



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 08:37 PM UTC

PDB ID : 1FEB / pdb\_00001feb  
Title : UNLIGANDED CRITHIDIA FASCICULATA TRYPTOPHANE REDUCTASE AT 2.0 ANGSTROM RESOLUTION  
Authors : Strickland, C.; Karplus, P.  
Deposited on : 1995-07-12  
Resolution : 2.00 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 : 4-5-2 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

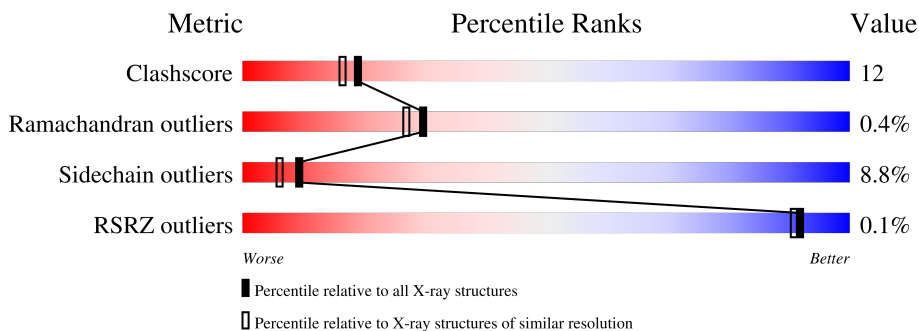
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	490	 66% 28% 5%
1	B	490	 67% 26% 6%

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 7818 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.

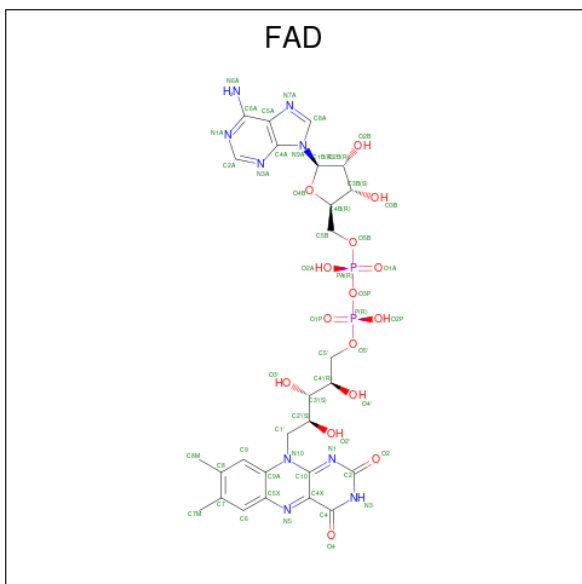
- Molecule 1 is a protein called TRYPANOTHIONE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	487	Total 3710	C 2334	N 643	O 713	S 20	0	0	0
1	B	484	Total 3685	C 2318	N 639	O 708	S 20	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	296	GLU	ASP	conflict	UNP P39040
A	478	GLU	GLN	conflict	UNP P39040
B	296	GLU	ASP	conflict	UNP P39040
B	478	GLU	GLN	conflict	UNP P39040

- 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		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

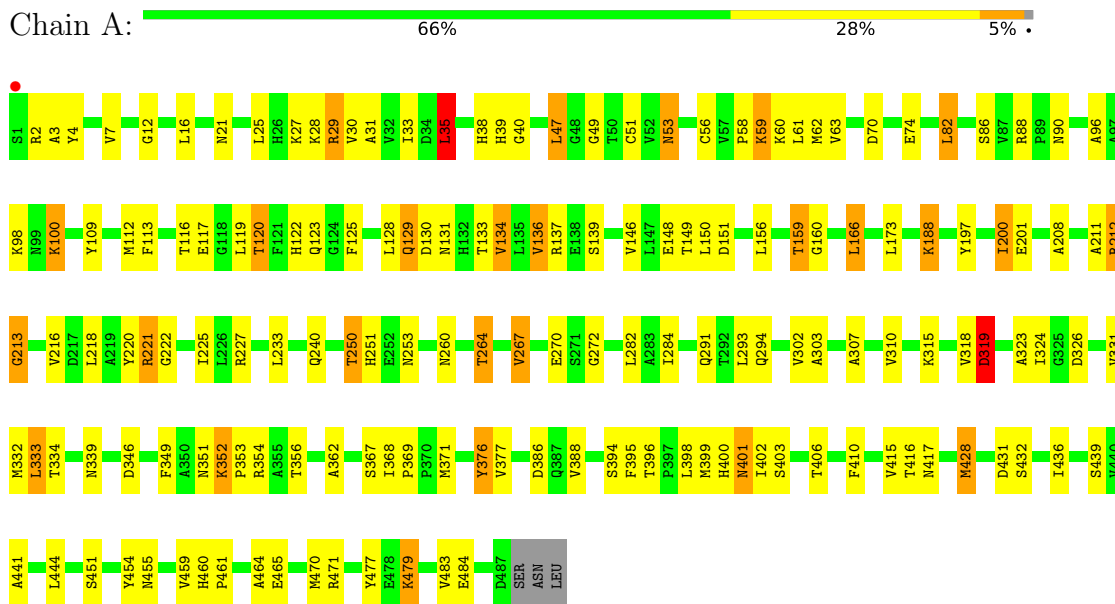
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	177	Total	O	0	0
			177	177		
3	B	140	Total	O	0	0
			140	140		

