



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:25 PM GMT

PDB ID : 1AOG  
Title : TRYPANOSOMA CRUZI TRYPANOTHIONE REDUCTASE (OXIDIZED FORM)  
Authors : Bond, C.S.; Zhang, Y.; Hunter, W.N.  
Deposited on : 1997-07-03  
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  
<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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

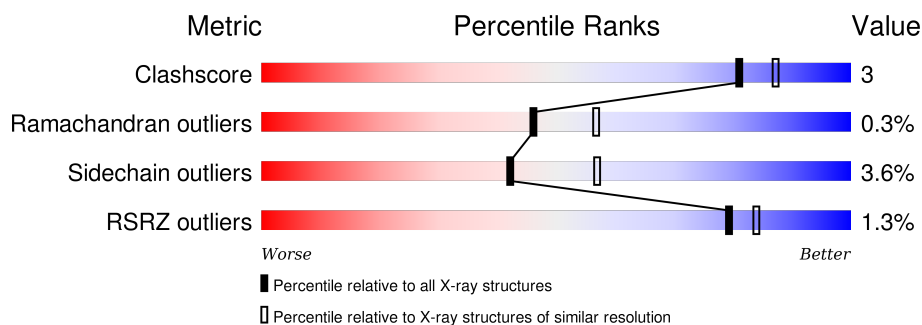
# 1 Overall quality at a glance

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	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (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. 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	485	<div> <div></div> <div>86%13%.</div> </div>
1	B	485	<div> <div></div> <div>84%15%.</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
3	MAE	A	500	-	-	-	X
3	MAE	A	501	-	-	-	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7988 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 TRYPTOPHAN REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	485	Total	C	N	O	S	0	0	0
			3731	2373	635	702	21			
1	B	483	Total	C	N	O	S	0	0	0
			3716	2364	632	699	21			

- 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 MALEIC ACID (three-letter code: MAE) (formula:  $C_4H_4O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	4	4		
3	A	1	Total	C	O	0	0
			8	4	4		

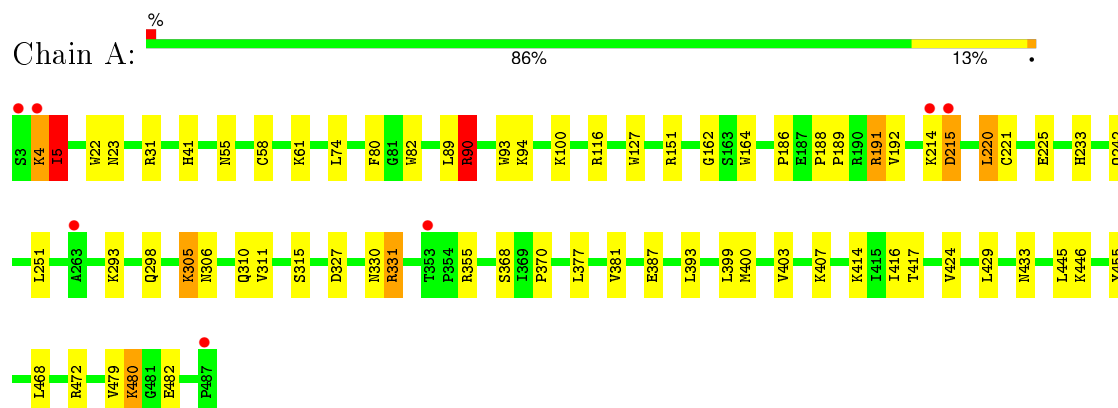
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	249	Total	O	0	0
			249	249		
4	B	170	Total	O	0	0
			170	170		

