



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 08:59 pm GMT

PDB ID : 2A87  
Title : Crystal Structure of M. tuberculosis Thioredoxin reductase  
Authors : Akif, M.; Suhre, K.; Verma, C.; Mande, S.C.; TB Structural Genomics Consortium (TBSGC)  
Deposited on : 2005-07-07  
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<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

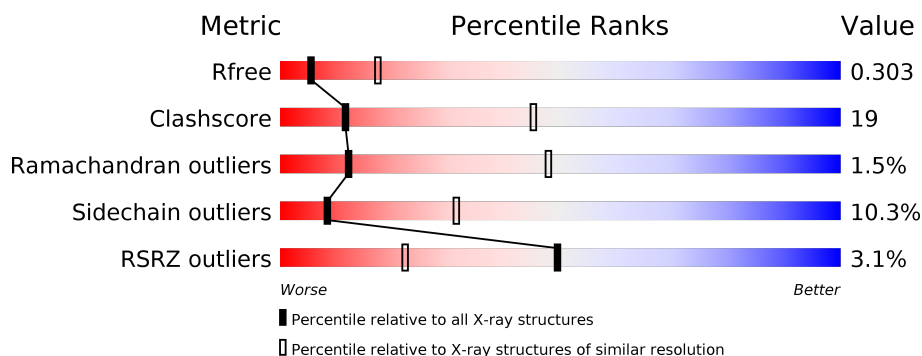
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	335	
1	B	335	

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	FAD	A	348	X	-	-	-
3	FAD	B	448	X	-	-	X
4	NAP	A	381	-	-	-	X
4	NAP	B	481	-	-	-	X

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4812 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.

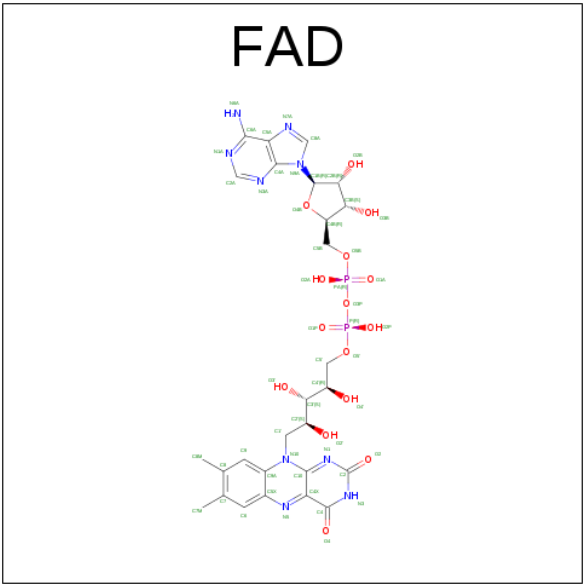
- Molecule 1 is a protein called Thioredoxin reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	313	Total	C	N	O	S	0	0	0
			2324	1437	428	449	10			
1	B	304	Total	C	N	O	S	0	0	0
			2268	1403	412	443	10			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

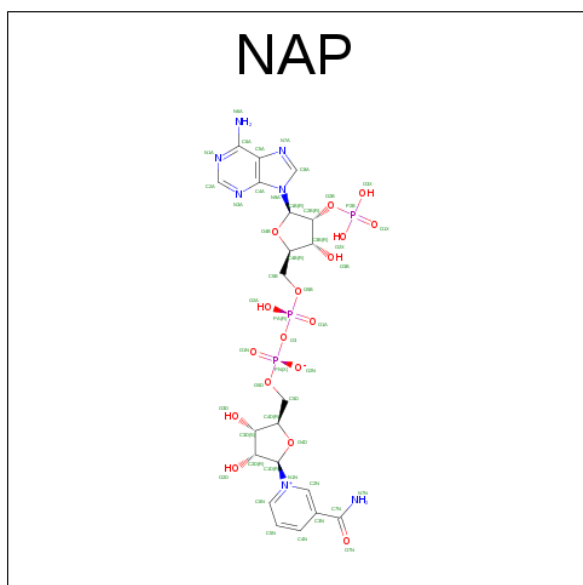
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C<sub>27</sub>H<sub>33</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 4 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula:  $C_{21}H_{28}N_7O_{17}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