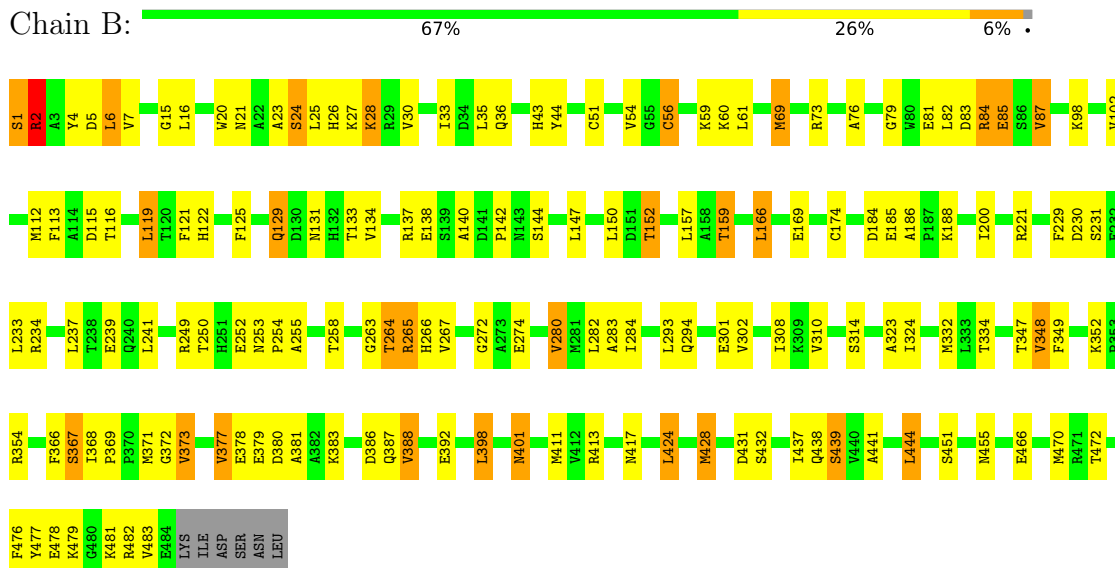
### 3 Residue-property plots [i](#)

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: TRYPANOTHIONE REDUCTASE



#### • Molecule 1: TRYPANOTHIONE REDUCTASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.90Å 169.60Å 60.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.00 8.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.00) 90.1 (8.00-2.00)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.40 (at 2.00Å)	Xtrriage
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.202 , (Not available) 0.201 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.3	Xtrriage
Anisotropy	0.363	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 86.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7818	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% 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: 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	1.01	5/3783 (0.1%)	1.28	30/5126 (0.6%)
1	B	0.96	3/3758 (0.1%)	1.24	34/5093 (0.7%)
All	All	0.99	8/7541 (0.1%)	1.26	64/10219 (0.6%)

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

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	208	ALA	CA-CB	-8.64	1.39	1.53
1	A	470	MET	SD-CE	-7.16	1.61	1.79
1	A	267	VAL	CA-CB	6.13	1.62	1.54
1	A	332	MET	SD-CE	-5.75	1.65	1.79
1	A	428	MET	SD-CE	-5.53	1.65	1.79
1	B	332	MET	SD-CE	5.28	1.92	1.79
1	B	102	VAL	CA-CB	-5.12	1.47	1.54
1	B	428	MET	SD-CE	-5.07	1.66	1.79

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	396	THR	CA-C-N	-9.70	109.79	119.78
1	A	396	THR	C-N-CA	-9.70	109.79	119.78
1	A	53	ASN	N-CA-C	8.65	122.33	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	40	GLY	CA-C-N	8.05	128.67	120.38
1	A	40	GLY	C-N-CA	8.05	128.67	120.38
1	A	129	GLN	N-CA-C	-7.93	102.13	112.68
1	A	166	LEU	N-CA-C	-7.62	98.61	110.42
1	B	472	THR	CA-C-N	7.48	127.41	119.85
1	B	472	THR	C-N-CA	7.48	127.41	119.85
1	A	291	GLN	N-CA-C	7.36	121.36	112.38
1	A	213	GLY	N-CA-C	-7.28	105.75	115.21
1	B	87	VAL	N-CA-C	6.83	118.59	109.37
1	B	24	SER	N-CA-C	6.71	119.59	111.40
1	B	129	GLN	N-CA-C	-6.60	104.87	113.12
1	A	123	GLN	N-CA-C	6.53	119.09	108.26
1	A	401	ASN	N-CA-C	-6.49	104.40	112.90
1	B	417	ASN	N-CA-C	-6.45	98.67	108.67
1	A	200	ILE	CB-CA-C	-6.23	103.86	112.02
1	B	401	ASN	N-CA-C	-6.16	104.47	112.23
1	A	352	LYS	CA-C-N	6.12	126.44	119.83
1	A	352	LYS	C-N-CA	6.12	126.44	119.83
1	A	417	ASN	N-CA-C	-6.07	98.64	108.41
1	B	348	VAL	N-CA-C	6.06	117.02	111.81
1	B	272	GLY	N-CA-C	-6.05	106.17	114.64
1	B	377	VAL	N-CA-C	-5.97	99.72	108.97
1	B	241	LEU	N-CA-C	-5.96	104.87	111.36
1	B	372	GLY	N-CA-C	-5.87	99.27	113.18
1	B	35	LEU	N-CA-C	5.85	118.43	111.71
1	B	144	SER	N-CA-C	-5.81	103.04	110.53
1	B	188	LYS	N-CA-C	-5.79	104.33	111.40
1	B	2	ARG	N-CA-C	-5.77	98.51	110.80
1	A	367	SER	N-CA-C	-5.75	102.41	110.35
1	A	459	VAL	N-CA-C	-5.73	100.15	108.17
1	B	324	ILE	CB-CA-C	-5.66	102.44	110.82
1	B	367	SER	N-CA-C	-5.65	102.55	110.35
1	A	349	PHE	N-CA-C	5.59	120.10	113.28
1	B	186	ALA	CA-C-N	-5.59	114.00	119.76
1	B	186	ALA	C-N-CA	-5.59	114.00	119.76
1	A	146	VAL	N-CA-C	-5.56	100.67	108.12
1	B	152	THR	N-CA-C	5.55	117.70	108.99
1	B	437	ILE	N-CA-C	5.54	118.82	111.17
1	B	347	THR	N-CA-C	5.54	117.32	111.28
1	B	483	VAL	N-CA-C	5.50	117.57	108.99
1	A	35	LEU	N-CA-C	5.47	119.05	112.38
1	A	319	ASP	N-CA-C	5.45	122.42	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	159	THR	N-CA-C	5.43	119.77	113.20
1	B	368	ILE	N-CA-C	-5.36	102.84	108.15
1	B	255	ALA	N-CA-C	-5.36	106.68	113.43
1	B	5	ASP	N-CA-C	-5.33	105.04	112.45
1	A	416	THR	CB-CA-C	-5.30	100.27	110.24
1	A	464	ALA	N-CA-C	5.26	117.70	111.33
1	B	15	GLY	N-CA-C	5.25	118.59	112.50
1	A	377	VAL	N-CA-C	-5.23	102.34	109.55
1	B	373	VAL	N-CA-CB	-5.23	102.26	111.93
1	A	173	LEU	N-CA-C	-5.18	106.65	113.17
1	B	131	ASN	N-CA-C	5.18	120.51	113.37
1	B	69	MET	N-CA-C	-5.16	105.35	110.97
1	A	376	TYR	N-CA-C	5.14	118.09	110.48
1	A	455	ASN	N-CA-C	-5.11	106.83	113.16
1	A	272	GLY	N-CA-C	-5.08	108.44	114.48
1	B	200	ILE	N-CA-C	5.06	115.78	110.62
1	A	264	THR	N-CA-C	-5.05	103.27	110.59
1	B	56	CYS	N-CA-C	5.03	117.15	111.11
1	A	159	THR	N-CA-C	5.01	119.37	113.16

