



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 07:18 PM BST

PDB ID : 1DNP  
Title : STRUCTURE OF DEOXYRIBODIPYRIMIDINE PHOTOLYASE  
Authors : Park, H.-W.; Sancar, A.; Deisenhofer, J.  
Deposited on : 1995-07-03  
Resolution : 2.30 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.

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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 : 2.13.1  
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) : 2.13.1

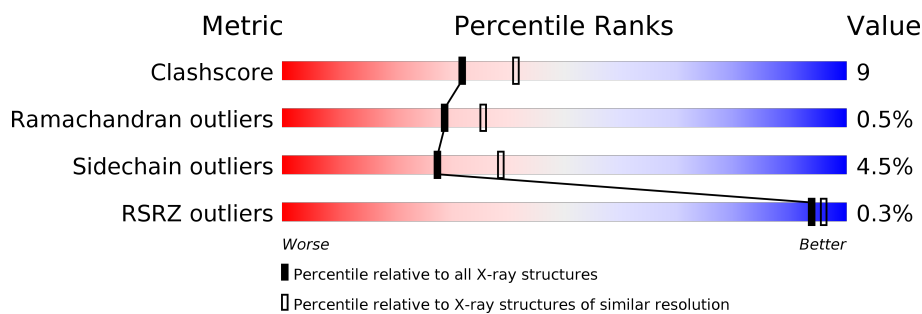
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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.

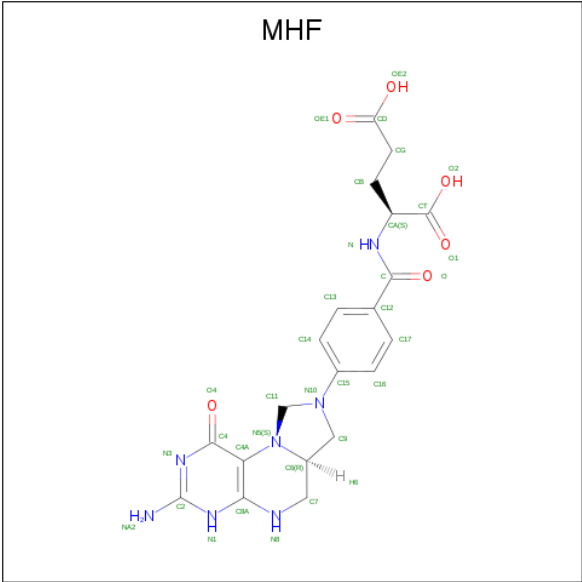


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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  $\geq 3$ , 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	471	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; bottom: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 18%, green 79%);"></div> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 18%, green 79%);"></div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 18%, green 79%);"></div> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 18%, green 79%);"></div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 18%, green 79%);"></div> <div style="position: absolute; 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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			33	20	7	6		
3	B	1	Total	C	N	O	0	0
			33	20	7	6		

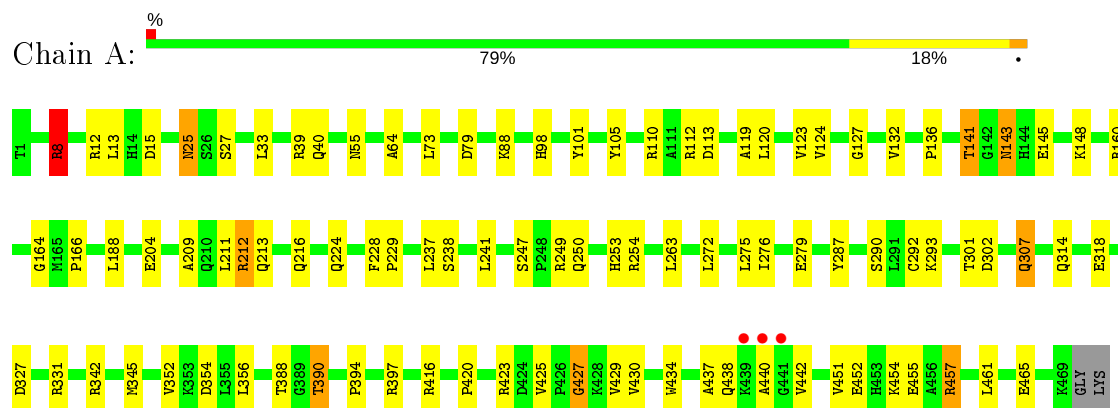
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	188	Total	O	0	0
			188	188		
4	B	185	Total	O	0	0
			185	185		

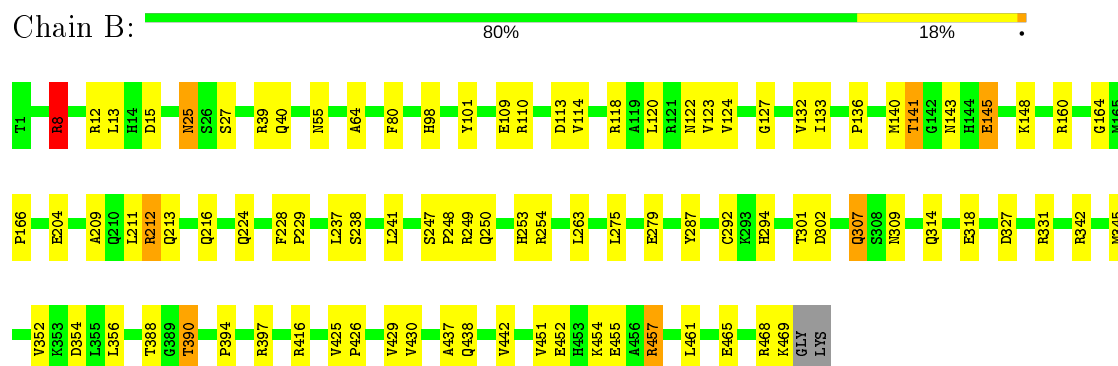
### 3 Residue-property plots

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: DNA PHOTOLYASE



#### • Molecule 1: DNA PHOTOLYASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.60Å 72.20Å 58.50Å 99.10° 101.50° 72.00°	Depositor
Resolution (Å)	10.00 – 2.30 24.70 – 2.25	Depositor EDS
% Data completeness (in resolution range)	78.3 (10.00-2.30) 74.3 (24.70-2.25)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.74 (at 2.26Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.172 , 0.246 0.160 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.2	Xtriage
Anisotropy	0.309	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 62.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8081	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.47% 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: MHF, 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	0.56	0/3871	0.73	1/5266 (0.0%)
1	B	0.56	0/3871	0.71	0/5266
All	All	0.56	0/7742	0.72	1/10532 (0.0%)

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	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	112	ARG	NE-CZ-NH2	-5.40	117.60	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	287	TYR	Sidechain
1	B	287	TYR	Sidechain

## 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	3768	0	3667	73	0
1	B	3768	0	3667	63	0
2	A	53	0	28	1	0
2	B	53	0	28	2	0
3	A	33	0	21	1	0
3	B	33	0	21	2	0
4	A	188	0	0	3	0
4	B	185	0	0	4	0
All	All	8081	0	7432	135	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 9.