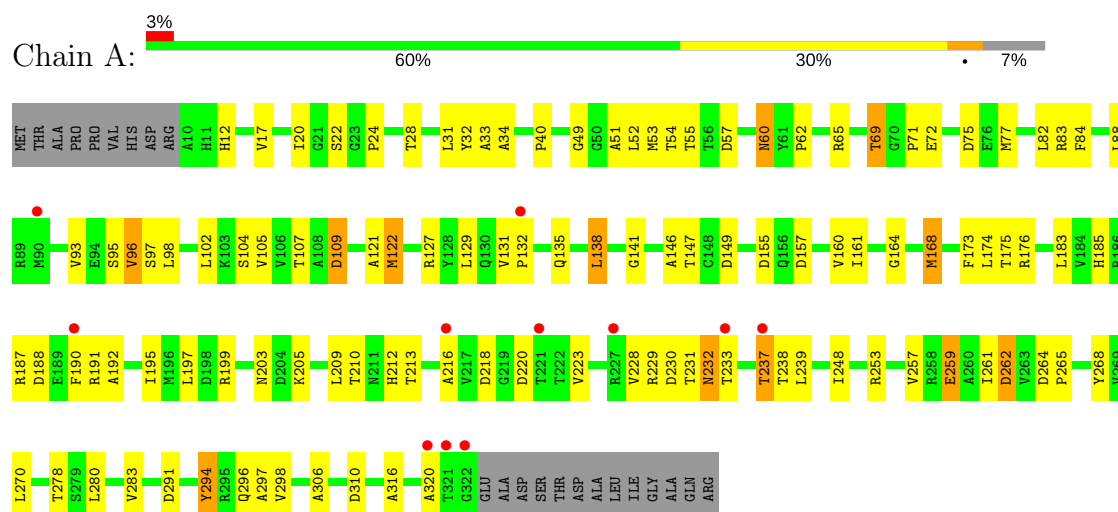
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	10	Total	O	0	0
			10	10		
5	B	6	Total	O	0	0
			6	6		

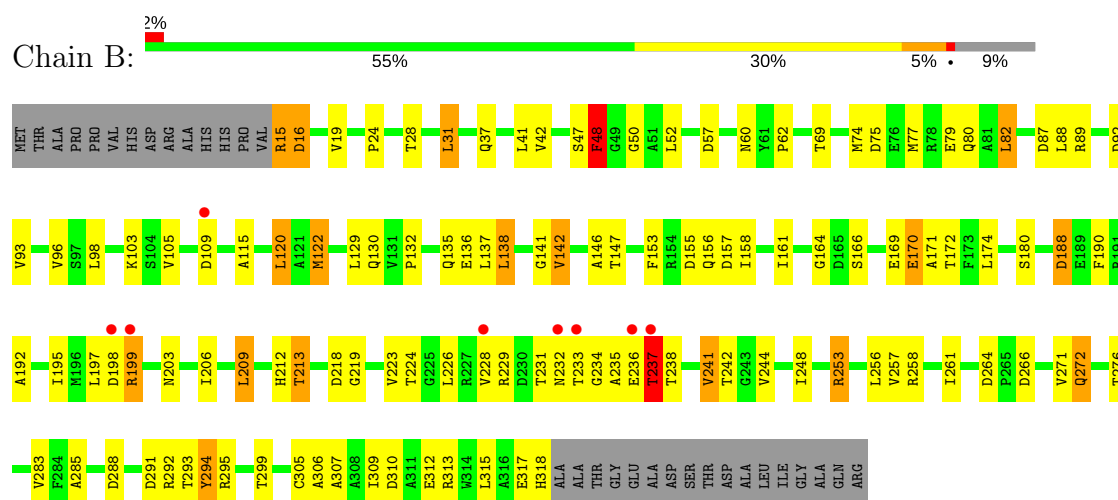
### 3 Residue-property plots

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: Thioredoxin reductase



#### • Molecule 1: Thioredoxin reductase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.40Å 107.40Å 118.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.00 – 3.00 33.96 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.9 (36.00-3.00) 97.8 (33.96-3.00)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.15 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.2.0016	Depositor
R, $R_{free}$	0.211 , 0.291 0.217 , 0.303	Depositor DCC
$R_{free}$ test set	707 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	74.8	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 65.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	4812	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% 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: NAP, MG, 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	0.49	0/2362	0.84	11/3205 (0.3%)
1	B	0.49	0/2303	0.88	14/3126 (0.4%)
All	All	0.49	0/4665	0.86	25/6331 (0.4%)