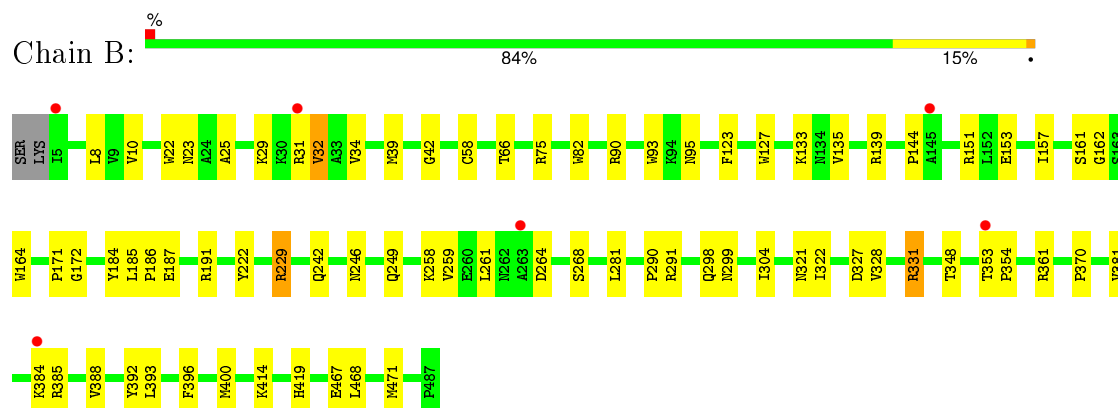
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.81Å 92.81Å 156.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.30 19.96 – 2.30	Depositor EDS
% Data completeness (in resolution range)	91.5 (8.00-2.30) 94.1 (19.96-2.30)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.35 (at 2.30Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.189 , (Not available) 0.173 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	31.0	Xtriage
Anisotropy	0.331	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 64.7	EDS
Estimated twinning fraction	0.042 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 55390 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7988	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.68% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAE, 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	0.74	2/3808 (0.1%)	1.39	42/5159 (0.8%)
1	B	0.73	0/3793	1.31	35/5140 (0.7%)
All	All	0.74	2/7601 (0.0%)	1.35	77/10299 (0.7%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	215	ASP	CA-CB	8.91	1.73	1.53
1	A	298	GLN	CG-CD	5.32	1.63	1.51

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	225	GLU	CA-CB-CG	18.04	153.08	113.40
1	A	480	LYS	CG-CD-CE	12.80	150.30	111.90
1	A	4	LYS	CA-C-N	-9.81	95.61	117.20
1	B	31	ARG	NE-CZ-NH2	-8.88	115.86	120.30
1	A	82	TRP	CD1-CG-CD2	8.81	113.35	106.30
1	A	22	TRP	CD1-CG-CD2	8.55	113.14	106.30
1	A	93	TRP	CD1-CG-CD2	8.46	113.06	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	215	ASP	CB-CG-OD1	8.31	125.78	118.30
1	A	164	TRP	CD1-CG-CD2	8.19	112.85	106.30
1	B	127	TRP	CD1-CG-CD2	8.17	112.84	106.30
1	B	164	TRP	CD1-CG-CD2	8.11	112.79	106.30
1	A	22	TRP	CE2-CD2-CG	-8.10	100.82	107.30
1	B	31	ARG	NE-CZ-NH1	8.03	124.32	120.30
1	B	22	TRP	CD1-CG-CD2	7.97	112.68	106.30
1	A	93	TRP	CE2-CD2-CG	-7.93	100.95	107.30
1	A	215	ASP	CB-CA-C	7.93	126.26	110.40
1	B	82	TRP	CD1-CG-CD2	7.84	112.57	106.30
1	A	127	TRP	CD1-CG-CD2	7.66	112.43	106.30
1	A	355	ARG	NE-CZ-NH1	7.63	124.11	120.30
1	B	93	TRP	CD1-CG-CD2	7.57	112.35	106.30
1	B	164	TRP	CE2-CD2-CG	-7.45	101.34	107.30
1	B	93	TRP	CE2-CD2-CG	-7.34	101.43	107.30
1	A	82	TRP	CE2-CD2-CG	-7.30	101.46	107.30
1	A	164	TRP	CE2-CD2-CG	-7.30	101.46	107.30
1	B	249	GLN	CA-CB-CG	7.19	129.23	113.40
1	A	220	LEU	CA-CB-CG	7.19	131.83	115.30
1	B	127	TRP	CE2-CD2-CG	-7.04	101.67	107.30
1	A	214	LYS	C-N-CA	-7.04	104.10	121.70
1	B	291	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	B	22	TRP	CE2-CD2-CG	-6.93	101.76	107.30
1	A	215	ASP	CA-C-N	-6.90	102.40	116.20
1	A	331	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	A	127	TRP	CE2-CD2-CG	-6.78	101.88	107.30
1	B	82	TRP	CE2-CD2-CG	-6.56	102.05	107.30
1	A	225	GLU	CB-CA-C	-6.53	97.35	110.40
1	A	4	LYS	N-CA-C	6.51	128.59	111.00
1	B	229	ARG	CG-CD-NE	-6.51	98.13	111.80
1	B	261	LEU	CA-CB-CG	6.49	130.23	115.30
1	B	229	ARG	NE-CZ-NH1	6.49	123.54	120.30
1	B	291	ARG	CB-CG-CD	-6.30	95.22	111.60
1	A	4	LYS	O-C-N	6.26	132.72	122.70
1	B	75	ARG	NE-CZ-NH2	-6.25	117.17	120.30
1	B	222	TYR	CB-CG-CD2	-6.24	117.25	121.00
1	A	90	ARG	CA-CB-CG	6.18	127.01	113.40
1	B	392	TYR	CB-CG-CD2	-6.15	117.31	121.00
1	A	305	LYS	CA-CB-CG	6.04	126.70	113.40
1	B	90	ARG	CA-CB-CG	6.01	126.63	113.40
1	B	291	ARG	CA-CB-CG	6.00	126.59	113.40
1	B	139	ARG	NE-CZ-NH1	5.99	123.30	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	116	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	A	164	TRP	CB-CG-CD1	-5.85	119.39	127.00
1	A	116	ARG	NE-CZ-NH2	-5.79	117.40	120.30
1	A	5	ILE	N-CA-C	5.75	126.52	111.00
1	A	151	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	B	361	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	B	385	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	A	191	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	A	82	TRP	CG-CD1-NE1	-5.59	104.51	110.10
1	A	225	GLU	CB-CG-CD	5.52	129.11	114.20
1	B	381	VAL	CG1-CB-CG2	5.48	119.67	110.90
1	B	75	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	B	281	LEU	CA-CB-CG	5.37	127.64	115.30
1	A	215	ASP	CA-C-O	5.35	131.33	120.10
1	A	164	TRP	CG-CD1-NE1	-5.29	104.81	110.10
1	A	433	ASN	CB-CG-ND2	5.28	129.38	116.70
1	A	293	LYS	CD-CE-NZ	5.25	123.77	111.70
1	B	82	TRP	CG-CD1-NE1	-5.20	104.90	110.10
1	A	433	ASN	CB-CG-OD1	-5.20	111.21	121.60
1	A	331	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	A	93	TRP	CG-CD2-CE3	5.19	138.57	133.90
1	B	191	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	B	127	TRP	CG-CD1-NE1	-5.11	104.99	110.10
1	B	187	GLU	CA-CB-CG	5.11	124.63	113.40
1	A	93	TRP	CG-CD1-NE1	-5.10	105.00	110.10
1	A	164	TRP	CG-CD2-CE3	5.10	138.49	133.90
1	B	164	TRP	CG-CD1-NE1	-5.04	105.06	110.10
1	B	22	TRP	CG-CD1-NE1	-5.00	105.10	110.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	215	ASP	Mainchain
1	B	299	ASN	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	3731	0	3743	24	0
1	B	3716	0	3725	26	0
2	A	53	0	27	0	0
2	B	53	0	31	0	0
3	A	16	0	4	0	0
4	A	249	0	0	2	0
4	B	170	0	0	2	0
All	All	7988	0	7530	49	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 3.