All (135) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:CYS:O	3:B:473:MHF:H111	1.85	0.77
1:A:425:VAL:HG12	1:A:429:VAL:HG23	1.65	0.77
1:A:292:CYS:O	3:A:473:MHF:H111	1.87	0.75
1:B:425:VAL:HG12	1:B:429:VAL:HG23	1.70	0.73
1:A:307:GLN:HA	1:A:307:GLN:HE21	1.54	0.72
1:B:307:GLN:HE21	1:B:307:GLN:HA	1.55	0.71
1:B:247:SER:H	1:B:250:GLN:HE21	1.41	0.69
1:A:420:PRO:HA	1:A:423:ARG:HG3	1.76	0.67
1:A:25:ASN:HD22	1:A:25:ASN:C	1.99	0.66
1:A:452:GLU:HB3	1:A:455:GLU:HG2	1.78	0.66
1:A:247:SER:H	1:A:250:GLN:HE21	1.43	0.65
1:B:247:SER:H	1:B:250:GLN:NE2	1.94	0.65
1:A:25:ASN:HD22	1:A:27:SER:H	1.46	0.64
1:B:25:ASN:C	1:B:25:ASN:HD22	2.01	0.64
1:A:101:TYR:O	1:A:127:GLY:HA2	1.97	0.64
1:A:394:PRO:HG2	1:A:397:ARG:HB2	1.80	0.64
1:B:394:PRO:HG2	1:B:397:ARG:HB2	1.80	0.64
1:A:314:GLN:O	1:A:318:GLU:HG3	1.98	0.63
1:A:247:SER:H	1:A:250:GLN:NE2	1.95	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:TYR:O	1:B:127:GLY:HA2	1.99	0.62
1:B:452:GLU:HB3	1:B:455:GLU:HG2	1.82	0.61
1:B:25:ASN:HD22	1:B:27:SER:H	1.49	0.61
1:B:110:ARG:HD3	4:B:805:HOH:O	2.01	0.60
1:A:425:VAL:CG1	1:A:429:VAL:HG23	2.32	0.60
1:A:211:LEU:HG	1:A:254:ARG:HG2	1.84	0.59
1:B:314:GLN:O	1:B:318:GLU:HG3	2.03	0.58
1:B:211:LEU:HG	1:B:254:ARG:HG2	1.85	0.58
1:B:425:VAL:CG1	1:B:429:VAL:HG23	2.34	0.58
1:B:342:ARG:HA	1:B:345:MET:CE	2.34	0.58
1:B:457:ARG:HH12	1:B:461:LEU:HD11	1.69	0.58
1:A:457:ARG:HH12	1:A:461:LEU:HD11	1.68	0.57
1:B:416:ARG:NH2	1:B:430:VAL:HG21	2.21	0.56
1:B:141:THR:HG22	1:B:145:GLU:H	1.71	0.56
1:B:148:LYS:O	1:B:390:THR:HG22	2.04	0.56
1:A:416:ARG:NH2	1:A:430:VAL:HG21	2.20	0.56
1:A:452:GLU:HB3	1:A:455:GLU:CG	2.34	0.56
1:A:8:ARG:HH22	1:A:113:ASP:CG	2.09	0.55
1:B:8:ARG:HH22	1:B:113:ASP:CG	2.10	0.55
1:A:416:ARG:HH22	1:A:427:GLY:HA2	1.71	0.55
1:A:342:ARG:HA	1:A:345:MET:CE	2.37	0.54
1:A:290:SER:HA	1:A:293:LYS:HD3	1.89	0.54
1:B:452:GLU:HB3	1:B:455:GLU:CG	2.38	0.53
1:A:437:ALA:O	1:A:442:VAL:HG22	2.07	0.53
1:B:98:HIS:CD2	1:B:124:VAL:HB	2.44	0.53
1:B:13:LEU:HD11	1:B:64:ALA:HB1	1.91	0.53
1:B:114:VAL:O	1:B:118:ARG:HG3	2.09	0.52
1:A:8:ARG:NH2	1:A:113:ASP:OD1	2.43	0.52
1:A:427:GLY:O	1:A:430:VAL:HG23	2.11	0.51
1:B:465:GLU:O	1:B:469:LYS:HG3	2.11	0.51
1:A:25:ASN:ND2	1:A:27:SER:H	2.07	0.50
1:A:39:ARG:HH12	1:B:309:ASN:HD22	1.59	0.50
1:B:25:ASN:ND2	1:B:27:SER:H	2.10	0.50
1:A:98:HIS:CD2	1:A:124:VAL:HB	2.46	0.50
1:B:8:ARG:NH2	1:B:113:ASP:OD1	2.44	0.50
1:A:88:LYS:HD2	1:A:119:ALA:HB1	1.94	0.50
1:A:148:LYS:O	1:A:390:THR:HG22	2.12	0.49
1:A:327:ASP:O	1:A:331:ARG:HG2	2.12	0.49
1:A:141:THR:HG22	1:A:145:GLU:H	1.77	0.49
1:A:461:LEU:O	1:A:465:GLU:HB2	2.13	0.49
1:A:15:ASP:OD1	1:A:249:ARG:NH1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:ARG:HG3	1:A:457:ARG:HH11	1.78	0.48
1:B:8:ARG:HB2	4:B:679:HOH:O	2.13	0.48
1:A:12:ARG:HB2	1:A:204:GLU:OE2	2.14	0.48
1:B:327:ASP:O	1:B:331:ARG:HG2	2.14	0.48
1:A:416:ARG:HH22	1:A:427:GLY:CA	2.26	0.48
1:B:342:ARG:HA	1:B:345:MET:HE3	1.95	0.48
1:A:13:LEU:HD11	1:A:64:ALA:HB1	1.95	0.48
1:A:272:LEU:O	1:A:276:ILE:HG13	2.14	0.48
1:B:209:ALA:O	1:B:213:GLN:HG3	2.14	0.48