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

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	198	ASP	CB-CG-OD2	6.83	124.45	118.30
1	B	288	ASP	CB-CG-OD2	6.66	124.29	118.30
1	B	264	ASP	CB-CG-OD2	6.57	124.21	118.30
1	A	149	ASP	CB-CG-OD2	6.46	124.11	118.30
1	A	262	ASP	CB-CG-OD2	6.41	124.06	118.30
1	A	310	ASP	CB-CG-OD2	6.22	123.89	118.30
1	A	157	ASP	CB-CG-OD2	6.09	123.78	118.30
1	B	75	ASP	CB-CG-OD2	6.03	123.72	118.30
1	B	266	ASP	CB-CG-OD2	6.01	123.71	118.30
1	A	109	ASP	CB-CG-OD2	6.01	123.71	118.30
1	B	218	ASP	CB-CG-OD2	5.89	123.60	118.30
1	B	310	ASP	CB-CG-OD2	5.75	123.48	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	92	ASP	CB-CG-OD2	5.68	123.41	118.30
1	B	16	ASP	CB-CG-OD2	5.58	123.32	118.30
1	B	155	ASP	CB-CG-OD2	5.52	123.27	118.30
1	A	220	ASP	CB-CG-OD2	5.39	123.15	118.30
1	B	157	ASP	CB-CG-OD2	5.38	123.14	118.30
1	A	75	ASP	CB-CG-OD2	5.36	123.12	118.30
1	A	57	ASP	CB-CG-OD2	5.31	123.08	118.30
1	A	155	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	218	ASP	CB-CG-OD2	5.28	123.05	118.30
1	B	87	ASP	CB-CG-OD2	5.18	122.96	118.30
1	A	230	ASP	CB-CG-OD2	5.10	122.89	118.30
1	B	57	ASP	CB-CG-OD2	5.08	122.87	118.30
1	B	109	ASP	CB-CG-OD2	5.02	122.82	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	259	GLU	Peptide
1	B	48	PHE	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	2324	0	2264	98	0
1	B	2268	0	2221	91	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	53	0	30	6	0
3	B	53	0	30	8	0
4	A	48	0	25	1	0
4	B	48	0	25	6	0
5	A	10	0	0	0	0
5	B	6	0	0	0	0
All	All	4812	0	4595	182	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 19.

