



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 10:56 am GMT

PDB ID : 1TYT  
Title : CRYSTAL AND MOLECULAR STRUCTURE OF CRITHIDIA FASCICULATA TRYPTOPHAN REDUCTASE AT 2.6 ANGSTROMS RESOLUTION  
Authors : Bailey, S.; Hunter, W.N.  
Deposited on : 1993-06-10  
Resolution : 2.60 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

<http://wwpdb.org/validation/2016/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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

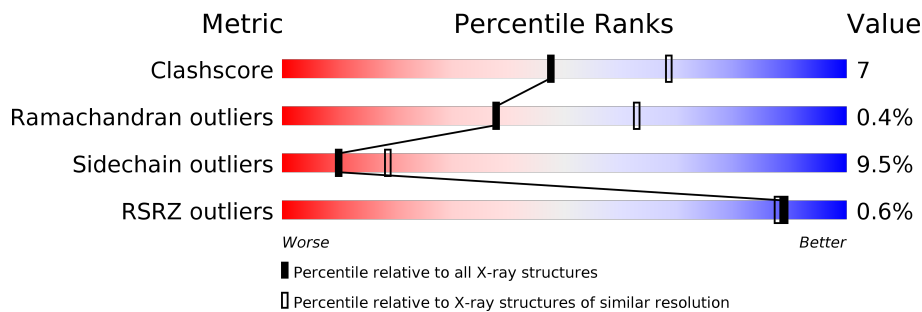
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

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. 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	487	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>71%</span> <span>23%</span> <span>6%</span> </div> </div>
1	B	487	<div> <div style="width: 100%; height: 10px; background-color: green;"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>72%</span> <span>22%</span> <span>5%</span> </div> </div>

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	A	493	X	-	-	-
2	FAD	B	493	X	-	-	-

## 2 Entry composition [i](#)

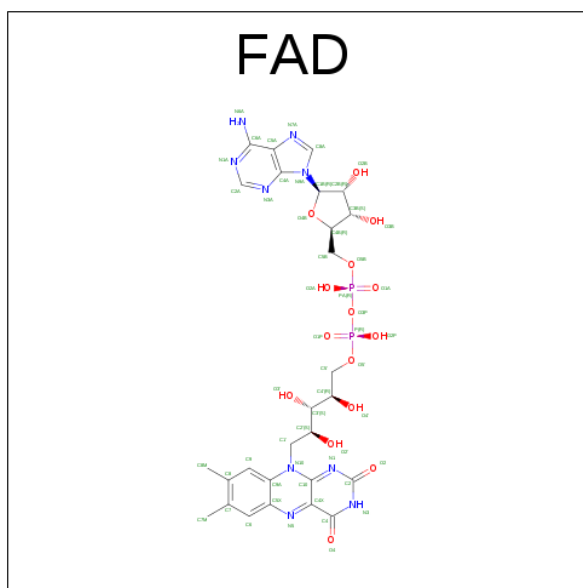
There are 3 unique types of molecules in this entry. The entry contains 7908 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 TRYPTANOTHIONE REDUCTASE, OXIDIZED FORM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	487	Total	C	N	O	S	0	0	0
			3710	2334	644	711	21			
1	B	486	Total	C	N	O	S	0	0	0
			3702	2329	643	710	20			

- 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
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		

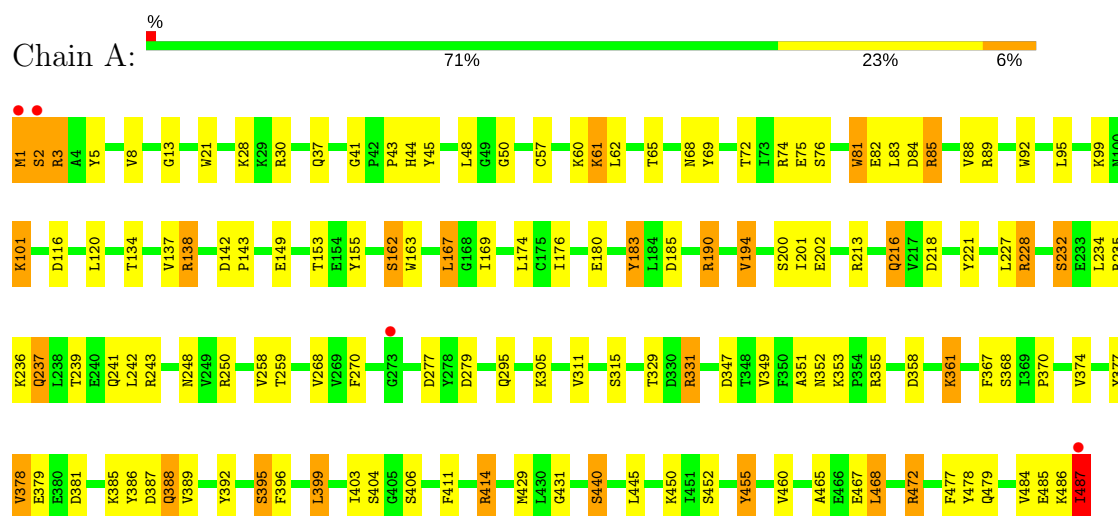
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	213	Total 213	O 213	0	0
3	B	177	Total 177	O 177	0	0