1:A:39:ARG:HH22	1:B:307:GLN:HG3	1.78	0.48
1:B:15:ASP:OD1	1:B:249:ARG:NH1	2.47	0.47
1:A:416:ARG:HH22	1:A:427:GLY:N	2.11	0.47
1:B:438:GLN:NE2	1:B:438:GLN:HA	2.30	0.46
1:A:209:ALA:O	1:A:213:GLN:HG3	2.15	0.46
1:B:437:ALA:HA	1:B:442:VAL:HG22	1.98	0.46
1:A:132:VAL:HG21	1:A:136:PRO:HD3	1.97	0.46
1:B:238:SER:HB3	2:B:472:FAD:H5'1	1.98	0.46
1:A:352:VAL:O	1:A:356:LEU:HA	2.16	0.45
1:B:12:ARG:HB2	1:B:204:GLU:OE2	2.15	0.45
1:B:120:LEU:HB3	1:B:123:VAL:HB	1.99	0.45
1:B:141:THR:HG23	1:B:143:ASN:H	1.81	0.45
1:A:237:LEU:O	1:A:241:LEU:HD23	2.16	0.45
1:A:120:LEU:HB3	1:A:123:VAL:HB	1.99	0.45
1:A:141:THR:CG2	1:A:143:ASN:OD1	2.65	0.45
1:B:133:ILE:HG13	1:B:248:PRO:HB2	1.99	0.45
1:B:457:ARG:HG3	1:B:457:ARG:HH11	1.82	0.45
1:A:457:ARG:HH11	1:A:457:ARG:CG	2.30	0.44
1:B:166:PRO:O	1:B:253:HIS:CE1	2.69	0.44
1:A:105:TYR:O	1:A:110:ARG:HD2	2.17	0.44
1:A:228:PHE:HA	1:A:229:PRO:HD2	1.92	0.44
1:B:237:LEU:O	1:B:241:LEU:HD23	2.16	0.44
1:B:461:LEU:O	1:B:465:GLU:HB2	2.18	0.44
1:B:275:LEU:O	1:B:279:GLU:HG2	2.18	0.44
1:A:440:ALA:O	1:A:442:VAL:HG13	2.18	0.44
1:B:140:MET:HA	1:B:140:MET:HE2	2.00	0.44
1:B:132:VAL:HG21	1:B:136:PRO:HD3	1.99	0.43
1:A:307:GLN:HG3	1:B:39:ARG:HH22	1.82	0.43
1:A:141:THR:HG23	1:A:143:ASN:H	1.84	0.43
1:B:307:GLN:HA	1:B:307:GLN:NE2	2.29	0.43
1:A:342:ARG:HA	1:A:345:MET:HE2	1.99	0.43
1:B:109:GLU:OE1	1:B:109:GLU:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:HIS:HA	4:B:681:HOH:O	2.18	0.43
1:A:238:SER:HB3	2:A:472:FAD:H5'1	2.00	0.43
1:A:301:THR:CB	1:A:388:THR:HG22	2.49	0.43
1:A:427:GLY:C	1:A:430:VAL:HG23	2.39	0.43
1:B:457:ARG:CG	1:B:457:ARG:HH11	2.31	0.43
1:A:166:PRO:O	1:A:253:HIS:CE1	2.71	0.43
1:A:275:LEU:O	1:A:279:GLU:HG2	2.18	0.43
1:A:397:ARG:HD2	1:A:397:ARG:HA	1.84	0.42
1:A:212:ARG:O	1:A:216:GLN:HG3	2.19	0.42
1:B:352:VAL:O	1:B:356:LEU:HA	2.19	0.42
1:B:212:ARG:O	1:B:216:GLN:HG3	2.20	0.42
1:A:188:LEU:HA	4:A:713:HOH:O	2.19	0.42
1:A:25:ASN:ND2	1:A:25:ASN:C	2.70	0.42
1:A:342:ARG:HA	1:A:345:MET:HE3	2.02	0.42
1:B:25:ASN:C	1:B:25:ASN:ND2	2.71	0.42
1:B:342:ARG:HA	1:B:345:MET:HE2	2.01	0.42
1:B:228:PHE:HA	1:B:229:PRO:HD2	1.89	0.42
3:B:473:MHF:H91	4:B:813:HOH:O	2.20	0.42
1:A:307:GLN:NE2	1:A:307:GLN:HA	2.27	0.41
1:A:254:ARG:HB2	4:A:793:HOH:O	2.19	0.41
1:A:437:ALA:HA	1:A:442:VAL:HG22	2.02	0.41
1:B:301:THR:CB	1:B:388:THR:HG22	2.51	0.41
1:B:301:THR:HB	1:B:388:THR:HG22	2.02	0.41
1:B:457:ARG:NH1	1:B:461:LEU:HD11	2.33	0.41
1:B:426:PRO:HB2	1:B:429:VAL:HG22	2.02	0.41
1:A:301:THR:HB	1:A:388:THR:HG22	2.02	0.41
1:A:434:TRP:HD1	4:A:739:HOH:O	2.03	0.41
1:A:457:ARG:NH1	1:A:461:LEU:HD11	2.34	0.41
1:A:416:ARG:NH2	1:A:427:GLY:N	2.68	0.40
1:A:40:GLN:NE2	1:A:79:ASP:HB2	2.36	0.40
1:B:40:GLN:NE2	1:B:80:PHE:H	2.19	0.40
1:A:212:ARG:HA	1:A:254:ARG:HD2	2.04	0.40
1:A:33:LEU:HD12	1:A:73:LEU:O	2.21	0.40
2:B:472:FAD:H9	2:B:472:FAD:H1'2	1.87	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	467/471 (99%)	450 (96%)	14 (3%)	3 (1%)	25	31
1	B	467/471 (99%)	454 (97%)	11 (2%)	2 (0%)	34	42
All	All	934/942 (99%)	904 (97%)	25 (3%)	5 (0%)	29	35

