



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2017 – 06:07 AM EDT

PDB ID : 3DGZ  
Title : Crystal Structure of Mouse Mitochondrial Thioredoxin Reductase, C-terminal 3-residue truncation  
Authors : Eckenroth, B.E.; Hondal, R.J.; Everse, S.J.  
Deposited on : unknown  
Resolution : 2.25 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 : rb-20030345  
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) : rb-20030345

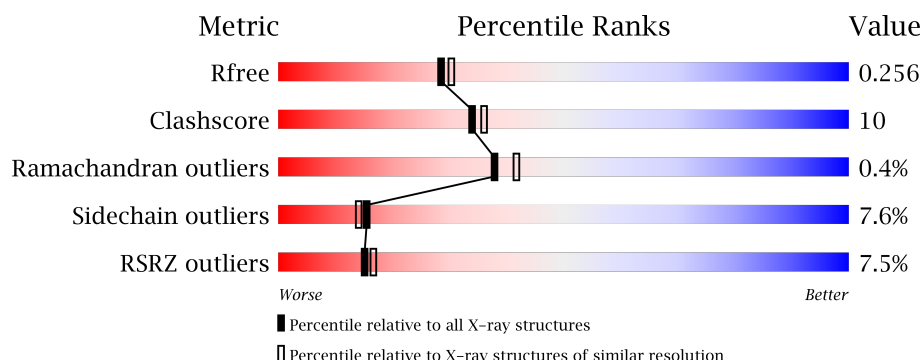
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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))
$R_{free}$	100719	1062 (2.26-2.26)
Clashscore	112137	1178 (2.26-2.26)
Ramachandran outliers	110173	1145 (2.26-2.26)
Sidechain outliers	110143	1146 (2.26-2.26)
RSRZ outliers	101464	1066 (2.26-2.26)

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	488	<div> <div>7%</div> <div>76%</div> <div>17%</div> <div>5%</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	NA7	A	501	-	-	-	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3960 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 Thioredoxin reductase 2.

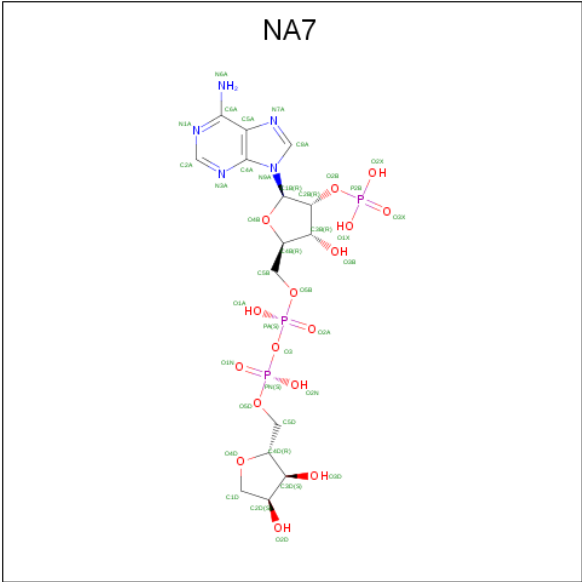
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	482	Total	C	N	O	S	0	0	0
			3679	2330	641	687	21			

- 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		

- Molecule 3 is [(2R,3R,4R,5R)-5-(6-AMINO-9H-PURIN-9-YL)-3-HYDROXY-4-(PHOSPHONOXY)TETRAHYDROFURAN-2-YL]METHYL [(2R,3S,4S)-3,4-DIHYDROXYTETRAHYDROFURAN-2-YL]METHYL DIHYDROGEN DIPHOSPHATE (three-letter code: NA7) (formula:  $C_{15}H_{24}N_5O_{16}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			39	15	5	16	3		

