



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 18, 2023 – 11:33 AM EDT

PDB ID : 1JEH  
Title : CRYSTAL STRUCTURE OF YEAST E3, LIPOAMIDE DEHYDROGENASE  
Authors : Toyoda, T.; Suzuki, K.; Sekigushi, T.; Reed, J.; Takenaka, A.  
Deposited on : 2001-06-18  
Resolution : 2.40 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](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)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

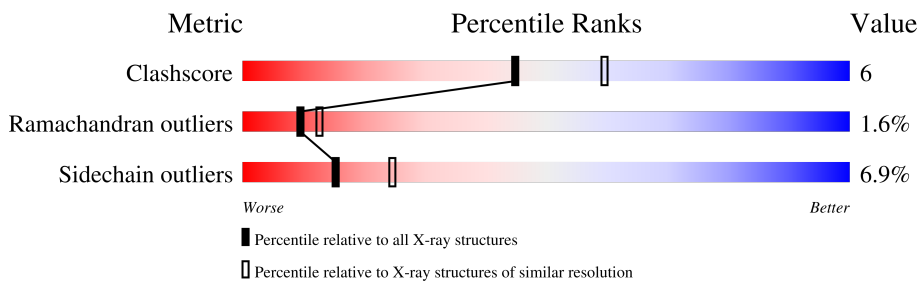
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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  $\geq 3$ , 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	478	
1	B	478	

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
2	FAD	B	580	X	-	-	-

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 7363 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 DIHYDROLIPOAMIDE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	478	Total 3588	2267	623	685	13	15	0	0
1	B	478	Total 3596	2270	625	688	13	10	0	0

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



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

- Molecule 3 is water.

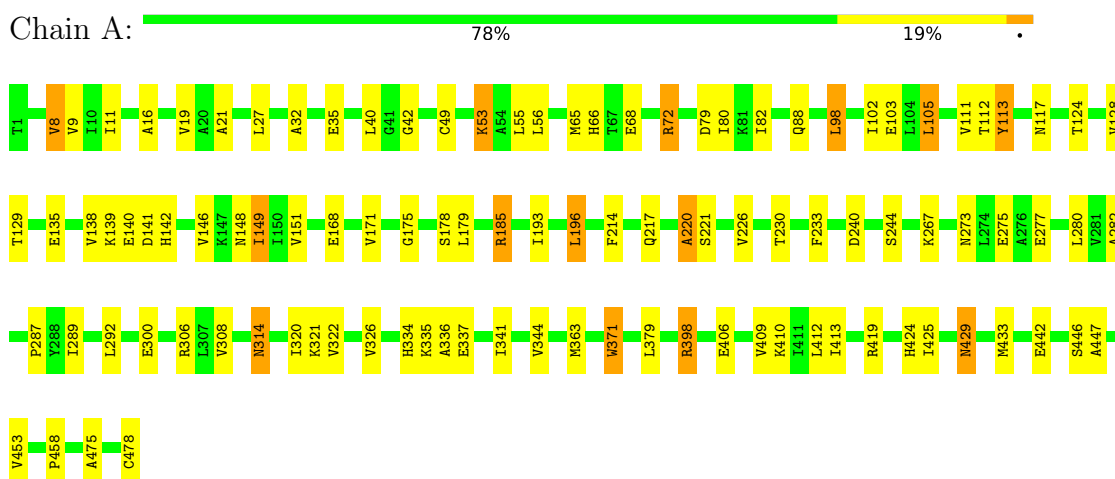
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	42	Total 42	O 42	0	0
3	B	31	Total 31	O 31	0	0