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	427	GLY
1	A	8	ARG
1	B	8	ARG
1	A	164	GLY
1	B	164	GLY

### 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	392/393 (100%)	375 (96%)	17 (4%)	29	40
1	B	392/393 (100%)	374 (95%)	18 (5%)	27	38
All	All	784/786 (100%)	749 (96%)	35 (4%)	27	39

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ARG

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Mol	Chain	Res	Type
1	A	25	ASN
1	A	55	ASN
1	A	141	THR
1	A	143	ASN
1	A	160	ARG
1	A	212	ARG
1	A	224	GLN
1	A	263	LEU
1	A	302	ASP
1	A	307	GLN
1	A	354	ASP
1	A	390	THR
1	A	438	GLN
1	A	451	VAL
1	A	454	LYS
1	A	457	ARG
1	B	8	ARG
1	B	25	ASN
1	B	55	ASN
1	B	122	ASN
1	B	141	THR
1	B	145	GLU
1	B	160	ARG
1	B	212	ARG
1	B	224	GLN
1	B	263	LEU
1	B	302	ASP
1	B	307	GLN
1	B	354	ASP
1	B	390	THR
1	B	451	VAL
1	B	454	LYS
1	B	457	ARG
1	B	468	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	14	HIS
1	A	25	ASN
1	A	40	GLN

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Mol	Chain	Res	Type
1	A	62	GLN
1	A	108	ASN
1	A	210	GLN
1	A	250	GLN
1	A	307	GLN
1	A	438	GLN
1	B	14	HIS
1	B	25	ASN
1	B	40	GLN
1	B	62	GLN
1	B	108	ASN
1	B	210	GLN
1	B	250	GLN
1	B	307	GLN
1	B	341	ASN
1	B	438	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](#)

4 ligands are modelled in this entry.

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	B	472	-	51,58,58	3.22	24 (47%)	60,89,89	2.85	18 (30%)
3	MHF	A	473	-	28,36,36	2.85	11 (39%)	30,52,52	1.98	6 (20%)
2	FAD	A	472	-	51,58,58	3.03	18 (35%)	60,89,89	2.83	17 (28%)
3	MHF	B	473	-	28,36,36	2.97	11 (39%)	30,52,52	2.01	6 (20%)

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	B	472	-	2/2/9/9	13/30/50/50	0/6/6/6
3	MHF	A	473	-	-	6/15/42/42	0/4/4/4
2	FAD	A	472	-	2/2/9/9	12/30/50/50	0/6/6/6
3	MHF	B	473	-	-	6/15/42/42	0/4/4/4

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	472	FAD	C1'-N10	-10.76	1.37	1.48
3	A	473	MHF	C11-N5	-9.13	1.24	1.45
2	A	472	FAD	C1'-N10	-8.44	1.39	1.48
3	B	473	MHF	C11-N5	-8.29	1.26	1.45
2	A	472	FAD	C10-N1	7.75	1.43	1.33
3	B	473	MHF	C4-N3	7.32	1.45	1.33
2	B	472	FAD	C10-N1	7.01	1.42	1.33
2	B	472	FAD	C4-C4X	6.61	1.52	1.41
2	B	472	FAD	C4X-C10	6.44	1.45	1.38
2	B	472	FAD	C5'-C4'	-6.15	1.43	1.51
3	A	473	MHF	C4-N3	6.14	1.43	1.33
2	A	472	FAD	C5'-C4'	-5.96	1.43	1.51
2	A	472	FAD	C4-C4X	5.84	1.51	1.41
2	A	472	FAD	C4X-C10	5.83	1.44	1.38
3	B	473	MHF	C7-C6	-5.66	1.45	1.52
2	B	472	FAD	C7M-C7	5.58	1.62	1.51
2	A	472	FAD	C4'-C3'	-5.26	1.43	1.53
2	A	472	FAD	C4X-N5	5.16	1.40	1.33
2	B	472	FAD	C4X-N5	4.91	1.40	1.33
2	A	472	FAD	C9A-N10	4.89	1.45	1.38
2	A	472	FAD	C7M-C7	4.70	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	472	FAD	C4'-C3'	-4.35	1.45	1.53
2	B	472	FAD	C9A-N10	4.23	1.44	1.38
3	B	473	MHF	C7-N8	4.13	1.51	1.44
2	A	472	FAD	C5X-N5	4.08	1.42	1.35
3	B	473	MHF	O-C	4.07	1.31	1.23
3	A	473	MHF	O-C	3.99	1.31	1.23
2	B	472	FAD	C5A-C4A	-3.85	1.30	1.40
2	A	472	FAD	C2B-C3B	-3.82	1.42	1.53
2	A	472	FAD	O3'-C3'	-3.66	1.34	1.43
3	B	473	MHF	C8A-N1	3.66	1.41	1.34
2	B	472	FAD	O2'-C2'	-3.64	1.35	1.43
2	A	472	FAD	O2'-C2'	-3.63	1.35	1.43
3	A	473	MHF	C7-C6	-3.61	1.47	1.52
3	A	473	MHF	CB-CA	3.55	1.57	1.53
3	A	473	MHF	C8A-N1	3.46	1.41	1.34
3	A	473	MHF	C9-N10	-3.42	1.42	1.46
3	A	473	MHF	C7-N8	3.33	1.50	1.44
2	B	472	FAD	C4-N3	3.24	1.38	1.33
2	B	472	FAD	C2B-C3B	-3.23	1.44	1.53
2	B	472	FAD	C5X-N5	3.09	1.40	1.35
2	B	472	FAD	C8A-N7A	-3.07	1.29	1.34
2	A	472	FAD	PA-O2A	-3.04	1.41	1.55
2	A	472	FAD	C4-N3	2.87	1.38	1.33
2	B	472	FAD	C4A-N3A	-2.86	1.31	1.35
2	B	472	FAD	C8M-C8	2.80	1.56	1.51
2	B	472	FAD	O3'-C3'	-2.78	1.36	1.43
3	B	473	MHF	CB-CA	2.74	1.56	1.53
2	B	472	FAD	C6-C5X	-2.72	1.37	1.41
3	B	473	MHF	C16-C15	2.66	1.44	1.39
2	B	472	FAD	O4'-C4'	-2.57	1.37	1.43
2	B	472	FAD	C2-N1	2.56	1.43	1.38
3	B	473	MHF	C9-N10	-2.53	1.43	1.46
2	B	472	FAD	P-O2P	-2.41	1.44	1.55
2	A	472	FAD	C5A-C4A	-2.40	1.34	1.40
3	A	473	MHF	C16-C15	2.39	1.44	1.39
3	A	473	MHF	CA-N	2.39	1.49	1.46
2	B	472	FAD	PA-O2A	-2.31	1.44	1.55
2	A	472	FAD	P-O2P	-2.19	1.45	1.55
2	A	472	FAD	O4B-C4B	-2.18	1.40	1.45
2	B	472	FAD	C2B-C1B	2.15	1.57	1.53
3	B	473	MHF	CA-N	2.12	1.49	1.46
3	A	473	MHF	C9-C6	-2.07	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	473	MHF	C4A-C8A	2.07	1.45	1.41