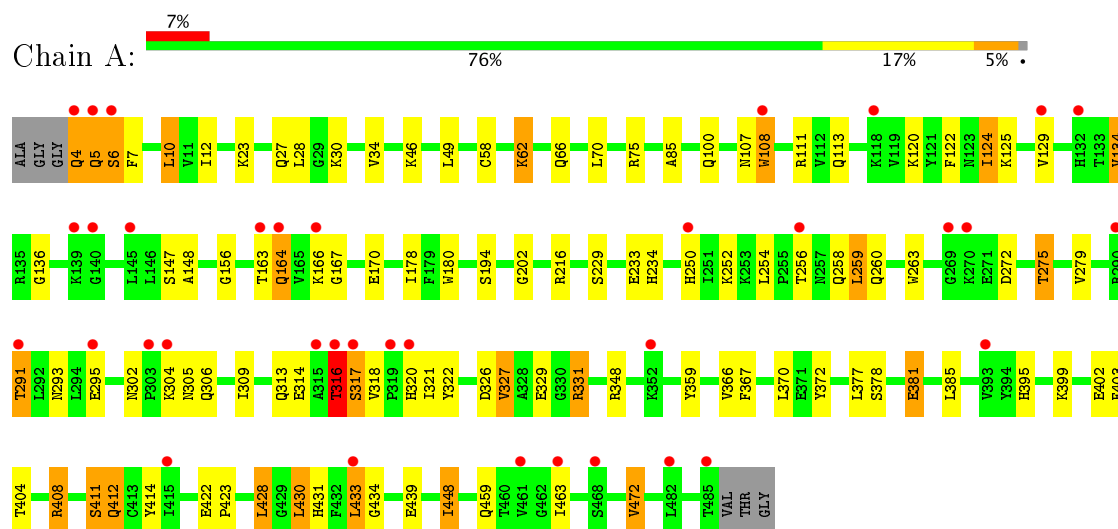
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	189	Total	O	0	0
			189	189		

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

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 ( $\text{RSRZ} > 2$ ). 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: Thioredoxin reductase 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.51Å 110.51Å 208.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.45 – 2.25 15.45 – 2.25	Depositor EDS
% Data completeness (in resolution range)	95.2 (15.45-2.25) 95.4 (15.45-2.25)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.01 (at 2.25Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.193 , 0.258 0.191 , 0.256	Depositor DCC
$R_{free}$ test set	2967 reflections (11.18%)	DCC
Wilson B-factor (Å <sup>2</sup> )	41.4	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 54.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	3960	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA7, 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	1.21	18/3761 (0.5%)	1.04	15/5101 (0.3%)

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 (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	6	SER	CB-OG	15.31	1.62	1.42
1	A	412	GLN	N-CA	9.80	1.66	1.46
1	A	108	TRP	CG-CD1	9.66	1.50	1.36
1	A	108	TRP	CB-CG	-8.18	1.35	1.50
1	A	317	SER	CB-OG	8.17	1.52	1.42
1	A	402	GLU	CD-OE1	7.02	1.33	1.25
1	A	7	PHE	CG-CD2	6.11	1.48	1.38
1	A	414	TYR	CG-CD1	5.79	1.46	1.39
1	A	439	GLU	CG-CD	5.74	1.60	1.51
1	A	408	ARG	CG-CD	5.71	1.66	1.51
1	A	316	THR	CB-OG1	5.67	1.54	1.43
1	A	202	GLY	N-CA	-5.35	1.38	1.46
1	A	381	GLU	CG-CD	5.32	1.59	1.51
1	A	6	SER	C-N	5.30	1.46	1.34
1	A	7	PHE	CE1-CZ	5.27	1.47	1.37
1	A	295	GLU	CG-CD	5.15	1.59	1.51
1	A	108	TRP	NE1-CE2	5.09	1.44	1.37
1	A	233	GLU	CG-CD	5.01	1.59	1.51

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	348	ARG	NE-CZ-NH2	-8.62	115.99	120.30
1	A	327	VAL	CB-CA-C	-7.75	96.67	111.40
1	A	62	LYS	CD-CE-NZ	7.63	129.25	111.70
1	A	411	SER	C-N-CA	-7.27	103.52	121.70
1	A	448	ILE	CG1-CB-CG2	-7.22	95.52	111.40
1	A	472	VAL	CG1-CB-CG2	7.04	122.17	110.90
1	A	430	LEU	CB-CG-CD2	6.78	122.53	111.00
1	A	433	LEU	CA-CB-CG	5.92	128.91	115.30
1	A	411	SER	O-C-N	-5.82	113.39	122.70
1	A	428	LEU	CA-CB-CG	5.71	128.43	115.30
1	A	433	LEU	CB-CG-CD1	5.55	120.44	111.00
1	A	412	GLN	N-CA-C	5.51	125.89	111.00
1	A	108	TRP	CB-CG-CD1	-5.32	120.09	127.00
1	A	108	TRP	CB-CG-CD2	5.25	133.43	126.60
1	A	463	ILE	CA-CB-CG1	5.20	120.89	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	85	ALA	Peptide

## 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	3679	0	3675	71	9
2	A	53	0	31	0	0
3	A	39	0	20	2	0
4	A	189	0	0	12	0
All	All	3960	0	3726	72	9

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 10.