All (49) 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:387:GLU:OE2	1:A:480:LYS:HD3	1.90	0.71
1:A:90:ARG:HH11	1:A:90:ARG:HB2	1.56	0.69
1:B:331:ARG:HB2	4:B:592:HOH:O	1.93	0.69
1:B:171:PRO:HG2	1:B:258:LYS:HB3	1.80	0.63
1:A:305:LYS:HE3	1:A:310:GLN:HG3	1.86	0.57
1:A:5:ILE:HG23	1:A:31:ARG:NH1	2.20	0.57
1:B:172:GLY:HA3	1:B:259:VAL:O	2.05	0.56
1:B:10:VAL:HB	1:B:34:VAL:HG12	1.90	0.53
1:A:233:HIS:HB3	4:A:732:HOH:O	2.08	0.53
1:B:348:THR:HG23	1:B:354:PRO:HB3	1.89	0.52
4:A:706:HOH:O	1:B:400:MET:HB3	2.09	0.52
1:A:417:THR:HG22	1:A:424:VAL:HA	1.92	0.51
1:B:290:PRO:HB3	1:B:328:VAL:HA	1.91	0.51
1:A:393:LEU:HD13	1:A:414:LYS:HD2	1.93	0.50
1:B:8:LEU:HB3	1:B:32:VAL:HB	1.94	0.50
1:A:41:HIS:HB3	1:A:55:ASN:OD1	2.13	0.48
1:B:157:ILE:HB	1:B:322:ILE:HG12	1.96	0.48
1:B:396:PHE:CE1	1:B:467:GLU:HG3	2.48	0.48
1:A:94:LYS:HE3	1:A:186:PRO:O	2.13	0.47
1:A:189:PRO:HB2	1:A:192:VAL:HB	1.97	0.47
1:A:5:ILE:HG23	1:A:31:ARG:HH12	1.79	0.47
1:B:39:MET:SD	1:B:123:PHE:CE2	3.09	0.45
1:B:8:LEU:O	1:B:32:VAL:HA	2.16	0.45
1:A:311:VAL:HB	1:A:315:SER:HA	1.98	0.45
1:B:133:LYS:O	1:B:321:ASN:ND2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:MET:SD	1:B:123:PHE:HE2	2.40	0.44
1:A:429:LEU:HD21	1:A:468:LEU:HD21	1.98	0.44
1:A:400:MET:HG3	1:B:66:THR:HG21	1.98	0.44
1:A:188:PRO:HA	1:A:189:PRO:HD3	1.82	0.44
1:A:221:CYS:HA	1:A:251:LEU:O	2.18	0.44
1:A:242:GLN:OE1	1:A:370:PRO:HG2	2.18	0.44
1:B:393:LEU:HD23	1:B:414:LYS:HD2	2.00	0.43
1:A:74:LEU:HD13	1:A:89:LEU:HD11	2.00	0.43
1:B:162:GLY:HA2	1:B:327:ASP:HB2	2.00	0.43
1:A:377:LEU:HG	1:A:381:VAL:HG22	2.00	0.43
1:B:468:LEU:HA	1:B:471:MET:HE3	2.00	0.42
1:B:135:VAL:HG22	1:B:153:GLU:HG2	2.01	0.42
1:B:419:HIS:HD2	4:B:578:HOH:O	2.03	0.42
1:B:388:VAL:HG22	1:B:419:HIS:HB3	2.02	0.42
1:B:25:ALA:O	1:B:29:LYS:HA	2.21	0.41
1:A:399:LEU:O	1:A:403:VAL:HG13	2.19	0.41
1:B:242:GLN:OE1	1:B:370:PRO:HG3	2.20	0.41
1:A:455:TYR:HB2	1:A:472:ARG:NH1	2.36	0.41
1:B:185:LEU:HA	1:B:186:PRO:HD3	1.89	0.41
1:A:479:VAL:O	1:A:482:GLU:HG2	2.21	0.41
1:B:42:GLY:HA2	1:B:184:TYR:CZ	2.56	0.41
1:B:353:THR:HA	1:B:354:PRO:HD3	1.70	0.40
1:A:80:PHE:CZ	1:A:403:VAL:HG22	2.56	0.40
1:A:162:GLY:HA2	1:A:327:ASP:HB2	2.03	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	483/485 (100%)	466 (96%)	15 (3%)	2 (0%)	39 48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	481/485 (99%)	464 (96%)	16 (3%)	1 (0%)	52 64
All	All	964/970 (99%)	930 (96%)	31 (3%)	3 (0%)	46 57