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	472	FAD	C4-N3-C2	12.87	126.01	115.14
2	B	472	FAD	C4-N3-C2	12.51	125.70	115.14
2	A	472	FAD	C4'-C3'-C2'	7.03	127.98	113.36
2	B	472	FAD	C4'-C3'-C2'	6.78	127.45	113.36
2	B	472	FAD	C1'-N10-C9A	6.38	123.32	118.29
3	B	473	MHF	N5-C11-N10	6.29	112.38	103.38
2	A	472	FAD	C1'-N10-C9A	6.28	123.23	118.29
3	A	473	MHF	N5-C11-N10	6.20	112.25	103.38
2	B	472	FAD	C9A-N10-C10	-5.77	114.35	121.91
2	B	472	FAD	C5X-C9A-N10	5.69	121.84	117.72
2	A	472	FAD	C9A-N10-C10	-5.52	114.68	121.91
2	A	472	FAD	C4X-C4-N3	-5.42	116.02	123.43
2	B	472	FAD	C4X-C4-N3	-5.38	116.07	123.43
2	B	472	FAD	C1'-C2'-C3'	5.31	124.61	109.79
2	A	472	FAD	C1'-C2'-C3'	5.23	124.42	109.79
2	A	472	FAD	C5X-C9A-N10	4.80	121.20	117.72
3	A	473	MHF	C11-N5-C4A	4.58	136.13	122.96
3	B	473	MHF	C11-N5-C4A	4.49	135.87	122.96
3	B	473	MHF	CG-CB-CA	3.88	120.88	113.04
3	A	473	MHF	CG-CB-CA	3.87	120.86	113.04
3	B	473	MHF	C11-N10-C15	3.82	131.25	120.09
3	A	473	MHF	C11-N10-C15	3.66	130.79	120.09
2	A	472	FAD	C4-C4X-C10	3.47	122.25	119.95
2	B	472	FAD	C2B-C3B-C4B	3.38	109.20	102.64
2	A	472	FAD	C2B-C3B-C4B	3.27	108.99	102.64
2	A	472	FAD	C4X-C10-N10	3.07	123.46	120.30
2	B	472	FAD	C8M-C8-C7	3.06	127.01	120.74
2	B	472	FAD	O5B-PA-O1A	3.03	120.89	109.07
2	A	472	FAD	O4B-C1B-C2B	2.89	111.15	106.93
2	B	472	FAD	C4X-C10-N10	2.85	123.23	120.30
2	B	472	FAD	C4-C4X-C10	2.83	121.83	119.95
2	B	472	FAD	O4B-C1B-C2B	2.81	111.03	106.93
2	A	472	FAD	C3B-C2B-C1B	-2.78	96.79	100.98
2	A	472	FAD	O5B-PA-O1A	2.78	119.92	109.07
2	B	472	FAD	C8M-C8-C9	-2.76	113.75	120.34
2	B	472	FAD	C3B-C2B-C1B	-2.71	96.90	100.98
2	B	472	FAD	N3A-C2A-N1A	-2.70	124.46	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	473	MHF	C14-C15-N10	-2.22	118.33	121.38
2	A	472	FAD	C1B-N9A-C4A	-2.17	122.83	126.64
2	A	472	FAD	C8M-C8-C9	-2.16	115.17	120.34
3	B	473	MHF	C9-C6-N5	2.15	105.40	101.69
2	B	472	FAD	C1'-N10-C10	2.14	120.32	118.41
3	A	473	MHF	C9-C6-N5	2.10	105.31	101.69
3	A	473	MHF	C14-C15-N10	-2.05	118.56	121.38
2	A	472	FAD	C8M-C8-C7	2.04	124.93	120.74
2	B	472	FAD	O5'-C5'-C4'	2.01	114.72	109.36
2	A	472	FAD	P-O5'-C5'	-2.00	109.94	121.68

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	472	FAD	C4'
2	B	472	FAD	C2'
2	A	472	FAD	C4'
2	A	472	FAD	C2'

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	472	FAD	N10-C1'-C2'-O2'
2	B	472	FAD	N10-C1'-C2'-C3'
2	B	472	FAD	C1'-C2'-C3'-O3'
2	B	472	FAD	O2'-C2'-C3'-O3'
2	B	472	FAD	C2'-C3'-C4'-O4'
2	B	472	FAD	O3'-C3'-C4'-O4'
2	B	472	FAD	O3'-C3'-C4'-C5'
2	A	472	FAD	N10-C1'-C2'-O2'
2	A	472	FAD	N10-C1'-C2'-C3'
2	A	472	FAD	C1'-C2'-C3'-O3'
2	A	472	FAD	O2'-C2'-C3'-O3'
2	A	472	FAD	C2'-C3'-C4'-O4'
2	A	472	FAD	O3'-C3'-C4'-O4'
2	A	472	FAD	O3'-C3'-C4'-C5'
3	A	473	MHF	C16-C15-N10-C9
3	B	473	MHF	C16-C15-N10-C9
2	B	472	FAD	O2'-C2'-C3'-C4'
2	A	472	FAD	O2'-C2'-C3'-C4'
3	A	473	MHF	C14-C15-N10-C9
3	B	473	MHF	C14-C15-N10-C9

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Mol	Chain	Res	Type	Atoms
3	B	473	MHF	C12-C-N-CA
3	A	473	MHF	C12-C-N-CA
3	A	473	MHF	C16-C15-N10-C11
2	B	472	FAD	C2'-C3'-C4'-C5'
2	A	472	FAD	C2'-C3'-C4'-C5'
3	A	473	MHF	C14-C15-N10-C11
3	B	473	MHF	C16-C15-N10-C11
3	B	473	MHF	C14-C15-N10-C11
3	A	473	MHF	O-C-N-CA
3	B	473	MHF	O-C-N-CA
2	A	472	FAD	C5'-O5'-P-O3P
2	B	472	FAD	C5B-O5B-PA-O3P
2	B	472	FAD	C5'-O5'-P-O3P
2	A	472	FAD	C5B-O5B-PA-O3P
2	B	472	FAD	P-O3P-PA-O2A
2	B	472	FAD	C5'-O5'-P-O1P
2	A	472	FAD	C5'-O5'-P-O1P

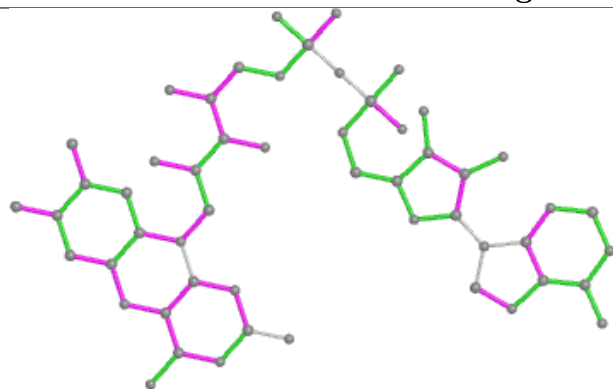
There are no ring outliers.