### 3 Residue-property plots

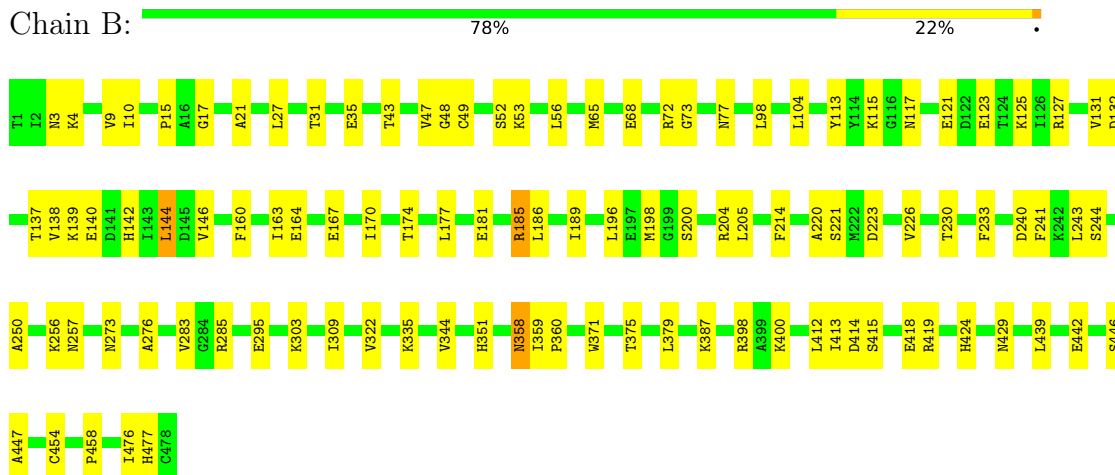
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

- Molecule 1: DIHYDROLIPOAMIDE DEHYDROGENASE



- Molecule 1: DIHYDROLIPOAMIDE DEHYDROGENASE



## 4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.10Å 158.70Å 67.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.40)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.202 , 0.260	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	7363	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

## 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: 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	0.59	0/3643	1.15	11/4912 (0.2%)
1	B	0.57	0/3652	1.08	8/4925 (0.2%)
All	All	0.58	0/7295	1.12	19/9837 (0.2%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	72	ARG	NE-CZ-NH1	15.83	128.22	120.30
1	A	72	ARG	NE-CZ-NH2	-13.38	113.61	120.30
1	B	371	TRP	CD1-CG-CD2	10.30	114.54	106.30
1	A	371	TRP	CD1-CG-CD2	9.78	114.12	106.30
1	A	113	TYR	CB-CG-CD2	-9.09	115.55	121.00
1	B	371	TRP	CE2-CD2-CG	-7.83	101.03	107.30
1	A	371	TRP	CE2-CD2-CG	-7.55	101.26	107.30
1	A	371	TRP	CB-CG-CD1	-7.24	117.59	127.00
1	A	398	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	B	220	ALA	CA-C-N	-6.96	101.88	117.20
1	B	371	TRP	CG-CD1-NE1	-6.37	103.73	110.10
1	A	371	TRP	CG-CD1-NE1	-6.27	103.83	110.10
1	A	371	TRP	CG-CD2-CE3	6.17	139.45	133.90
1	B	371	TRP	CB-CG-CD1	-6.02	119.18	127.00
1	A	220	ALA	N-CA-C	5.88	126.88	111.00
1	B	185	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	B	285	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	B	371	TRP	CG-CD2-CE3	5.14	138.53	133.90
1	A	292	LEU	CA-CB-CG	5.03	126.87	115.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3588	0	3621	58	0
1	B	3596	0	3623	45	0
2	A	53	0	31	1	0
2	B	53	0	31	0	0
3	A	42	0	0	11	0
3	B	31	0	0	4	0
All	All	7363	0	7306	94	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 6.