All (72) 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:75:ARG:HD2	4:A:681:HOH:O	1.59	1.00
1:A:23:LYS:HZ3	1:A:113:GLN:NE2	1.62	0.95
1:A:23:LYS:HZ3	1:A:113:GLN:HE21	0.95	0.94
1:A:75:ARG:CD	4:A:681:HOH:O	2.15	0.92
1:A:411:SER:O	1:A:412:GLN:HB2	1.67	0.92
1:A:4:GLN:N	1:A:122:PHE:CZ	2.41	0.89
1:A:124:ILE:HG23	1:A:136:GLY:HA3	1.58	0.85
1:A:331:ARG:HG3	1:A:331:ARG:HH11	1.40	0.85
1:A:302:ASN:O	1:A:305:ASN:O	1.97	0.82
1:A:331:ARG:CG	1:A:331:ARG:HH11	1.91	0.81
1:A:378:SER:OG	1:A:381:GLU:HG3	1.81	0.79
1:A:23:LYS:NZ	1:A:113:GLN:NE2	2.32	0.78
1:A:411:SER:O	1:A:412:GLN:CB	2.27	0.75
1:A:66:GLN:O	1:A:70:LEU:HD23	1.89	0.72
1:A:163:THR:O	1:A:164:GLN:HB2	1.91	0.71
1:A:163:THR:O	1:A:164:GLN:CB	2.40	0.70
1:A:459:GLN:NE2	4:A:634:HOH:O	2.25	0.70
1:A:377:LEU:O	1:A:431:HIS:HE1	1.75	0.69
1:A:306:GLN:NE2	4:A:686:HOH:O	2.24	0.68
1:A:4:GLN:N	1:A:122:PHE:HZ	1.89	0.67
1:A:124:ILE:CG2	1:A:136:GLY:HA3	2.24	0.67
1:A:166:LYS:HZ2	1:A:250:HIS:HB2	1.62	0.64
1:A:372:TYR:OH	1:A:431:HIS:HD2	1.81	0.63
1:A:320:HIS:CD2	1:A:321:ILE:HG13	2.34	0.63
1:A:291:THR:HG22	4:A:684:HOH:O	1.99	0.62
1:A:62:LYS:HE3	1:A:367:PHE:CE2	2.35	0.62
1:A:194:SER:HB3	3:A:501:NA7:HC4'	1.84	0.60
1:A:316:THR:HG23	1:A:318:VAL:H	1.68	0.59
1:A:234:HIS:HE1	4:A:632:HOH:O	1.86	0.58
1:A:124:ILE:HD13	1:A:136:GLY:C	2.24	0.57
1:A:331:ARG:CG	1:A:331:ARG:NH1	2.61	0.57
1:A:66:GLN:O	1:A:70:LEU:CD2	2.52	0.55
1:A:124:ILE:HG23	1:A:136:GLY:CA	2.33	0.55
1:A:403:PHE:CG	1:A:408:ARG:HG3	2.44	0.53
1:A:30:LYS:NZ	4:A:568:HOH:O	2.43	0.52
1:A:260:GLN:HE22	1:A:275:THR:CG2	2.22	0.52
1:A:75:ARG:HD3	4:A:681:HOH:O	1.98	0.52
3:A:501:NA7:HC1'	4:A:582:HOH:O	2.10	0.51
1:A:291:THR:CG2	4:A:684:HOH:O	2.55	0.49
1:A:372:TYR:HB2	1:A:433:LEU:HD13	1.94	0.49
1:A:6:SER:HA	1:A:147:SER:O	2.13	0.49
1:A:260:GLN:NE2	1:A:275:THR:HB	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:ILE:HD11	1:A:134:VAL:HG21	1.96	0.47
1:A:23:LYS:NZ	1:A:113:GLN:HE21	1.81	0.47
1:A:322:TYR:CD1	1:A:322:TYR:N	2.81	0.47
1:A:370:LEU:HD11	1:A:434:GLY:HA2	1.97	0.47
1:A:5:GLN:HA	4:A:578:HOH:O	2.15	0.46
1:A:331:ARG:HD2	1:A:359:TYR:CZ	2.51	0.46
1:A:167:GLY:HA2	1:A:170:GLU:CG	2.47	0.45
1:A:316:THR:OG1	1:A:317:SER:N	2.41	0.45
1:A:399:LYS:HD3	1:A:404:THR:HG22	1.97	0.45
1:A:293:ASN:HD22	1:A:293:ASN:N	2.15	0.44
1:A:254:LEU:HD11	1:A:260:GLN:HE21	1.82	0.44
1:A:263:TRP:CE2	1:A:272:ASP:HB3	2.52	0.44
1:A:259:LEU:HD23	1:A:279:VAL:HG23	2.00	0.44
1:A:422:GLU:HA	1:A:423:PRO:HD3	1.90	0.43
1:A:107:ASN:HB3	1:A:111:ARG:HH12	1.83	0.43
1:A:313:GLN:C	1:A:314:GLU:HG2	2.40	0.42
1:A:156:GLY:HA2	1:A:326:ASP:HB2	2.00	0.42
1:A:66:GLN:OE1	1:A:70:LEU:HD21	2.19	0.42
1:A:314:GLU:OE2	1:A:331:ARG:NH1	2.53	0.42
1:A:302:ASN:C	1:A:302:ASN:OD1	2.58	0.42
1:A:23:LYS:O	1:A:27:GLN:HG3	2.20	0.42
1:A:331:ARG:HA	1:A:331:ARG:HD3	1.80	0.42
1:A:309:ILE:O	1:A:316:THR:HA	2.20	0.42
1:A:49:LEU:H	1:A:111:ARG:NH2	2.18	0.42
1:A:10:LEU:HB2	1:A:148:ALA:HB2	2.01	0.41
1:A:293:ASN:ND2	1:A:293:ASN:N	2.68	0.41
1:A:113:GLN:NE2	4:A:598:HOH:O	2.53	0.41
1:A:100:GLN:HG2	1:A:180:TRP:CZ3	2.56	0.41
1:A:256:THR:CB	1:A:258:GLN:HE21	2.34	0.40
1:A:293:ASN:H	1:A:293:ASN:HD22	1.70	0.40