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	376	TYR	Sidechain

## 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	3710	0	3652	92	0
1	B	3685	0	3624	90	0
2	A	53	0	31	3	0
2	B	53	0	30	2	0
3	A	177	0	0	5	0
3	B	140	0	0	4	0
All	All	7818	0	7337	175	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 12.

All (175) 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:388:VAL:HG23	1:A:477:TYR:HB2	1.41	1.01
1:A:188:LYS:HG3	1:A:211:ALA:HB3	1.56	0.85
1:B:16:LEU:HD22	1:B:112:MET:HE1	1.57	0.85
1:A:82:LEU:HB3	1:B:87:VAL:HG22	1.60	0.83
1:A:388:VAL:CG2	1:A:477:TYR:HB2	2.12	0.79
1:B:231:SER:HA	1:B:234:ARG:HD3	1.68	0.76
1:A:212:ARG:NE	1:A:212:ARG:HA	2.02	0.74
1:B:378:GLU:HG3	3:B:612:HOH:O	1.91	0.70
1:B:380:ASP:HA	1:B:383:LYS:HE2	1.74	0.70
1:A:31:ALA:HA	1:A:120:THR:HG23	1.74	0.70
1:B:1:SER:O	1:B:2:ARG:HB2	1.93	0.69
1:B:233:LEU:HD23	1:B:371:MET:HE3	1.73	0.69
1:A:188:LYS:CG	1:A:211:ALA:HB3	2.23	0.68
1:B:60:LYS:HE3	1:B:366:PHE:CE2	2.29	0.67
1:A:96:ALA:O	1:A:100:LYS:HD2	1.95	0.67
1:A:428:MET:HE1	1:A:436:ILE:HG22	1.77	0.67
1:A:212:ARG:HA	1:A:212:ARG:HE	1.60	0.66
1:B:388:VAL:HG22	1:B:477:TYR:HB2	1.76	0.66
1:A:3:ALA:HB3	1:A:151:ASP:O	1.96	0.66
1:A:428:MET:HE1	1:A:436:ILE:CG2	2.26	0.65
1:B:138:GLU:HB3	1:B:147:LEU:HD21	1.77	0.65
1:A:2:ARG:HB3	1:A:151:ASP:OD2	1.96	0.65
1:A:315:LYS:HD2	1:A:319:ASP:HA	1.78	0.65
1:A:402:ILE:HD12	1:B:61:LEU:HD22	1.80	0.64
1:A:16:LEU:HD22	1:A:112:MET:HE1	1.80	0.63
1:A:439:SER:HB2	1:B:439:SER:HB2	1.81	0.63
1:A:166:LEU:HD12	1:A:284:ILE:HD13	1.83	0.61
1:B:137:ARG:HH22	1:B:294:GLN:HE22	1.51	0.59
1:A:116:THR:HB	1:A:119:LEU:HB3	1.85	0.58
1:B:36:GLN:OE1	1:B:43:HIS:HB2	2.04	0.58
1:B:310:VAL:HB	1:B:314:SER:HA	1.85	0.57
1:B:387:GLN:HA	1:B:477:TYR:O	2.04	0.57
1:A:398:LEU:HD12	1:A:401:ASN:HD22	1.69	0.57
1:B:113:PHE:CE1	1:B:119:LEU:HD22	2.40	0.57
1:B:21:ASN:O	1:B:25:LEU:HB2	2.05	0.57
1:A:221:ARG:HD2	1:A:253:ASN:HB2	1.88	0.56
1:B:33:ILE:HG22	2:B:499:FAD:H2A	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:HIS:HB3	1:A:53:ASN:OD1	2.05	0.56
1:B:4:TYR:CE2	1:B:150:LEU:HD22	2.40	0.56
1:B:73:ARG:NH1	3:B:586:HOH:O	2.37	0.56
1:A:362:ALA:HB2	1:A:441:ALA:HB2	1.87	0.55
1:A:399:MET:HE2	1:A:400:HIS:CE1	2.41	0.55
1:B:444:LEU:HD23	1:B:444:LEU:N	2.20	0.55
1:A:4:TYR:CE2	1:A:150:LEU:HD22	2.41	0.55
1:A:31:ALA:HB1	1:A:122:HIS:CD2	2.41	0.55
1:A:431:ASP:O	1:A:432:SER:HB2	2.06	0.55
1:A:125:PHE:HB3	3:A:666:HOH:O	2.07	0.55
1:A:197:TYR:O	1:A:201:GLU:HG3	2.07	0.55
1:B:266:HIS:NE2	1:B:274:GLU:HB3	2.22	0.55
1:B:174:CYS:HA	1:B:280:VAL:HG13	1.87	0.55
1:A:59:LYS:HD3	1:A:60:LYS:N	2.22	0.54
1:A:129:GLN:NE2	1:A:133:THR:HG21	2.22	0.54
1:A:21:ASN:O	1:A:25:LEU:HB2	2.08	0.54
1:A:302:VAL:HG12	1:A:303:ALA:O	2.08	0.53
1:B:282:LEU:HB3	1:B:284:ILE:HD13	1.90	0.53
1:B:36:GLN:OE1	1:B:43:HIS:ND1	2.42	0.53
1:B:20:TRP:HZ3	1:B:116:THR:HG1	1.55	0.53
1:B:76:ALA:HB2	1:B:84:ARG:NH1	2.23	0.53
1:B:7:VAL:HG11	1:B:134:VAL:HG21	1.91	0.53
1:A:59:LYS:O	1:A:63:VAL:HG23	2.08	0.52
1:A:29:ARG:HH11	1:A:29:ARG:HG2	1.74	0.52
1:A:112:MET:HE3	1:A:119:LEU:HD21	1.92	0.52
1:A:302:VAL:HG13	1:A:307:ALA:O	2.09	0.52
1:A:212:ARG:CZ	1:A:213:GLY:H	2.23	0.52
1:B:98:LYS:HD2	1:B:98:LYS:C	2.34	0.52
1:B:431:ASP:O	1:B:432:SER:HB2	2.09	0.52
1:A:212:ARG:NH2	1:A:213:GLY:H	2.07	0.52
1:A:200:ILE:CD1	1:A:225:ILE:HD12	2.41	0.51
1:A:233:LEU:HD23	1:A:371:MET:HE3	1.92	0.51
1:B:478:GLU:O	1:B:481:LYS:HB3	2.11	0.51
1:B:23:ALA:O	1:B:27:LYS:HA	2.11	0.51
1:B:267:VAL:O	1:B:274:GLU:HA	2.11	0.51
1:B:451:SER:O	1:B:455:ASN:HB2	2.11	0.51
1:A:58:PRO:O	1:A:62:MET:HG3	2.11	0.51
1:B:381:ALA:HB1	1:B:424:LEU:HD23	1.92	0.50
1:B:60:LYS:HE3	1:B:366:PHE:HE2	1.75	0.50
1:B:221:ARG:HG3	1:B:221:ARG:HH11	1.75	0.50
1:B:386:ASP:CG	1:B:387:GLN:H	2.19	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:VAL:HG22	1:A:31:ALA:HB3	1.93	0.50
1:A:351:ASN:O	1:A:353:PRO:HD3	2.11	0.50
1:B:20:TRP:HZ3	1:B:116:THR:OG1	1.94	0.49
1:A:74:GLU:HB3	1:A:403:SER:HB2	1.93	0.49
1:A:166:LEU:CD1	1:A:284:ILE:HD13	2.42	0.49
1:A:394:SER:HA	1:A:410:PHE:O	2.11	0.49
1:B:352:LYS:HG3	1:B:352:LYS:O	2.13	0.49