All (94) 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:A:151:VAL:HA	3:A:495:HOH:O	1.62	0.98
1:A:9:VAL:HG22	1:A:32:ALA:HB3	1.54	0.90
1:A:32:ALA:HA	3:A:503:HOH:O	1.73	0.88
1:A:453:VAL:HG22	1:B:442:GLU:HG3	1.63	0.80
1:A:287:PRO:HG2	1:A:306:ARG:HG2	1.65	0.79
1:A:453:VAL:HG21	1:B:439:LEU:HD23	1.65	0.76
1:A:105:LEU:HD21	1:B:477:HIS:HA	1.76	0.67
3:A:522:HOH:O	1:B:476:ILE:HG12	1.95	0.66
1:B:35:GLU:HB3	1:B:113:TYR:HE1	1.62	0.65
1:A:35:GLU:HB3	1:A:113:TYR:HE1	1.62	0.64
1:A:128:VAL:HB	1:A:142:HIS:HB2	1.79	0.64
1:A:112:THR:N	3:A:503:HOH:O	2.32	0.63
1:B:413:ILE:HG21	1:B:447:ALA:HB2	1.81	0.63
1:A:429:ASN:HB2	3:A:481:HOH:O	2.00	0.61
1:B:335:LYS:HG3	1:B:359:ILE:HD13	1.85	0.59
1:A:419:ARG:HA	1:A:446:SER:HA	1.86	0.58
1:A:409:VAL:HG13	1:A:425:ILE:HG12	1.86	0.57
1:B:4:LYS:O	1:B:144:LEU:HA	2.04	0.57
1:B:379:LEU:HD23	3:B:600:HOH:O	2.03	0.57
1:A:79:ASP:HB2	1:B:77:ASN:HB3	1.87	0.57
1:A:334:HIS:HD2	1:B:454:CYS:SG	2.27	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:ILE:HD12	1:B:250:ALA:HB3	1.88	0.55
1:B:9:VAL:HB	1:B:146:VAL:HG11	1.89	0.54
1:A:19:VAL:HG21	1:A:337:GLU:HG2	1.90	0.54
1:B:3:ASN:HB2	3:B:593:HOH:O	2.08	0.53
1:A:9:VAL:HG23	1:A:146:VAL:HG11	1.91	0.53
1:B:200:SER:O	1:B:204:ARG:HG3	2.09	0.53
1:B:379:LEU:HA	3:B:600:HOH:O	2.08	0.53
1:A:11:ILE:HB	3:A:495:HOH:O	2.10	0.51
1:A:103:GLU:HG3	3:A:488:HOH:O	2.11	0.51
1:A:68:GLU:O	1:A:72:ARG:HG3	2.11	0.51
1:B:52:SER:O	1:B:56:LEU:HB2	2.12	0.50
1:A:65:MET:HG2	1:B:65:MET:SD	2.52	0.50
1:A:458:PRO:HD3	1:B:49:CYS:HB3	1.94	0.49
1:B:223:ASP:HA	1:B:375:THR:HG23	1.94	0.49
1:B:226:VAL:HG21	1:B:424:HIS:HB3	1.95	0.49
1:B:358:ASN:OD1	1:B:442:GLU:HG2	2.13	0.49
1:B:47:VAL:HB	1:B:174:THR:HG22	1.95	0.48
1:B:163:ILE:HG22	1:B:170:ILE:HG21	1.96	0.48
1:B:419:ARG:HA	1:B:446:SER:HA	1.95	0.47
1:A:314:ASN:HA	1:A:321:LYS:HA	1.95	0.47
1:B:68:GLU:O	1:B:72:ARG:HG2	2.15	0.47
1:A:171:VAL:HB	1:A:175:GLY:HA3	1.97	0.47
1:A:413:ILE:HG21	1:A:447:ALA:HB2	1.96	0.47
1:A:149:ILE:HG23	1:A:320:ILE:HG12	1.97	0.47
1:B:121:GLU:HB2	1:B:125:LYS:HG3	1.96	0.47
1:A:40:LEU:HB2	3:A:488:HOH:O	2.14	0.47
1:A:8:VAL:HA	1:A:148:ASN:O	2.15	0.46
1:A:196:LEU:HD23	1:A:363:MET:SD	2.55	0.46