All (182) 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:20:ILE:HB	1:A:122:MET:HE1	1.44	0.99
1:B:50:GLY:HA2	3:B:448:FAD:H52A	1.49	0.94
1:B:236:GLU:O	1:B:237:THR:HG23	1.74	0.86
1:A:127:ARG:HE	1:A:248:ILE:HG22	1.47	0.80
1:A:69:THR:HG23	1:A:71:PRO:HD2	1.64	0.80
1:A:168:MET:HE2	1:A:197:LEU:HD23	1.66	0.78
1:A:69:THR:HG22	1:A:72:GLU:H	1.48	0.77
1:A:129:LEU:HD23	1:A:248:ILE:HD11	1.67	0.76
1:B:141:GLY:HA3	1:B:223:VAL:HG23	1.67	0.76
1:B:50:GLY:HA2	3:B:448:FAD:C5B	2.16	0.74
1:B:50:GLY:CA	3:B:448:FAD:H52A	2.17	0.74
1:B:129:LEU:HD21	1:B:161:ILE:HG21	1.70	0.73
1:B:52:LEU:HD12	1:B:74:MET:CE	2.19	0.72
1:A:190:PHE:HB2	1:A:197:LEU:HD11	1.69	0.72
1:A:129:LEU:CD2	1:A:248:ILE:HD11	2.20	0.71
1:A:122:MET:HE3	1:A:122:MET:N	2.05	0.71
1:B:231:THR:O	1:B:231:THR:HG23	1.90	0.71
1:A:173:PHE:O	1:A:176:ARG:HG2	1.91	0.71
1:A:188:ASP:HA	1:A:210:THR:CG2	2.21	0.70
1:B:158:ILE:HA	1:B:241:VAL:HG12	1.73	0.70
1:A:54:THR:HG21	1:A:138:LEU:HD13	1.76	0.68
1:B:137:LEU:O	1:B:142:VAL:HG23	1.94	0.68
1:B:93:VAL:CG2	1:B:105:VAL:HG13	2.24	0.67
1:A:212:HIS:HE1	1:A:231:THR:HG23	1.61	0.64
1:A:96:VAL:CG2	1:A:105:VAL:HG22	2.28	0.64
1:A:122:MET:HG3	1:A:253:ARG:O	1.99	0.63
1:B:24:PRO:HA	1:B:77:MET:HE3	1.80	0.62
1:A:261:ILE:HD11	1:A:280:LEU:HD12	1.80	0.62
1:A:60:ASN:N	1:A:60:ASN:HD22	1.96	0.62
1:B:52:LEU:HD12	1:B:74:MET:HE1	1.80	0.62
1:A:294:TYR:HB3	1:B:309:ILE:HD12	1.82	0.62
1:A:141:GLY:HA3	1:A:223:VAL:HG23	1.81	0.62
1:B:129:LEU:HD11	1:B:161:ILE:HD13	1.82	0.62
1:B:231:THR:HG22	1:B:234:GLY:HA3	1.82	0.61
1:A:20:ILE:HB	1:A:122:MET:CE	2.24	0.61
1:A:60:ASN:H	1:A:60:ASN:HD22	1.48	0.61
1:A:175:THR:HG23	1:A:205:LYS:HD2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:LEU:HD11	1:B:257:VAL:HG22	1.84	0.60
1:B:52:LEU:HD12	1:B:74:MET:HE3	1.83	0.60
1:B:93:VAL:HG21	1:B:105:VAL:HG13	1.82	0.60
1:B:129:LEU:HD23	1:B:248:ILE:HD11	1.85	0.59
1:B:226:LEU:HD22	1:B:244:VAL:HG22	1.84	0.58
1:B:31:LEU:C	1:B:31:LEU:HD13	2.24	0.58
1:B:258:ARG:O	1:B:258:ARG:HG2	2.03	0.57
1:A:24:PRO:HA	1:A:77:MET:CE	2.35	0.57
1:B:129:LEU:HD11	1:B:161:ILE:CD1	2.34	0.57
1:A:96:VAL:HG22	1:A:105:VAL:HG22	1.87	0.57
1:B:231:THR:HG22	1:B:234:GLY:CA	2.36	0.56
1:B:295:ARG:HH21	4:B:481:NAP:H1D	1.70	0.56
1:A:65:ARG:NH1	1:B:79:GLU:HG2	2.20	0.56
1:A:60:ASN:ND2	3:A:348:FAD:C4	2.64	0.56
1:A:62:PRO:HG3	1:B:28:THR:HG23	1.87	0.55
1:A:62:PRO:HD3	1:A:298:VAL:HG21	1.86	0.55
1:B:135:GLN:HA	1:B:138:LEU:HD12	1.90	0.54
1:A:20:ILE:HG22	1:A:122:MET:HE2	1.89	0.54
1:A:131:VAL:HG12	1:A:216:ALA:HA	1.90	0.53
1:B:137:LEU:C	1:B:142:VAL:HG23	2.28	0.53
1:B:228:VAL:HG23	1:B:237:THR:OG1	2.09	0.53
1:B:295:ARG:O	3:B:448:FAD:H1'2	2.09	0.53
1:B:93:VAL:HG13	1:B:256:LEU:CD1	2.38	0.53
1:B:19:VAL:HB	1:B:42:VAL:HG22	1.92	0.52