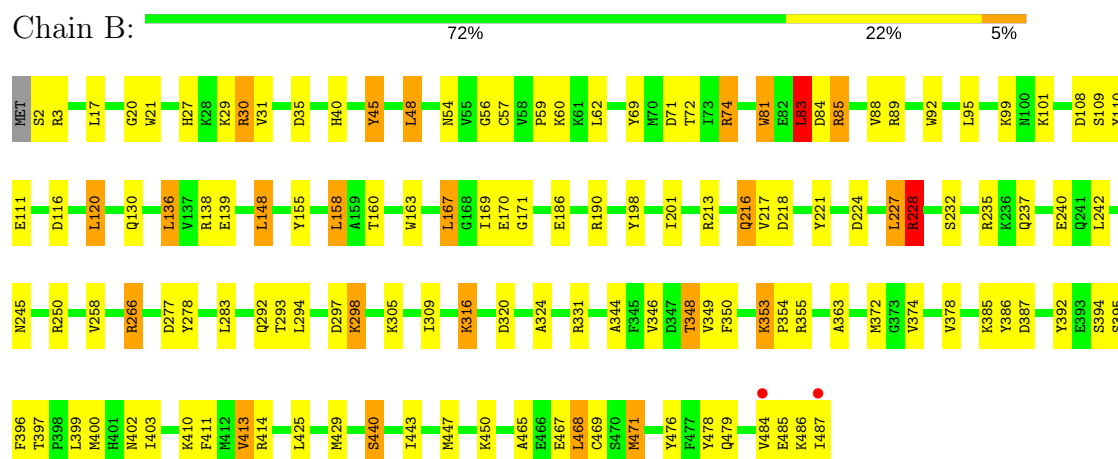
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: TRYPTANOTHIONE REDUCTASE, OXIDIZED FORM



#### • Molecule 1: TRYPTANOTHIONE REDUCTASE, OXIDIZED FORM



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	128.80Å 128.80Å 92.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.60 43.53 – 2.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.60) 58.2 (43.53-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.80 (at 2.61Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.161 , (Not available) 0.164 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	22.4	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 63.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.044 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7908	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.71% 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	0.96	6/3783 (0.2%)	1.68	66/5124 (1.3%)
1	B	0.92	5/3775 (0.1%)	1.71	79/5114 (1.5%)
All	All	0.94	11/7558 (0.1%)	1.69	145/10238 (1.4%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	395	SER	CA-CB	-13.23	1.33	1.52
1	A	138	ARG	CZ-NH1	8.87	1.44	1.33
1	A	162	SER	CA-CB	-6.27	1.43	1.52
1	A	468	LEU	CB-CG	-5.79	1.35	1.52
1	B	394	SER	CA-CB	-5.65	1.44	1.52
1	B	83	LEU	CB-CG	-5.46	1.36	1.52
1	B	218	ASP	CA-CB	-5.42	1.42	1.53
1	B	374	VAL	CB-CG1	-5.22	1.41	1.52
1	B	148	LEU	CB-CG	-5.21	1.37	1.52
1	A	82	GLU	CB-CG	-5.06	1.42	1.52
1	A	194	VAL	CA-CB	5.01	1.65	1.54

