



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 02:49 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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

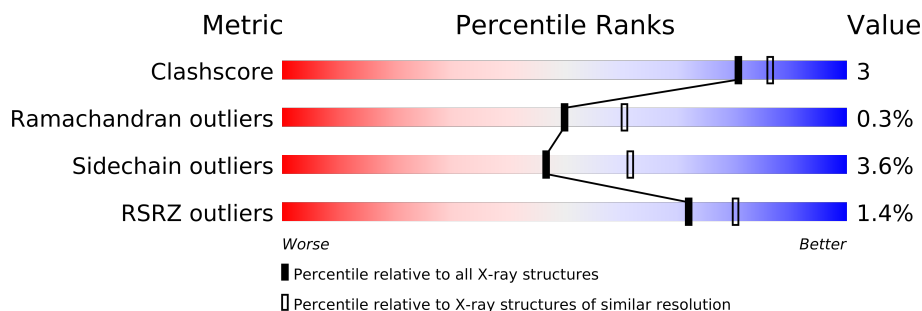
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	485	
1	B	485	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	MAE	A	500	-	X
3	MAE	A	501	-	X

2 Entry composition i

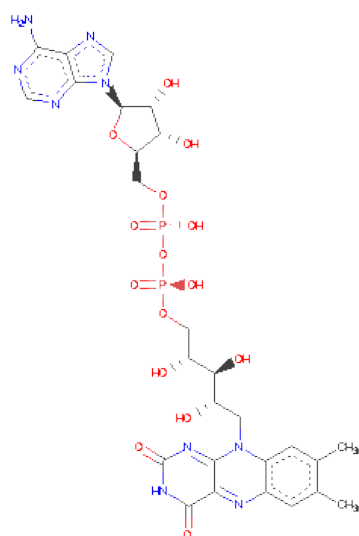
There are 4 unique types of molecules in this entry. The entry contains 7988 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

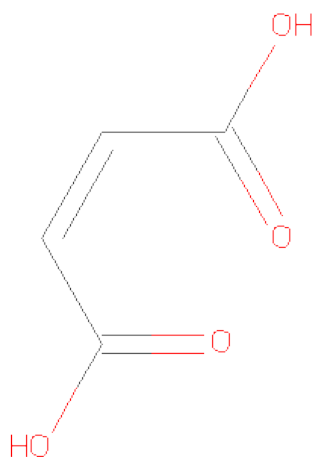
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	485	Total	C	N	O	S	0	0	0
			3731	2373	635	702	21			
1	B	483	Total	C	N	O	S	0	0	0
			3716	2364	632	699	21			

- 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		

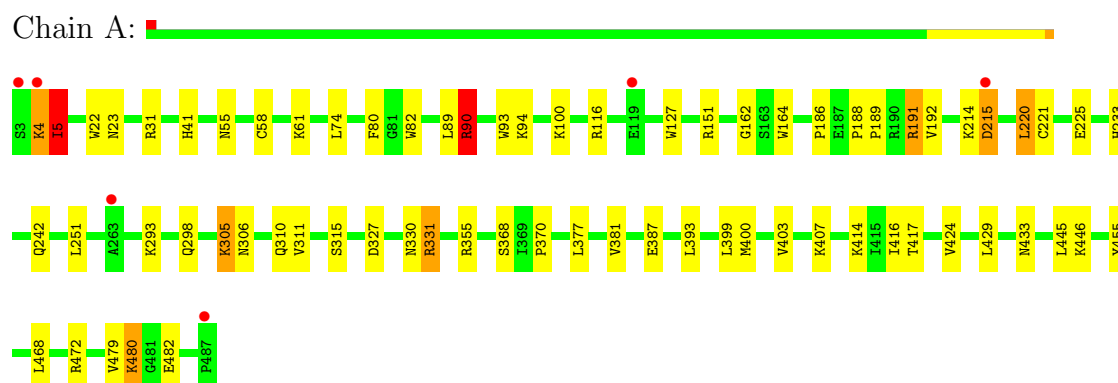
- Molecule 4 is water.

