



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 10, 2022 – 10:57 PM EST

PDB ID : 3UXE  
Title : Design, Synthesis and Biological Evaluation of Potent Quinoline and Pyrrolo-quinoline Ammosamide Analogues as Inhibitors for Quinone Reductase 2  
Authors : Reddy, N.P.; Jensen, K.C.; Mesecar, A.D.; Fanwick, P.E.; Cushman, M.  
Deposited on : 2011-12-05  
Resolution : 1.50 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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.31.2  
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) : 2.31.2

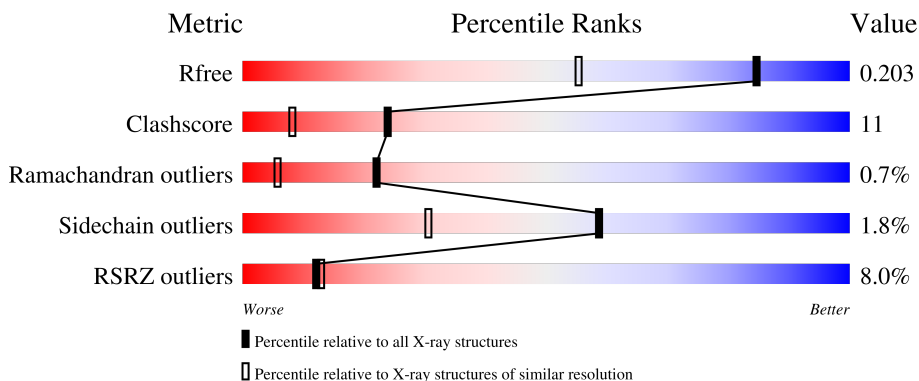
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.50 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))
$R_{free}$	130704	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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  $\geq 3$ , 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	230	
1	B	230	

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
4	465	A	303	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4216 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
			Total	C	N	O	S			
1	A	230	1829	1178	304	338	9	0	1	0
1	B	230	1837	1183	304	341	9	0	3	0

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 ZINC ION (three-letter code: ZN) (formula: Zn).

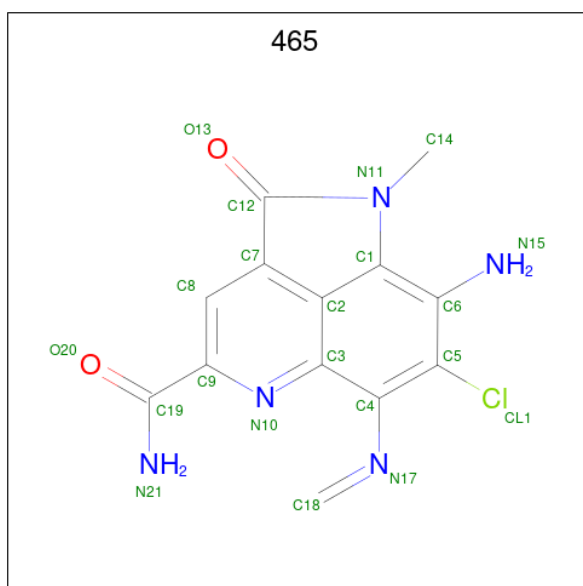
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C<sub>27</sub>H<sub>33</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>).



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

- Molecule 4 is 8-amino-7-chloro-1-methyl-6-(methylideneamino)-2-oxo-1,2-dihydropyrrolo[4,3,2-de]quinoline-4-carboxamide (three-letter code: 465) (formula: C<sub>13</sub>H<sub>10</sub>ClN<sub>5</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Cl	N			O
4	A	1	21	13	1	5	2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Cl	N			O
4	B	1	21	13	1	5	2	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	B	1	6	3	0	0

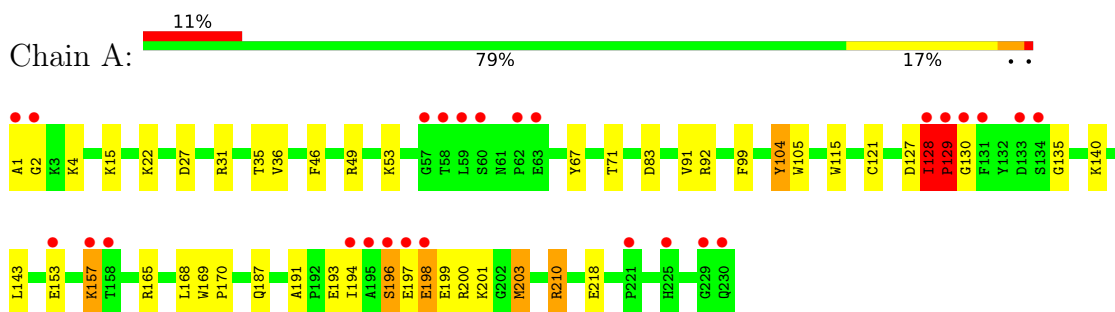
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	168	168	168	0	0
6	B	226	226	226	0	0

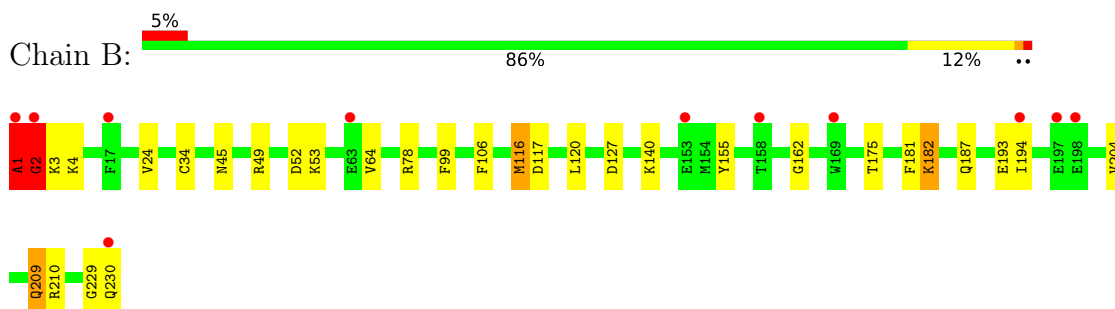
### 3 Residue-property plots [i](#)

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]



- Molecule 1: Ribosyldihyronicotinamide dehydrogenase [quinone]



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.55Å 83.95Å 106.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.68 – 1.50 19.68 – 1.50	Depositor EDS
% Data completeness (in resolution range)	99.2 (19.68-1.50) 99.3 (19.68-1.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.37 (at 1.50Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.177 , 0.197 0.183 , 0.203	Depositor DCC
$R_{free}$ test set	4080 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.8	Xtrriage
Anisotropy	0.046	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 42.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	4216	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.61% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: GOL, FAD, 465, 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	1.31	3/1882 (0.2%)	1.20	11/2552 (0.4%)
1	B	1.32	6/1896 (0.3%)	1.29	17/2571 (0.7%)
All	All	1.31	9/3778 (0.2%)	1.25	28/5123 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	2
All	All	0	5