All (145) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	414	ARG	NE-CZ-NH2	-13.35	113.63	120.30
1	A	138	ARG	NE-CZ-NH1	12.52	126.56	120.30
1	B	414	ARG	NE-CZ-NH1	11.73	126.16	120.30
1	B	331	ARG	NE-CZ-NH1	11.59	126.09	120.30
1	B	136	LEU	CA-CB-CG	11.33	141.37	115.30
1	A	138	ARG	NE-CZ-NH2	-10.47	115.06	120.30
1	A	190	ARG	NE-CZ-NH2	-10.06	115.27	120.30
1	B	402	ASN	CB-CA-C	-9.89	90.62	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	402	ASN	CA-CB-CG	9.70	134.75	113.40
1	A	414	ARG	NE-CZ-NH1	9.51	125.05	120.30
1	B	81	TRP	CD1-CG-CD2	9.40	113.82	106.30
1	A	1	MET	CA-CB-CG	9.35	129.19	113.30
1	A	355	ARG	NE-CZ-NH1	9.16	124.88	120.30
1	B	3	ARG	NE-CZ-NH2	-9.15	115.73	120.30
1	A	414	ARG	NE-CZ-NH2	-8.99	115.80	120.30
1	B	92	TRP	CD1-CG-CD2	8.96	113.47	106.30
1	B	163	TRP	CD1-CG-CD2	8.89	113.41	106.30
1	B	74	ARG	NE-CZ-NH1	8.88	124.74	120.30
1	B	478	TYR	CB-CG-CD2	-8.85	115.69	121.00
1	B	138	ARG	NE-CZ-NH1	8.84	124.72	120.30
1	A	89	ARG	NE-CZ-NH2	-8.78	115.91	120.30
1	A	155	TYR	CB-CG-CD1	-8.72	115.77	121.00
1	B	402	ASN	N-CA-CB	8.59	126.06	110.60
1	B	213	ARG	NE-CZ-NH2	-8.45	116.08	120.30
1	A	81	TRP	CD1-CG-CD2	8.42	113.04	106.30
1	A	84	ASP	CB-CG-OD1	8.32	125.79	118.30
1	A	392	TYR	CB-CG-CD2	-8.28	116.03	121.00
1	B	92	TRP	CE2-CD2-CG	-8.20	100.74	107.30
1	A	74	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	B	30	ARG	NE-CZ-NH1	8.00	124.30	120.30
1	B	81	TRP	CE2-CD2-CG	-7.91	100.97	107.30
1	B	331	ARG	NE-CZ-NH2	-7.90	116.35	120.30
1	A	331	ARG	NE-CZ-NH1	7.79	124.19	120.30
1	B	476	TYR	CB-CG-CD1	-7.65	116.41	121.00
1	B	167	LEU	CA-CB-CG	7.65	132.89	115.30
1	B	163	TRP	CE2-CD2-CG	-7.52	101.28	107.30
1	B	218	ASP	CB-CG-OD1	7.49	125.04	118.30
1	A	81	TRP	CE2-CD2-CG	-7.47	101.32	107.30
1	B	429	MET	CG-SD-CE	-7.46	88.26	100.20
1	A	84	ASP	CB-CG-OD2	-7.45	111.60	118.30
1	A	163	TRP	CG-CD2-CE3	7.44	140.59	133.90
1	A	163	TRP	CD1-CG-CD2	7.34	112.18	106.30
1	A	163	TRP	CE2-CD2-CG	-7.33	101.43	107.30
1	A	92	TRP	CD1-CG-CD2	7.31	112.15	106.30
1	B	250	ARG	NE-CZ-NH2	-7.28	116.66	120.30
1	A	190	ARG	NE-CZ-NH1	7.18	123.89	120.30
1	B	136	LEU	N-CA-CB	-7.13	96.13	110.40
1	B	74	ARG	CG-CD-NE	7.12	126.75	111.80
1	B	228	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	A	92	TRP	CE2-CD2-CG	-7.04	101.67	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	395	SER	N-CA-CB	-7.01	99.99	110.50
1	A	21	TRP	CE2-CD2-CG	-6.96	101.73	107.30
1	B	228	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	A	61	LYS	CA-CB-CG	-6.87	98.29	113.40
1	A	228	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	A	270	PHE	CB-CG-CD1	-6.82	116.03	120.80
1	A	228	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	A	349	VAL	CG1-CB-CG2	-6.77	100.06	110.90
1	A	21	TRP	CD1-CG-CD2	6.72	111.68	106.30
1	B	89	ARG	NE-CZ-NH1	6.65	123.62	120.30
1	B	278	TYR	CB-CG-CD2	-6.64	117.01	121.00
1	B	402	ASN	CB-CG-ND2	6.62	132.60	116.70
1	A	174	LEU	CA-CB-CG	6.57	130.41	115.30
1	B	21	TRP	CD1-CG-CD2	6.54	111.53	106.30
1	B	218	ASP	CB-CG-OD2	-6.53	112.42	118.30
1	B	138	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	B	81	TRP	CG-CD1-NE1	-6.37	103.73	110.10
1	B	190	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	B	190	ARG	CG-CD-NE	-6.32	98.53	111.80
1	B	213	ARG	NE-CZ-NH1	6.29	123.45	120.30
1	B	21	TRP	CE2-CD2-CG	-6.26	102.29	107.30
1	B	30	ARG	NE-CZ-NH2	-6.25	117.18	120.30
1	A	270	PHE	CB-CG-CD2	6.24	125.17	120.80
1	A	455	TYR	CB-CG-CD2	-6.14	117.32	121.00