All (9) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:TRP:CZ3	1:A:108:TRP:CZ3[16_664]	0.90	1.30
1:A:108:TRP:CE3	1:A:108:TRP:CE3[16_664]	1.10	1.10
1:A:108:TRP:CE3	1:A:108:TRP:CZ3[16_664]	1.11	1.09
1:A:108:TRP:CZ3	1:A:108:TRP:CH2[16_664]	1.54	0.66
1:A:108:TRP:CD2	1:A:108:TRP:CZ3[16_664]	1.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:TRP:CE3	1:A:108:TRP:CH2[16_664]	1.83	0.37
1:A:108:TRP:CD2	1:A:108:TRP:CE3[16_664]	1.87	0.33
1:A:108:TRP:CZ2	1:A:108:TRP:CZ3[16_664]	2.10	0.10
1:A:108:TRP:CE2	1:A:108:TRP:CZ3[16_664]	2.16	0.04

## 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	480/488 (98%)	458 (95%)	20 (4%)	2 (0%)	38	42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	316	THR
1	A	304	LYS

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	394/396 (100%)	364 (92%)	30 (8%)	15	14

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	5	GLN
1	A	10	LEU
1	A	28	LEU
1	A	34	VAL
1	A	46	LYS
1	A	58	CYS
1	A	120	LYS
1	A	124	ILE
1	A	125	LYS
1	A	129	VAL
1	A	134	VAL
1	A	164	GLN
1	A	178	ILE
1	A	216	ARG
1	A	229	SER
1	A	252	LYS
1	A	259	LEU
1	A	275	THR
1	A	291	THR
1	A	327	VAL
1	A	329	GLU
1	A	331	ARG
1	A	366	VAL
1	A	385	LEU
1	A	395	HIS
1	A	428	LEU
1	A	430	LEU
1	A	448	ILE
1	A	472	VAL

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

Mol	Chain	Res	Type
1	A	27	GLN
1	A	78	HIS
1	A	107	ASN
1	A	113	GLN
1	A	164	GLN
1	A	234	HIS
1	A	250	HIS
1	A	258	GLN
1	A	260	GLN