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	2	GLY	N-CA	7.74	1.57	1.46
1	B	1	ALA	C-O	6.64	1.35	1.23
1	B	99	PHE	CE1-CZ	5.73	1.48	1.37
1	B	106	PHE	CD1-CE1	5.27	1.49	1.39
1	B	193	GLU	CB-CG	5.18	1.62	1.52
1	A	115	TRP	CZ3-CH2	5.18	1.48	1.40
1	A	99	PHE	CD2-CE2	5.16	1.49	1.39
1	B	182	LYS	CE-NZ	5.09	1.61	1.49
1	A	121	CYS	CB-SG	-5.08	1.73	1.81

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203	MET	CG-SD-CE	-11.49	81.82	100.20
1	B	78	ARG	NE-CZ-NH1	11.19	125.89	120.30
1	B	49	ARG	NE-CZ-NH1	10.05	125.33	120.30
1	B	78	ARG	NE-CZ-NH2	-9.87	115.36	120.30
1	B	127[A]	ASP	CB-CG-OD1	7.33	124.89	118.30
1	B	127[B]	ASP	CB-CG-OD1	7.33	124.89	118.30
1	B	2	GLY	N-CA-C	-7.32	94.79	113.10
1	B	181	PHE	CB-CG-CD1	-7.28	115.71	120.80
1	B	182	LYS	CD-CE-NZ	7.13	128.09	111.70
1	B	1	ALA	C-N-CA	7.09	137.18	122.30
1	B	117	ASP	CB-CG-OD1	6.97	124.58	118.30
1	B	49	ARG	NE-CZ-NH2	-6.85	116.88	120.30
1	A	27	ASP	CB-CG-OD2	-6.62	112.34	118.30
1	B	127[A]	ASP	CB-CG-OD2	-6.29	112.64	118.30
1	B	127[B]	ASP	CB-CG-OD2	-6.29	112.64	118.30
1	B	116[A]	MET	CG-SD-CE	-6.22	90.24	100.20
1	B	116[B]	MET	CG-SD-CE	-6.22	90.24	100.20
1	A	143	LEU	CB-CG-CD1	-6.13	100.57	111.00
1	A	104	TYR	CB-CG-CD2	-5.85	117.49	121.00
1	A	210	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	A	46	PHE	CB-CG-CD1	-5.80	116.74	120.80
1	B	52	ASP	CB-CG-OD1	5.73	123.46	118.30
1	A	49	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	A	31	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	A	128	ILE	CG1-CB-CG2	5.48	123.45	111.40
1	A	36	VAL	CG1-CB-CG2	-5.37	102.31	110.90
1	B	49	ARG	CG-CD-NE	5.29	122.91	111.80
1	A	83	ASP	CB-CG-OD1	5.12	122.91	118.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	128	ILE	Peptide
1	A	129	PRO	Peptide
1	A	196	SER	Peptide
1	B	1	ALA	Peptide
1	B	2	GLY	Peptide

## 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	1829	0	1788	49	0
1	B	1837	0	1797	26	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	53	0	31	3	0
3	B	53	0	31	0	0
4	A	21	0	10	8	0
4	B	21	0	10	4	0
5	B	6	0	8	0	0
6	A	168	0	0	12	1
6	B	226	0	0	11	1
All	All	4216	0	3675	83	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 11.

All (83) 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)
6:A:498:HOH:O	4:B:304:465:C18	1.86	1.22
1:B:1:ALA:O	1:B:34:CYS:SG	2.00	1.19
6:A:498:HOH:O	4:B:304:465:H18A	1.39	1.17
4:A:303:465:C18	6:B:541:HOH:O	1.90	1.16
4:B:304:465:H18	4:B:304:465:N10	1.73	1.02
1:A:197:GLU:H	1:A:198:GLU:CB	1.73	1.01
1:B:182:LYS:CE	6:B:582:HOH:O	2.10	0.99
1:B:182:LYS:HE3	6:B:582:HOH:O	1.63	0.97
1:A:197:GLU:H	1:A:198:GLU:HB2	1.34	0.93
1:A:128:ILE:HG12	6:A:565:HOH:O	1.67	0.92
1:B:116[B]:MET:HG3	1:B:120:LEU:HD12	1.49	0.91
1:A:197:GLU:N	1:A:198:GLU:HB2	1.88	0.89
4:A:303:465:H18	6:B:541:HOH:O	1.61	0.86
1:A:198:GLU:H	1:A:201:LYS:HG2	1.43	0.83
4:A:303:465:H18	4:A:303:465:N10	1.93	0.82
1:B:230:GLN:NE2	1:B:230:GLN:HA	1.98	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:GLY:O	1:A:135:GLY:HA2	1.87	0.75
4:B:304:465:C18	4:B:304:465:N10	2.48	0.74
1:A:199:GLU:O	1:A:203:MET:HG3	1.88	0.74
1:A:197:GLU:H	1:A:198:GLU:CA	1.99	0.73
4:A:303:465:H18A	6:B:541:HOH:O	1.71	0.73
1:A:53:LYS:HE2	6:A:512:HOH:O	1.89	0.72
1:A:127:ASP:H	1:A:130:GLY:HA3	1.54	0.72
1:A:197:GLU:CA	1:A:198:GLU:HB2	2.21	0.70
1:A:198:GLU:N	1:A:201:LYS:HG2	2.05	0.70
1:B:2:GLY:H	1:B:3:LYS:HG2	1.56	0.70
1:A:105:TRP:CZ3	4:A:303:465:H18A	2.28	0.68
1:A:187:GLN:HE21	1:A:210:ARG:HH11	1.41	0.68
1:B:187:GLN:HE21	1:B:210:ARG:HH11	1.43	0.66
1:A:198:GLU:H	1:A:201:LYS:H	1.41	0.66
1:A:2:GLY:HA2	6:A:518:HOH:O	1.96	0.66
1:A:15:LYS:HE3	6:A:519:HOH:O	1.95	0.66
1:B:116[B]:MET:HG2	1:B:175:THR:HG21	1.78	0.65
1:A:218:GLU:OE2	6:A:540:HOH:O	2.15	0.65
1:A:1:ALA:N	6:A:463:HOH:O	2.25	0.64
1:B:45:ASN:OD1	6:B:578:HOH:O	2.16	0.61
1:B:24:VAL:HG13	6:B:445:HOH:O	2.01	0.60
1:A:105:TRP:CE3	4:A:303:465:H18A	2.37	0.60
1:B:230:GLN:HA	1:B:230:GLN:HE21	1.67	0.59
1:A:1:ALA:HA	6:A:518:HOH:O	2.03	0.59
4:A:303:465:C18	4:A:303:465:N10	2.65	0.59
1:B:140:LYS:HE2	6:B:569:HOH:O	2.03	0.59
1:B:116[B]:MET:HG3	1:B:120:LEU:CD1	2.29	0.58
1:A:197:GLU:N	1:A:198:GLU:CB	2.51	0.56
1:A:198:GLU:N	1:A:201:LYS:H	2.02	0.56
1:A:197:GLU:CB	1:A:198:GLU:HB2	2.36	0.55
1:B:1:ALA:HB1	1:B:2:GLY:HA2	1.88	0.55
1:A:153:GLU:HG2	6:A:526:HOH:O	2.05	0.54
1:B:1:ALA:CB	1:B:2:GLY:CA	2.86	0.54
1:B:182:LYS:HE2	6:B:582:HOH:O	1.92	0.54
1:A:165:ARG:HA	1:A:168:LEU:HD12	1.90	0.53
1:B:230:GLN:HE21	1:B:230:GLN:CA	2.21	0.53
1:A:127:ASP:HB3	1:A:129:PRO:HD2	1.89	0.52
1:A:196:SER:OG	1:A:197:GLU:N	2.43	0.52
1:A:187:GLN:NE2	1:A:210:ARG:HH11	2.08	0.51
1:A:191:ALA:HB1	1:A:194:ILE:HG12	1.92	0.51
1:B:4:LYS:HD2	6:B:601:HOH:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:ASP:N	1:A:130:GLY:HA3	2.25	0.50
1:A:200:ARG:NH1	6:A:548:HOH:O	2.43	0.50
1:A:127:ASP:H	1:A:130:GLY:CA	2.24	0.49
1:A:197:GLU:N	1:A:198:GLU:CA	2.73	0.49
1:B:2:GLY:H	1:B:3:LYS:CG	2.26	0.48
1:A:15:LYS:HD2	1:B:64:VAL:HG22	1.96	0.48
1:A:198:GLU:H	1:A:201:LYS:CG	2.21	0.47
1:A:200:ARG:HD3	3:A:302:FAD:O4B	2.15	0.47
1:B:24:VAL:HG11	1:B:204:VAL:CG1	2.46	0.46
1:A:4:LYS:HG2	1:A:35:THR:HB	1.98	0.46
1:B:209:GLN:HG3	6:B:579:HOH:O	2.14	0.46
1:A:92:ARG:HD2	6:A:470:HOH:O	2.17	0.45
1:A:157:LYS:HE3	1:A:157:LYS:HB2	1.56	0.45
1:A:105:TRP:CZ3	4:A:303:465:C18	2.97	0.45
1:A:91:VAL:O	1:A:140:LYS:HE3	2.17	0.44
1:B:187:GLN:NE2	1:B:210:ARG:HH11	2.10	0.44
1:A:128:ILE:O	1:A:128:ILE:HG23	2.17	0.43
1:A:200:ARG:HB3	3:A:302:FAD:C2A	2.49	0.43
1:B:155:TYR:HA	1:B:162:GLY:O	2.18	0.43
1:A:196:SER:O	1:A:200:ARG:N	2.48	0.42
1:B:229:GLY:O	1:B:230:GLN:CB	2.68	0.42
1:A:1:ALA:HA	1:A:2:GLY:HA2	1.98	0.42
1:B:1:ALA:CB	1:B:2:GLY:HA2	2.51	0.41
1:A:104:TYR:HA	3:A:302:FAD:C5X	2.51	0.41
1:A:67:TYR:CZ	1:A:71:THR:HG21	2.56	0.41
1:A:169:TRP:HB3	1:A:170:PRO:HD3	2.03	0.40