1	A	241	GLN	CA-CB-CG	-6.12	99.93	113.40
1	B	190	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	A	429	MET	CG-SD-CE	-6.03	90.55	100.20
1	B	155	TYR	CB-CG-CD1	-6.03	117.38	121.00
1	A	250	ARG	NE-CZ-NH2	-6.01	117.29	120.30
1	B	163	TRP	CG-CD1-NE1	-6.01	104.09	110.10
1	B	186	GLU	CA-CB-CG	5.99	126.57	113.40
1	B	120	LEU	CA-CB-CG	5.95	128.99	115.30
1	A	374	VAL	N-CA-CB	-5.93	98.46	111.50
1	A	388	GLN	CA-CB-CG	5.92	126.43	113.40
1	A	85	ARG	NE-CZ-NH2	-5.89	117.35	120.30
1	B	250	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	B	447	MET	CG-SD-CE	-5.89	90.77	100.20
1	B	110	TYR	CB-CG-CD2	-5.88	117.47	121.00
1	B	250	ARG	CB-CG-CD	-5.85	96.38	111.60
1	A	468	LEU	CB-CG-CD2	-5.83	101.09	111.00
1	A	213	ARG	CA-C-N	5.77	127.73	116.20
1	A	487	ILE	N-CA-C	5.76	126.55	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	387	ASP	CA-CB-CG	5.72	125.99	113.40
1	B	120	LEU	CB-CG-CD1	-5.70	101.32	111.00
1	B	378	VAL	N-CA-CB	-5.69	98.98	111.50
1	B	469	CYS	CA-CB-SG	-5.68	103.77	114.00
1	B	27	HIS	CA-CB-CG	-5.68	103.94	113.60
1	A	81	TRP	CG-CD1-NE1	-5.67	104.43	110.10
1	B	92	TRP	CG-CD2-CE3	5.64	138.98	133.90
1	A	358	ASP	CB-CG-OD2	-5.60	113.26	118.30
1	B	120	LEU	CA-C-N	5.59	129.51	117.20
1	B	266	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	B	84	ASP	CB-CG-OD1	5.59	123.33	118.30
1	A	74	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	A	386	TYR	CB-CG-CD1	-5.57	117.66	121.00
1	B	346	VAL	CG1-CB-CG2	-5.56	102.00	110.90
1	B	392	TYR	CB-CG-CD2	-5.49	117.71	121.00
1	B	221	TYR	CB-CG-CD2	-5.45	117.73	121.00
1	B	471	MET	CG-SD-CE	-5.42	91.53	100.20
1	A	235	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	B	136	LEU	CB-CA-C	5.39	120.44	110.20
1	A	174	LEU	CB-CG-CD2	-5.39	101.84	111.00
1	B	81	TRP	CG-CD2-CE3	5.38	138.74	133.90
1	A	213	ARG	O-C-N	-5.36	114.08	123.20
1	B	277	ASP	CB-CG-OD1	-5.35	113.48	118.30
1	B	348	THR	CA-CB-CG2	5.33	119.86	112.40
1	A	202	GLU	OE1-CD-OE2	-5.33	116.91	123.30
1	B	83	LEU	CA-CB-CG	5.32	127.53	115.30
1	A	378	VAL	N-CA-CB	-5.31	99.81	111.50
1	B	81	TRP	CB-CG-CD1	-5.31	120.10	127.00
1	A	69	TYR	CG-CD2-CE2	-5.27	117.09	121.30
1	B	92	TRP	CG-CD1-NE1	-5.25	104.85	110.10
1	A	163	TRP	CB-CG-CD1	-5.24	120.18	127.00
1	A	138	ARG	CB-CG-CD	-5.24	97.98	111.60
1	B	349	VAL	CG1-CB-CG2	-5.20	102.58	110.90
1	A	361	LYS	CA-CB-CG	-5.18	102.01	113.40
1	B	45	TYR	CA-CB-CG	-5.15	103.61	113.40
1	B	186	GLU	CB-CA-C	-5.14	100.13	110.40
1	A	237	GLN	OE1-CD-NE2	-5.13	110.09	121.90
1	A	486	LYS	CA-CB-CG	-5.13	102.11	113.40
1	A	183	TYR	CB-CG-CD1	-5.10	117.94	121.00
1	B	48	LEU	CA-CB-CG	5.10	127.04	115.30
1	A	1	MET	CG-SD-CE	5.10	108.36	100.20
1	B	92	TRP	CB-CG-CD1	-5.10	120.37	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	92	TRP	CG-CD2-CE3	5.09	138.48	133.90
1	A	89	ARG	CA-CB-CG	5.07	124.55	113.40
1	A	472	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	B	425	LEU	CA-CB-CG	5.05	126.91	115.30
1	A	167	LEU	CA-CB-CG	5.04	126.90	115.30
1	A	486	LYS	N-CA-C	5.03	124.57	111.00
1	B	109	SER	CA-CB-OG	-5.03	97.63	111.20
1	A	85	ARG	CG-CD-NE	-5.01	101.28	111.80
1	B	148	LEU	CB-CG-CD2	-5.01	102.48	111.00
1	B	198	TYR	CB-CG-CD2	-5.01	117.99	121.00
1	A	82	GLU	CG-CD-OE2	-5.01	108.28	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3710	0	3657	60	0
1	B	3702	0	3645	54	0
2	A	53	0	31	0	0
2	B	53	0	31	2	0
3	A	213	0	0	6	0
3	B	177	0	0	4	0
All	All	7908	0	7364	104	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 7.