4 monomers are involved in 6 short contacts:

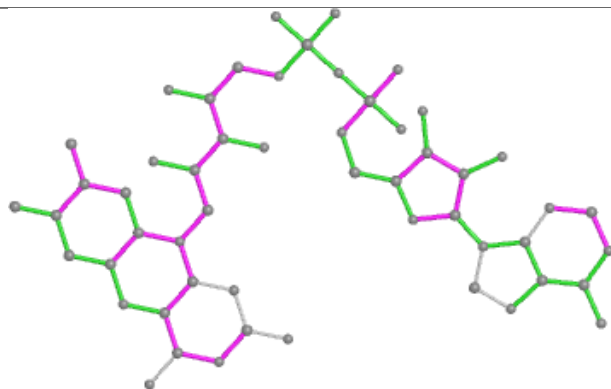
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	472	FAD	2	0
3	A	473	MHF	1	0
2	A	472	FAD	1	0
3	B	473	MHF	2	0

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

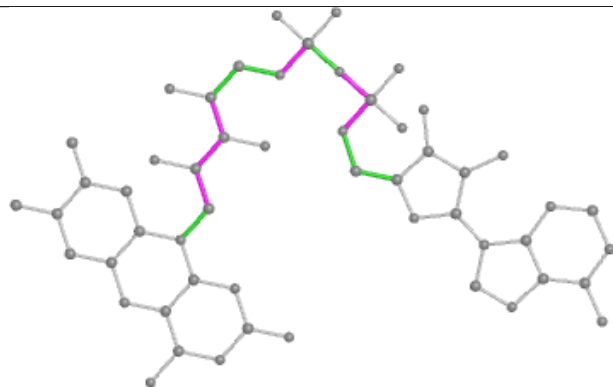
## Ligand FAD B 472



Bond lengths



Bond angles

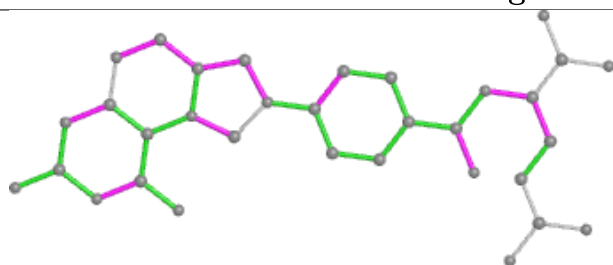


Torsions

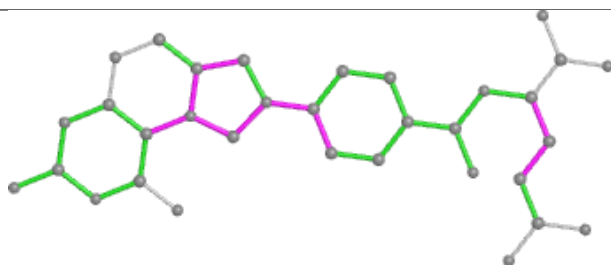


Rings

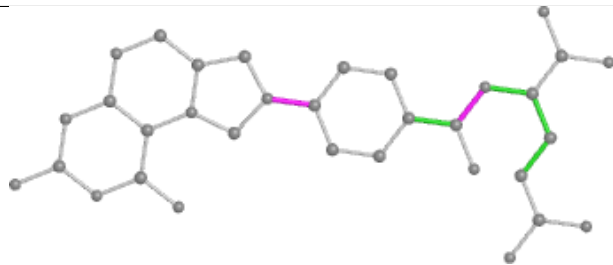
## Ligand MHF A 473



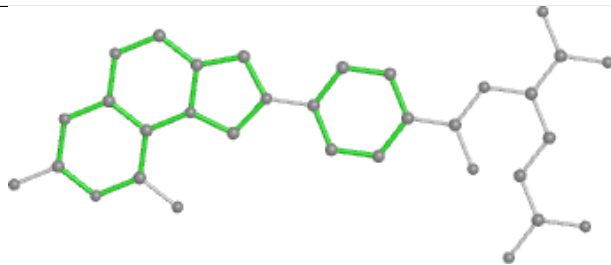
Bond lengths



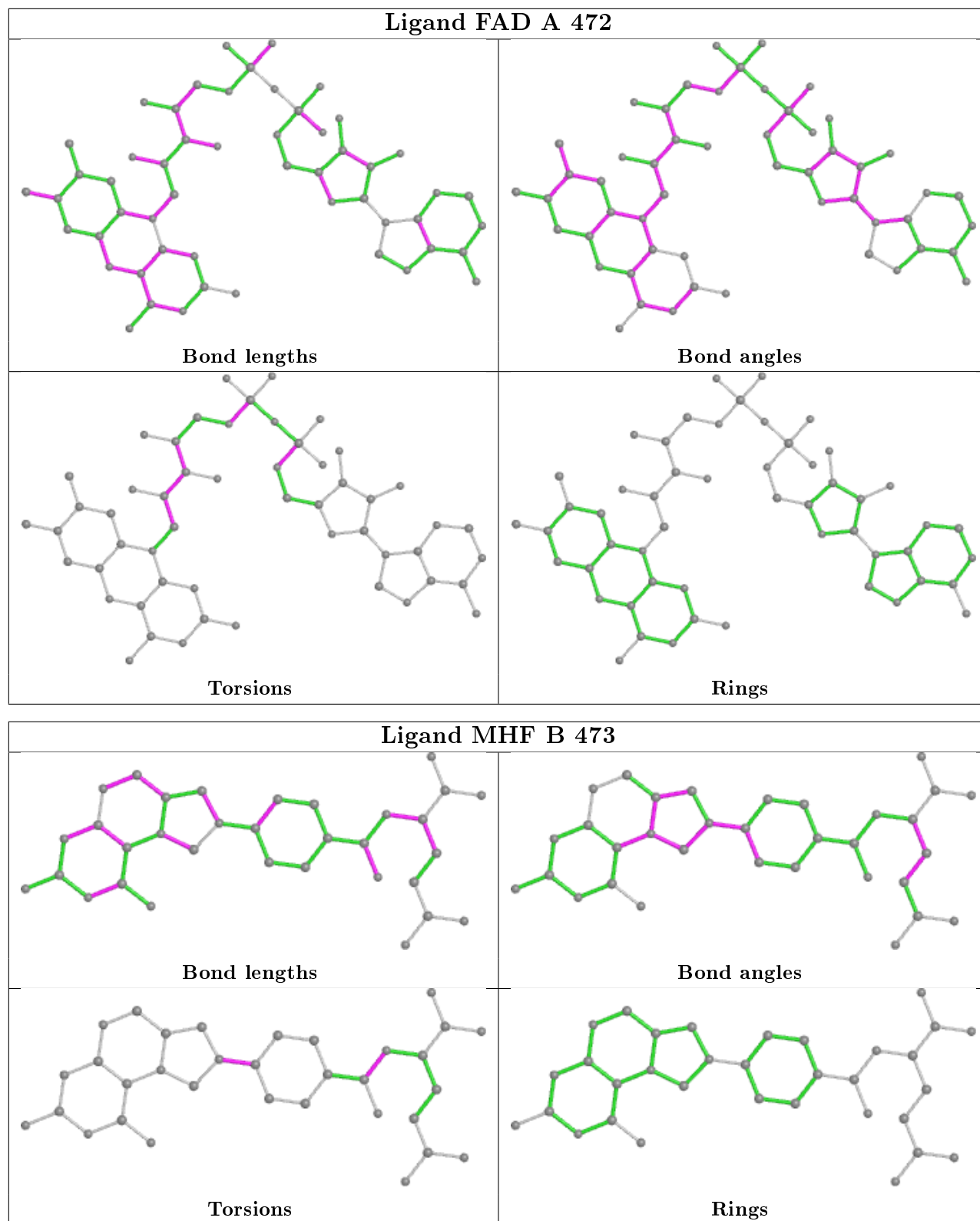
Bond angles



Torsions



Rings