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)
6:A:568:HOH:O	6:B:465:HOH:O[2_555]	1.81	0.39

## 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	229/230 (100%)	218 (95%)	8 (4%)	3 (1%)	12	2
1	B	231/230 (100%)	223 (96%)	8 (4%)	0	100	100
All	All	460/460 (100%)	441 (96%)	16 (4%)	3 (1%)	22	6

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	129	PRO
1	A	198	GLU
1	A	128	ILE

### 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	195/194 (100%)	191 (98%)	4 (2%)	53	23
1	B	197/194 (102%)	194 (98%)	3 (2%)	65	39
All	All	392/388 (101%)	385 (98%)	7 (2%)	59	30

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LYS
1	A	128	ILE
1	A	157	LYS
1	A	193	GLU
1	B	53	LYS
1	B	194	ILE
1	B	209	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	A	172	GLN
1	A	187	GLN
1	A	212	GLN
1	B	172	GLN
1	B	187	GLN
1	B	230	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 monosaccharides 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
3	FAD	B	303	-	53,58,58	1.74	12 (22%)	68,89,89	2.37	25 (36%)
5	GOL	B	302	-	5,5,5	0.34	0	5,5,5	0.65	0
3	FAD	A	302	-	53,58,58	2.04	11 (20%)	68,89,89	1.91	15 (22%)
4	465	A	303	-	19,23,23	3.09	10 (52%)	26,36,36	3.73	11 (42%)
4	465	B	304	-	19,23,23	3.53	8 (42%)	26,36,36	4.88	15 (57%)

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
3	FAD	B	303	-	-	6/30/50/50	0/6/6/6
5	GOL	B	302	-	-	2/4/4/4	-
3	FAD	A	302	-	-	2/30/50/50	0/6/6/6
4	465	A	303	-	-	0/4/6/6	0/3/3/3
4	465	B	304	-	-	0/4/6/6	0/3/3/3

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	303	465	C1-C6	8.05	1.48	1.39
4	B	304	465	C6-C5	7.89	1.49	1.41
4	B	304	465	C1-C6	7.84	1.48	1.39
3	A	302	FAD	C1'-C2'	6.22	1.61	1.52
3	A	302	FAD	C10-N1	6.16	1.45	1.33
4	B	304	465	O13-C12	5.96	1.34	1.22
4	A	303	465	C6-C5	5.88	1.47	1.41
3	A	302	FAD	C4X-N5	5.22	1.40	1.30
4	B	304	465	C4-N17	-5.07	1.34	1.42
4	A	303	465	C4-N17	-5.04	1.34	1.42
3	B	303	FAD	C2A-N3A	4.19	1.38	1.32
4	B	304	465	C4-C5	4.13	1.45	1.40
3	B	303	FAD	C4X-N5	4.08	1.38	1.30
3	A	302	FAD	C2B-C1B	-3.93	1.47	1.53
4	A	303	465	C4-C5	3.74	1.45	1.40
3	A	302	FAD	O2-C2	3.45	1.30	1.24
4	B	304	465	C5-CL1	3.40	1.80	1.72
3	A	302	FAD	C2A-N3A	3.33	1.37	1.32
3	B	303	FAD	C10-N1	3.33	1.40	1.33
3	B	303	FAD	C6-C7	3.28	1.44	1.39
3	B	303	FAD	C2B-C1B	-3.13	1.49	1.53
3	A	302	FAD	C2A-N1A	3.10	1.39	1.33
3	A	302	FAD	C4-N3	3.00	1.44	1.38
3	B	303	FAD	O2-C2	2.77	1.29	1.24
3	B	303	FAD	C9-C8	2.60	1.43	1.39
3	B	303	FAD	C4-N3	2.55	1.43	1.38
4	A	303	465	C9-N10	2.48	1.40	1.33
3	B	303	FAD	C4'-C3'	2.35	1.57	1.53
3	A	302	FAD	C1'-N10	2.34	1.54	1.48
3	B	303	FAD	P-O5'	-2.34	1.49	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	303	465	O13-C12	2.34	1.27	1.22
4	B	304	465	C14-N11	2.26	1.50	1.46
3	B	303	FAD	C1'-C2'	2.26	1.55	1.52
4	A	303	465	C3-N10	-2.19	1.32	1.37
4	A	303	465	C1-N11	-2.17	1.37	1.40
4	A	303	465	C9-C19	-2.11	1.48	1.50
4	B	304	465	C7-C2	2.11	1.44	1.42
3	A	302	FAD	PA-O1A	2.10	1.58	1.50
3	A	302	FAD	P-O5'	-2.08	1.50	1.59
4	A	303	465	C14-N11	2.03	1.50	1.46
3	B	303	FAD	C2A-N1A	2.02	1.37	1.33