All (104) 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:396:PHE:CE1	1:A:467:GLU:HG3	2.18	0.79
1:B:237:GLN:HG2	3:B:643:HOH:O	1.89	0.71
1:B:228:ARG:HH11	1:B:228:ARG:HB2	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:GLN:HB2	1:A:484:VAL:HG21	1.77	0.66
1:B:353:LYS:NZ	1:B:355:ARG:HD3	2.11	0.66
1:A:101:LYS:NZ	1:B:403:ILE:HG12	2.11	0.65
1:B:344:ALA:HA	1:B:355:ARG:HE	1.62	0.65
1:A:347:ASP:HA	1:A:351:ALA:HB3	1.78	0.64
1:A:388:GLN:HA	1:A:487:ILE:HD11	1.80	0.64
1:B:201:ILE:HD12	1:B:227:LEU:HD13	1.80	0.63
1:B:316:LYS:HE3	1:B:320:ASP:HA	1.82	0.62
1:B:130:GLN:HB2	1:B:136:LEU:HD22	1.82	0.62
1:B:108:ASP:HA	1:B:111:GLU:HG2	1.86	0.58
1:A:62:LEU:HD22	1:B:403:ILE:HD12	1.86	0.57
1:A:65:THR:HG21	1:B:400:MET:HG3	1.86	0.57
1:B:158:LEU:HD13	1:B:309:ILE:HD13	1.85	0.57
1:A:138:ARG:NH2	1:A:295:GLN:HE22	2.04	0.56
1:A:361:LYS:HD2	1:A:445:LEU:HB3	1.87	0.56
1:A:477:PHE:CD2	1:A:487:ILE:HG21	2.42	0.55
1:A:138:ARG:HD2	3:A:658:HOH:O	2.05	0.55
1:A:228:ARG:HG2	3:A:666:HOH:O	2.06	0.55
1:A:75:GLU:HG2	1:A:404:SER:HB2	1.89	0.55
1:B:397:THR:OG1	1:B:410:LYS:HD2	2.06	0.55
1:B:353:LYS:HZ2	1:B:355:ARG:HD3	1.72	0.54
1:B:158:LEU:HD12	1:B:324:ALA:HB2	1.90	0.54
1:A:477:PHE:HB3	1:A:487:ILE:HD13	1.90	0.53
1:B:240:GLU:HG2	3:B:607:HOH:O	2.08	0.53
1:B:167:LEU:HD23	1:B:283:LEU:HD22	1.91	0.53
1:B:465:ALA:O	1:B:468:LEU:HB2	2.09	0.53
1:A:72:THR:HG21	3:A:549:HOH:O	2.09	0.52
1:A:138:ARG:HH22	1:A:295:GLN:HE22	1.56	0.52
1:A:76:SER:HB2	1:A:81:TRP:HB2	1.91	0.52
1:B:293:THR:HG21	3:B:525:HOH:O	2.10	0.51
1:A:5:TYR:CD1	1:A:30:ARG:HG2	2.45	0.51
1:B:81:TRP:O	1:B:85:ARG:NH2	2.43	0.51
1:A:403:ILE:HD12	1:B:62:LEU:HD22	1.91	0.51
1:A:101:LYS:HZ3	1:B:403:ILE:HG12	1.74	0.51
1:B:160:THR:HG21	1:B:294:LEU:HD21	1.93	0.51
1:A:329:THR:HB	1:A:331:ARG:HD2	1.94	0.50
1:B:228:ARG:HD2	3:B:657:HOH:O	2.12	0.50
1:A:8:VAL:HG23	1:A:153:THR:HB	1.93	0.50
1:B:40:HIS:HB3	1:B:54:ASN:OD1	2.11	0.50
1:A:1:MET:HB2	1:A:3:ARG:O	2.11	0.50
1:A:399:LEU:HD13	1:B:62:LEU:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:SER:HB2	1:B:440:SER:HB2	1.93	0.49
1:B:385:LYS:HB2	1:B:386:TYR:CD1	2.47	0.49
1:B:353:LYS:HZ3	1:B:355:ARG:HD3	1.78	0.49
1:B:413:VAL:HG13	1:B:471:MET:HE1	1.95	0.49
1:A:137:VAL:HB	1:A:149:GLU:HB2	1.94	0.49
1:A:88:VAL:HG22	1:B:83:LEU:CD1	2.43	0.48
1:B:29:LYS:HE2	1:B:350:PHE:CD1	2.47	0.48
1:A:101:LYS:HZ1	1:B:403:ILE:HG12	1.79	0.47
1:B:35:ASP:OD2	2:B:493:FAD:H3B	2.14	0.47