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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<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	469/471 (99%)	-0.54	3 (0%) 89 92	2, 14, 47, 73	0
1	B	469/471 (99%)	-0.56	0 100 100	3, 14, 40, 81	0
All	All	938/942 (99%)	-0.55	3 (0%) 94 96	2, 14, 42, 81	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	440	ALA	3.1
1	A	441	GLY	2.7
1	A	439	LYS	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.

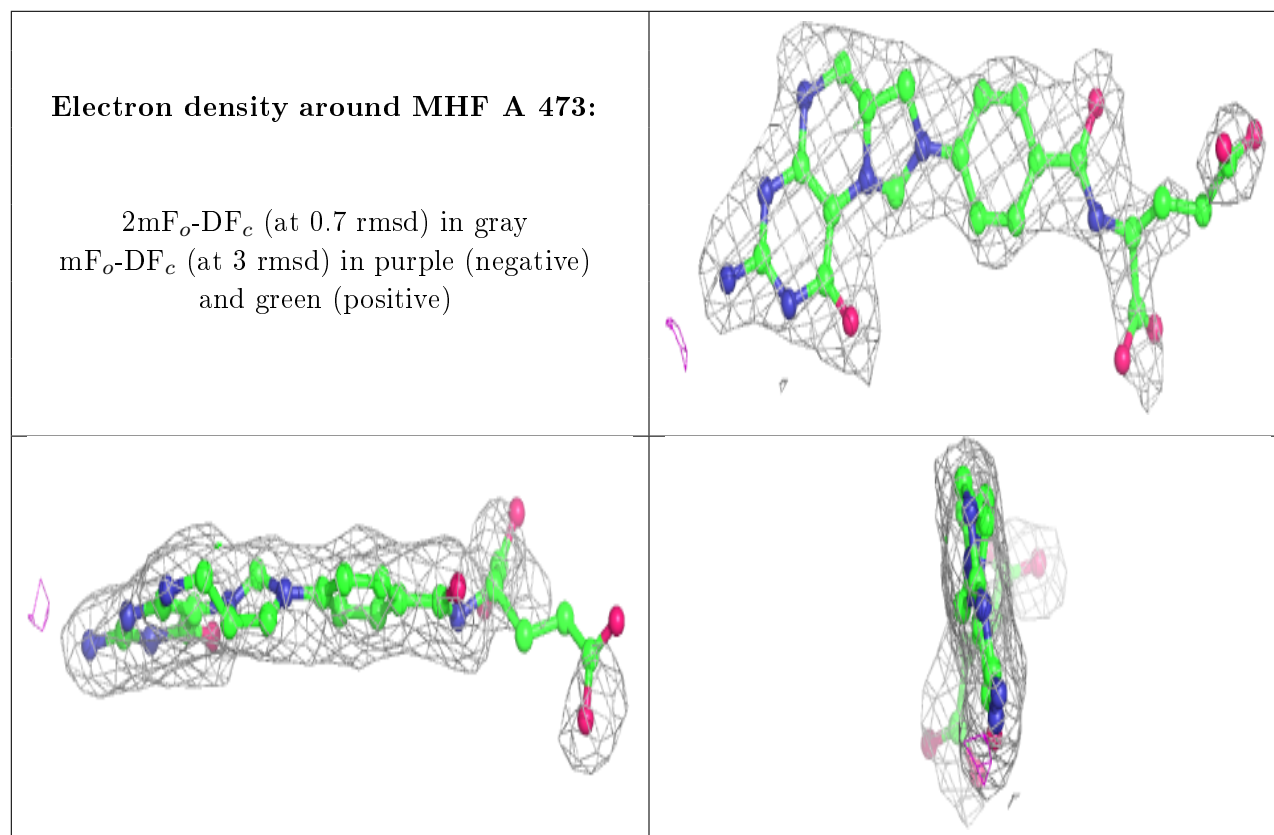
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	MHF	A	473	33/33	0.90	0.21	4,21,60,67	0
3	MHF	B	473	33/33	0.91	0.20	4,16,62,67	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	FAD	A	472	53/53	0.98	0.10	2,6,14,17	0
2	FAD	B	472	53/53	0.99	0.10	2,5,11,14	0