1:A:369:PRO:HG3	3:A:574:HOH:O	2.13	0.49
1:B:166:LEU:H	1:B:166:LEU:HD23	1.77	0.49
1:B:69:MET:HE3	3:B:586:HOH:O	2.12	0.49
1:B:44:TYR:HB3	1:B:54:VAL:HG11	1.94	0.49
1:B:26:HIS:O	1:B:28:LYS:HD2	2.13	0.49
1:B:378:GLU:HB2	1:B:379:GLU:OE1	2.13	0.49
1:B:20:TRP:CZ3	1:B:116:THR:OG1	2.66	0.48
1:A:90:ASN:N	1:B:79:GLY:O	2.43	0.48
1:A:136:VAL:HG13	1:A:148:GLU:HG3	1.96	0.48
1:A:250:THR:O	1:A:251:HIS:HB2	2.13	0.48
1:A:35:LEU:HD13	2:A:499:FAD:C2A	2.44	0.48
1:B:466:GLU:O	1:B:470:MET:HE2	2.13	0.48
1:A:12:GLY:HA2	1:A:49:GLY:CA	2.45	0.47
1:A:471:ARG:HD2	3:A:651:HOH:O	2.14	0.47
1:B:184:ASP:O	1:B:185:GLU:HG3	2.15	0.47
1:B:283:ALA:H	1:B:284:ILE:HD12	1.79	0.47
1:B:438:GLN:O	1:B:441:ALA:HB3	2.15	0.47
1:B:310:VAL:HG11	1:B:323:ALA:O	2.14	0.47
1:A:51:CYS:HB3	3:A:548:HOH:O	2.14	0.47
1:A:29:ARG:HG2	1:A:29:ARG:NH1	2.29	0.47
1:B:229:PHE:O	1:B:234:ARG:HD2	2.15	0.47
1:B:129:GLN:HB3	1:B:133:THR:HB	1.97	0.46
1:A:33:ILE:HG22	2:A:499:FAD:H2A	1.97	0.46
1:A:149:THR:O	1:A:150:LEU:HD23	2.15	0.46
1:B:85:GLU:CD	1:B:85:GLU:H	2.24	0.46
1:A:61:LEU:HD11	1:B:398:LEU:HD13	1.98	0.46
1:A:188:LYS:HG3	1:A:211:ALA:CB	2.39	0.46
1:A:451:SER:HA	1:A:454:TYR:CZ	2.51	0.46
1:B:137:ARG:HH12	1:B:294:GLN:NE2	2.14	0.45
1:B:137:ARG:HH22	1:B:294:GLN:NE2	2.12	0.45
1:A:200:ILE:HD12	1:A:225:ILE:HD12	1.97	0.45
1:A:460:HIS:HA	1:A:461:PRO:HA	1.59	0.45
2:B:499:FAD:H9	2:B:499:FAD:H1'1	1.78	0.45
1:A:166:LEU:HD13	1:A:282:LEU:HD22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:SER:HB2	1:B:439:SER:CB	2.46	0.45
1:A:113:PHE:CD1	1:A:119:LEU:HG	2.51	0.45
1:A:212:ARG:HD2	3:A:566:HOH:O	2.17	0.45
1:B:6:LEU:HB3	1:B:30:VAL:HG13	1.99	0.45
1:A:156:LEU:HD11	1:A:324:ILE:HG12	1.98	0.44
1:A:130:ASP:OD1	1:A:133:THR:HB	2.17	0.44
1:A:260:ASN:HB2	1:A:264:THR:O	2.18	0.44
1:A:331:VAL:HG12	1:A:333:LEU:HD22	1.99	0.44
1:A:253:ASN:O	1:A:270:GLU:HG3	2.18	0.44
2:A:499:FAD:H1'1	2:A:499:FAD:H9	1.71	0.44
1:A:70:ASP:O	1:A:74:GLU:HG3	2.18	0.43
1:A:346:ASP:HB3	1:A:352:LYS:O	2.17	0.43
1:B:392:GLU:HG3	1:B:413:ARG:HD2	2.01	0.43
1:B:398:LEU:HD23	1:B:401:ASN:HD22	1.83	0.43
1:B:479:LYS:C	1:B:481:LYS:H	2.26	0.43
1:B:249:ARG:HB3	1:B:252:GLU:HG3	2.00	0.43
1:B:265:ARG:HG3	1:B:280:VAL:HG12	2.00	0.43
1:B:221:ARG:HG3	1:B:221:ARG:NH1	2.34	0.43
1:B:263:GLY:O	1:B:264:THR:O	2.36	0.43
1:A:302:VAL:CG1	1:A:303:ALA:N	2.81	0.43
1:A:310:VAL:HG11	1:A:323:ALA:HB3	2.01	0.43
1:B:159:THR:HG21	1:B:293:LEU:HD21	2.00	0.43
1:A:200:ILE:HD13	1:A:218:LEU:HD11	2.01	0.42
1:A:439:SER:CB	1:B:439:SER:HB2	2.48	0.42
1:A:220:TYR:CE2	1:A:222:GLY:HA3	2.54	0.42
1:B:157:LEU:HD13	1:B:308:ILE:HD13	2.01	0.42
1:A:128:LEU:HD23	1:A:134:VAL:HB	2.02	0.42
1:A:240:GLN:OE1	1:A:369:PRO:HG3	2.20	0.42
1:A:160:GLY:HA2	1:A:326:ASP:HB2	2.02	0.42
1:A:465:GLU:HA	1:B:438:GLN:OE1	2.19	0.42
1:B:4:TYR:O	1:B:152:THR:HA	2.20	0.42
1:A:159:THR:HG21	1:A:293:LEU:HD21	2.02	0.42
1:B:83:ASP:OD1	1:B:85:GLU:HG2	2.20	0.42
1:A:339:ASN:OD1	1:A:356:THR:HG23	2.20	0.42
1:B:230:ASP:OD1	1:B:233:LEU:HD13	2.20	0.42
1:B:282:LEU:HB3	1:B:284:ILE:CD1	2.50	0.42
1:A:98:LYS:HE3	1:A:98:LYS:HB3	1.89	0.42
1:B:476:PHE:CD1	1:B:476:PHE:N	2.87	0.42
1:B:28:LYS:HE3	1:B:349:PHE:CD1	2.55	0.41
1:B:230:ASP:O	1:B:234:ARG:HG3	2.20	0.41
1:A:395:PHE:CD1	1:A:395:PHE:N	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:LEU:HD13	1:A:109:TYR:HB3	2.02	0.41
1:A:109:TYR:O	1:A:112:MET:HB3	2.19	0.41
1:B:2:ARG:HH11	1:B:2:ARG:HG3	1.84	0.41
1:B:59:LYS:HD2	1:B:60:LYS:N	2.35	0.41
1:A:137:ARG:HH22	1:A:294:GLN:HE22	1.67	0.41
1:B:51:CYS:HB3	3:B:553:HOH:O	2.20	0.41
1:B:137:ARG:NH2	1:B:294:GLN:HE22	2.17	0.41
1:A:88:ARG:N	1:B:81:GLU:O	2.46	0.41
1:B:121:PHE:C	1:B:122:HIS:CD2	2.99	0.41
1:A:386:ASP:OD1	1:A:479:LYS:HG3	2.20	0.40
1:B:125:PHE:CE2	1:B:140:ALA:HB2	2.56	0.40
1:B:137:ARG:NH1	1:B:142:PRO:HA	2.37	0.40
1:B:253:ASN:OD1	1:B:254:PRO:HD2	2.22	0.40
1:B:411:MET:O	1:B:428:MET:HA	2.21	0.40
1:B:113:PHE:HE1	1:B:119:LEU:HD22	1.83	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	485/490 (99%)	463 (96%)	20 (4%)	2 (0%)	30	27
1	B	482/490 (98%)	453 (94%)	27 (6%)	2 (0%)	30	27
All	All	967/980 (99%)	916 (95%)	47 (5%)	4 (0%)	30	27