1:A:379:GLU:OE2	1:A:414:ARG:NH2	2.48	0.47
1:A:83:LEU:HB3	1:B:88:VAL:HG22	1.97	0.46
1:B:59:PRO:HB3	1:B:99:LYS:HD2	1.97	0.46
1:A:347:ASP:HB3	1:A:353:LYS:O	2.14	0.46
1:A:377:TYR:HA	3:A:628:HOH:O	2.16	0.46
1:A:239:THR:O	1:A:243:ARG:HG3	2.15	0.46
1:A:1:MET:HB3	1:A:2:SER:H	1.49	0.46
1:B:20:GLY:HA2	1:B:31:VAL:HG11	1.98	0.45
1:A:138:ARG:HH22	1:A:295:GLN:NE2	2.13	0.45
1:B:298:LYS:HB3	1:B:298:LYS:HZ2	1.81	0.45
1:A:258:VAL:HG22	1:A:268:VAL:HG22	1.99	0.45
1:A:232:SER:O	1:A:236:LYS:HG3	2.16	0.45
1:A:37:GLN:OE1	1:A:44:HIS:HB2	2.17	0.45
1:B:396:PHE:CE1	1:B:467:GLU:HG3	2.52	0.45
1:B:17:LEU:HD12	1:B:17:LEU:HA	1.84	0.44
1:A:167:LEU:HB3	1:A:169:ILE:HG12	2.00	0.44
1:B:29:LYS:HE2	1:B:350:PHE:HD1	1.82	0.44
1:B:395:SER:HA	1:B:411:PHE:O	2.18	0.44
1:A:142:ASP:HA	1:A:143:PRO:HD2	1.73	0.43
1:A:81:TRP:O	1:A:85:ARG:NH2	2.52	0.43
1:B:232:SER:HA	1:B:235:ARG:HD3	2.00	0.43
1:A:460:VAL:HG22	1:B:363:ALA:HB3	2.00	0.43
1:B:69:TYR:HA	1:B:72:THR:OG1	2.18	0.43
1:A:201:ILE:HG22	1:A:368:SER:HB3	1.99	0.43
1:B:385:LYS:HB2	1:B:386:TYR:CE1	2.54	0.43
1:B:216:GLN:HG3	1:B:217:VAL:N	2.34	0.43
1:B:348:THR:OG1	1:B:354:PRO:HA	2.19	0.43
1:B:74:ARG:NH2	1:B:245:ASN:OD1	2.51	0.43
1:A:190:ARG:HA	1:A:216:GLN:O	2.19	0.42
1:A:176:ILE:HB	1:A:180:GLU:HB2	2.01	0.42
1:A:13:GLY:HA2	1:A:50:GLY:HA3	2.01	0.42
1:B:171:GLY:HA3	1:B:258:VAL:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:GLN:HA	3:A:674:HOH:O	2.18	0.42
1:B:56:GLY:O	1:B:59:PRO:HD2	2.20	0.42
1:A:311:VAL:HB	1:A:315:SER:HA	2.01	0.42
1:A:411:PHE:CD1	1:A:431:GLY:HA3	2.55	0.42
1:A:465:ALA:O	1:A:468:LEU:HB2	2.20	0.42
1:B:139:GLU:N	1:B:148:LEU:HD13	2.35	0.42
1:A:43:PRO:HG2	1:A:44:HIS:CD2	2.55	0.42
2:B:493:FAD:H9	2:B:493:FAD:H1'1	1.88	0.42
1:A:138:ARG:NH1	1:A:143:PRO:HA	2.35	0.41
1:A:44:HIS:O	1:A:45:TYR:HB2	2.20	0.41
1:A:218:ASP:OD1	1:A:248:ASN:HB3	2.20	0.41
1:A:389:VAL:HB	1:A:478:TYR:HB2	2.03	0.41
1:A:41:GLY:HA2	1:A:183:TYR:CZ	2.56	0.41
1:B:479:GLN:HB2	1:B:484:VAL:HG11	2.02	0.41
1:A:295:GLN:NE2	3:A:653:HOH:O	2.55	0.40
1:A:455:TYR:HB2	1:A:472:ARG:NH1	2.36	0.40
1:B:443:ILE:HG21	1:B:443:ILE:HD13	1.85	0.40
1:A:221:TYR:OH	1:A:228:ARG:HD2	2.22	0.40
1:A:61:LYS:HE3	1:A:367:PHE:CE1	2.56	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	485/487 (100%)	456 (94%)	28 (6%)	1 (0%)	51	76
1	B	484/487 (99%)	465 (96%)	16 (3%)	3 (1%)	28	53
All	All	969/974 (100%)	921 (95%)	44 (4%)	4 (0%)	38	63