1:A:280:LEU:HD22	1:A:282:ALA:HB2	1.98	0.46
1:A:410:LYS:HE2	1:A:412:LEU:HD11	1.98	0.46
1:A:88:GLN:NE2	1:A:178:SER:HA	2.31	0.45
1:A:151:VAL:HG13	1:A:322:VAL:HG13	1.98	0.45
1:A:300:GLU:HB3	1:A:308:VAL:HG22	1.99	0.45
1:A:287:PRO:HB3	1:A:326:VAL:HA	1.99	0.45
1:A:226:VAL:HG21	1:A:424:HIS:HB3	1.99	0.45
1:A:27:LEU:HD22	1:A:344:VAL:HG12	1.99	0.45
1:B:115:LYS:O	1:B:137:THR:HA	2.17	0.45
1:A:16:ALA:HB2	1:A:336:ALA:HB1	2.00	0.44
1:A:49:CYS:O	1:A:53:LYS:HE2	2.17	0.44
1:A:117:ASN:HB3	1:A:129:THR:HB	2.00	0.44
1:B:214:PHE:O	1:B:244:SER:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:PHE:HB3	1:B:243:LEU:HD13	2.00	0.44
1:A:9:VAL:CG2	1:A:146:VAL:HG11	2.48	0.44
1:A:98:LEU:O	1:A:102:ILE:HG12	2.18	0.44
1:A:193:ILE:HD11	1:A:371:TRP:HH2	1.83	0.44
1:A:49:CYS:HB3	1:B:458:PRO:HD3	2.00	0.43
1:B:10:ILE:HG21	1:B:17:GLY:HA2	2.00	0.43
1:B:414:ASP:O	1:B:418:GLU:HA	2.19	0.43
1:A:88:GLN:HE22	1:A:178:SER:HA	1.83	0.42
1:A:214:PHE:O	1:A:244:SER:HA	2.19	0.42
1:B:230:THR:HA	1:B:233:PHE:CE1	2.54	0.42
1:B:185:ARG:HD2	1:B:276:ALA:HA	2.00	0.42
1:B:21:ALA:HA	1:B:31:THR:HG21	2.01	0.42
1:A:42:GLY:HA2	2:A:480:FAD:O3B	2.19	0.42
1:B:359:ILE:HA	1:B:360:PRO:HD2	1.90	0.42
1:B:27:LEU:HD12	1:B:344:VAL:HG12	2.01	0.42
1:B:160:PHE:HD1	1:B:283:VAL:HG21	1.84	0.42
1:A:21:ALA:HB1	1:A:111:VAL:HG11	2.02	0.41
1:A:341:ILE:HG12	3:A:522:HOH:O	2.20	0.41
1:B:387:LYS:HE2	1:B:415:SER:HA	2.03	0.41
1:A:72:ARG:NH2	3:A:512:HOH:O	2.54	0.41
1:A:11:ILE:CB	3:A:495:HOH:O	2.68	0.41
1:A:82:ILE:HG13	1:B:73:GLY:O	2.20	0.41
1:A:185:ARG:NH2	1:A:275:GLU:HB3	2.36	0.41
1:B:181:GLU:HG2	3:B:609:HOH:O	2.19	0.41
1:B:309:ILE:CG2	1:B:322:VAL:HB	2.51	0.41
1:B:127:ARG:HA	1:B:142:HIS:O	2.20	0.41
1:A:9:VAL:CG2	1:A:32:ALA:HB3	2.39	0.40
1:A:475:ALA:HB3	1:A:478:CYS:HB3	2.03	0.40
1:A:151:VAL:CG1	1:A:322:VAL:HG22	2.51	0.40
1:A:230:THR:HA	1:A:233:PHE:CE1	2.56	0.40
1:B:43:THR:O	1:B:48:GLY:N	2.54	0.40
1:A:425:ILE:HD13	1:A:433:MET:SD	2.61	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	476/478 (100%)	443 (93%)	24 (5%)	9 (2%)	8 10
1	B	476/478 (100%)	442 (93%)	28 (6%)	6 (1%)	12 17
All	All	952/956 (100%)	885 (93%)	52 (6%)	15 (2%)	9 13