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

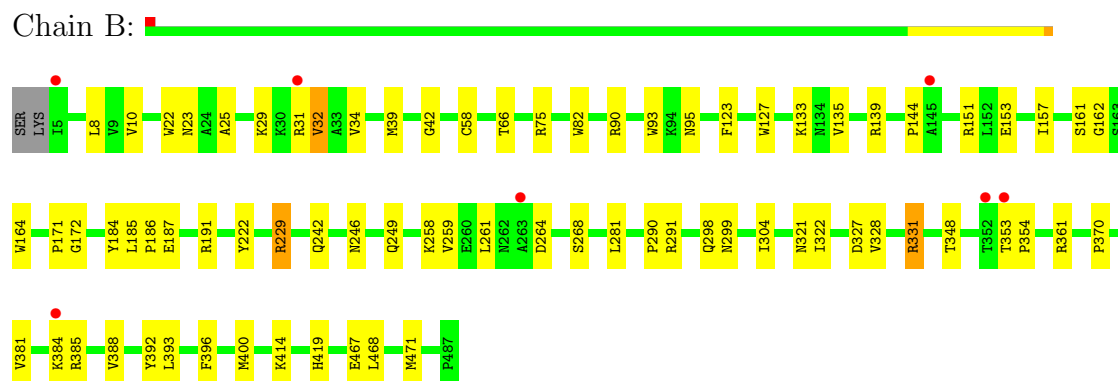
3 Residue-property plots

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: TRYPTANOTHIONE REDUCTASE



• Molecule 1: TRYPTANOTHIONE REDUCTASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	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) 94.2 (19.96-2.30)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	31.0	Xtriage
Anisotropy	0.331	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 53.5	EDS
Estimated twinning fraction	0.042 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit,

and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

All (49) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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	Distance(Å)	Clash(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

5.3.1 Protein backbone ⓘ

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%)	43	52
1	B	481/485 (99%)	464 (96%)	16 (3%)	1 (0%)	56	68
All	All	964/970 (99%)	930 (96%)	31 (3%)	3 (0%)	50	60

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%)	45	60
1	B	404/406 (100%)	390 (96%)	14 (4%)	48	63
All	All	810/812 (100%)	781 (96%)	29 (4%)	47	61

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
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

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Mol	Chain	Res	Type
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 chains 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	-	58,58,58	1.80	6 (10%)	85,89,89	2.34	18 (21%)
3	MAE	A	500	-	7,7,7	1.91	3 (42%)	8,8,8	2.79	4 (50%)
3	MAE	A	501	-	7,7,7	1.88	4 (57%)	8,8,8	1.94	3 (37%)
2	FAD	B	492	-	58,58,58	1.38	8 (13%)	85,89,89	2.06	16 (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	-	-	0/34/50/50	0/1/6/6
3	MAE	A	500	-	-	0/5/5/5	0/0/0/0
3	MAE	A	501	-	-	0/5/5/5	0/0/0/0
2	FAD	B	492	-	-	0/34/50/50	0/1/6/6

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	492	FAD	O2B-C2B	-6.85	1.26	1.43
2	A	492	FAD	C4-C4X	6.04	1.51	1.41
2	A	492	FAD	C1'-C2'	-5.42	1.46	1.51
2	B	492	FAD	C4-C4X	4.62	1.48	1.41
2	B	492	FAD	C1'-N10	3.97	1.52	1.48
2	A	492	FAD	C1'-N10	3.10	1.51	1.48
2	B	492	FAD	O3B-C3B	2.87	1.49	1.43
3	A	500	MAE	O2-C1	-2.81	1.22	1.30
2	B	492	FAD	C2'-C3'	-2.56	1.48	1.53
2	B	492	FAD	C3B-C4B	-2.50	1.46	1.53
3	A	501	MAE	C3-C4	-2.50	1.42	1.48
3	A	500	MAE	O4-C4	-2.47	1.23	1.30
2	A	492	FAD	C2'-C3'	-2.47	1.48	1.53
2	A	492	FAD	C8A-N7A	-2.42	1.29	1.34
3	A	501	MAE	O2-C1	-2.29	1.23	1.30
2	B	492	FAD	C8A-N7A	-2.25	1.30	1.34
2	B	492	FAD	C5X-N5	-2.19	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500	MAE	C3-C2	2.18	1.39	1.32
3	A	501	MAE	O4-C4	-2.17	1.23	1.30
3	A	501	MAE	C2-C1	-2.05	1.43	1.48
2	B	492	FAD	C2B-C1B	-2.03	1.50	1.53