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	485	GLU
1	A	352	ASN
1	B	45	TYR
1	B	169	ILE

### 5.3.2 Protein sidechains ⓘ

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	390/390 (100%)	350 (90%)	40 (10%)	8	15
1	B	389/390 (100%)	355 (91%)	34 (9%)	12	23
All	All	779/780 (100%)	705 (90%)	74 (10%)	10	19

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	3	ARG
1	A	28	LYS
1	A	48	LEU
1	A	57	CYS
1	A	60	LYS
1	A	68	ASN
1	A	95	LEU
1	A	99	LYS
1	A	101	LYS
1	A	116	ASP
1	A	120	LEU
1	A	134	THR
1	A	162	SER
1	A	185	ASP
1	A	194	VAL
1	A	200	SER
1	A	216	GLN
1	A	227	LEU
1	A	232	SER

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Mol	Chain	Res	Type
1	A	234	LEU
1	A	237	GLN
1	A	242	LEU
1	A	259	THR
1	A	277	ASP
1	A	279	ASP
1	A	305	LYS
1	A	370	PRO
1	A	378	VAL
1	A	381	ASP
1	A	385	LYS
1	A	387	ASP
1	A	395	SER
1	A	399	LEU
1	A	406	SER
1	A	440	SER
1	A	450	LYS
1	A	452	SER
1	A	485	GLU
1	A	487	ILE
1	B	2	SER
1	B	30	ARG
1	B	48	LEU
1	B	57	CYS
1	B	60	LYS
1	B	71	ASP
1	B	83	LEU
1	B	85	ARG
1	B	95	LEU
1	B	101	LYS
1	B	116	ASP
1	B	120	LEU
1	B	158	LEU
1	B	170	GLU
1	B	216	GLN
1	B	224	ASP
1	B	227	LEU
1	B	228	ARG
1	B	242	LEU
1	B	266	ARG
1	B	292	GLN
1	B	297	ASP