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	304	465	C1-N11-C12	-10.22	104.98	110.97
4	B	304	465	C6-C5-C4	9.47	135.17	118.66
4	B	304	465	C5-C4-C3	-9.18	112.39	119.61
4	A	303	465	O13-C12-C7	-8.81	121.29	129.78
4	B	304	465	C8-C7-C12	8.29	144.06	129.41
4	A	303	465	C1-N11-C12	-8.03	106.27	110.97
4	A	303	465	C8-C7-C12	7.85	143.28	129.41
4	B	304	465	C9-C19-N21	7.34	123.51	116.25
4	B	304	465	O13-C12-C7	-7.23	122.81	129.78
4	B	304	465	C4-C5-CL1	-7.04	107.18	119.16
3	B	303	FAD	C4X-C10-N10	6.52	126.02	116.48
4	A	303	465	C2-C7-C12	-6.47	96.17	105.80
4	B	304	465	O20-C19-C9	-6.29	114.35	119.61
3	A	302	FAD	N3-C2-N1	6.26	131.66	119.38
3	A	302	FAD	C4-N3-C2	-6.15	114.27	125.64
4	A	303	465	C6-C5-C4	6.00	129.11	118.66
3	B	303	FAD	C9A-C5X-N5	5.70	128.63	122.43
3	A	302	FAD	N3A-C2A-N1A	-5.59	119.94	128.68
4	A	303	465	C4-C5-CL1	-5.38	110.01	119.16
3	B	303	FAD	C4A-C5A-N7A	-5.09	104.09	109.40
3	B	303	FAD	C5X-C9A-N10	-4.99	112.80	117.95
3	A	302	FAD	O2-C2-N1	-4.92	113.68	121.83
3	B	303	FAD	C4-N3-C2	-4.54	117.25	125.64
3	B	303	FAD	O4B-C1B-C2B	-4.49	100.37	106.93
4	B	304	465	C2-C7-C12	-4.47	99.14	105.80
3	B	303	FAD	N3-C2-N1	4.21	127.64	119.38
3	B	303	FAD	C4-C4X-C10	4.13	123.73	116.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	303	FAD	C8M-C8-C7	4.01	128.95	120.74
4	A	303	465	C7-C8-C9	-3.98	114.01	120.33
4	B	304	465	C2-C1-N11	3.56	109.74	106.63
3	B	303	FAD	O2-C2-N3	-3.51	111.82	118.65
3	B	303	FAD	C10-C4X-N5	-3.45	117.53	124.86
3	B	303	FAD	N3A-C2A-N1A	-3.39	123.38	128.68
3	A	302	FAD	C4X-C10-N10	3.25	121.23	116.48
4	B	304	465	C5-C4-N17	3.19	127.24	121.78
3	A	302	FAD	C1B-N9A-C4A	-3.02	121.34	126.64
3	A	302	FAD	P-O3P-PA	-3.01	122.51	132.83
3	B	303	FAD	O3B-C3B-C4B	-2.95	102.51	111.05
3	A	302	FAD	C10-C4X-N5	-2.80	118.91	124.86
3	A	302	FAD	O5'-P-O1P	2.70	119.63	109.07
4	B	304	465	C8-C9-C19	2.67	126.94	118.59
3	A	302	FAD	C4X-C4-N3	2.59	119.78	113.19
4	A	303	465	C4-C3-N10	2.59	124.26	118.29
4	B	304	465	C4-C3-C2	-2.58	114.83	119.17
3	B	303	FAD	C8M-C8-C9	-2.52	114.83	119.49
4	B	304	465	C8-C9-N10	-2.44	118.55	124.50
3	B	303	FAD	C9-C8-C7	-2.42	116.19	119.67
3	B	303	FAD	P-O3P-PA	-2.42	124.51	132.83
3	B	303	FAD	O4'-C4'-C5'	-2.36	104.61	109.92
3	B	303	FAD	C5A-C6A-N6A	2.33	123.89	120.35
3	A	302	FAD	O4-C4-N3	-2.29	115.72	120.12
3	A	302	FAD	C4-C4X-C10	2.28	120.62	116.79
3	B	303	FAD	O4-C4-N3	-2.26	115.78	120.12
3	B	303	FAD	O4B-C4B-C5B	2.26	116.79	109.37
4	A	303	465	C5-C4-N17	-2.23	117.95	121.78
3	B	303	FAD	C5A-C6A-N1A	-2.22	115.33	120.35
3	A	302	FAD	O4'-C4'-C5'	2.21	114.88	109.92
4	A	303	465	C4-N17-C18	2.20	122.40	118.41
3	B	303	FAD	C1B-N9A-C4A	-2.19	122.79	126.64
4	A	303	465	C4-C3-C2	-2.18	115.50	119.17
3	B	303	FAD	C6-C5X-C9A	-2.17	115.86	118.94
3	B	303	FAD	C9-C9A-C5X	2.14	124.16	120.11
3	A	302	FAD	O2-C2-N3	-2.07	114.63	118.65
3	B	303	FAD	O5B-C5B-C4B	-2.06	101.89	108.99
4	B	304	465	C7-C8-C9	2.05	123.57	120.33
3	A	302	FAD	C4X-C10-N1	-2.01	120.08	124.73

There are no chirality outliers.

All (10) torsion outliers are listed below:

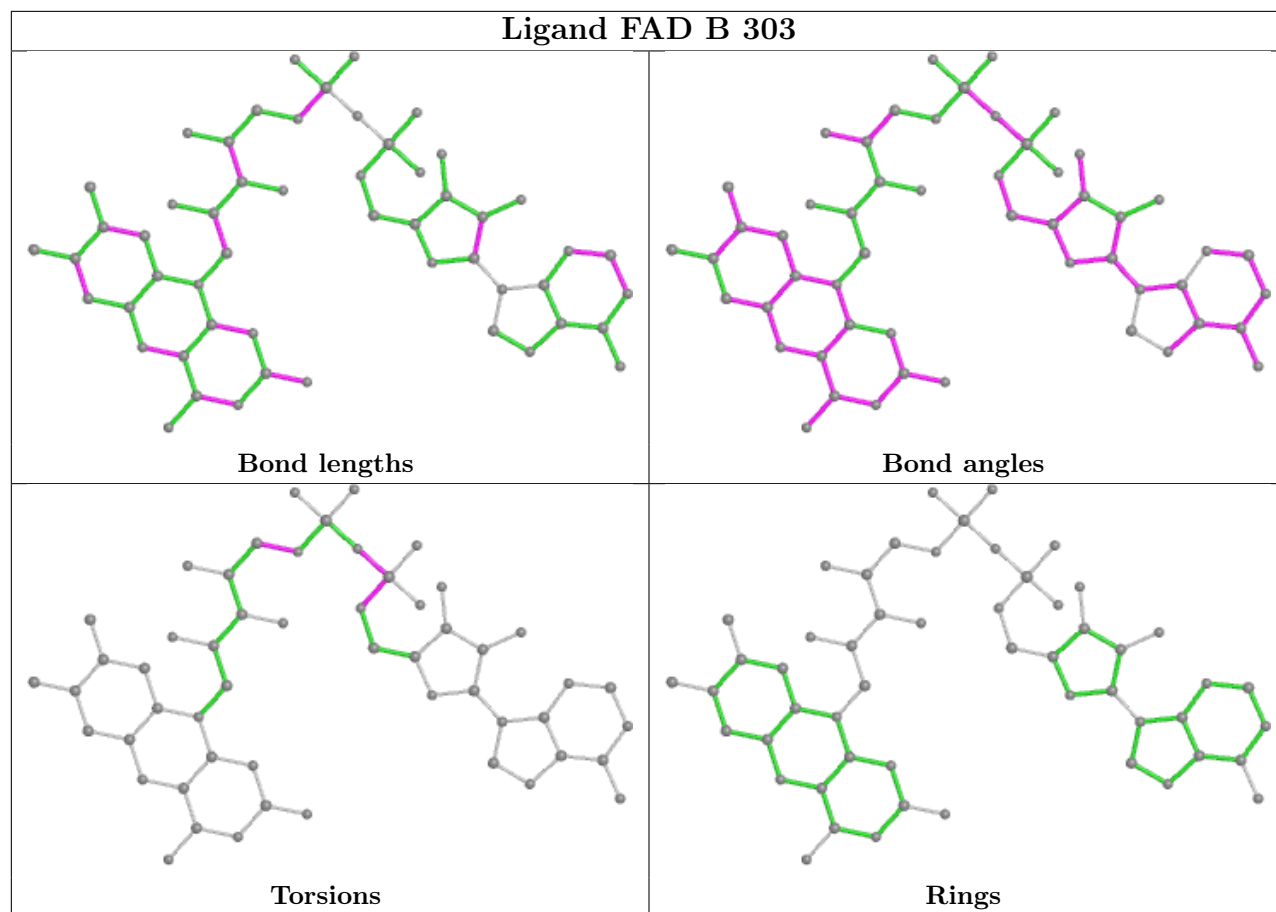
Mol	Chain	Res	Type	Atoms
3	B	303	FAD	C5B-O5B-PA-O1A
5	B	302	GOL	O1-C1-C2-C3
5	B	302	GOL	O1-C1-C2-O2
3	B	303	FAD	C5B-O5B-PA-O2A
3	B	303	FAD	C4'-C5'-O5'-P
3	A	302	FAD	C4'-C5'-O5'-P
3	B	303	FAD	P-O3P-PA-O2A
3	B	303	FAD	C5B-O5B-PA-O3P
3	B	303	FAD	P-O3P-PA-O1A
3	A	302	FAD	C5B-O5B-PA-O2A

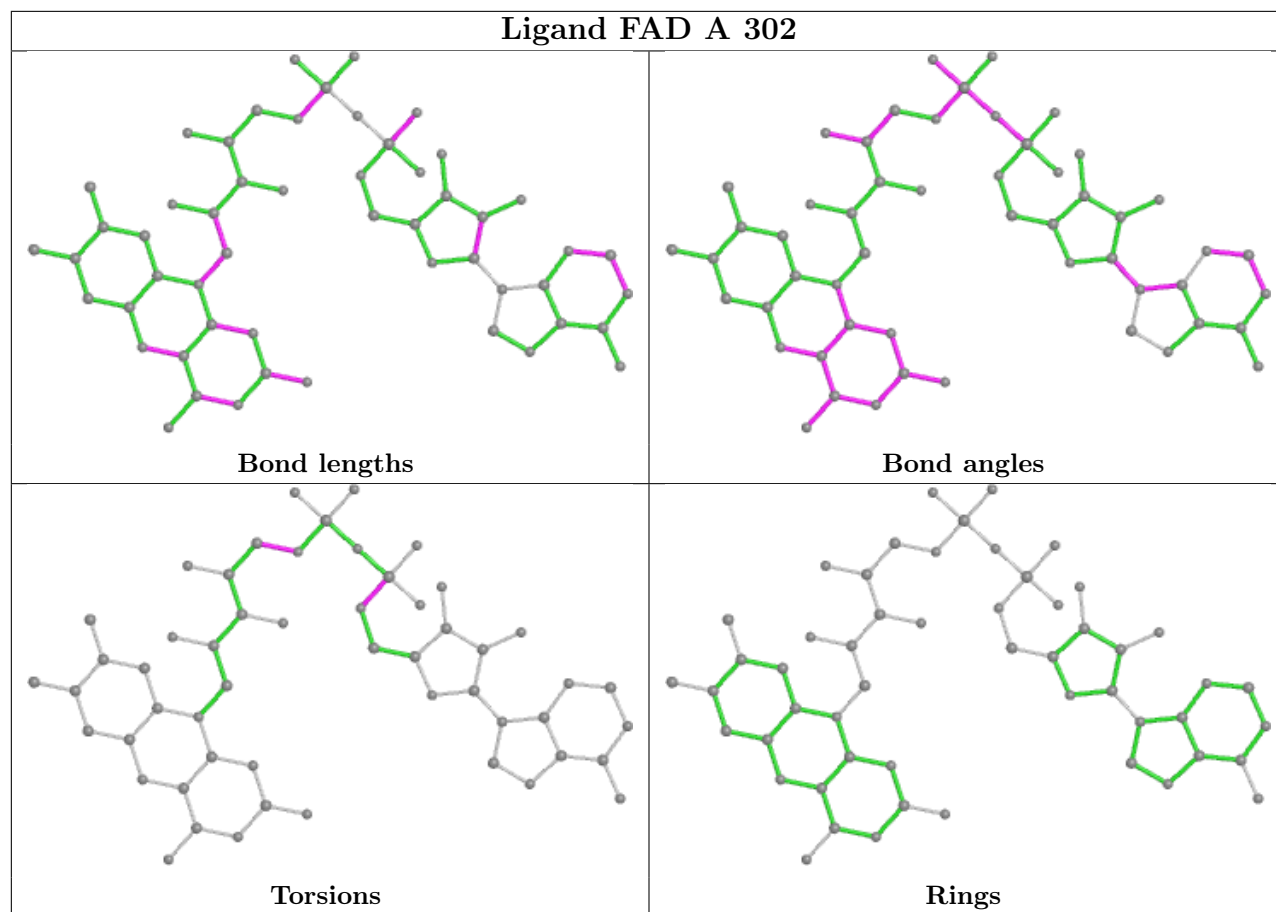
There are no ring outliers.