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Mol	Chain	Res	Type
1	A	293	ASN
1	A	431	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 ⓘ

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	500	-	51,58,58	1.56	8 (15%)	54,89,89	2.25	12 (22%)
3	NA7	A	501	-	36,42,42	1.20	3 (8%)	40,65,65	2.26	5 (12%)

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	500	-	-	0/28/50/50	0/6/6/6
3	NA7	A	501	-	-	0/23/56/56	0/4/4/4

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	FAD	C9-C9A	2.03	1.45	1.40
2	A	500	FAD	C2A-N1A	2.19	1.38	1.33
3	A	501	NA7	C2A-N1A	2.44	1.38	1.33
2	A	500	FAD	C5X-N5	2.62	1.39	1.35
3	A	501	NA7	O4B-C1B	2.73	1.45	1.41
2	A	500	FAD	C4-N3	3.50	1.39	1.33
2	A	500	FAD	C2A-N3A	3.56	1.38	1.32
2	A	500	FAD	C10-N1	3.61	1.38	1.33
2	A	500	FAD	C4X-N5	4.17	1.39	1.33
3	A	501	NA7	C2A-N3A	4.38	1.39	1.32
2	A	500	FAD	C1'-N10	4.56	1.53	1.48

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	NA7	N3A-C2A-N1A	-12.17	118.26	128.86
2	A	500	FAD	N3A-C2A-N1A	-11.52	118.83	128.86
2	A	500	FAD	O3B-C3B-C4B	-3.22	101.69	111.09
2	A	500	FAD	C4X-C4-N3	-3.01	119.19	123.48
2	A	500	FAD	C10-C4X-N5	-2.77	117.41	120.59
2	A	500	FAD	O4'-C4'-C3'	2.12	114.34	109.09
3	A	501	NA7	C4B-O4B-C1B	2.14	112.05	109.77
2	A	500	FAD	C1'-N10-C10	2.29	120.85	118.50
2	A	500	FAD	C4B-O4B-C1B	2.45	112.38	109.77
3	A	501	NA7	O3B-C3B-C2B	2.46	118.17	111.18
3	A	501	NA7	O2B-C2B-C3B	2.60	121.24	111.63
3	A	501	NA7	C1D-C2D-C3D	2.60	105.66	101.67
2	A	500	FAD	C2A-N1A-C6A	2.70	123.49	118.77
2	A	500	FAD	C4-C4X-N5	3.18	122.16	118.68
2	A	500	FAD	O3'-C3'-C4'	3.24	116.85	108.82
2	A	500	FAD	C4X-N5-C5X	3.64	120.61	116.76
2	A	500	FAD	C4-N3-C2	4.89	119.44	115.16

There are no chirality outliers.

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
3	A	501	NA7	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 ⓘ

### 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, 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	482/488 (98%)	0.49	36 (7%) 15 17	29, 39, 45, 59	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	108	TRP	3.7
1	A	164	GLN	3.6
1	A	163	THR	3.5
1	A	290	ARG	3.4
1	A	485	THR	3.4
1	A	463	ILE	3.3
1	A	433	LEU	3.2
1	A	129	VAL	3.1
1	A	303	PRO	3.0
1	A	132	HIS	3.0
1	A	269	GLY	2.9
1	A	4	GLN	2.7
1	A	139	LYS	2.7
1	A	118	LYS	2.7
1	A	270	LYS	2.6
1	A	320	HIS	2.6
1	A	145	LEU	2.5
1	A	317	SER	2.5
1	A	352	LYS	2.5
1	A	256	THR	2.5
1	A	6	SER	2.5
1	A	140	GLY	2.4
1	A	166	LYS	2.3
1	A	5	GLN	2.3
1	A	393	VAL	2.3
1	A	415	ILE	2.3
1	A	316	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	304	LYS	2.1
1	A	291	THR	2.1
1	A	319	PRO	2.1
1	A	468	SER	2.1
1	A	250	HIS	2.1
1	A	482	LEU	2.1
1	A	461	VAL	2.1
1	A	295	GLU	2.0
1	A	315	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	NA7	A	501	39/39	0.80	0.29	2.42	70,80,111,112	0
2	FAD	A	500	53/53	0.94	0.12	-0.65	28,35,39,40	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.