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Mol	Chain	Res	Type
1	B	298	LYS
1	B	305	LYS
1	B	316	LYS
1	B	353	LYS
1	B	372	MET
1	B	399	LEU
1	B	413	VAL
1	B	440	SER
1	B	450	LYS
1	B	468	LEU
1	B	486	LYS
1	B	487	ILE

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

Mol	Chain	Res	Type
1	A	39	HIS
1	A	68	ASN
1	A	179	ASN
1	B	179	ASN
1	B	292	GLN
1	B	419	HIS
1	B	479	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 carbohydrates 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	A	493	-	51,58,58	1.33	4 (7%)	54,89,89	2.37	11 (20%)
2	FAD	B	493	-	51,58,58	1.37	4 (7%)	54,89,89	2.30	14 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	A	493	-	1/1/9/9	0/28/50/50	0/6/6/6
2	FAD	B	493	-	1/1/9/9	0/28/50/50	0/6/6/6

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	493	FAD	C2'-C3'	-2.82	1.47	1.53
2	A	493	FAD	C8A-N7A	-2.07	1.30	1.34
2	A	493	FAD	C5'-C4'	-2.04	1.48	1.51
2	A	493	FAD	C1'-N10	2.28	1.50	1.48
2	B	493	FAD	C1'-N10	3.54	1.52	1.48
2	B	493	FAD	C4-N3	3.73	1.39	1.33
2	B	493	FAD	C4-C4X	5.12	1.51	1.41
2	A	493	FAD	C4-C4X	5.84	1.52	1.41

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	493	FAD	C4X-C4-N3	-6.03	114.90	123.48
2	B	493	FAD	C4X-C4-N3	-5.55	115.58	123.48
2	B	493	FAD	O4B-C4B-C3B	-5.14	94.95	105.17
2	A	493	FAD	O2'-C2'-C1'	-4.30	99.84	109.79
2	A	493	FAD	C4B-O4B-C1B	-3.17	106.39	109.77
2	B	493	FAD	O2'-C2'-C1'	-3.05	102.74	109.79
2	A	493	FAD	O4B-C4B-C3B	-2.89	99.43	105.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	493	FAD	O4'-C4'-C5'	-2.51	104.40	110.00
2	A	493	FAD	O3'-C3'-C4'	-2.16	103.46	108.82
2	B	493	FAD	C4-C4X-C10	-2.11	118.26	119.96
2	B	493	FAD	C5X-C9A-N10	2.15	119.25	117.66
2	B	493	FAD	O3B-C3B-C4B	2.17	117.42	111.09
2	B	493	FAD	C4-C4X-N5	2.39	121.30	118.68
2	B	493	FAD	C1'-N10-C9A	2.65	120.77	118.35
2	A	493	FAD	C4'-C3'-C2'	2.82	119.47	113.41
2	B	493	FAD	C2B-C3B-C4B	2.82	108.11	102.62
2	A	493	FAD	C4-C4X-N5	2.93	121.89	118.68
2	B	493	FAD	O3B-C3B-C2B	3.13	121.85	111.83
2	B	493	FAD	O4'-C4'-C3'	3.16	116.94	109.09
2	B	493	FAD	C4X-N5-C5X	3.42	120.37	116.76
2	A	493	FAD	O3B-C3B-C4B	3.65	121.74	111.09
2	A	493	FAD	C1'-N10-C9A	3.95	121.96	118.35
2	A	493	FAD	C4X-N5-C5X	5.74	122.83	116.76
2	A	493	FAD	C4-N3-C2	10.17	124.05	115.16
2	B	493	FAD	C4-N3-C2	10.43	124.28	115.16

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	493	FAD	C3B
2	A	493	FAD	C3B

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	493	FAD	2	0

## 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	487/487 (100%)	-0.86	4 (0%) 86 83	3, 11, 33, 57	0
1	B	486/487 (99%)	-1.05	2 (0%) 92 91	3, 9, 34, 59	0
All	All	973/974 (99%)	-0.95	6 (0%) 89 88	3, 10, 34, 59	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	487	ILE	4.1
1	A	1	MET	3.1
1	A	2	SER	2.4
1	A	273	GLY	2.2
1	B	487	ILE	2.1
1	B	484	VAL	2.1

### 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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	FAD	B	493	53/53	0.99	0.10	0.36	3,4,10,12	0
2	FAD	A	493	53/53	0.99	0.11	-0.12	3,4,9,12	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.