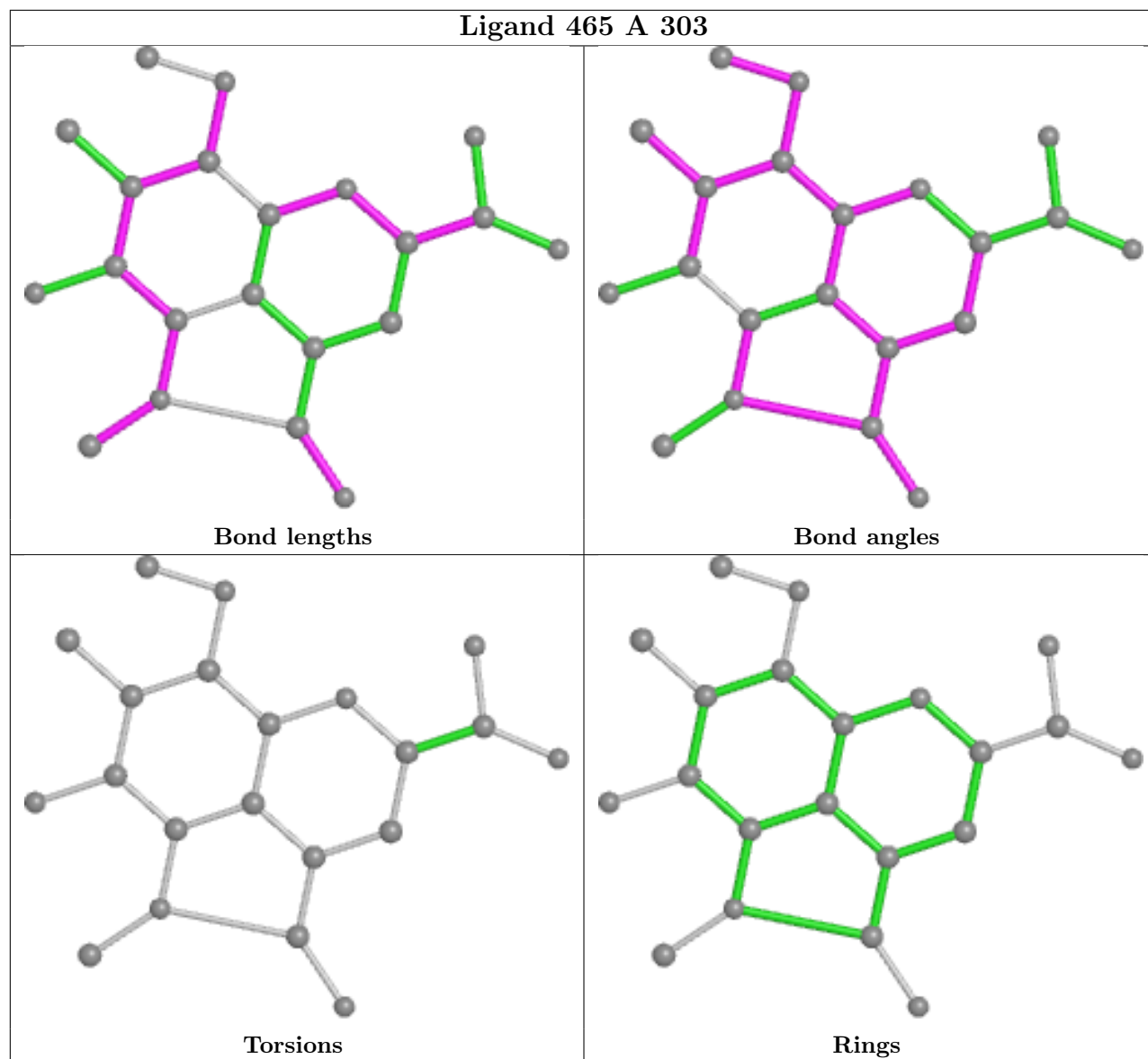
3 monomers are involved in 15 short contacts:

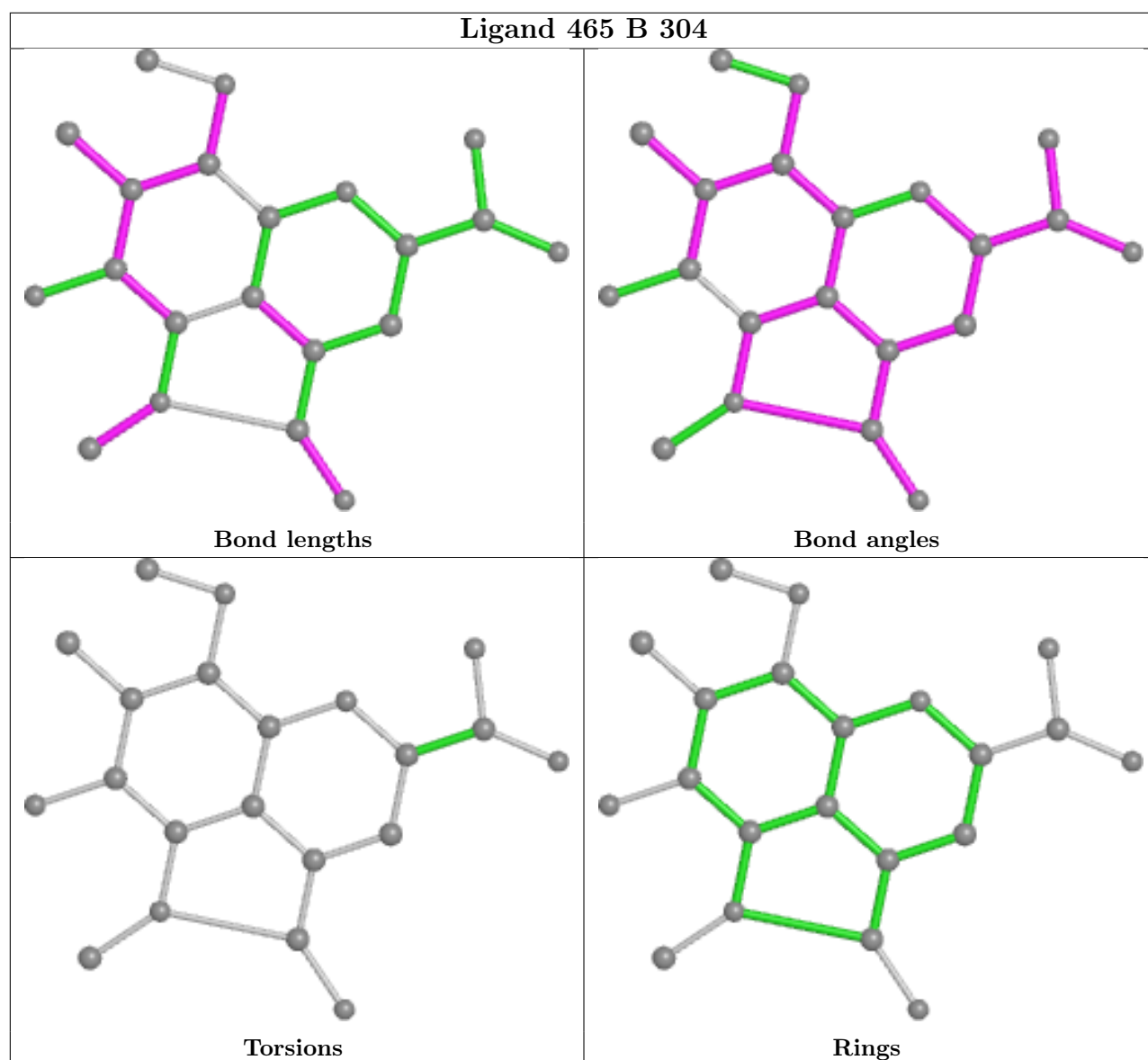
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	302	FAD	3	0
4	A	303	465	8	0
4	B	304	465	4	0