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	4	LYS
1	B	144	PRO

### 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	406/406 (100%)	391 (96%)	15 (4%)	41 55
1	B	404/406 (100%)	390 (96%)	14 (4%)	43 58
All	All	810/812 (100%)	781 (96%)	29 (4%)	42 57

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	58	CYS
1	A	61	LYS
1	A	90	ARG
1	A	100	LYS
1	A	191	ARG
1	A	220	LEU
1	A	306	ASN
1	A	330	ASN
1	A	331	ARG
1	A	368	SER
1	A	407	LYS
1	A	416	ILE

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Mol	Chain	Res	Type
1	A	445	LEU
1	A	446	LYS
1	B	23	ASN
1	B	32	VAL
1	B	58	CYS
1	B	95	ASN
1	B	151	ARG
1	B	161	SER
1	B	229	ARG
1	B	246	ASN
1	B	264	ASP
1	B	268	SER
1	B	298	GLN
1	B	304	ILE
1	B	331	ARG
1	B	384	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	180	ASN
1	A	233	HIS
1	B	69	GLN
1	B	180	ASN
1	B	246	ASN
1	B	249	GLN
1	B	419	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

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	A	492	-	48,58,58	1.76	7 (14%)	54,89,89	3.17	14 (25%)
3	MAE	A	500	-	1,7,7	1.55	0	0,8,8	0.00	-
3	MAE	A	501	-	1,7,7	1.42	0	0,8,8	0.00	-
2	FAD	B	492	-	48,58,58	1.45	9 (18%)	54,89,89	2.32	10 (18%)