1:B:291:ASP:OD2	1:B:294:TYR:O	2.27	0.52
1:B:231:THR:O	1:B:231:THR:CG2	2.58	0.51
1:B:96:VAL:HG12	1:B:98:LEU:HG	1.92	0.51
1:A:131:VAL:CG1	1:A:132:PRO:HD2	2.40	0.51
1:A:49:GLY:HA3	1:A:53:MET:HG3	1.92	0.51
1:A:297:ALA:H	3:A:348:FAD:C2	2.24	0.51
1:A:291:ASP:OD2	1:A:294:TYR:O	2.30	0.50
1:B:93:VAL:HG23	1:B:105:VAL:HG13	1.92	0.50
1:A:60:ASN:H	1:A:60:ASN:ND2	2.09	0.50
1:A:195:ILE:O	1:A:199:ARG:HG3	2.12	0.50
1:B:226:LEU:HD22	1:B:244:VAL:CG2	2.42	0.50
1:A:231:THR:O	1:A:233:THR:N	2.44	0.49
1:B:188:ASP:C	1:B:188:ASP:OD1	2.51	0.49
1:B:235:ALA:O	1:B:236:GLU:HG2	2.13	0.49
1:A:82:LEU:HG	1:A:88:LEU:HD12	1.95	0.49
1:A:257:VAL:HG12	1:A:257:VAL:O	2.12	0.49
1:B:213:THR:HG22	1:B:229:ARG:CB	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:ASN:N	1:A:60:ASN:ND2	2.60	0.49
1:A:60:ASN:OD1	1:A:296:GLN:NE2	2.45	0.49
4:B:481:NAP:C5D	4:B:481:NAP:H2N	2.43	0.49
1:A:237:THR:HG22	1:A:238:THR:N	2.27	0.49
1:A:127:ARG:NE	1:A:248:ILE:HG22	2.21	0.49
1:A:82:LEU:HG	1:A:88:LEU:CD1	2.43	0.49
1:B:261:ILE:HD11	1:B:283:VAL:HG11	1.93	0.48
1:A:51:ALA:HB3	3:A:348:FAD:HO2'	1.79	0.48
1:B:219:GLY:HA3	1:B:224:THR:HG23	1.96	0.48
1:A:24:PRO:HA	1:A:77:MET:HE2	1.96	0.48
1:A:51:ALA:HB3	3:A:348:FAD:O2'	2.14	0.48
1:A:93:VAL:HG13	1:A:105:VAL:HG13	1.95	0.48
1:B:120:LEU:HG	1:B:122:MET:HE2	1.96	0.47
1:A:257:VAL:O	1:A:257:VAL:CG1	2.63	0.47
1:B:16:ASP:HB3	1:B:315:LEU:HD13	1.95	0.47
1:B:48:PHE:O	3:B:448:FAD:O3B	2.33	0.47
1:A:32:TYR:CZ	1:B:60:ASN:ND2	2.82	0.47
1:A:168:MET:CE	1:A:197:LEU:HD23	2.42	0.47
1:B:24:PRO:HA	1:B:77:MET:CE	2.45	0.47
1:A:209:LEU:HD12	1:A:239:LEU:HD11	1.96	0.47
1:A:28:THR:HG23	1:B:62:PRO:HG3	1.96	0.47
1:B:153:PHE:HA	1:B:156:GLN:NE2	2.30	0.46
1:B:257:VAL:HG13	1:B:261:ILE:HB	1.97	0.46
1:A:209:LEU:HD22	1:A:212:HIS:CD2	2.50	0.46
1:A:65:ARG:HA	1:B:80:GLN:HG3	1.97	0.46
1:A:175:THR:HG21	1:A:203:ASN:HD21	1.80	0.46
1:B:93:VAL:HG13	1:B:256:LEU:HD11	1.97	0.46
1:A:316:ALA:O	1:A:320:ALA:HB2	2.14	0.46
1:A:294:TYR:CZ	1:B:306:ALA:HB1	2.50	0.46
1:A:320:ALA:HB1	1:B:199:ARG:CG	2.46	0.45
1:A:135:GLN:HE21	1:A:138:LEU:HD12	1.80	0.45
1:B:292:ARG:HH21	4:B:481:NAP:H3D	1.81	0.45
1:B:24:PRO:HG3	1:B:77:MET:HE1	1.99	0.45
1:B:122:MET:O	1:B:253:ARG:HG3	2.17	0.45
1:A:49:GLY:HA3	1:A:53:MET:CG	2.47	0.45
1:B:318:HIS:CG	1:B:318:HIS:O	2.68	0.45
1:A:121:ALA:H	1:A:122:MET:HE3	1.81	0.45
1:B:231:THR:O	1:B:233:THR:N	2.49	0.45
1:B:47:SER:O	3:B:448:FAD:O2B	2.26	0.45
1:B:272:GLN:HE21	1:B:272:GLN:HB2	1.65	0.45
1:A:129:LEU:HD11	1:A:161:ILE:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:481:NAP:H2N	4:B:481:NAP:H52N	1.98	0.45
1:A:264:ASP:OD2	1:A:268:TYR:HB2	2.17	0.45
1:B:52:LEU:CD1	1:B:74:MET:HE3	2.46	0.45
1:B:171:ALA:HA	1:B:174:LEU:HD12	1.99	0.45
1:A:102:LEU:HA	1:A:102:LEU:HD12	1.82	0.44