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

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	230/230 (100%)	0.67	26 (11%) <b>5</b> <b>5</b>	12, 25, 50, 73	0
1	B	230/230 (100%)	0.24	11 (4%) 30 33	12, 20, 37, 58	0
All	All	460/460 (100%)	0.46	37 (8%) <b>12</b> <b>13</b>	12, 22, 47, 73	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	230	GLN	8.1
1	A	1	ALA	7.6
1	B	2	GLY	7.2
1	A	130	GLY	7.1
1	A	129	PRO	6.2
1	A	2	GLY	6.0
1	B	230	GLN	5.8
1	A	58	THR	5.6
1	A	57	GLY	5.3
1	A	229	GLY	5.2
1	A	128	ILE	5.1
1	A	197	GLU	4.6
1	A	194	ILE	4.3
1	A	59	LEU	4.2
1	A	196	SER	4.1
1	A	158	THR	3.9
1	A	131	PHE	3.6
1	A	225	HIS	3.5
1	A	198	GLU	3.5
1	A	157	LYS	3.4
1	A	134	SER	3.3
1	A	153	GLU	3.3
1	B	198	GLU	3.2
1	B	63	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	195	ALA	3.2
1	B	158	THR	2.8
1	A	63	GLU	2.7
1	B	194	ILE	2.7
1	B	1	ALA	2.7
1	A	62	PRO	2.5
1	B	17	PHE	2.4
1	B	153	GLU	2.3
1	B	197	GLU	2.3
1	A	221	PRO	2.1
1	A	133	ASP	2.1
1	A	60	SER	2.1
1	B	169	TRP	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

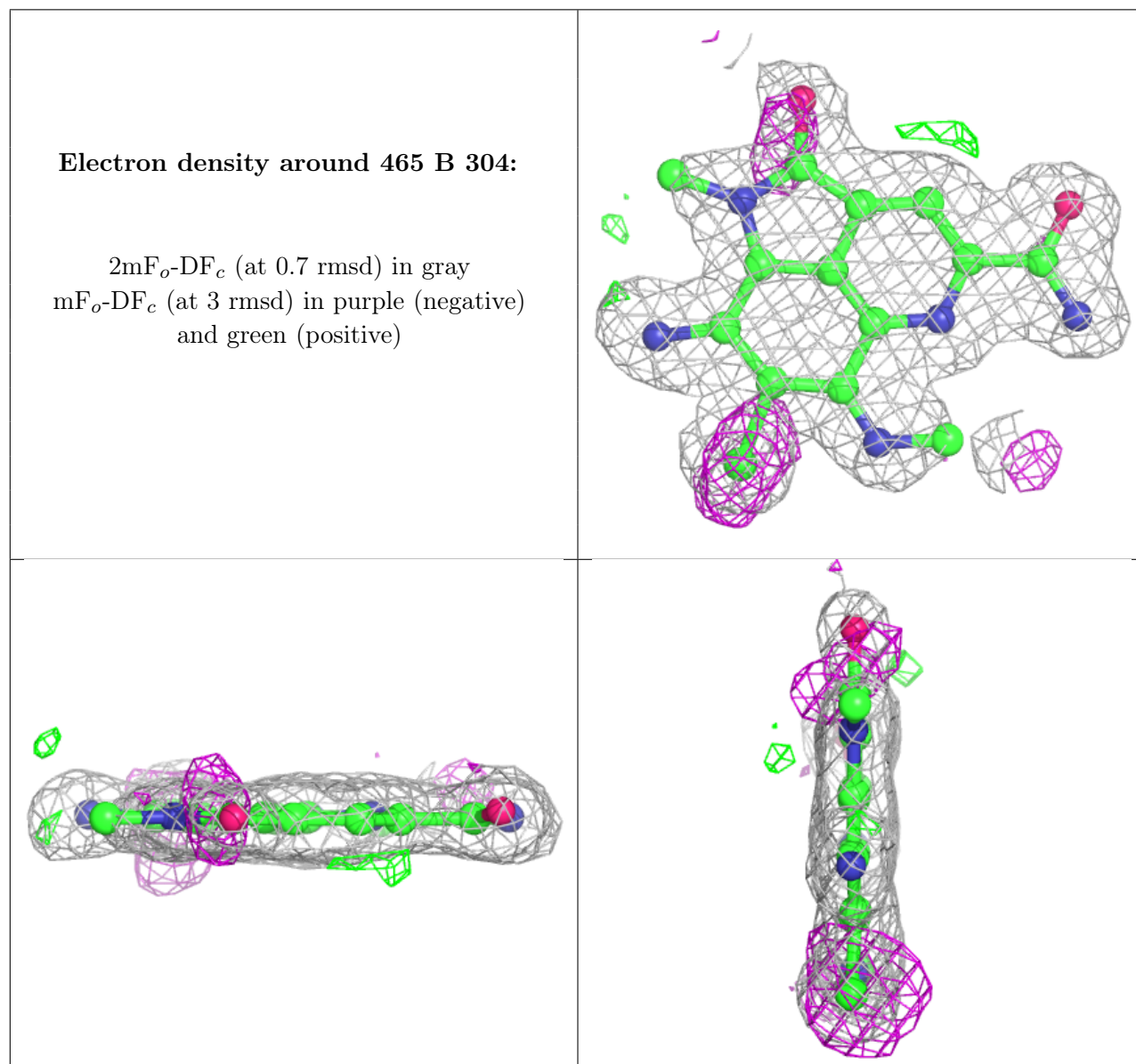
## 6.4 Ligands [i](#)