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	124	THR
1	A	141	ASP
1	A	220	ALA
1	B	138	VAL
1	B	139	LYS
1	A	140	GLU
1	A	139	LYS
1	A	168	GLU
1	A	221	SER
1	B	131	VAL
1	B	132	ASP
1	A	138	VAL
1	B	221	SER
1	A	135	GLU
1	B	256	LYS

### 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	374/386 (97%)	349 (93%)	25 (7%)	16 26
1	B	376/386 (97%)	349 (93%)	27 (7%)	14 23
All	All	750/772 (97%)	698 (93%)	52 (7%)	15 25

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	VAL
1	A	53	LYS
1	A	55	LEU
1	A	56	LEU
1	A	66	HIS
1	A	80	ILE
1	A	98	LEU
1	A	105	LEU
1	A	149	ILE
1	A	179	LEU
1	A	185	ARG
1	A	196	LEU
1	A	217	GLN
1	A	240	ASP
1	A	267	LYS
1	A	273	ASN
1	A	277	GLU
1	A	289	ILE
1	A	314	ASN
1	A	335	LYS
1	A	379	LEU
1	A	398	ARG
1	A	406	GLU
1	A	429	ASN
1	A	442	GLU
1	B	15	PRO
1	B	53	LYS
1	B	98	LEU
1	B	104	LEU
1	B	117	ASN
1	B	123	GLU
1	B	140	GLU
1	B	144	LEU
1	B	164	GLU
1	B	167	GLU
1	B	177	LEU
1	B	186	LEU
1	B	189	ILE
1	B	196	LEU
1	B	198	MET
1	B	205	LEU
1	B	240	ASP

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Mol	Chain	Res	Type
1	B	257	ASN
1	B	273	ASN
1	B	295	GLU
1	B	303	LYS
1	B	351	HIS
1	B	358	ASN
1	B	398	ARG
1	B	400	LYS
1	B	412	LEU
1	B	429	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	HIS
1	A	88	GLN
1	A	271	GLN
1	A	319	HIS
1	A	334	HIS
1	B	6	HIS
1	B	46	ASN
1	B	109	ASN
1	B	237	GLN
1	B	257	ASN
1	B	273	ASN
1	B	319	HIS
1	B	424	HIS
1	B	468	ASN

### 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

2 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	580	-	53,58,58	1.58	7 (13%)	68,89,89	1.35	10 (14%)
2	FAD	A	480	-	53,58,58	1.62	9 (16%)	68,89,89	1.30	8 (11%)

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	580	-	1/1/9/9	5/30/50/50	0/6/6/6
2	FAD	A	480	-	-	2/30/50/50	0/6/6/6

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	580	FAD	O4B-C1B	4.30	1.47	1.41
2	A	480	FAD	PA-O2A	-4.30	1.35	1.55
2	B	580	FAD	PA-O2A	-4.27	1.35	1.55
2	A	480	FAD	O5'-C5'	4.08	1.60	1.44
2	B	580	FAD	O5'-C5'	4.04	1.60	1.44
2	A	480	FAD	O4B-C1B	4.03	1.46	1.41
2	A	480	FAD	P-O2P	-3.48	1.39	1.55
2	B	580	FAD	P-O2P	-3.43	1.39	1.55
2	A	480	FAD	O2-C2	-3.09	1.18	1.24
2	B	580	FAD	O2-C2	-3.04	1.18	1.24
2	A	480	FAD	C1'-C2'	2.88	1.56	1.52
2	B	580	FAD	C1'-C2'	2.72	1.56	1.52
2	A	480	FAD	C2B-C1B	-2.51	1.50	1.53
2	A	480	FAD	C4X-N5	2.30	1.35	1.30
2	A	480	FAD	C6-C7	-2.18	1.36	1.39

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	580	FAD	C6-C7	-2.13	1.36	1.39

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	480	FAD	O5B-PA-O1A	-3.51	95.36	109.07
2	B	580	FAD	O5B-PA-O1A	-3.02	97.27	109.07
2	B	580	FAD	C5'-C4'-C3'	-2.91	106.58	112.20
2	B	580	FAD	C3B-C2B-C1B	2.91	105.36	100.98
2	A	480	FAD	O4B-C1B-C2B	-2.55	103.21	106.93
2	B	580	FAD	O5'-P-O1P	-2.54	99.16	109.07
2	A	480	FAD	C2A-N1A-C6A	2.50	123.02	118.75
2	B	580	FAD	C5A-C6A-N1A	-2.47	114.74	120.35
2	A	480	FAD	C5A-C6A-N1A	-2.39	114.94	120.35
2	A	480	FAD	C4-N3-C2	-2.29	121.41	125.64
2	B	580	FAD	C2A-N1A-C6A	2.27	122.64	118.75
2	A	480	FAD	C5A-C6A-N6A	2.27	123.80	120.35
2	B	580	FAD	C5A-C6A-N6A	2.23	123.73	120.35
2	B	580	FAD	C4X-C10-N1	-2.21	119.61	124.73
2	B	580	FAD	C4-N3-C2	-2.20	121.58	125.64
2	B	580	FAD	C10-N1-C2	2.20	121.30	116.90
2	A	480	FAD	C4'-C3'-C2'	-2.05	109.09	113.36
2	A	480	FAD	C4A-C5A-N7A	2.02	111.50	109.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	580	FAD	C2B