1:A:264:ASP:HB2	1:A:265:PRO:CD	2.47	0.44
1:A:96:VAL:HG13	1:A:98:LEU:HD21	1.99	0.44
1:A:96:VAL:HG22	1:A:105:VAL:CG2	2.47	0.44
1:A:107:THR:OG1	1:A:109:ASP:OD2	2.31	0.44
1:A:191:ARG:NE	4:A:381:NAP:O3B	2.48	0.44
1:A:96:VAL:HG12	1:A:96:VAL:O	2.17	0.44
1:A:96:VAL:HG13	1:A:98:LEU:CD2	2.47	0.44
1:A:264:ASP:HB3	1:A:270:LEU:HD11	1.99	0.44
1:B:203:ASN:HB3	1:B:206:ILE:HG13	2.00	0.44
1:A:20:ILE:CG2	1:A:122:MET:HE2	2.47	0.44
1:B:122:MET:HG3	1:B:253:ARG:O	2.17	0.44
1:B:219:GLY:CA	1:B:224:THR:HG23	2.47	0.43
1:B:190:PHE:HB2	1:B:197:LEU:HD11	1.99	0.43
1:B:41:LEU:HD11	1:B:89:ARG:HG3	2.00	0.43
1:B:209:LEU:CD1	1:B:212:HIS:CD2	3.01	0.43
1:B:169:GLU:O	1:B:172:THR:HG22	2.18	0.43
1:B:60:ASN:OD1	3:B:448:FAD:O4	2.36	0.43
1:A:261:ILE:CD1	1:A:280:LEU:HD12	2.48	0.43
1:A:98:LEU:HB3	1:A:283:VAL:HG21	2.00	0.43
1:A:22:SER:O	3:A:348:FAD:H52A	2.18	0.43
1:B:223:VAL:O	1:B:242:THR:HA	2.19	0.43
1:A:20:ILE:O	1:A:122:MET:CE	2.67	0.42
1:B:276:THR:HG21	1:B:307:ALA:N	2.34	0.42
1:B:93:VAL:CG1	3:B:448:FAD:H62A	2.31	0.42
1:B:295:ARG:NH2	4:B:481:NAP:H1D	2.34	0.42
1:A:135:GLN:NE2	1:A:138:LEU:HD12	2.34	0.42
1:A:261:ILE:HG22	1:A:262:ASP:N	2.34	0.42
1:A:33:ALA:CB	1:A:40:PRO:HG3	2.49	0.42
1:B:146:ALA:HB2	1:B:170:GLU:HG3	2.02	0.42
1:A:237:THR:CG2	1:A:238:THR:N	2.82	0.42
1:A:164:GLY:CA	1:A:192:ALA:HB2	2.50	0.42
1:A:146:ALA:HB1	1:A:174:LEU:HD21	2.00	0.42
1:B:120:LEU:HB3	1:B:122:MET:HE2	2.01	0.42
1:A:60:ASN:HD21	3:A:348:FAD:C4	2.20	0.42
1:B:213:THR:O	1:B:229:ARG:N	2.53	0.42
1:A:138:LEU:CD2	1:A:138:LEU:C	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:VAL:CG1	1:A:229:ARG:N	2.83	0.41
1:B:271:VAL:CG1	1:B:285:ALA:HB3	2.51	0.41
1:A:185:HIS:CE1	1:A:187:ARG:HG2	2.54	0.41
1:B:248:ILE:HG22	1:B:248:ILE:O	2.20	0.41
1:A:187:ARG:O	1:A:210:THR:HG23	2.19	0.41
1:A:231:THR:HG22	1:A:231:THR:O	2.21	0.41
1:B:82:LEU:HG	1:B:88:LEU:CD1	2.51	0.41
1:A:34:ALA:HB1	1:A:84:PHE:O	2.20	0.41
1:A:131:VAL:HG12	1:A:132:PRO:HD2	2.02	0.41
1:A:168:MET:HE3	1:A:183:LEU:CD2	2.50	0.41
1:B:315:LEU:O	1:B:318:HIS:HA	2.21	0.41
1:B:212:HIS:CE1	1:B:231:THR:HB	2.56	0.41
1:A:306:ALA:HB1	1:B:294:TYR:CZ	2.56	0.41
1:B:292:ARG:HH21	4:B:481:NAP:C3D	2.34	0.41
1:A:146:ALA:CB	1:A:174:LEU:HD21	2.50	0.41
1:B:15:ARG:HH11	1:B:41:LEU:HD22	1.85	0.41
1:A:160:VAL:C	1:A:161:ILE:HD13	2.42	0.40
1:A:52:LEU:HD22	1:A:55:THR:HG21	2.03	0.40
1:B:103:LYS:N	1:B:115:ALA:O	2.50	0.40
1:B:164:GLY:CA	1:B:192:ALA:HB2	2.51	0.40
1:B:82:LEU:HG	1:B:88:LEU:HD13	2.02	0.40
1:A:131:VAL:CG1	1:A:216:ALA:HA	2.51	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	311/335 (93%)	284 (91%)	22 (7%)	5 (2%)	11	46
1	B	302/335 (90%)	275 (91%)	23 (8%)	4 (1%)	14	51
All	All	613/670 (92%)	559 (91%)	45 (7%)	9 (2%)	12	48