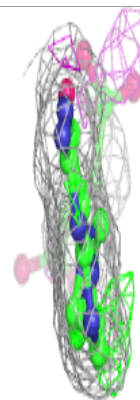
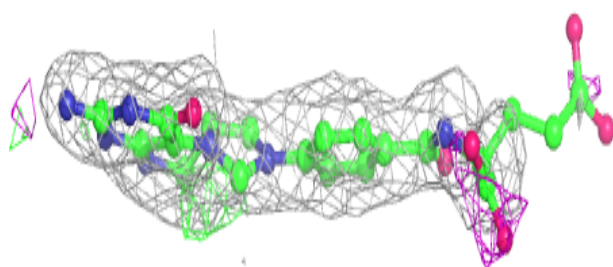
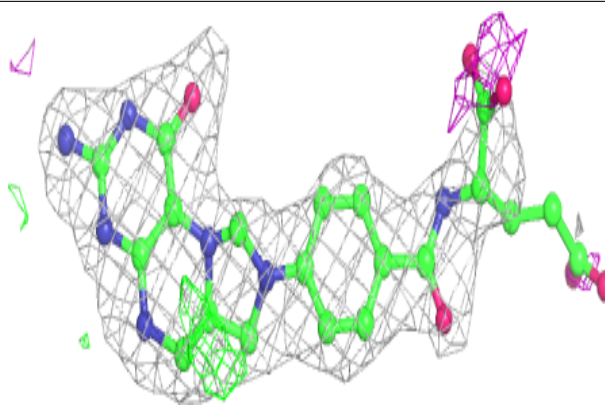
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



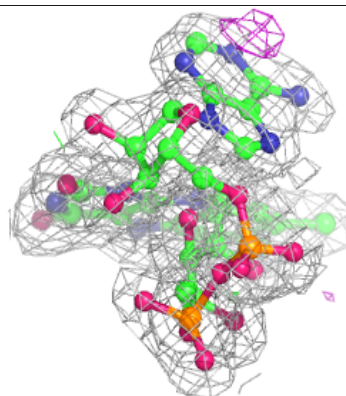
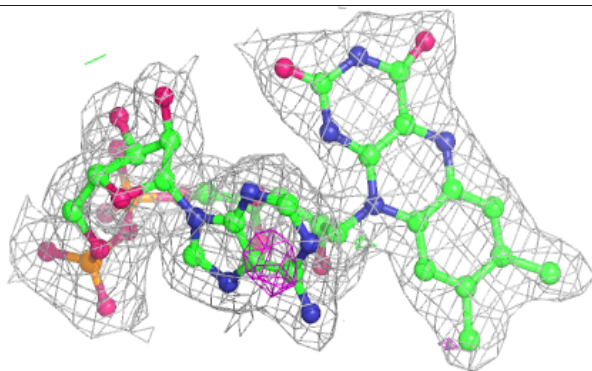
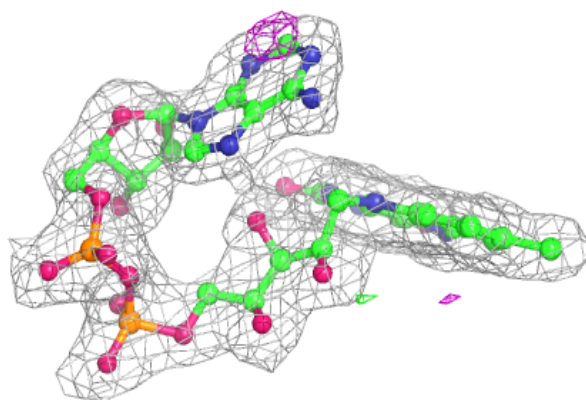


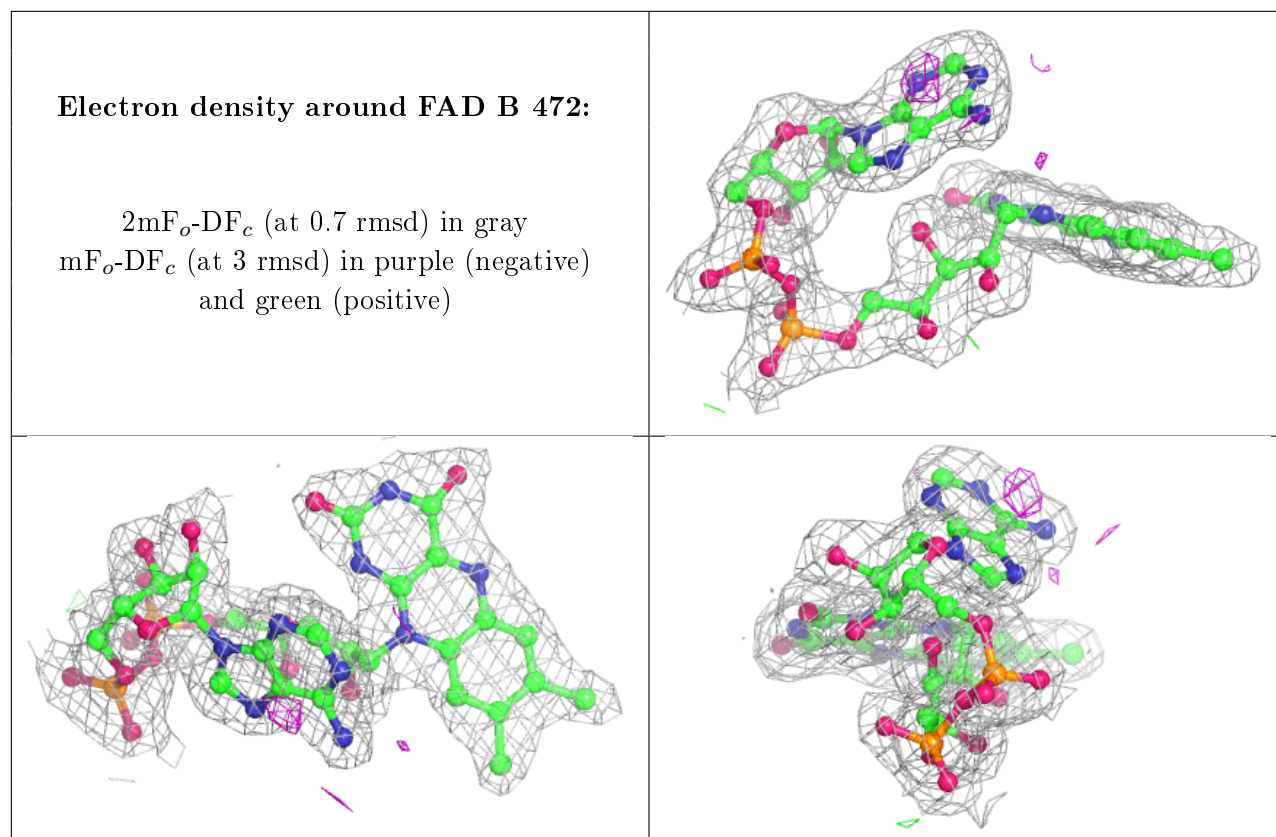
**Electron density around MHF B 473:**

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

**Electron density around FAD A 472:**

$2mF_o-DF_c$  (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.