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	131	ASN
1	B	264	THR
1	A	319	ASP

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Mol	Chain	Res	Type
1	B	2	ARG

### 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	390/393 (99%)	355 (91%)	35 (9%)	9 6
1	B	387/393 (98%)	354 (92%)	33 (8%)	10 7
All	All	777/786 (99%)	709 (91%)	68 (9%)	9 6

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LYS
1	A	28	LYS
1	A	29	ARG
1	A	30	VAL
1	A	35	LEU
1	A	38	HIS
1	A	47	LEU
1	A	56	CYS
1	A	59	LYS
1	A	82	LEU
1	A	86	SER
1	A	100	LYS
1	A	117	GLU
1	A	120	THR
1	A	134	VAL
1	A	136	VAL
1	A	139	SER
1	A	188	LYS
1	A	212	ARG
1	A	216	VAL
1	A	221	ARG
1	A	227	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	250	THR
1	A	267	VAL
1	A	318	VAL
1	A	333	LEU
1	A	334	THR
1	A	354	ARG
1	A	368	ILE
1	A	406	THR
1	A	415	VAL
1	A	444	LEU
1	A	479	LYS
1	A	483	VAL
1	A	484	GLU
1	B	1	SER
1	B	6	LEU
1	B	24	SER
1	B	28	LYS
1	B	56	CYS
1	B	82	LEU
1	B	84	ARG
1	B	85	GLU
1	B	115	ASP
1	B	119	LEU
1	B	166	LEU
1	B	169	GLU
1	B	237	LEU
1	B	239	GLU
1	B	250	THR
1	B	258	THR
1	B	265	ARG
1	B	280	VAL
1	B	301	GLU
1	B	302	VAL
1	B	334	THR
1	B	348	VAL
1	B	354	ARG
1	B	367	SER
1	B	369	PRO
1	B	373	VAL
1	B	377	VAL
1	B	388	VAL
1	B	398	LEU

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Mol	Chain	Res	Type
1	B	424	LEU
1	B	439	SER
1	B	444	LEU
1	B	482	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	HIS
1	A	38	HIS
1	A	67	ASN
1	A	123	GLN
1	A	129	GLN
1	A	401	ASN
1	B	26	HIS
1	B	207	ASN
1	B	247	ASN
1	B	294	GLN
1	B	401	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 oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

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	499	-	58,58,58	1.82	21 (36%)	85,89,89	0.97	6 (7%)
2	FAD	A	499	-	58,58,58	2.57	16 (27%)	85,89,89	0.99	3 (3%)

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	499	-	-	3/34/50/50	0/6/6/6
2	FAD	A	499	-	-	3/34/50/50	0/6/6/6