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	259	GLU
1	A	232	ASN
1	B	232	ASN
1	B	237	THR
1	A	12	HIS
1	A	278	THR
1	A	237	THR
1	B	48	PHE
1	B	132	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	234/256 (91%)	218 (93%)	16 (7%)	18	54
1	B	232/256 (91%)	200 (86%)	32 (14%)	4	19
All	All	466/512 (91%)	418 (90%)	48 (10%)	8	31

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	VAL
1	A	31	LEU
1	A	60	ASN
1	A	69	THR
1	A	83	ARG
1	A	95	SER
1	A	96	VAL
1	A	97	SER
1	A	104	SER
1	A	122	MET
1	A	138	LEU
1	A	147	THR
1	A	168	MET
1	A	213	THR

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Mol	Chain	Res	Type
1	A	232	ASN
1	A	294	TYR
1	B	15	ARG
1	B	31	LEU
1	B	37	GLN
1	B	69	THR
1	B	82	LEU
1	B	120	LEU
1	B	122	MET
1	B	130	GLN
1	B	136	GLU
1	B	138	LEU
1	B	142	VAL
1	B	147	THR
1	B	166	SER
1	B	170	GLU
1	B	180	SER
1	B	188	ASP
1	B	195	ILE
1	B	199	ARG
1	B	209	LEU
1	B	213	THR
1	B	237	THR
1	B	238	THR
1	B	241	VAL
1	B	253	ARG
1	B	272	GLN
1	B	293	THR
1	B	294	TYR
1	B	299	THR
1	B	305	CYS
1	B	312	GLU
1	B	313	ARG
1	B	317	GLU

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	99	HIS
1	A	135	GLN
1	A	185	HIS
1	A	202	ASN

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Mol	Chain	Res	Type
1	A	211	ASN
1	A	232	ASN
1	A	250	HIS
1	A	296	GLN
1	B	37	GLN
1	B	156	GLN
1	B	272	GLN

### 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 ⓘ

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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	$\# Z  > 2$
3	FAD	A	348	1	51,58,58	1.93	13 (25%)	54,89,89	2.06	10 (18%)
4	NAP	A	381	2	44,52,52	1.61	3 (6%)	51,80,80	1.60	2 (3%)
3	FAD	B	448	-	51,58,58	2.05	10 (19%)	54,89,89	2.04	9 (16%)
4	NAP	B	481	2	44,52,52	1.62	3 (6%)	51,80,80	1.65	3 (5%)

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
3	FAD	A	348	1	1/1/9/9	0/28/50/50	0/6/6/6
4	NAP	A	381	2	-	0/27/67/67	0/5/5/5
3	FAD	B	448	-	1/1/9/9	0/28/50/50	0/6/6/6
4	NAP	B	481	2	-	0/27/67/67	0/5/5/5

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	348	FAD	O4B-C4B	-4.51	1.34	1.45
3	B	448	FAD	O4B-C4B	-2.95	1.38	1.45
3	A	348	FAD	C7M-C7	2.12	1.55	1.51
3	A	348	FAD	C8M-C8	2.20	1.55	1.51
3	B	448	FAD	C2B-C1B	2.21	1.57	1.53
3	A	348	FAD	C9A-N10	2.38	1.41	1.38
4	B	481	NAP	C2A-N1A	2.46	1.38	1.33
4	A	381	NAP	C2A-N1A	2.61	1.38	1.33
3	A	348	FAD	C2-N1	2.61	1.43	1.38
3	A	348	FAD	C2A-N1A	2.72	1.39	1.33
3	B	448	FAD	C2-N1	2.74	1.43	1.38
3	A	348	FAD	C5'-C4'	2.77	1.55	1.51
3	A	348	FAD	C5X-N5	3.04	1.40	1.35
3	A	348	FAD	O4B-C1B	3.36	1.45	1.41
3	B	448	FAD	C2A-N1A	3.41	1.40	1.33
4	B	481	NAP	C2A-N3A	3.77	1.38	1.32
3	B	448	FAD	C9A-N10	3.90	1.43	1.38
3	B	448	FAD	C5X-N5	4.01	1.41	1.35
4	A	381	NAP	C2A-N3A	4.06	1.38	1.32
3	A	348	FAD	C4-N3	4.16	1.40	1.33
3	B	448	FAD	O4B-C1B	4.59	1.47	1.41
3	A	348	FAD	C1'-N10	4.67	1.53	1.48
3	A	348	FAD	C4X-N5	4.79	1.40	1.33
3	B	448	FAD	C4-N3	4.87	1.41	1.33
3	A	348	FAD	C10-N1	5.13	1.40	1.33
3	B	448	FAD	C4X-N5	5.49	1.41	1.33
3	B	448	FAD	C10-N1	6.15	1.41	1.33
4	A	381	NAP	O7N-C7N	8.29	1.41	1.24
4	B	481	NAP	O7N-C7N	8.44	1.41	1.24

