
All	All	456/462 (98%)	0.54	58 (12%) 8 8	5, 18, 39, 60	26 (5%)

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	131[A]	PHE	6.0
1	B	128[A]	ILE	5.3
1	A	2	GLY	4.4
1	B	194	ILE	4.1
1	B	58	THR	4.1
1	B	130[A]	GLY	3.7
1	B	229	GLY	3.5
1	B	198	GLU	3.4
1	B	202	GLY	3.4
1	B	146[A]	VAL	3.3
1	A	160	VAL	3.3
1	B	228	PHE	3.3
1	B	59	LEU	3.2
1	B	153	GLU	3.2
1	B	135[A]	GLY	3.2
1	B	195	ALA	3.2
1	B	214	ILE	3.2
1	B	151	THR	3.1
1	B	204	VAL	3.0
1	B	64	VAL	3.0
1	A	194	ILE	3.0
1	B	62	PRO	3.0
1	B	205	ALA	2.9
1	B	209	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	156	THR	2.8
1	B	57	GLY	2.8
1	B	226	TRP	2.8
1	A	198	GLU	2.8
1	B	123	GLY	2.7
1	B	63	GLU	2.7
1	B	203	MET	2.6
1	A	229	GLY	2.6
1	B	2	GLY	2.5
1	B	196	SER	2.4
1	A	195	ALA	2.4
1	B	134[A]	SER	2.4
1	B	152	ALA	2.4
1	B	159	GLY	2.4
1	B	185	ALA	2.4
1	B	158	THR	2.4
1	B	224	ALA	2.3
1	B	225	HIS	2.3
1	B	190	PHE	2.3
1	A	158	THR	2.3
1	B	79	SER	2.3
1	B	188	ILE	2.2
1	B	206	ALA	2.2
1	B	222	CYS	2.2
1	B	150	GLY	2.2
1	B	157	LYS	2.2
1	B	223	THR	2.1
1	B	197	GLU	2.1
1	B	199	GLU	2.1
1	A	63	GLU	2.1
1	B	69	VAL	2.0
1	B	166	TYR	2.0
1	B	183	VAL	2.0
1	A	196	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

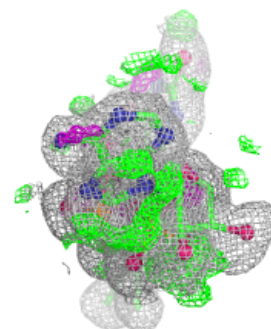
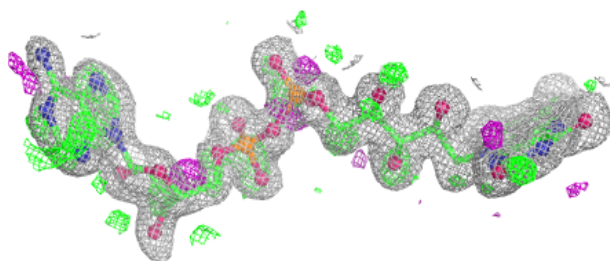
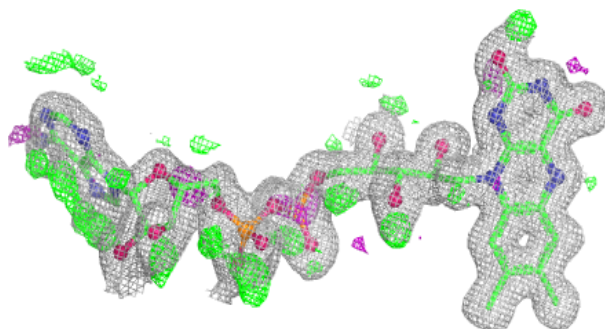
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ML1	B	302[A]	17/17	0.72	0.20	21,25,37,43	17
3	ML1	B	302[B]	17/17	0.72	0.20	23,28,39,41	17
3	ML1	A	302	17/17	0.88	0.14	19,28,52,53	0
4	ZN	B	303	1/1	0.88	0.10	24,24,24,24	0
2	FAD	B	301	53/53	0.95	0.09	10,17,31,35	0
2	FAD	A	301	53/53	0.97	0.07	12,16,31,38	0
4	ZN	A	303	1/1	0.98	0.04	15,15,15,15	0

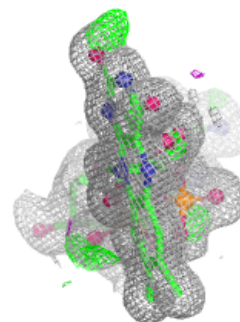
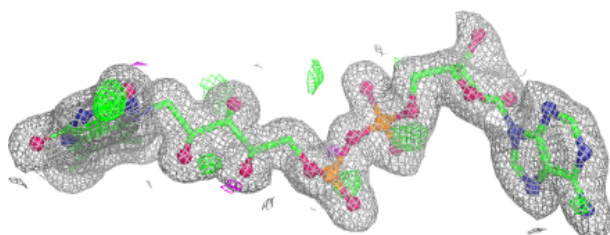
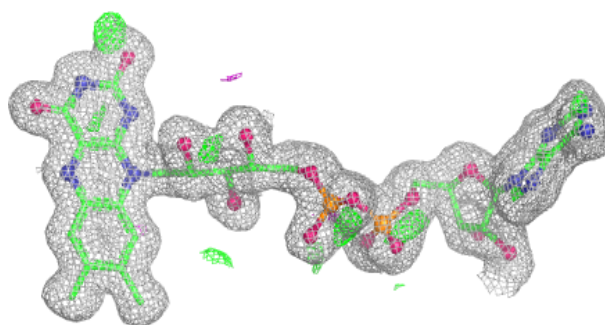
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD B 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 FAD A 301:**

$2mF_o-DF_c$ (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.