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	492	FAD	C2B-C1B-N9A	9.15	136.75	113.27
2	A	492	FAD	C2-N1-C10	8.43	123.48	114.98
2	B	492	FAD	C2-N1-C10	8.36	123.41	114.98
2	B	492	FAD	O4B-C1B-N9A	7.47	115.39	108.44
2	A	492	FAD	O3B-C3B-C4B	7.39	132.85	111.08
2	A	492	FAD	O4B-C1B-N9A	-6.82	102.10	108.44
2	B	492	FAD	O3B-C3B-C4B	6.78	131.06	111.08
2	A	492	FAD	O2B-C2B-C3B	6.18	131.95	111.83
2	A	492	FAD	C2'-C1'-N10	5.45	119.68	112.45
2	B	492	FAD	O2A-PA-O3P	5.24	130.01	105.14
3	A	500	MAE	O2-C1-O1	-5.24	110.55	122.54
3	A	500	MAE	O4-C4-O3	-4.29	112.73	122.54
2	B	492	FAD	O4B-C1B-C2B	-4.09	100.50	106.77
2	A	492	FAD	C4X-N5-C5X	4.06	121.25	116.69
2	B	492	FAD	C4X-N5-C5X	3.98	121.16	116.69
2	B	492	FAD	C4X-C10-N10	-3.82	118.60	120.51
2	B	492	FAD	C5B-C4B-C3B	-3.73	100.28	115.21
2	B	492	FAD	C4X-C10-N1	-3.71	119.03	122.73
2	A	492	FAD	C4X-C10-N10	-3.46	118.78	120.51
3	A	501	MAE	O2-C1-O1	-3.27	115.06	122.54
2	A	492	FAD	C4X-C10-N1	-3.22	119.51	122.73
2	A	492	FAD	C1B-N9A-C4A	3.18	132.12	126.64
3	A	501	MAE	O4-C4-O3	-3.08	115.50	122.54
2	B	492	FAD	C8A-N9A-C4A	-2.97	104.63	106.90
2	A	492	FAD	O2A-PA-O3P	2.89	118.85	105.14
2	B	492	FAD	O3P-PA-O1A	-2.70	91.92	111.28
2	A	492	FAD	O4'-C4'-C5'	-2.58	104.82	110.12
3	A	500	MAE	O4-C4-C3	2.57	126.56	116.57
2	A	492	FAD	C8A-N9A-C4A	-2.55	104.95	106.90
2	B	492	FAD	O2B-C2B-C3B	2.53	120.05	111.83
2	B	492	FAD	O4'-C4'-C5'	-2.44	105.11	110.12
2	B	492	FAD	C9A-N10-C10	-2.43	119.38	121.77
2	B	492	FAD	N1-C10-N10	2.41	122.31	115.97
2	A	492	FAD	C5X-C9A-N10	2.34	119.11	116.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	MAE	O1-C1-C2	2.32	128.22	120.75
2	B	492	FAD	C5X-C9A-N10	2.28	119.05	116.80
2	A	492	FAD	O2'-C2'-C1'	-2.28	104.06	109.71
2	A	492	FAD	O2B-C2B-C1B	2.27	118.10	111.23
2	A	492	FAD	C2B-C3B-C4B	2.19	107.03	102.65
2	A	492	FAD	N1-C10-N10	2.13	121.57	115.97
3	A	500	MAE	O1-C1-C2	2.10	127.51	120.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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, 95th 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 ²)	Q<0.9
1	A	485/485 (100%)	-0.60	6 (1%) 75 83	7, 23, 51, 80	0
1	B	483/485 (99%)	-0.43	7 (1%) 72 80	6, 31, 73, 90	0
All	All	968/970 (99%)	-0.52	13 (1%) 72 82	6, 26, 68, 90	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	SER	9.3
1	A	4	LYS	6.4
1	B	353	THR	3.4
1	A	215	ASP	2.9
1	A	487	PRO	2.7
1	A	119	GLU	2.6
1	B	5	ILE	2.5
1	A	263	ALA	2.3
1	B	352	THR	2.3
1	B	31	ARG	2.2
1	B	263	ALA	2.1
1	B	145	ALA	2.1
1	B	384	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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, 95th 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	MAE	A	501	8/8	0.59	35.20	67,69,74,79	0
3	MAE	A	500	8/8	0.13	2.07	31,37,39,39	0
2	FAD	A	492	53/53	0.07	-0.30	3,14,21,25	0
2	FAD	B	492	53/53	0.07	-0.81	10,20,39,42	0

6.5 Other polymers ⓘ

There are no such residues in this entry.