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	481	NAP	N3A-C2A-N1A	-9.98	120.17	128.86
4	A	381	NAP	N3A-C2A-N1A	-9.86	120.27	128.86
3	B	448	FAD	N3A-C2A-N1A	-9.74	120.38	128.86
3	A	348	FAD	N3A-C2A-N1A	-9.50	120.59	128.86
4	B	481	NAP	C4B-O4B-C1B	-3.15	106.41	109.77
3	A	348	FAD	C4A-C5A-N7A	-2.36	107.13	109.41
3	B	448	FAD	C4A-C5A-N7A	-2.21	107.27	109.41
3	B	448	FAD	C4X-C4-N3	-2.02	120.61	123.48
3	A	348	FAD	C1'-C2'-C3'	2.18	116.06	109.82
4	A	381	NAP	C4D-O4D-C1D	2.24	112.16	109.77
3	B	448	FAD	C5B-C4B-C3B	2.44	124.58	115.29
3	B	448	FAD	C1'-N10-C10	2.73	121.31	118.50
3	A	348	FAD	C4X-N5-C5X	2.83	119.75	116.76
3	A	348	FAD	C5X-C9A-N10	2.84	119.77	117.66
3	A	348	FAD	C5B-C4B-C3B	3.24	127.63	115.29
3	A	348	FAD	O4B-C4B-C5B	3.28	120.47	109.40
4	B	481	NAP	C1B-N9A-C4A	3.32	132.38	126.64
3	A	348	FAD	O4B-C4B-C3B	3.39	111.90	105.17
3	B	448	FAD	C4X-N5-C5X	3.54	120.50	116.76
3	B	448	FAD	O4B-C4B-C5B	3.77	122.12	109.40
3	B	448	FAD	O4B-C4B-C3B	4.08	113.29	105.17
3	A	348	FAD	C4-N3-C2	4.40	119.01	115.16
3	A	348	FAD	C1'-N10-C10	5.79	124.44	118.50
3	B	448	FAD	C4-N3-C2	5.89	120.31	115.16

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	448	FAD	C4B
3	A	348	FAD	C4B

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	348	FAD	6	0
4	A	381	NAP	1	0
3	B	448	FAD	8	0
4	B	481	NAP	6	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	313/335 (93%)	0.08	11 (3%)	44	19	61, 69, 77, 97	0
1	B	304/335 (90%)	-0.12	8 (2%)	56	27	62, 70, 76, 83	0
All	All	617/670 (92%)	-0.02	19 (3%)	49	22	61, 70, 77, 97	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	232	ASN	5.4
1	A	322	GLY	3.6
1	A	321	THR	3.5
1	B	233	THR	3.3
1	A	190	PHE	3.2
1	A	216	ALA	2.9
1	A	233	THR	2.9
1	A	227	ARG	2.8
1	A	90	MET	2.8
1	B	236	GLU	2.6
1	B	109	ASP	2.6
1	B	237	THR	2.6
1	A	221	THR	2.6
1	A	320	ALA	2.3
1	B	198	ASP	2.2
1	B	228	VAL	2.2
1	A	132	PRO	2.1
1	A	237	THR	2.1
1	B	199	ARG	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(Å <sup>2</sup> )	Q<0.9
3	FAD	B	448	53/53	0.83	0.48	5.29	52,107,120,120	0
4	NAP	B	481	48/48	0.71	0.43	4.59	44,72,107,119	48
4	NAP	A	381	48/48	0.69	0.47	3.32	35,72,94,98	48
3	FAD	A	348	53/53	0.90	0.29	1.18	38,75,106,111	0
2	MG	B	336	1/1	0.84	0.10	-	59,59,59,59	0
2	MG	A	336	1/1	0.72	0.20	-	75,75,75,75	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.