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	499	FAD	P-O3P	-12.65	1.45	1.59
2	A	499	FAD	C9A-N10	-5.38	1.31	1.41
2	A	499	FAD	C8-C7	5.31	1.53	1.40
2	B	499	FAD	C1'-C2'	-4.39	1.46	1.52
2	A	499	FAD	C5A-N7A	-4.05	1.31	1.39
2	A	499	FAD	C9-C8	-3.78	1.34	1.39
2	B	499	FAD	C9-C8	3.73	1.44	1.39
2	A	499	FAD	C7M-C7	-3.55	1.44	1.51
2	A	499	FAD	C6-C7	-3.38	1.35	1.39
2	A	499	FAD	C5'-C4'	-3.36	1.47	1.51
2	A	499	FAD	PA-O2A	-3.20	1.40	1.55
2	B	499	FAD	C8-C7	3.19	1.48	1.40
2	B	499	FAD	C10-N10	3.01	1.43	1.37
2	B	499	FAD	O3'-C3'	-2.95	1.35	1.43
2	A	499	FAD	PA-O3P	2.91	1.62	1.59
2	A	499	FAD	C2-N3	2.90	1.45	1.39
2	B	499	FAD	C4'-C3'	-2.89	1.48	1.53
2	B	499	FAD	C4X-N5	2.88	1.37	1.30
2	A	499	FAD	PA-O5B	-2.68	1.48	1.59
2	B	499	FAD	C2'-C3'	2.60	1.58	1.53
2	B	499	FAD	O5'-C5'	2.57	1.54	1.44
2	B	499	FAD	PA-O3P	2.55	1.62	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	499	FAD	C9A-C5X	2.48	1.45	1.41
2	B	499	FAD	C6-C7	-2.47	1.36	1.39
2	B	499	FAD	P-O5'	-2.44	1.49	1.59
2	A	499	FAD	C2A-N1A	2.41	1.38	1.33
2	B	499	FAD	C8A-N9A	2.34	1.41	1.37
2	B	499	FAD	O4B-C1B	2.26	1.47	1.42
2	B	499	FAD	C2B-C1B	-2.23	1.46	1.53
2	A	499	FAD	C5X-N5	-2.22	1.35	1.39
2	B	499	FAD	P-O3P	2.15	1.61	1.59
2	B	499	FAD	C8M-C8	2.15	1.55	1.51
2	B	499	FAD	PA-O2A	-2.10	1.45	1.55
2	A	499	FAD	C9A-C5X	2.08	1.44	1.41
2	B	499	FAD	C1B-N9A	-2.08	1.40	1.46
2	A	499	FAD	P-O1P	-2.06	1.43	1.50
2	B	499	FAD	PA-O1A	-2.02	1.43	1.50

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	499	FAD	C5A-N7A-C8A	3.57	109.06	103.45
2	A	499	FAD	C4-N3-C2	-2.62	120.99	125.64
2	B	499	FAD	C4-N3-C2	-2.47	121.25	125.64
2	B	499	FAD	C5A-N7A-C8A	2.37	107.18	103.45
2	B	499	FAD	C4A-C5A-N7A	-2.37	107.87	110.58
2	A	499	FAD	C4A-C5A-N7A	-2.30	107.95	110.58
2	B	499	FAD	C5A-C4A-N9A	2.09	108.09	105.81
2	B	499	FAD	C4X-C10-N10	2.03	119.39	116.48
2	B	499	FAD	N9A-C8A-N7A	-2.02	111.07	113.94

There are no chirality outliers.

All (6) torsion outliers are listed below:

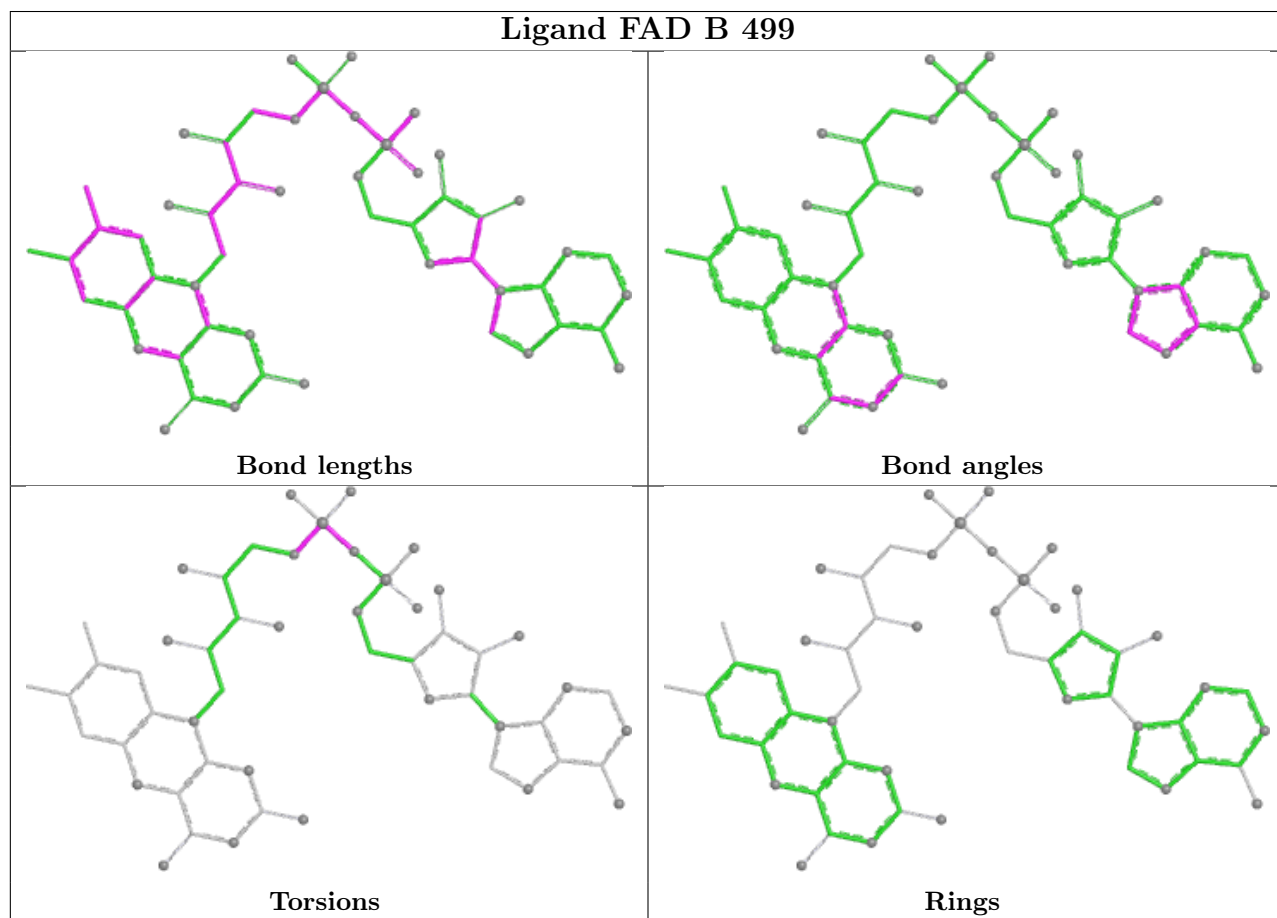
Mol	Chain	Res	Type	Atoms
2	A	499	FAD	PA-O3P-P-O5'
2	B	499	FAD	PA-O3P-P-O5'
2	B	499	FAD	C5'-O5'-P-O2P
2	B	499	FAD	PA-O3P-P-O2P
2	A	499	FAD	O4B-C4B-C5B-O5B
2	A	499	FAD	PA-O3P-P-O2P