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	492	-	-	0/30/50/50	0/6/6/6
3	MAE	A	500	-	-	0/0/5/5	0/0/0/0
3	MAE	A	501	-	-	0/0/5/5	0/0/0/0
2	FAD	B	492	-	-	0/30/50/50	0/6/6/6

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	492	FAD	O2B-C2B	-6.91	1.26	1.43
2	B	492	FAD	C2'-C3'	-2.59	1.48	1.53
2	B	492	FAD	C3B-C4B	-2.55	1.46	1.53
2	A	492	FAD	C2'-C3'	-2.50	1.48	1.53
2	A	492	FAD	C8A-N7A	-2.49	1.29	1.34
2	B	492	FAD	C8A-N7A	-2.31	1.30	1.34
2	B	492	FAD	C5X-N5	-2.14	1.31	1.35
2	B	492	FAD	C10-N10	-2.08	1.36	1.39
2	A	492	FAD	C7M-C7	2.03	1.55	1.51
2	B	492	FAD	C4-N3	2.48	1.37	1.33
2	B	492	FAD	O3B-C3B	2.89	1.49	1.43
2	A	492	FAD	C4-N3	2.90	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	492	FAD	C1'-N10	3.10	1.51	1.48
2	B	492	FAD	C4-C4X	3.76	1.48	1.41
2	B	492	FAD	C1'-N10	4.03	1.52	1.48
2	A	492	FAD	C4-C4X	4.91	1.51	1.41

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	492	FAD	C4X-C4-N3	-5.45	116.13	123.59
2	B	492	FAD	C4X-C4-N3	-5.25	116.40	123.59
2	B	492	FAD	C5B-C4B-C3B	-3.76	100.28	115.21
2	B	492	FAD	C4X-C10-N10	-3.25	118.60	120.52
2	A	492	FAD	C4X-C10-N10	-2.95	118.78	120.52
2	A	492	FAD	O4B-C1B-N9A	-2.87	102.10	108.10
2	A	492	FAD	O4'-C4'-C5'	-2.47	104.82	110.19
2	A	492	FAD	O2'-C2'-C1'	-2.40	104.06	109.94
2	A	492	FAD	C4-C4X-C10	-2.34	118.44	119.94
2	B	492	FAD	O4'-C4'-C5'	-2.33	105.11	110.19
2	A	492	FAD	C2B-C3B-C4B	2.15	107.03	102.61
2	B	492	FAD	O2B-C2B-C3B	2.53	120.05	111.83
2	A	492	FAD	O2A-PA-O3P	3.03	118.85	105.09
2	A	492	FAD	C1B-N9A-C4A	3.44	132.12	126.94
2	B	492	FAD	O4B-C1B-N9A	3.48	115.39	108.10
2	B	492	FAD	C4X-N5-C5X	3.83	121.16	116.76
2	A	492	FAD	C4X-N5-C5X	3.90	121.25	116.76
2	B	492	FAD	O2A-PA-O3P	5.49	130.01	105.09
2	A	492	FAD	O2B-C2B-C3B	6.19	131.95	111.83
2	B	492	FAD	O3B-C3B-C4B	6.67	131.06	111.05
2	A	492	FAD	O3B-C3B-C4B	7.27	132.85	111.05
2	B	492	FAD	C4-N3-C2	9.55	123.50	115.25
2	A	492	FAD	C4-N3-C2	10.08	123.96	115.25
2	A	492	FAD	C2B-C1B-N9A	14.70	136.75	114.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	485/485 (100%)	-0.59	7 (1%) 78 83	7, 23, 51, 80	0
1	B	483/485 (99%)	-0.44	6 (1%) 81 85	6, 31, 73, 90	0
All	All	968/970 (99%)	-0.52	13 (1%) 79 84	6, 26, 68, 90	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	SER	8.9
1	A	4	LYS	7.1
1	A	215	ASP	3.6
1	B	353	THR	3.5
1	A	487	PRO	3.0
1	B	31	ARG	2.7
1	B	145	ALA	2.5
1	B	5	ILE	2.5
1	B	263	ALA	2.3
1	A	214	LYS	2.3
1	A	353	THR	2.2
1	B	384	LYS	2.1
1	A	263	ALA	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 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(Å <sup>2</sup> )	Q<0.9
3	MAE	A	501	8/8	0.78	0.51	28.69	67,69,74,79	0
3	MAE	A	500	8/8	0.92	0.15	2.37	31,37,39,39	0
2	FAD	A	492	53/53	0.98	0.07	-0.36	3,14,21,25	0
2	FAD	B	492	53/53	0.98	0.07	-0.82	10,20,39,42	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.