All (7) torsion outliers are listed below:

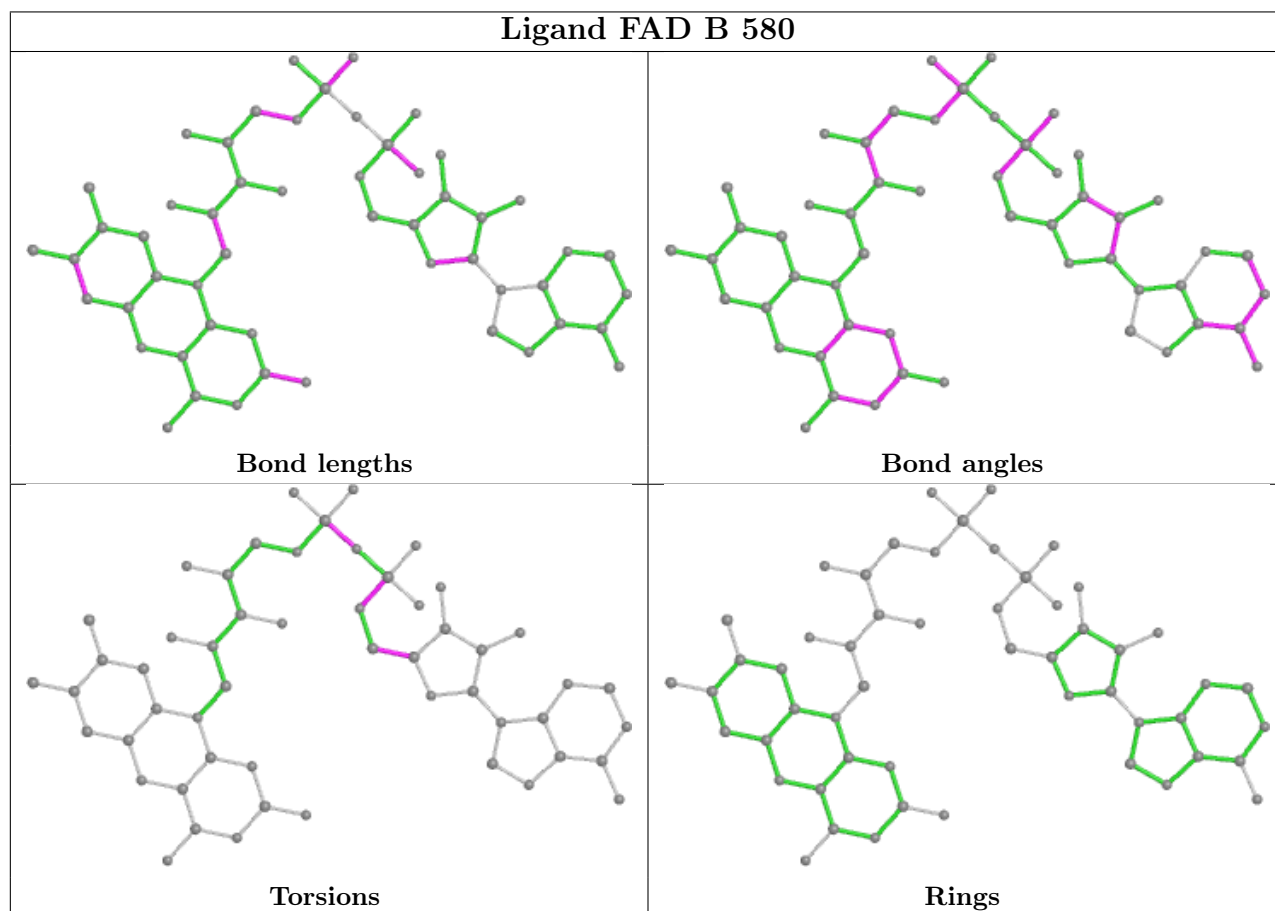
Mol	Chain	Res	Type	Atoms
2	A	480	FAD	PA-O3P-P-O5'
2	B	580	FAD	C5B-O5B-PA-O3P
2	B	580	FAD	PA-O3P-P-O5'
2	B	580	FAD	C5B-O5B-PA-O2A
2	B	580	FAD	O4B-C4B-C5B-O5B
2	B	580	FAD	C5B-O5B-PA-O1A
2	A	480	FAD	O4B-C4B-C5B-O5B

There are no ring outliers.