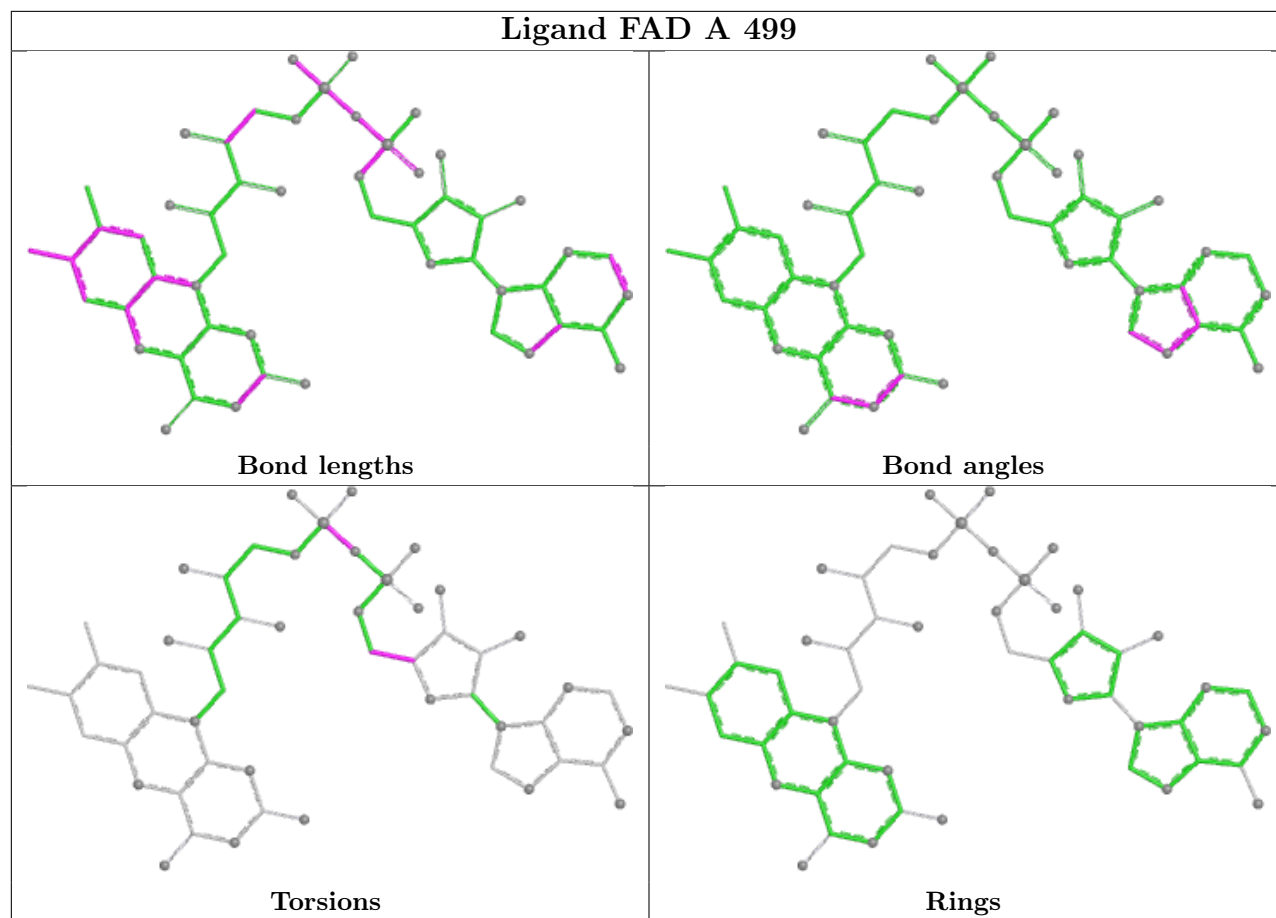
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	499	FAD	2	0
2	A	499	FAD	3	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 [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	487/490 (99%)	-0.67	1 (0%) 91 90	7, 25, 56, 89	0
1	B	484/490 (98%)	-0.60	0 100 100	8, 27, 56, 90	0
All	All	971/980 (99%)	-0.63	1 (0%) 92 91	7, 26, 57, 90	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	SER	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 oligosaccharides in this entry.