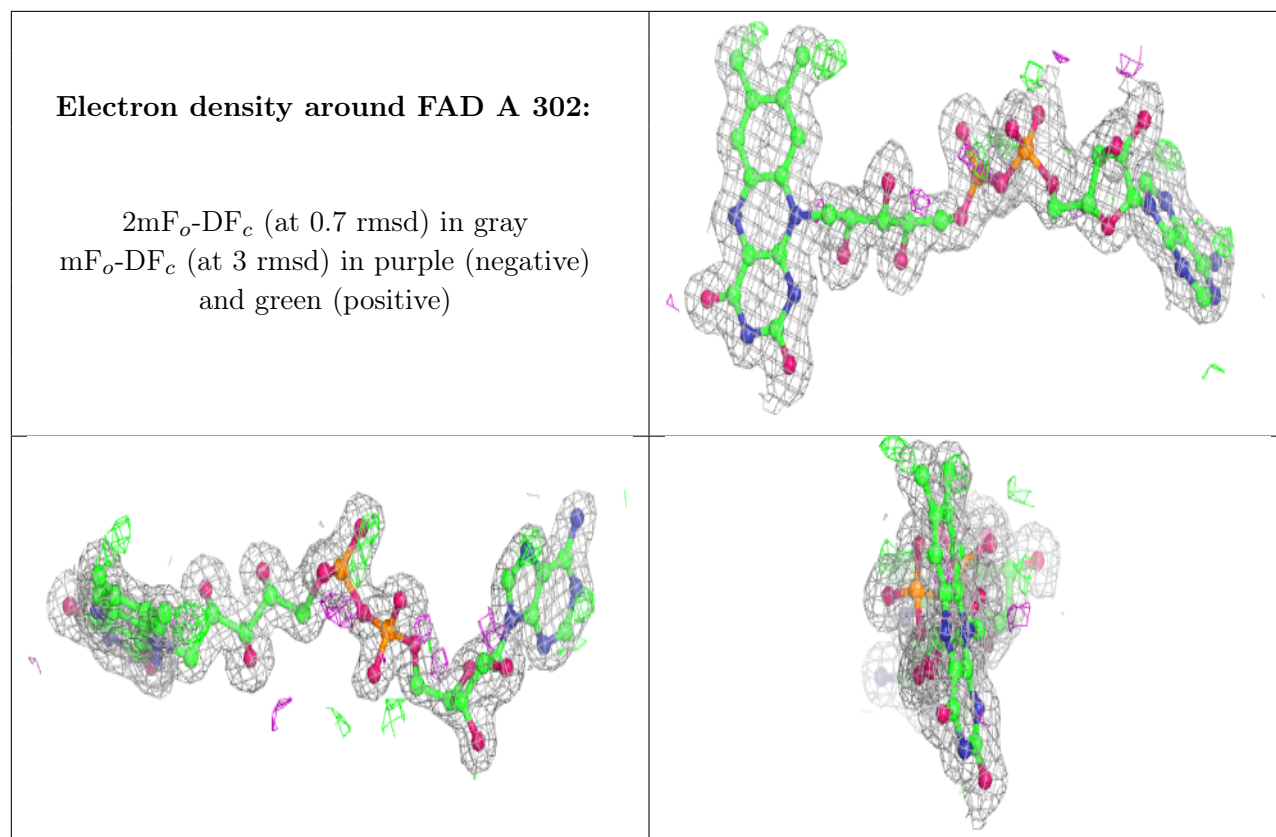
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	GOL	B	302	6/6	0.80	0.24	49,53,53,53	0
4	465	B	304	21/21	0.89	0.13	20,25,31,37	0
3	FAD	A	302	53/53	0.94	0.09	12,19,35,38	0
4	465	A	303	21/21	0.94	0.09	17,24,31,37	0
3	FAD	B	303	53/53	0.95	0.08	13,19,31,35	0
2	ZN	B	301	1/1	1.00	0.05	22,22,22,22	0
2	ZN	A	301	1/1	1.00	0.07	29,29,29,29	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

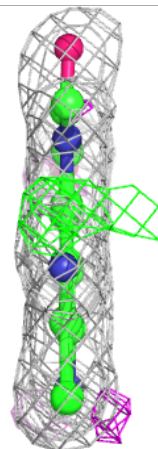
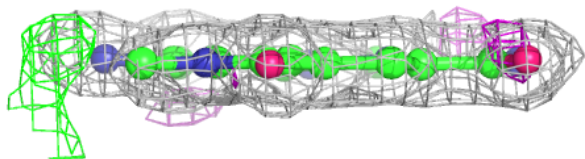
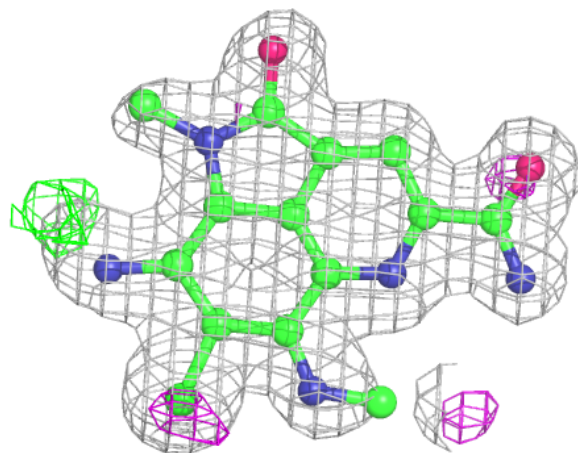
as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

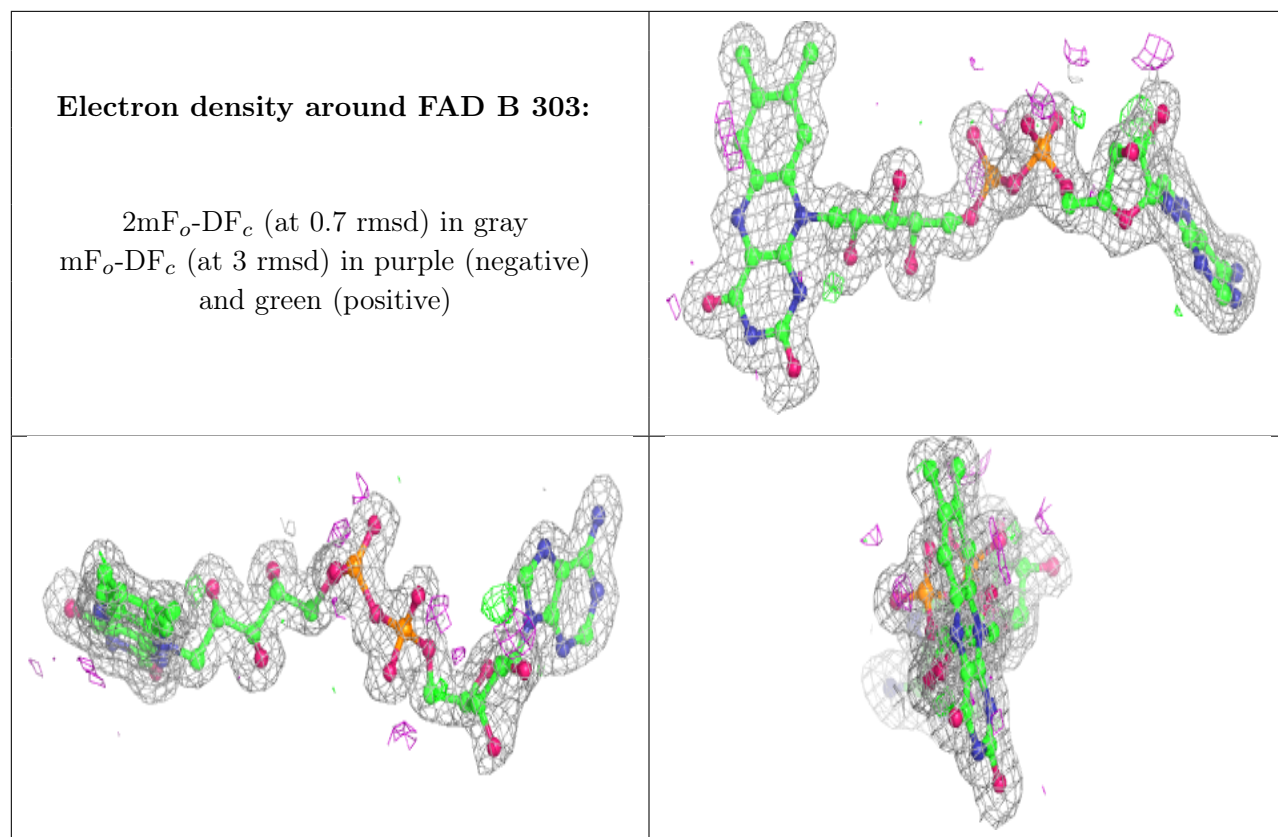




**Electron density around 465 A 303:**

$2mF_o-DF_c$  (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.