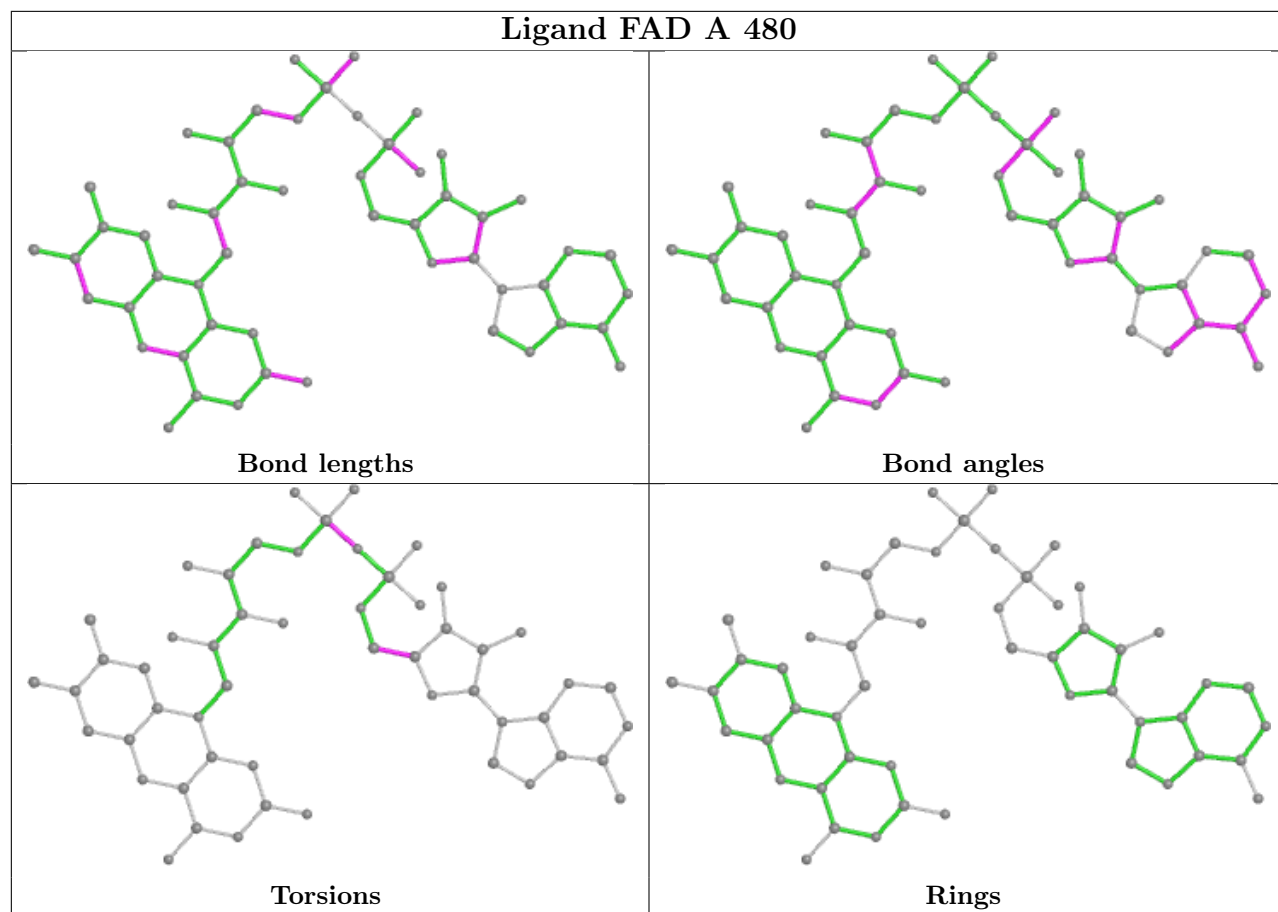
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	480	FAD	1	0

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







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.