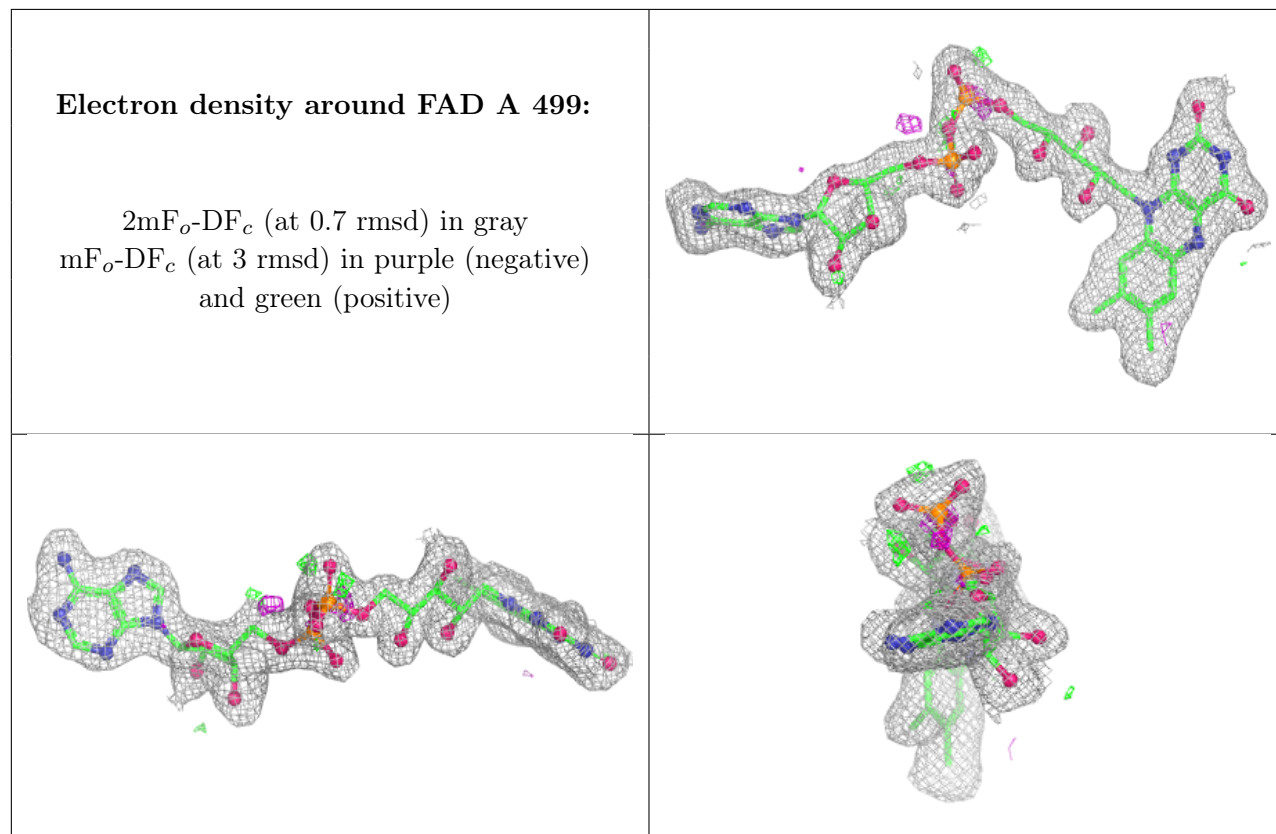
### 6.4 Ligands [i](#)

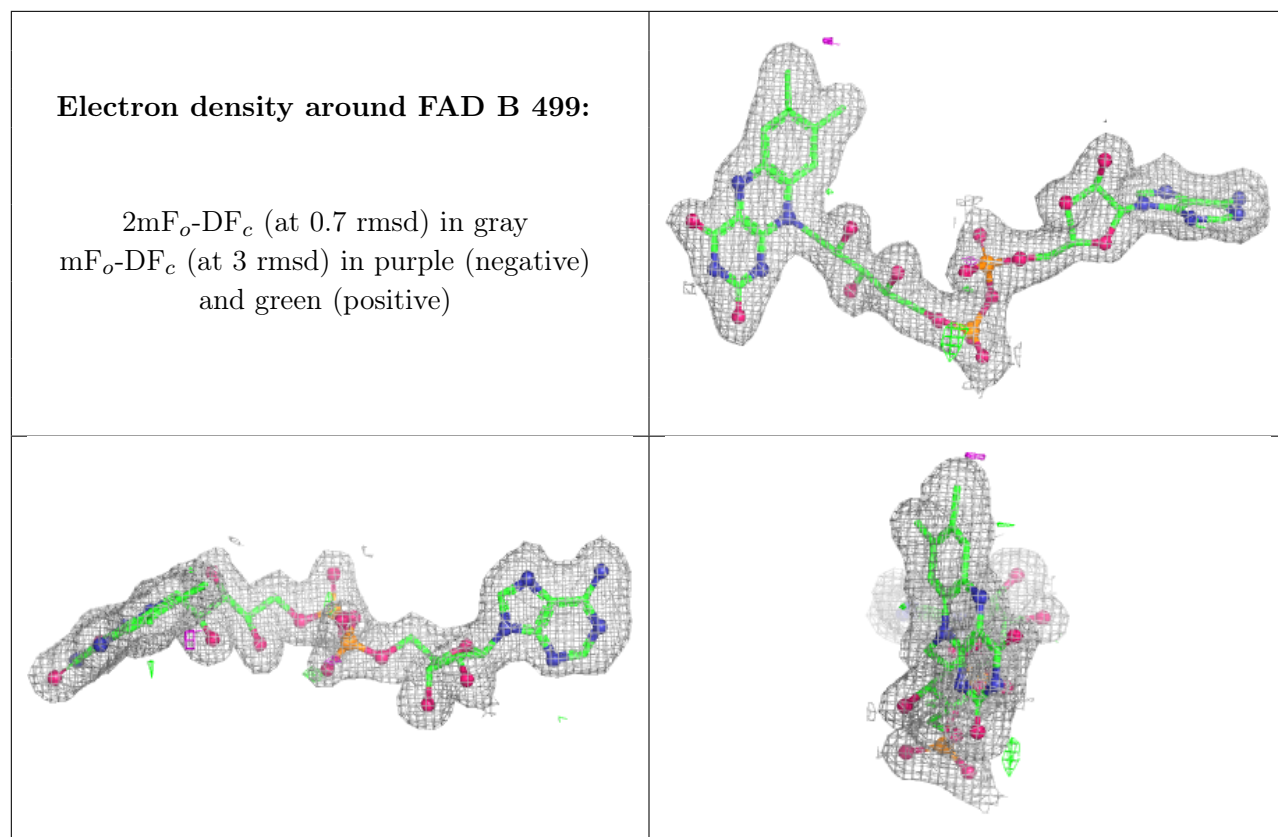
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 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
2	FAD	A	499	53/53	0.97	0.04	6,18,24,29	0
2	FAD	B	499	53/53	0.98	0.04	6,15,20,21	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.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.